



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:01 AM UTC

PDB ID : 7K6V / pdb_00007k6v
Title : Crystal Structure of Virus-like Particles of GII.4 Norovirus Houston virus (HOV)
Authors : Hu, L.; Prasad, B.V.V.
Deposited on : 2020-09-21
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

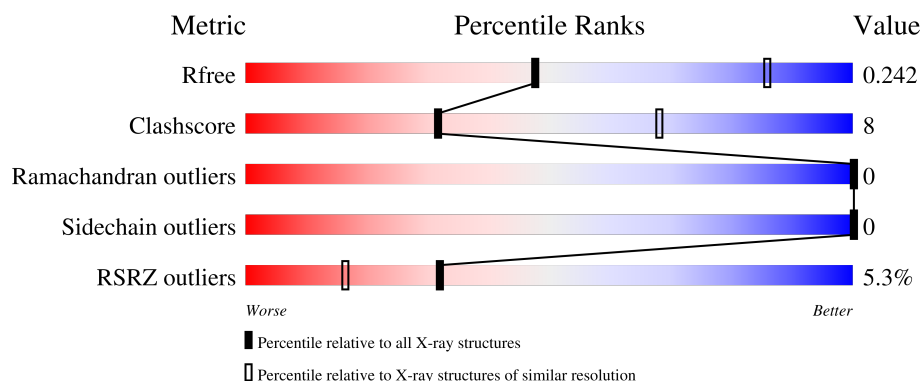
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	540	 3% 76% 16% 7%
1	AB	540	 3% 79% 18% .
1	AC	540	 3% 77% 17% 6%
1	BA	540	 3% 76% 16% 8%
1	BB	540	 4% 78% 19% .

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Mol	Chain	Length	Quality of chain
1	BC	540	
1	CA	540	
1	CB	540	
1	CC	540	
1	DA	540	
1	DB	540	
1	DC	540	
1	EA	540	
1	EB	540	
1	EC	540	
1	FA	540	
1	FB	540	
1	FC	540	
1	GA	540	
1	GB	540	
1	GC	540	
1	HA	540	
1	HB	540	
1	HC	540	
1	IA	540	
1	IB	540	
1	IC	540	
1	JA	540	
1	JB	540	
1	JC	540	

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Mol	Chain	Length	Quality of chain
1	KA	540	
1	KB	540	
1	KC	540	
1	LA	540	
1	LB	540	
1	LC	540	
1	MA	540	
1	MB	540	
1	MC	540	
1	NA	540	
1	NB	540	
1	NC	540	
1	OA	540	
1	OB	540	
1	OC	540	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 176522 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	500	Total	C	N	O	S	0	0	0
			3860	2474	656	715	15			
1	AB	523	Total	C	N	O	S	0	0	0
			4013	2560	681	757	15			
1	AC	508	Total	C	N	O	S	0	0	0
			3921	2506	668	732	15			
1	BA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	BB	523	Total	C	N	O	S	0	0	0
			4019	2563	684	757	15			
1	BC	507	Total	C	N	O	S	0	0	0
			3913	2502	666	730	15			
1	CA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	CB	523	Total	C	N	O	S	0	0	0
			4013	2560	681	757	15			
1	CC	507	Total	C	N	O	S	0	0	0
			3913	2502	666	730	15			
1	DA	498	Total	C	N	O	S	0	0	0
			3845	2464	654	713	14			
1	DB	523	Total	C	N	O	S	0	0	0
			4013	2560	681	757	15			
1	DC	506	Total	C	N	O	S	0	0	0
			3906	2497	665	730	14			
1	EA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	EB	523	Total	C	N	O	S	0	0	0
			4013	2560	681	757	15			
1	EC	493	Total	C	N	O	S	0	0	0
			3814	2442	651	709	12			
1	FA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	FB	523	Total	C	N	O	S	0	0	0
			4019	2563	684	757	15			
1	FC	509	Total	C	N	O	S	0	0	0
			3928	2511	669	733	15			
1	GA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	GB	523	Total	C	N	O	S	0	0	0
			4016	2562	684	755	15			
1	GC	507	Total	C	N	O	S	0	0	0
			3913	2502	666	730	15			
1	HA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	HB	523	Total	C	N	O	S	0	0	0
			4015	2561	684	755	15			
1	HC	507	Total	C	N	O	S	0	0	0
			3913	2502	666	730	15			
1	IA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	IB	523	Total	C	N	O	S	0	0	0
			4019	2564	685	755	15			
1	IC	503	Total	C	N	O	S	0	0	0
			3885	2487	660	723	15			
1	JA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	JB	523	Total	C	N	O	S	0	0	0
			4007	2558	681	753	15			
1	JC	506	Total	C	N	O	S	0	0	0
			3906	2497	665	730	14			
1	KA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	KB	523	Total	C	N	O	S	0	0	0
			4009	2558	681	755	15			
1	KC	507	Total	C	N	O	S	0	0	0
			3913	2502	666	730	15			
1	LA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	LB	523	Total	C	N	O	S	0	0	0
			4003	2556	681	751	15			
1	LC	502	Total	C	N	O	S	0	0	0
			3865	2474	657	719	15			
1	MA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	MB	523	Total	C	N	O	S	0	0	0
			4010	2559	681	755	15			
1	MC	506	Total	C	N	O	S	0	0	0
			3906	2497	665	730	14			
1	NA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	NB	523	Total	C	N	O	S	0	0	0
			4017	2564	685	753	15			
1	NC	506	Total	C	N	O	S	0	0	0
			3899	2494	665	726	14			
1	OA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	OB	523	Total	C	N	O	S	0	0	0
			4017	2564	685	753	15			
1	OC	498	Total	C	N	O	S	0	0	0
			3851	2464	656	719	12			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AA	3	Total	Cl	0	0
			3	3		
2	AB	1	Total	Cl	0	0
			1	1		
2	AC	1	Total	Cl	0	0
			1	1		
2	BA	2	Total	Cl	0	0
			2	2		
2	BC	1	Total	Cl	0	0
			1	1		
2	CA	2	Total	Cl	0	0
			2	2		
2	CC	3	Total	Cl	0	0
			3	3		
2	DA	1	Total	Cl	0	0
			1	1		
2	DB	1	Total	Cl	0	0
			1	1		
2	DC	2	Total	Cl	0	0
			2	2		
2	EA	3	Total	Cl	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	FA	2	Total 2	Cl 2	0	0
2	GA	1	Total 1	Cl 1	0	0
2	GC	2	Total 2	Cl 2	0	0
2	HA	1	Total 1	Cl 1	0	0
2	HC	1	Total 1	Cl 1	0	0
2	IA	3	Total 3	Cl 3	0	0
2	JA	3	Total 3	Cl 3	0	0
2	KA	2	Total 2	Cl 2	0	0
2	KC	2	Total 2	Cl 2	0	0
2	LA	1	Total 1	Cl 1	0	0
2	LC	2	Total 2	Cl 2	0	0
2	MA	3	Total 3	Cl 3	0	0
2	MC	2	Total 2	Cl 2	0	0
2	NA	2	Total 2	Cl 2	0	0
2	NC	1	Total 1	Cl 1	0	0
2	OA	2	Total 2	Cl 2	0	0

- Molecule 3 is CADMIUM ION (CCD ID: CD) (formula: Cd) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AC	1	Total 1	Cd 1	0	0
3	BA	1	Total 1	Cd 1	0	0
3	BC	1	Total 1	Cd 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	CA	1	Total	Cd	0	0
			1	1		
3	DA	1	Total	Cd	0	0
			1	1		
3	EA	1	Total	Cd	0	0
			1	1		
3	EB	1	Total	Cd	0	0
			1	1		
3	EC	1	Total	Cd	0	0
			1	1		
3	FA	1	Total	Cd	0	0
			1	1		
3	FC	1	Total	Cd	0	0
			1	1		
3	GA	1	Total	Cd	0	0
			1	1		
3	GB	1	Total	Cd	0	0
			1	1		
3	HC	1	Total	Cd	0	0
			1	1		
3	IA	1	Total	Cd	0	0
			1	1		
3	JA	1	Total	Cd	0	0
			1	1		
3	JC	1	Total	Cd	0	0
			1	1		
3	KA	1	Total	Cd	0	0
			1	1		
3	KB	1	Total	Cd	0	0
			1	1		
3	MA	1	Total	Cd	0	0
			1	1		
3	MB	1	Total	Cd	0	0
			1	1		
3	NC	1	Total	Cd	0	0
			1	1		
3	OA	1	Total	Cd	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	JA	1	Total	C	O	0	0
			4	2	2		

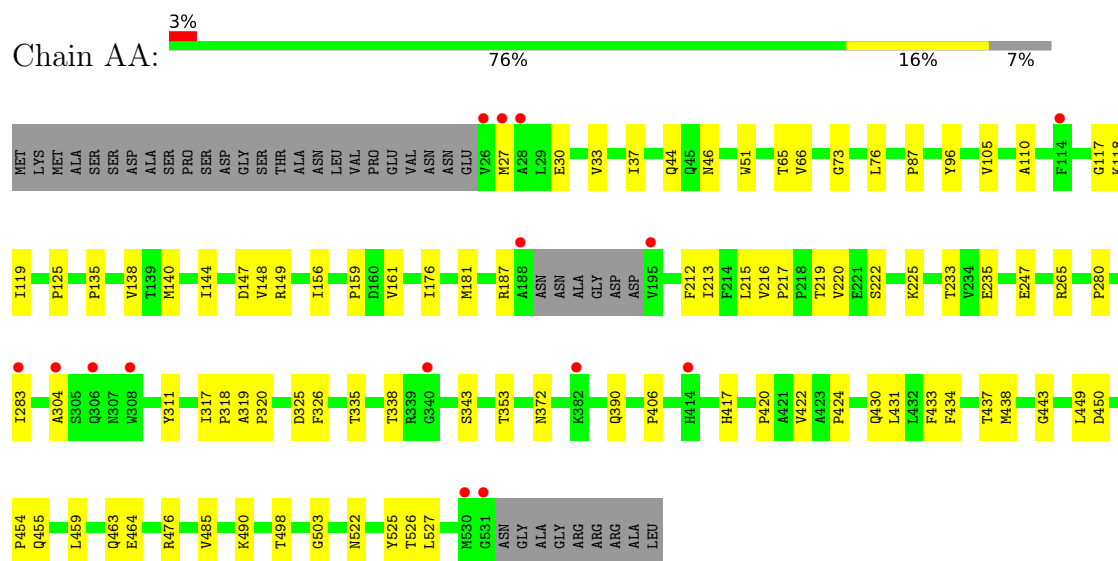
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	HC	1	Total	O	0	0
			1	1		
5	OA	1	Total	O	0	0
			1	1		
5	OB	1	Total	O	0	0
			1	1		

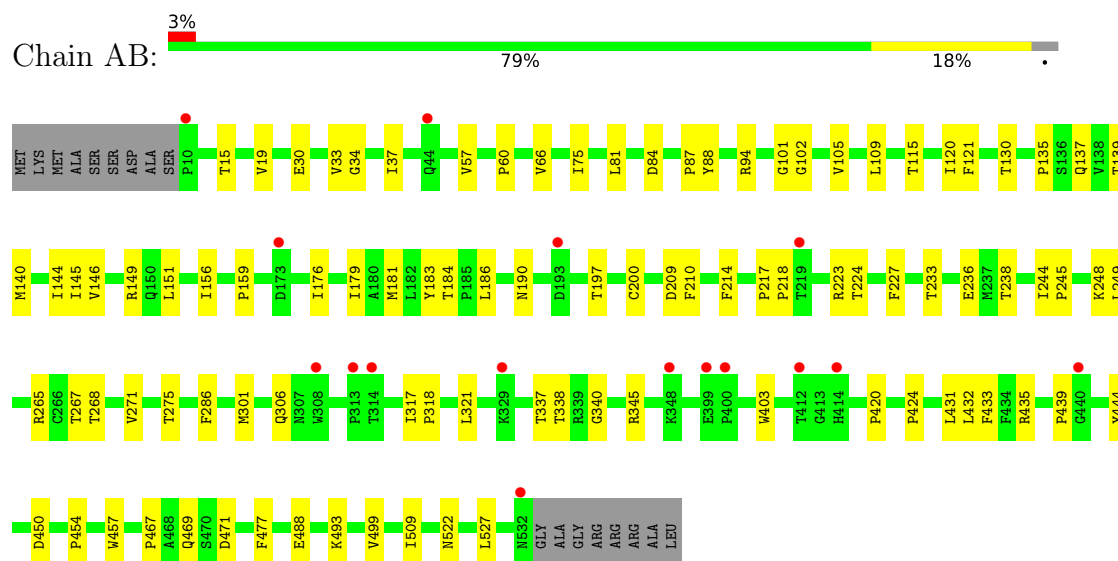
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Capsid protein VP1

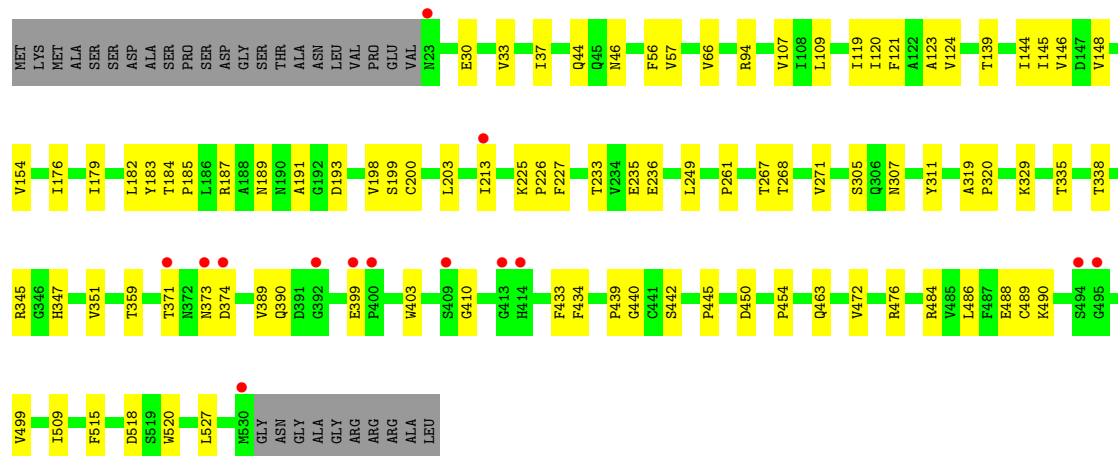


• Molecule 1: Capsid protein VP1



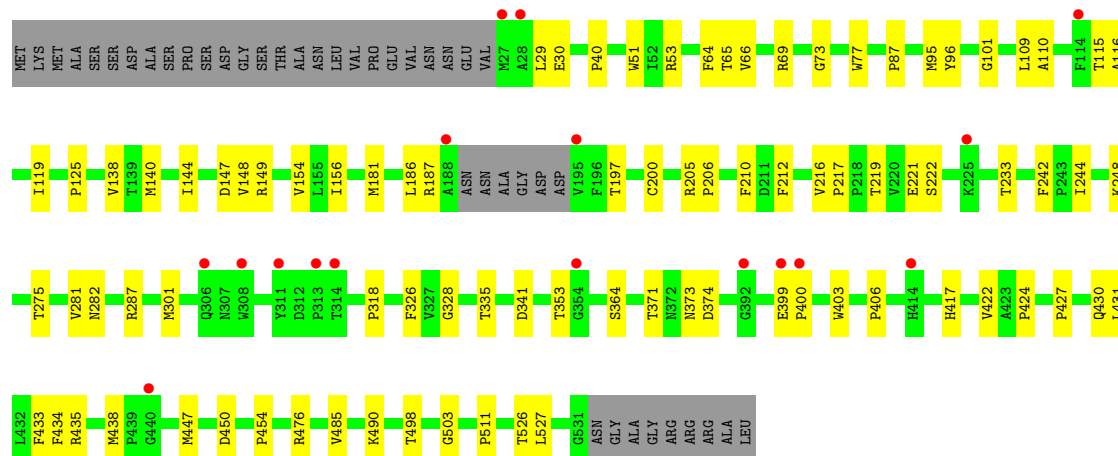
• Molecule 1: Capsid protein VP1

Chain AC: 



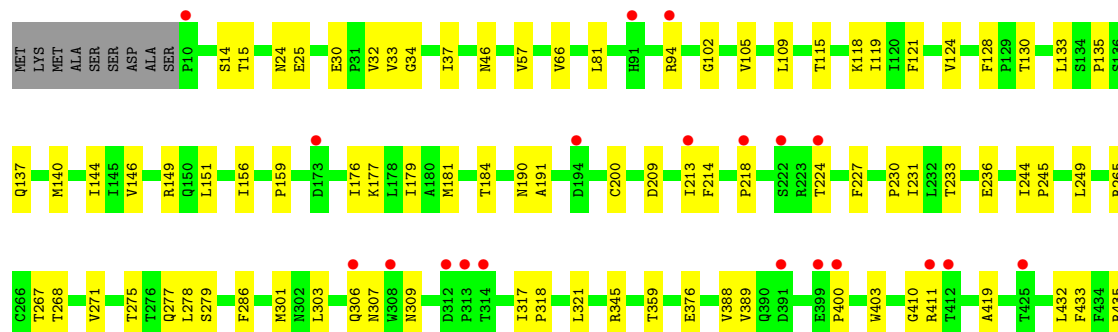
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Chain BA: 



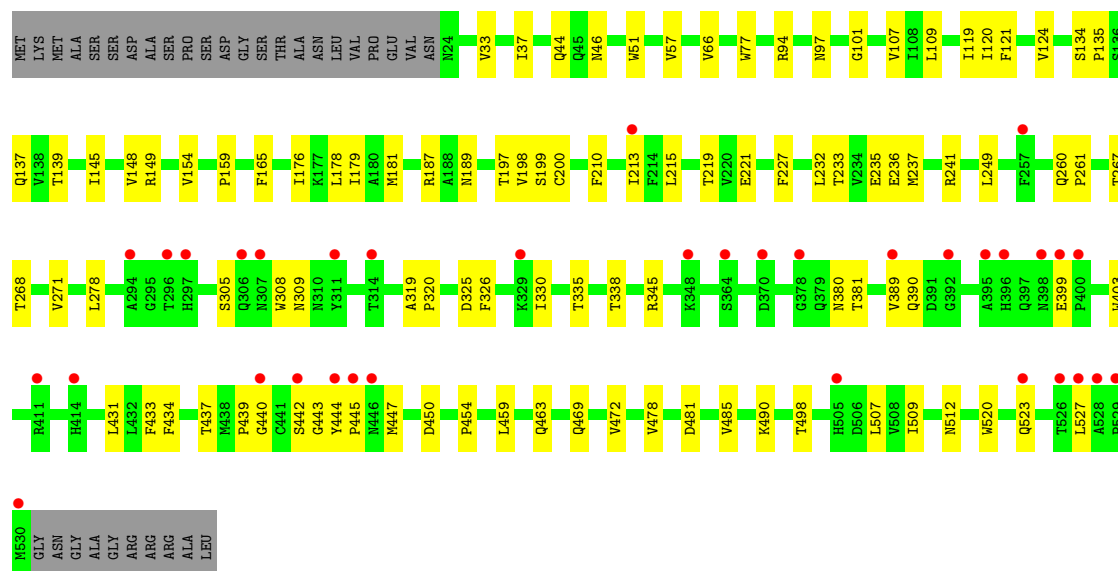
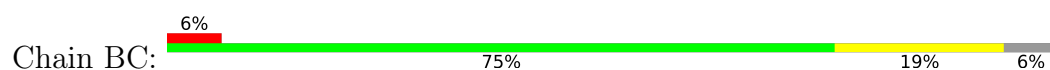
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Chain BB: 

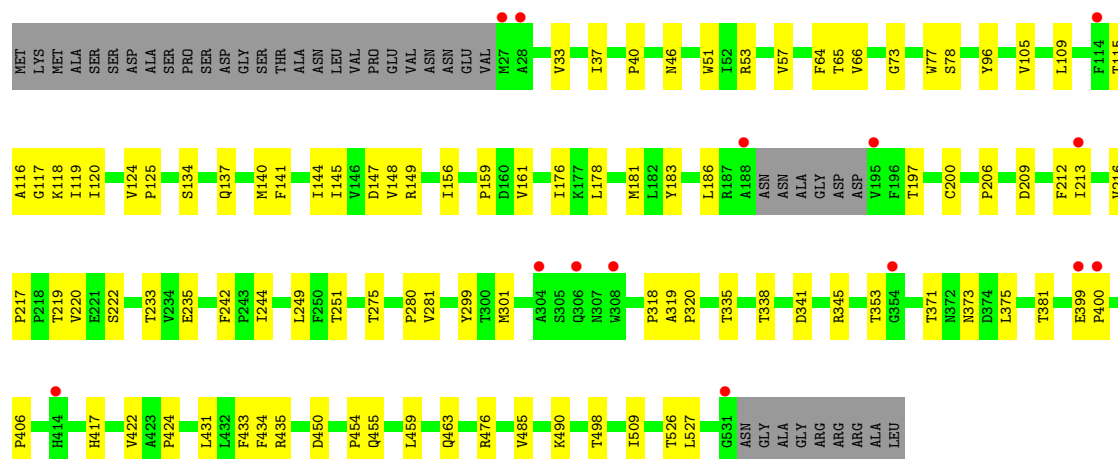
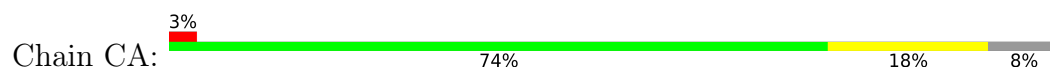




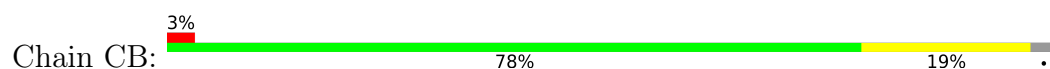
- Molecule 1: Capsid protein VP1

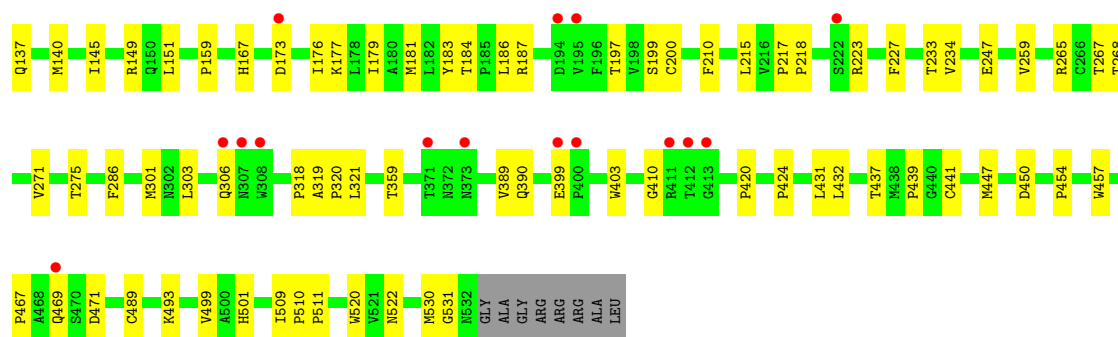


- Molecule 1: Capsid protein VP1

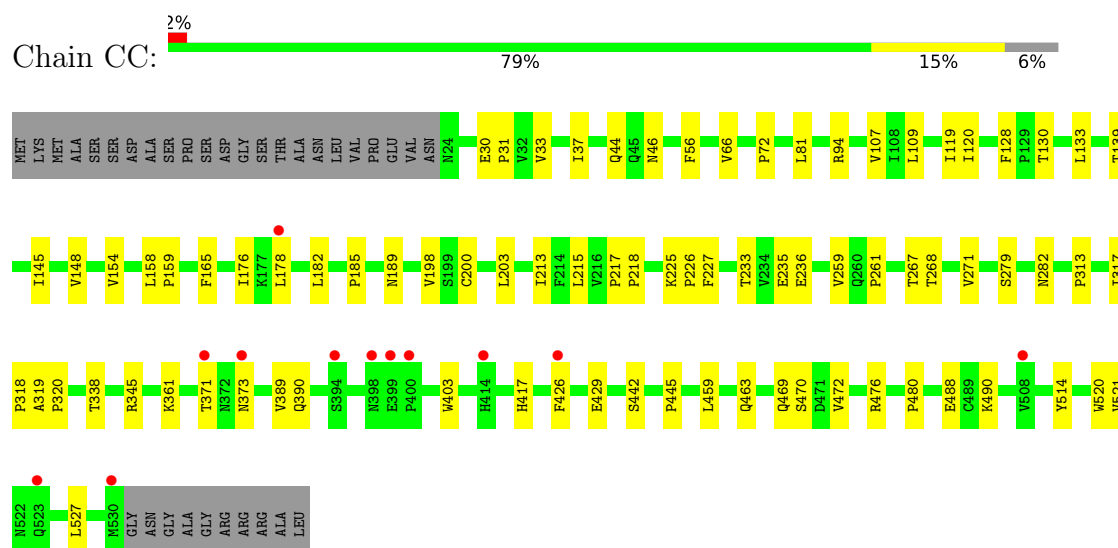


- Molecule 1: Capsid protein VP1

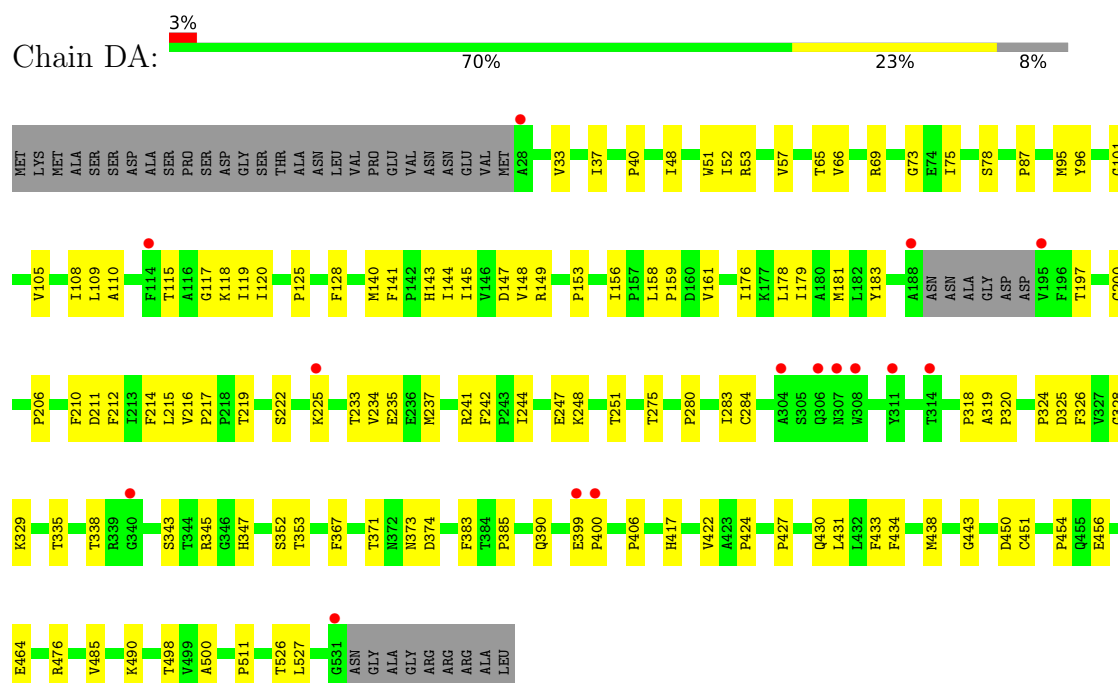




• Molecule 1: Capsid protein VP1



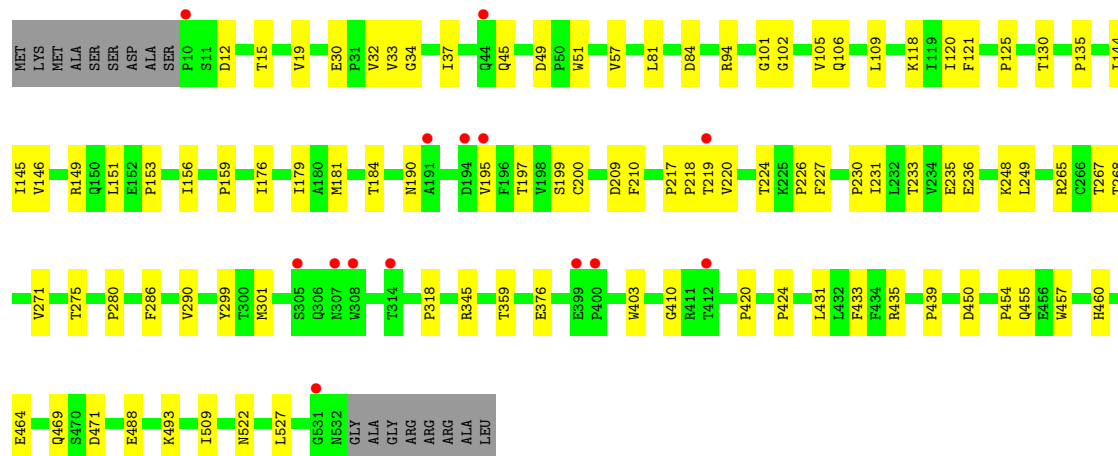
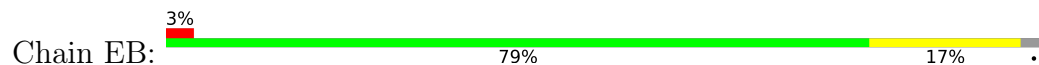
• Molecule 1: Capsid protein VP1



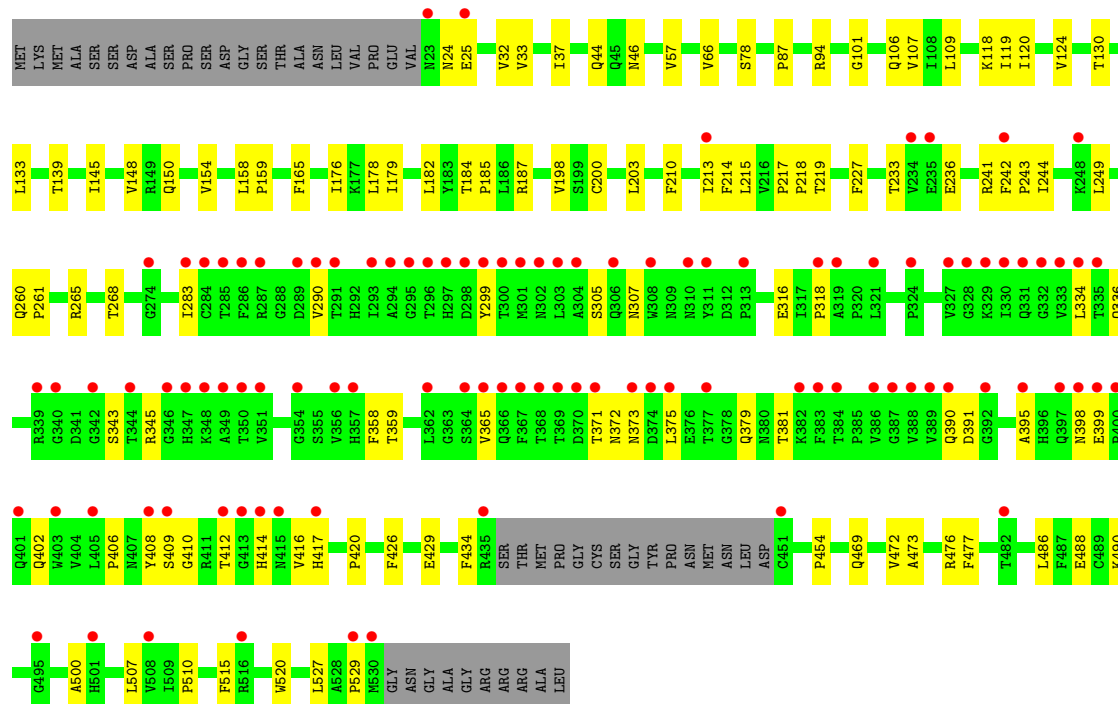
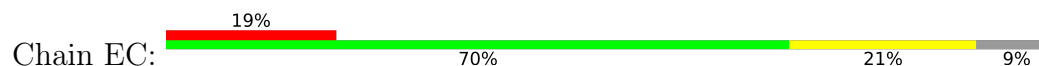
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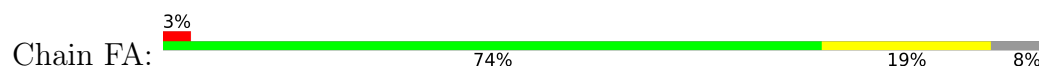
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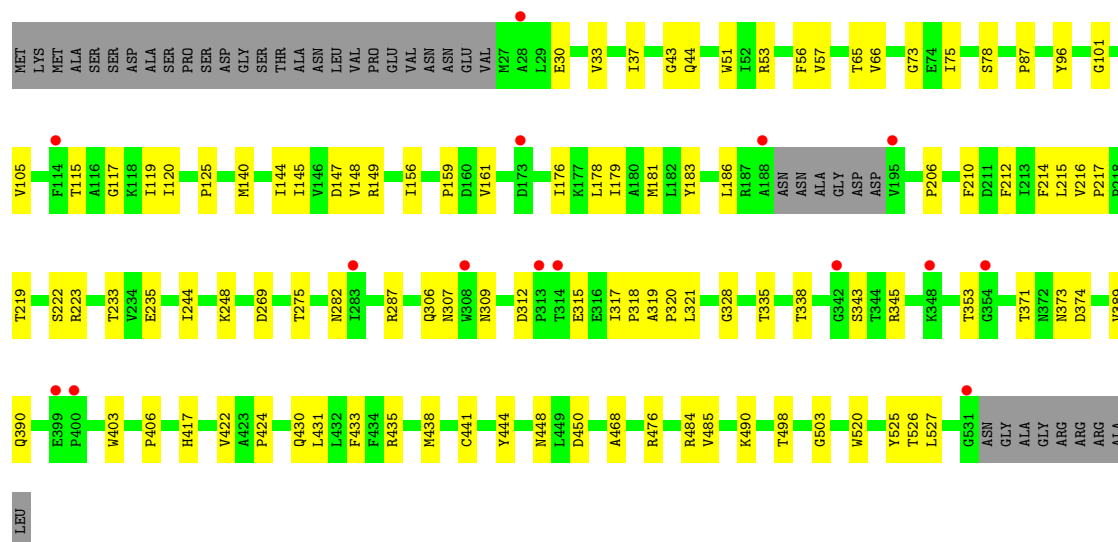


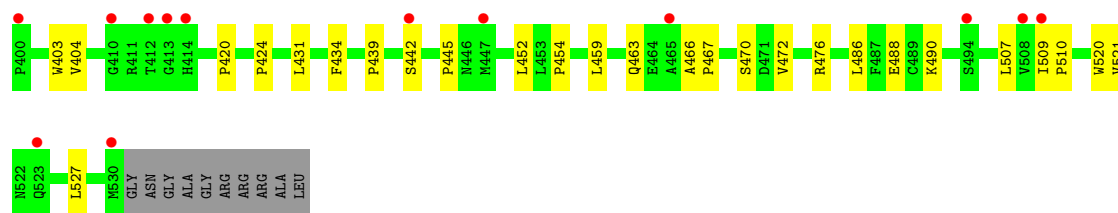
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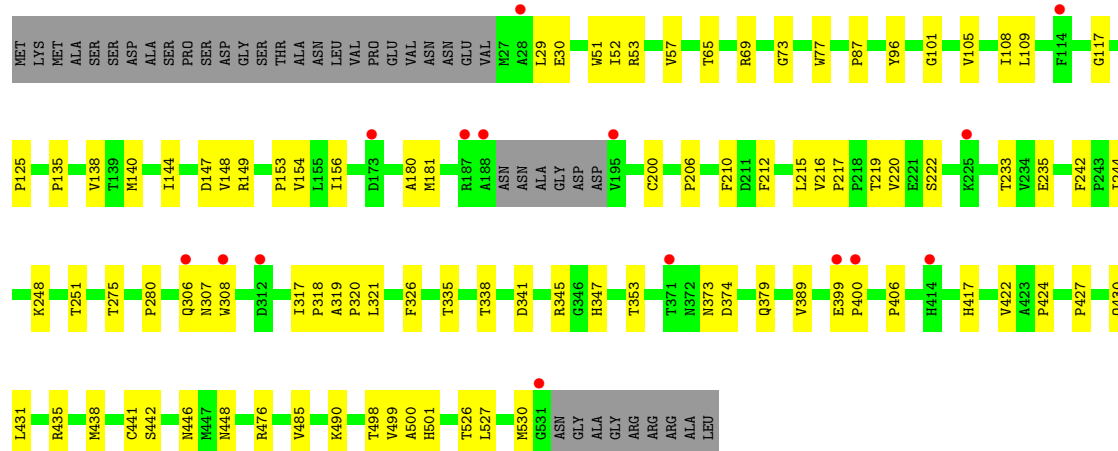
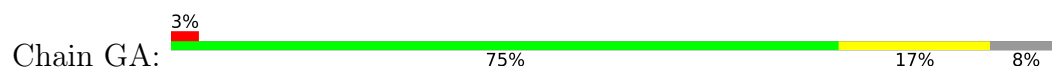
• Molecule 1: Capsid protein VP1



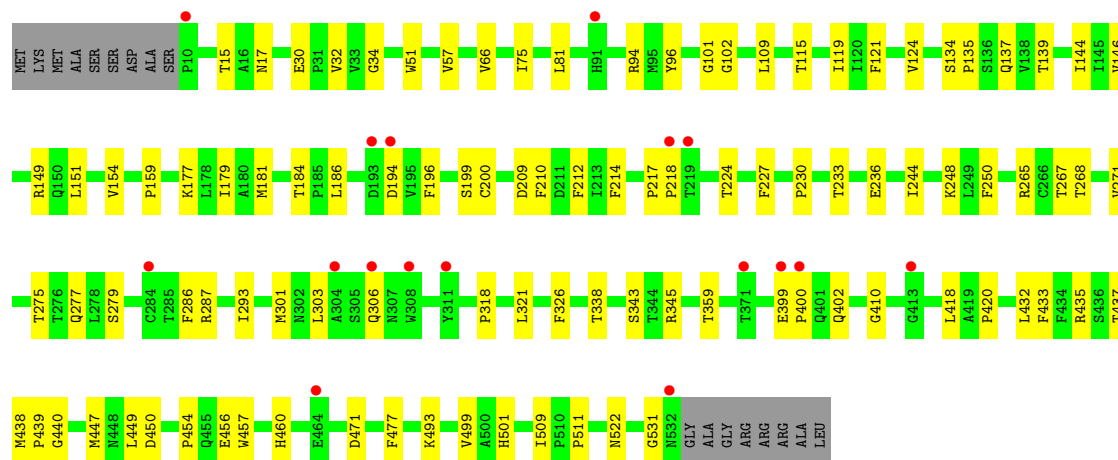
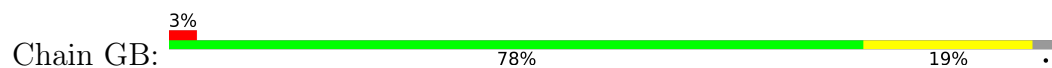




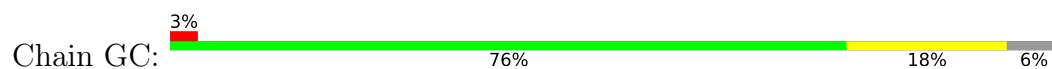
• Molecule 1: Capsid protein VP1

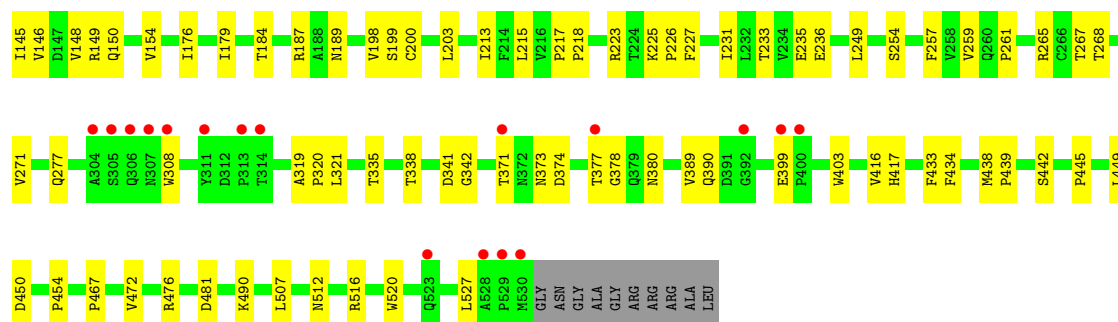


• Molecule 1: Capsid protein VP1

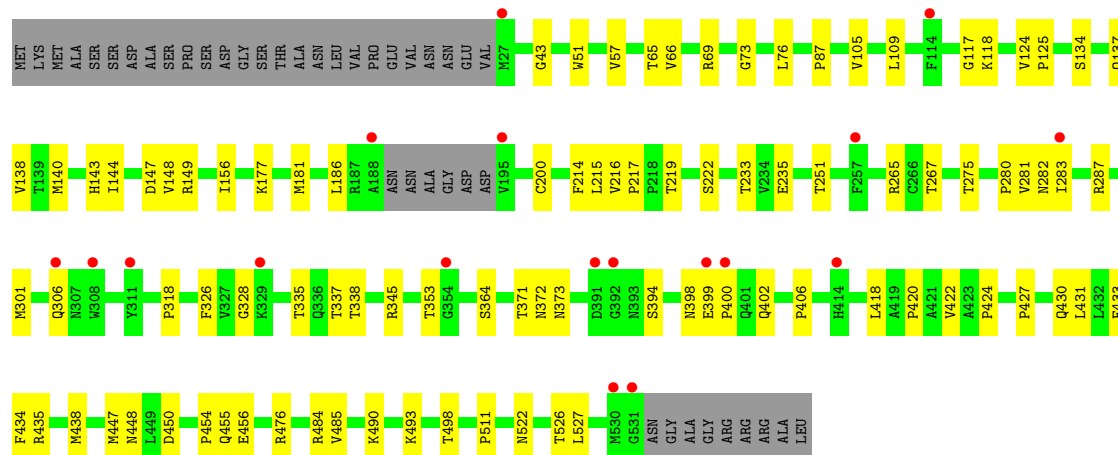
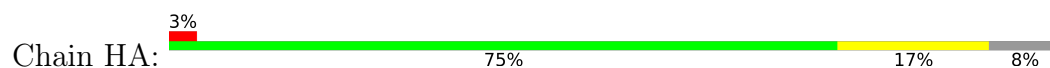


• Molecule 1: Capsid protein VP1

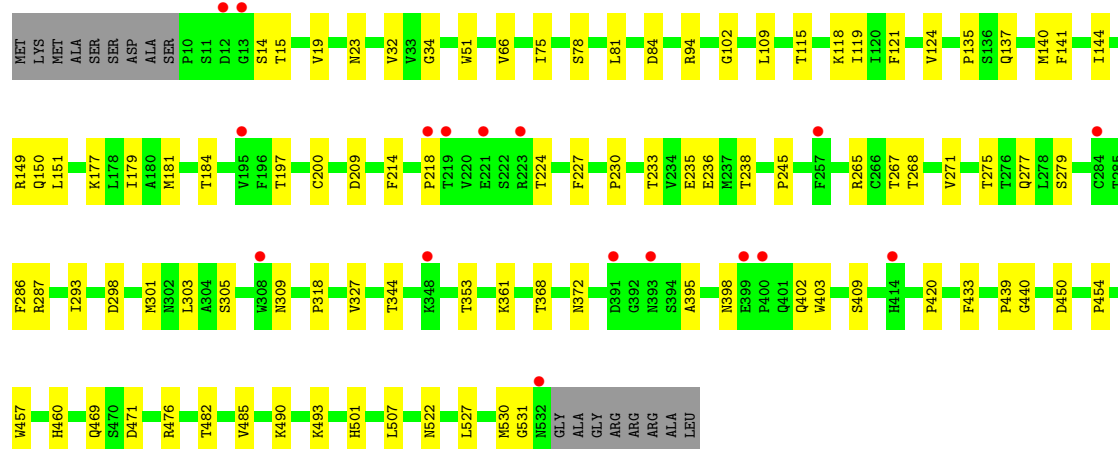
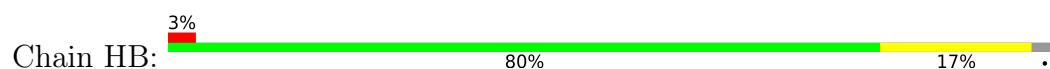




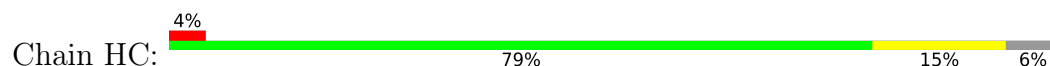
• Molecule 1: Capsid protein VP1

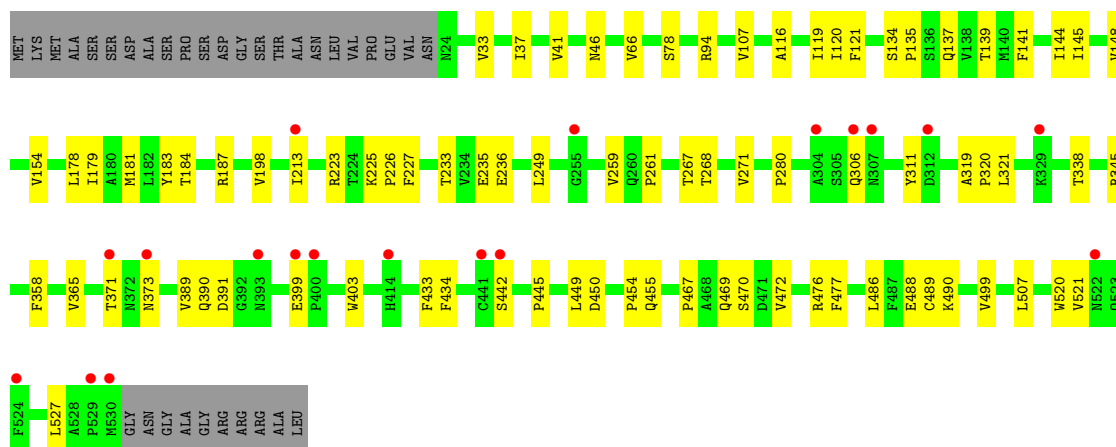


• Molecule 1: Capsid protein VP1

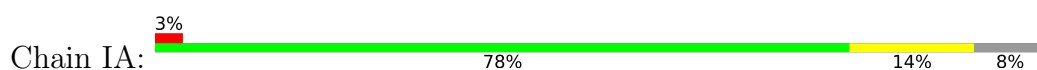


• Molecule 1: Capsid protein VP1

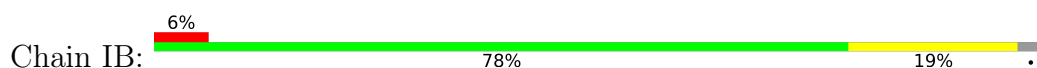




• Molecule 1: Capsid protein VP1

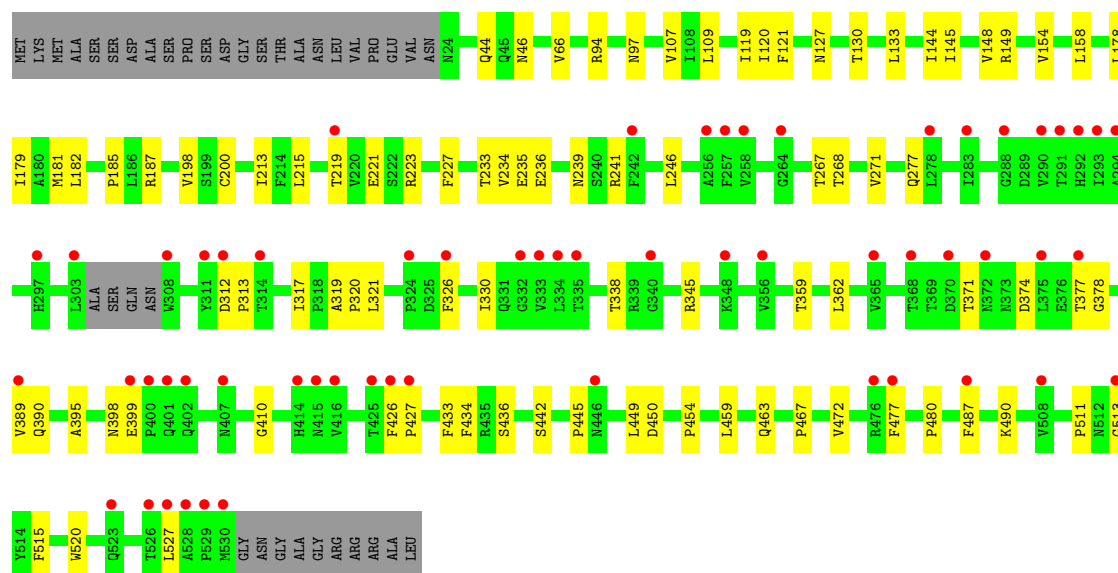


• Molecule 1: Capsid protein VP1



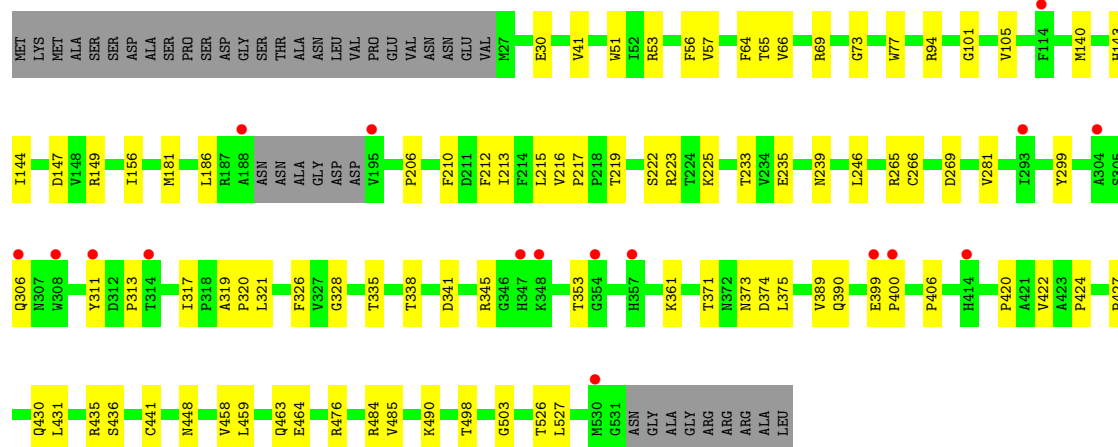
• Molecule 1: Capsid protein VP1

Chain IC: 



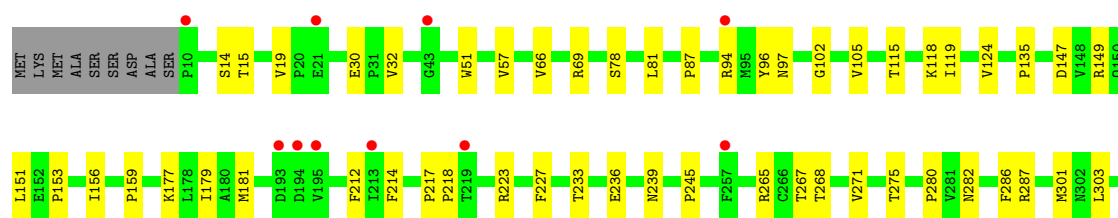
• Molecule 1: Capsid protein VP1

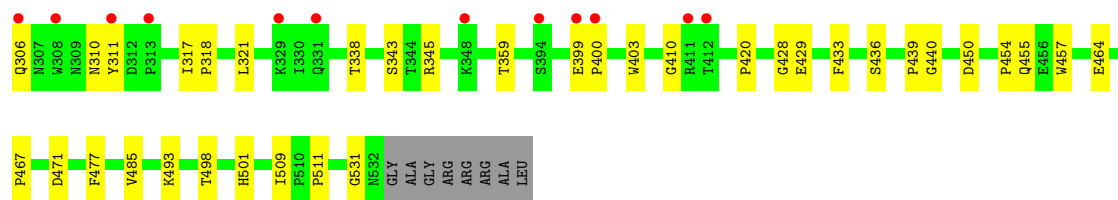
Chain JA: 



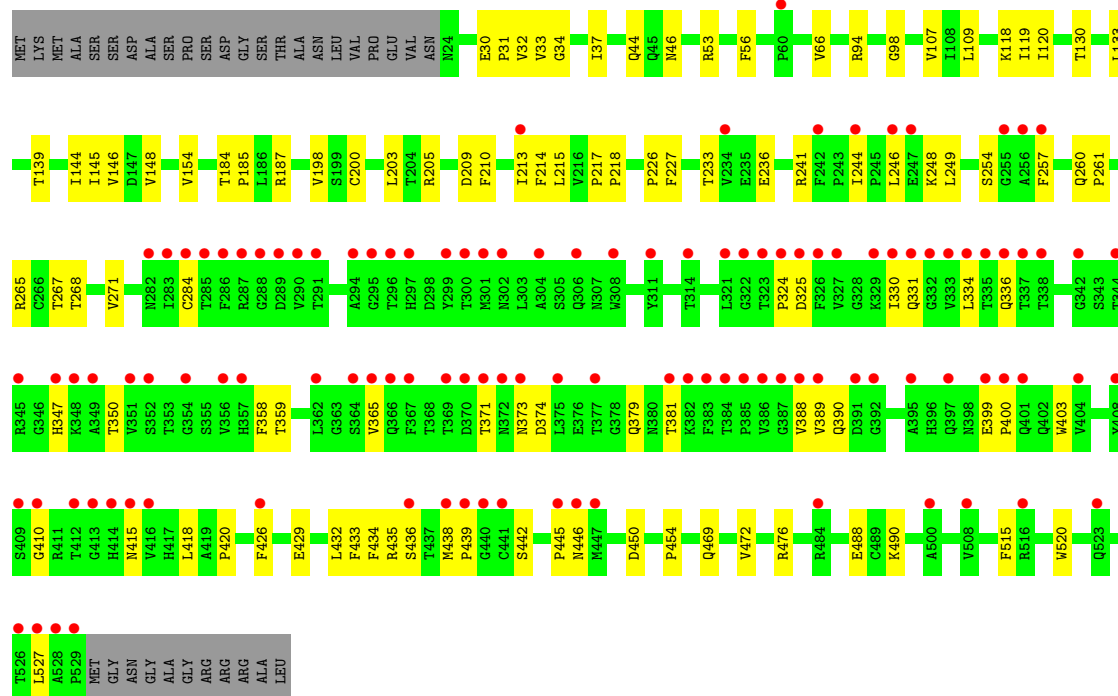
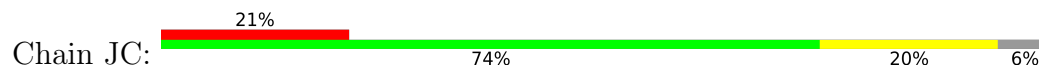
• Molecule 1: Capsid protein VP1

Chain JB: 

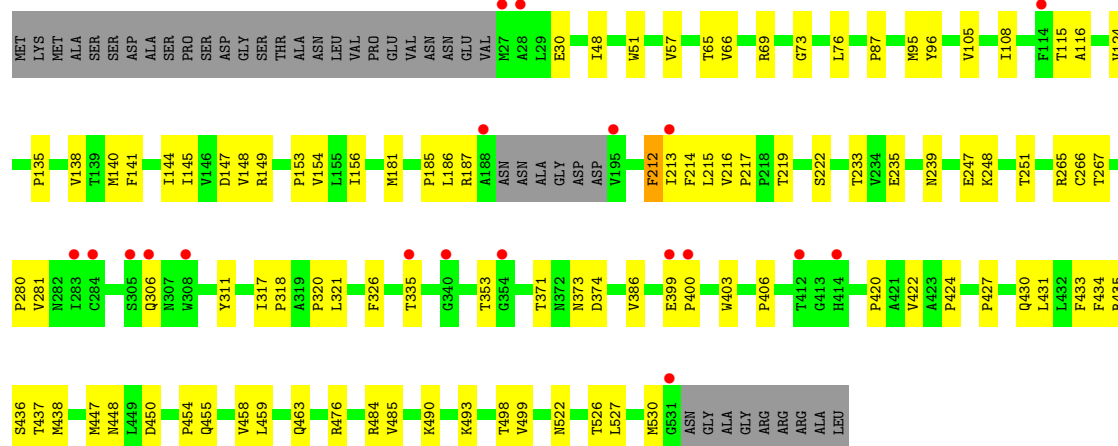
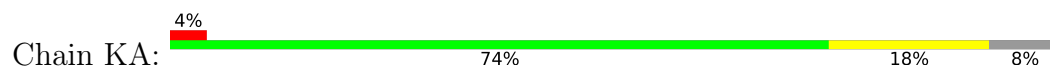




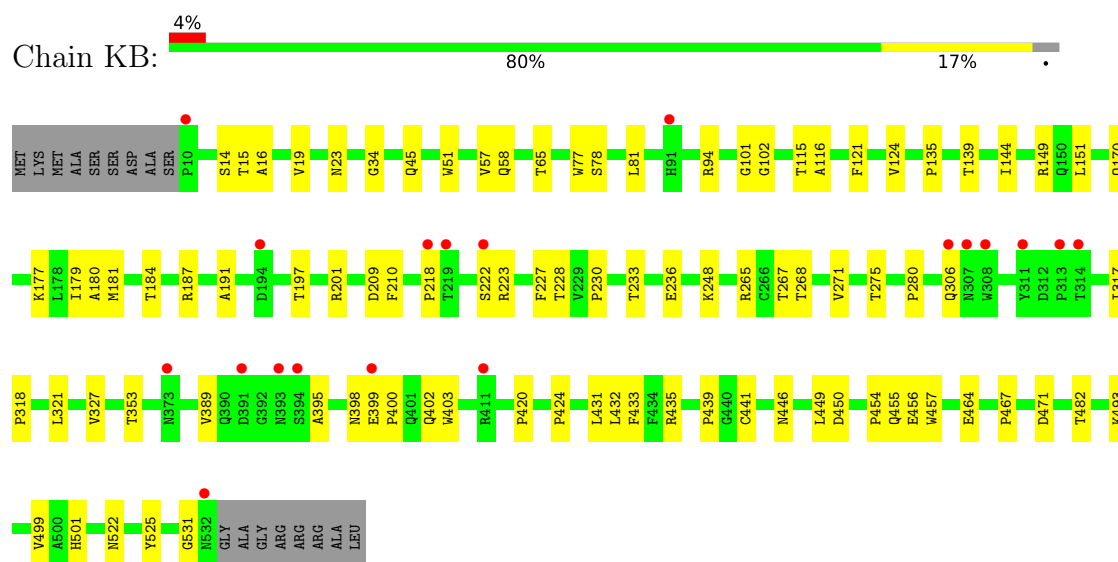
• Molecule 1: Capsid protein VP1



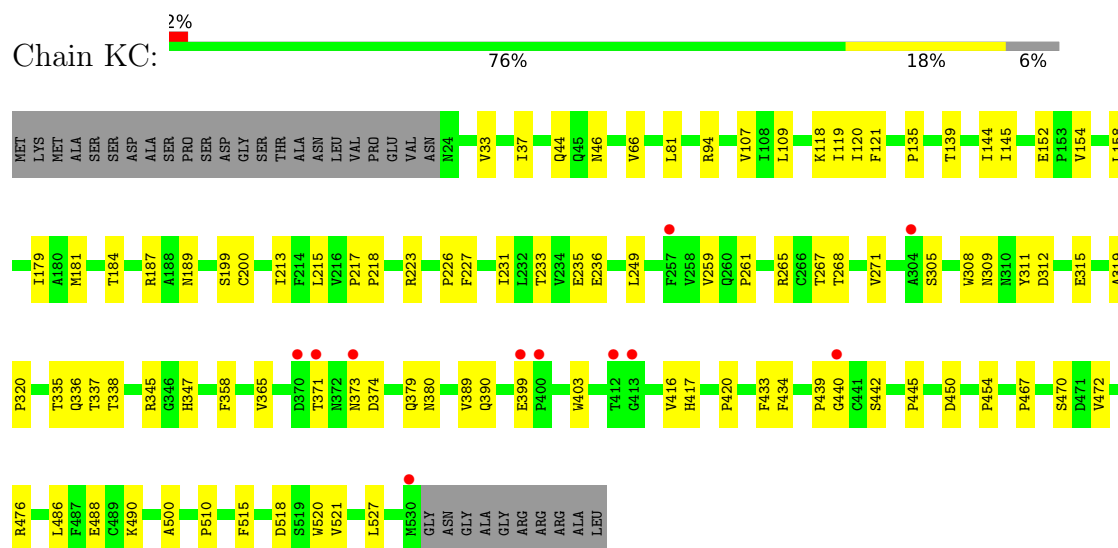
• Molecule 1: Capsid protein VP1



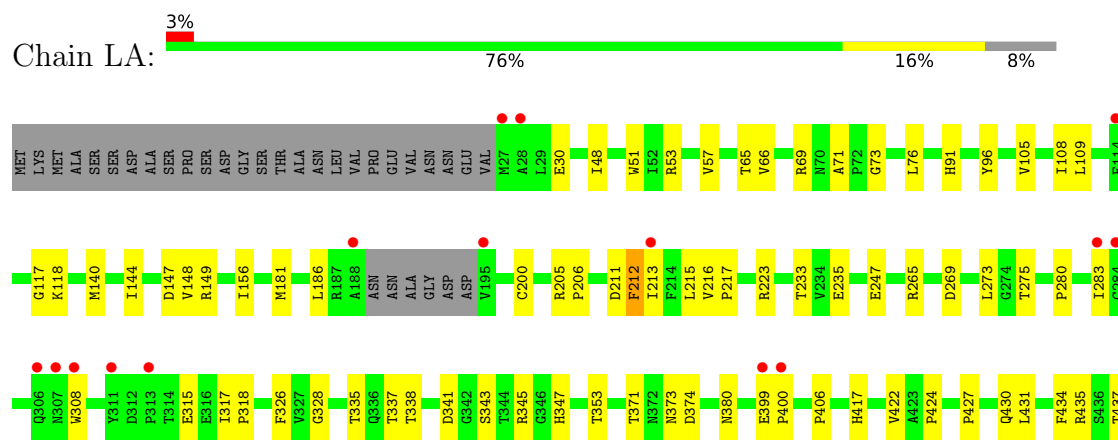
• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1

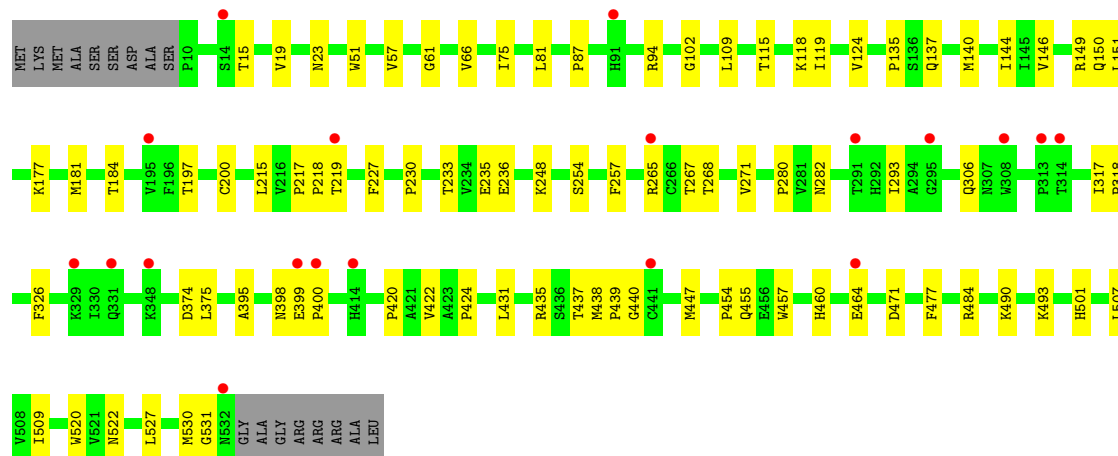
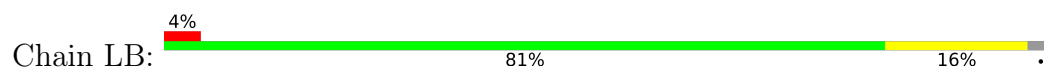


• Molecule 1: Capsid protein VP1

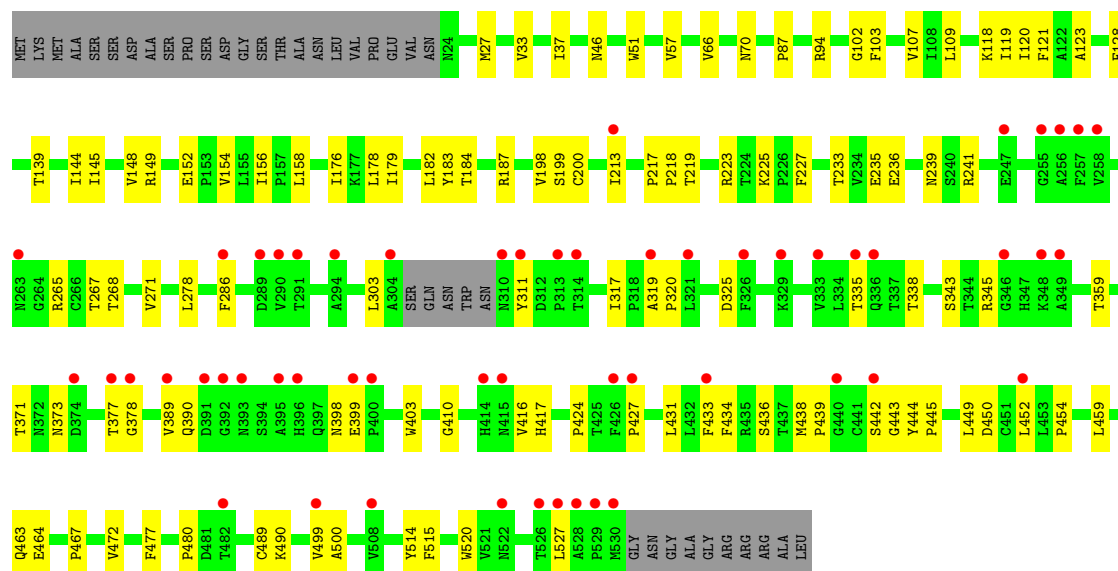
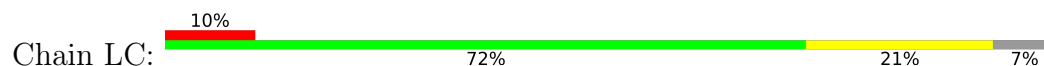




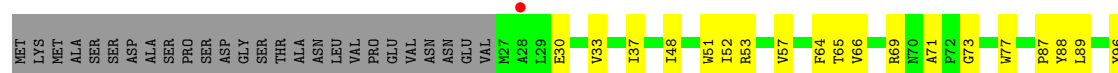
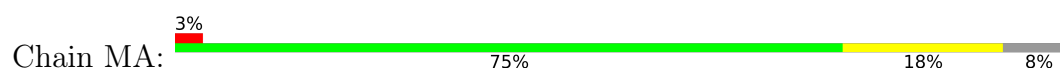
• Molecule 1: Capsid protein VP1

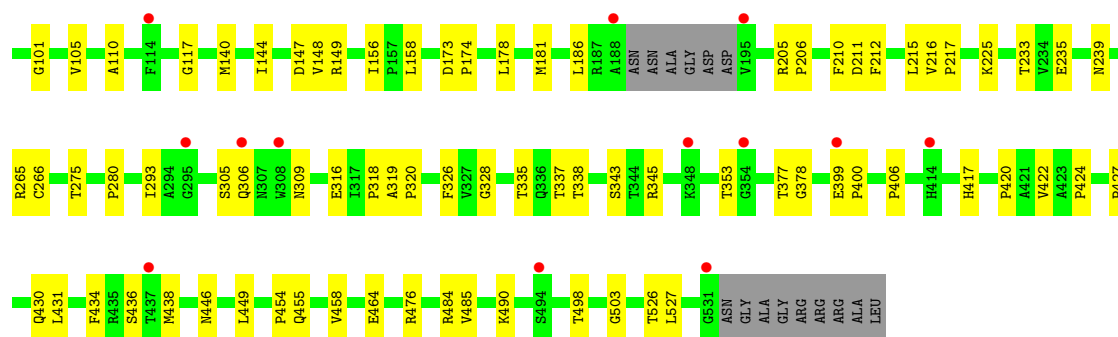


• Molecule 1: Capsid protein VP1

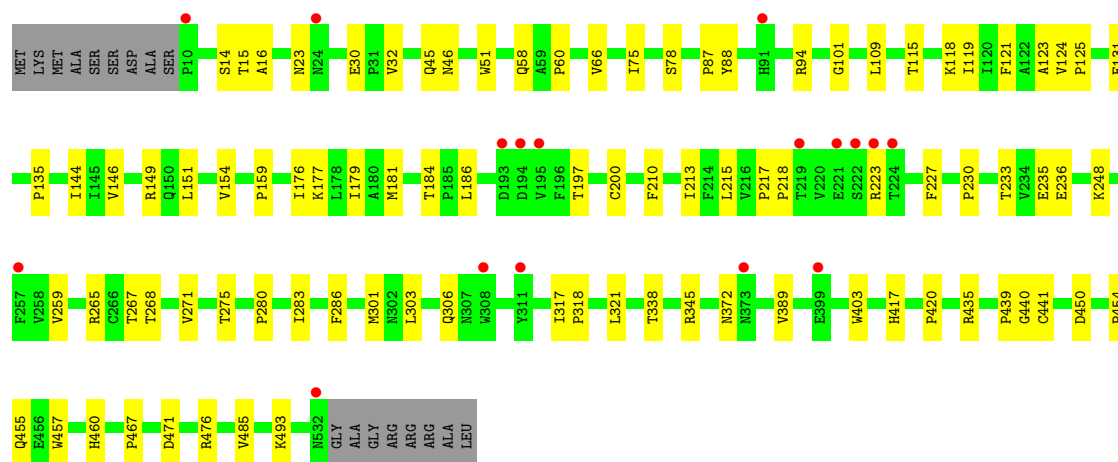
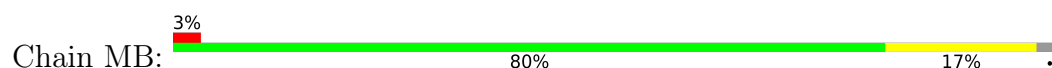


• Molecule 1: Capsid protein VP1

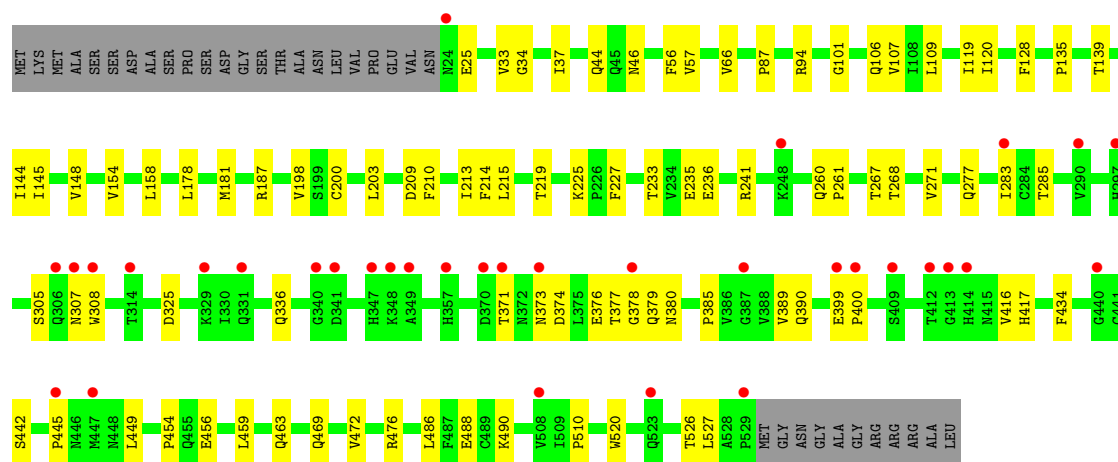
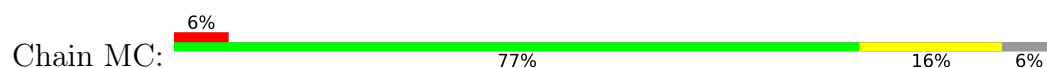




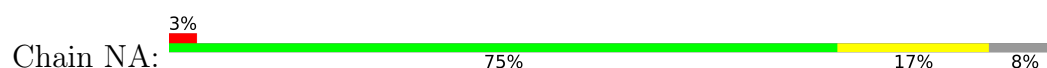
• Molecule 1: Capsid protein VP1



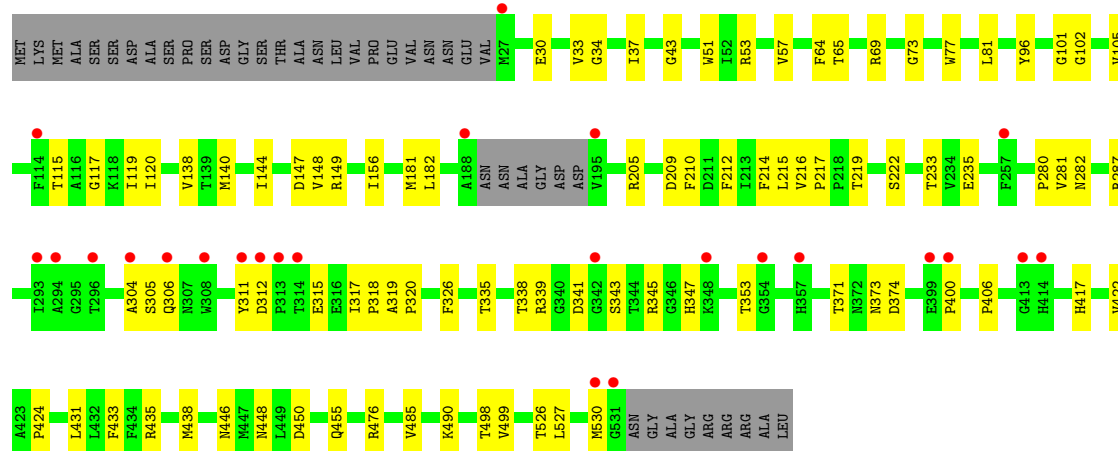
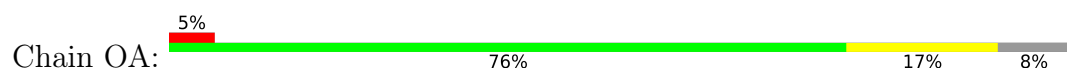
• Molecule 1: Capsid protein VP1



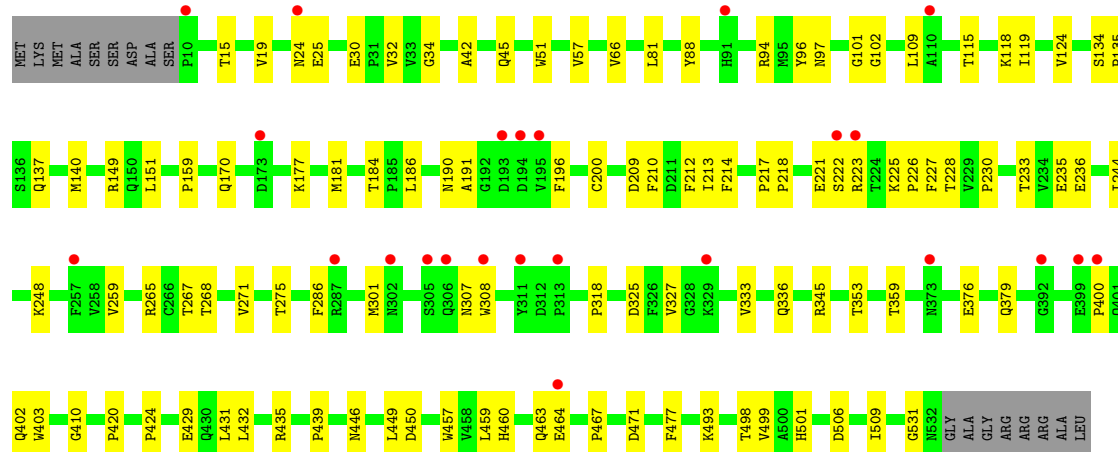
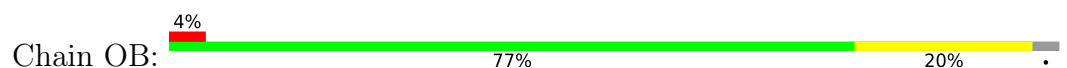
• Molecule 1: Capsid protein VP1



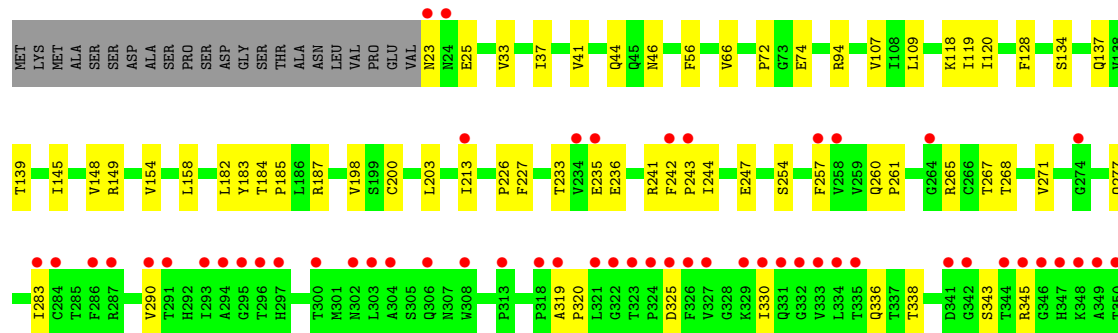
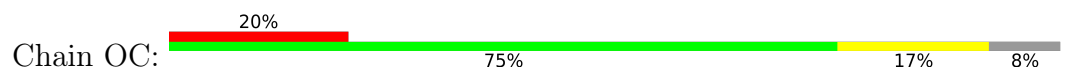
WORLDWIDE
PDB
PROTEIN DATA BANK

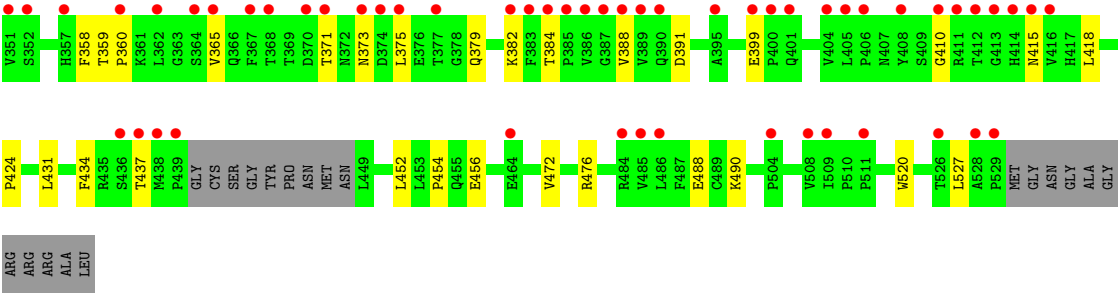


• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	420.17Å 446.60Å 463.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (30.00-3.00) 95.7 (30.00-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.207 , 0.242 0.207 , 0.242	Depositor DCC
R_{free} test set	40728 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	176522	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CL, CD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.16	0/3978	0.43	0/5458
1	AB	0.16	0/4134	0.43	0/5677
1	AC	0.16	0/4040	0.45	0/5545
1	BA	0.15	0/3971	0.42	0/5448
1	BB	0.16	0/4140	0.46	0/5684
1	BC	0.15	0/4032	0.44	0/5534
1	CA	0.16	0/3971	0.44	0/5448
1	CB	0.16	0/4134	0.45	0/5677
1	CC	0.16	0/4032	0.44	0/5534
1	DA	0.16	0/3963	0.43	0/5438
1	DB	0.17	0/4134	0.46	0/5677
1	DC	0.15	0/4025	0.45	0/5525
1	EA	0.16	0/3971	0.45	1/5448 (0.0%)
1	EB	0.16	0/4134	0.45	0/5677
1	EC	0.16	0/3929	0.45	0/5392
1	FA	0.16	0/3971	0.43	0/5448
1	FB	0.16	0/4140	0.46	1/5684 (0.0%)
1	FC	0.16	0/4047	0.44	0/5555
1	GA	0.16	0/3971	0.43	0/5448
1	GB	0.16	0/4137	0.46	0/5680
1	GC	0.16	0/4032	0.43	0/5534
1	HA	0.15	0/3971	0.42	0/5448
1	HB	0.16	0/4136	0.45	0/5679
1	HC	0.15	0/4032	0.42	0/5534
1	IA	0.16	0/3971	0.42	0/5448
1	IB	0.17	0/4140	0.45	0/5683
1	IC	0.16	0/4003	0.44	0/5493
1	JA	0.16	0/3971	0.45	3/5448 (0.1%)
1	JB	0.15	0/4128	0.44	0/5669
1	JC	0.15	0/4025	0.43	0/5525
1	KA	0.16	0/3971	0.45	3/5448 (0.1%)
1	KB	0.16	0/4130	0.43	0/5672

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	KC	0.15	0/4032	0.43	0/5534
1	LA	0.16	0/3971	0.45	3/5448 (0.1%)
1	LB	0.16	0/4124	0.44	0/5664
1	LC	0.16	0/3981	0.44	0/5462
1	MA	0.15	0/3971	0.43	0/5448
1	MB	0.29	1/4131 (0.0%)	0.46	0/5673
1	MC	0.15	0/4025	0.43	0/5525
1	NA	0.16	0/3971	0.44	0/5448
1	NB	0.16	0/4138	0.44	0/5680
1	NC	0.15	0/4018	0.42	0/5516
1	OA	0.15	0/3971	0.43	0/5448
1	OB	0.16	0/4138	0.44	0/5680
1	OC	0.15	0/3967	0.43	0/5445
All	All	0.16	1/181802 (0.0%)	0.44	11/249529 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	MB	217	PRO	N-CD	-15.10	1.26	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	LA	213	ILE	N-CA-C	7.75	117.74	111.62
1	KA	213	ILE	N-CA-C	7.13	117.26	111.62
1	JA	213	ILE	N-CA-C	6.97	117.13	111.62
1	JA	212	PHE	CA-C-N	-6.55	116.22	123.16
1	JA	212	PHE	C-N-CA	-6.55	116.22	123.16
1	KA	212	PHE	CA-C-N	-6.17	116.62	123.16
1	KA	212	PHE	C-N-CA	-6.17	116.62	123.16
1	LA	212	PHE	CA-C-N	-6.04	116.75	123.16
1	LA	212	PHE	C-N-CA	-6.04	116.75	123.16
1	FB	61	GLY	N-CA-C	-5.25	100.75	113.18
1	EA	61	GLY	N-CA-C	-5.24	100.76	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	3860	0	3758	69	0
1	AB	4013	0	3874	69	0
1	AC	3921	0	3802	65	0
1	BA	3853	0	3749	67	0
1	BB	4019	0	3885	68	0
1	BC	3913	0	3796	74	0
1	CA	3853	0	3749	79	0
1	CB	4013	0	3874	68	0
1	CC	3913	0	3796	57	0
1	DA	3845	0	3740	89	0
1	DB	4013	0	3874	78	0
1	DC	3906	0	3787	70	0
1	EA	3853	0	3749	68	0
1	EB	4013	0	3874	66	0
1	EC	3814	0	3705	76	0
1	FA	3853	0	3749	82	0
1	FB	4019	0	3885	75	0
1	FC	3928	0	3811	70	0
1	GA	3853	0	3749	75	0
1	GB	4016	0	3883	74	0
1	GC	3913	0	3796	68	0
1	HA	3853	0	3749	70	0
1	HB	4015	0	3881	71	0
1	HC	3913	0	3796	58	0
1	IA	3853	0	3749	58	0
1	IB	4019	0	3892	73	0
1	IC	3885	0	3771	63	0
1	JA	3853	0	3749	70	0
1	JB	4007	0	3870	61	0
1	JC	3906	0	3787	72	0
1	KA	3853	0	3749	76	0
1	KB	4009	0	3870	70	0
1	KC	3913	0	3796	63	0
1	LA	3853	0	3749	69	0
1	LB	4003	0	3866	60	0
1	LC	3865	0	3758	84	0
1	MA	3853	0	3749	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	MB	4010	0	3872	71	0
1	MC	3906	0	3787	62	0
1	NA	3853	0	3749	69	0
1	NB	4017	0	3892	58	0
1	NC	3899	0	3781	66	0
1	OA	3853	0	3749	67	0
1	OB	4017	0	3892	77	0
1	OC	3851	0	3739	62	0
2	AA	3	0	0	0	0
2	AB	1	0	0	0	0
2	AC	1	0	0	0	0
2	BA	2	0	0	0	0
2	BC	1	0	0	0	0
2	CA	2	0	0	0	0
2	CC	3	0	0	1	0
2	DA	1	0	0	0	0
2	DB	1	0	0	0	0
2	DC	2	0	0	0	0
2	EA	3	0	0	0	0
2	FA	2	0	0	0	0
2	GA	1	0	0	0	0
2	GC	2	0	0	0	0
2	HA	1	0	0	0	0
2	HC	1	0	0	0	0
2	IA	3	0	0	0	0
2	JA	3	0	0	0	0
2	KA	2	0	0	0	0
2	KC	2	0	0	0	0
2	LA	1	0	0	0	0
2	LC	2	0	0	0	0
2	MA	3	0	0	0	0
2	MC	2	0	0	1	0
2	NA	2	0	0	0	0
2	NC	1	0	0	0	0
2	OA	2	0	0	0	0
3	AC	1	0	0	0	0
3	BA	1	0	0	0	0
3	BC	1	0	0	0	0
3	CA	1	0	0	0	0
3	DA	1	0	0	0	0
3	EA	1	0	0	0	0
3	EB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	EC	1	0	0	0	0
3	FA	1	0	0	0	0
3	FC	1	0	0	0	0
3	GA	1	0	0	0	0
3	GB	1	0	0	0	0
3	HC	1	0	0	0	0
3	IA	1	0	0	0	0
3	JA	1	0	0	0	0
3	JC	1	0	0	0	0
3	KA	1	0	0	0	0
3	KB	1	0	0	0	0
3	MA	1	0	0	0	0
3	MB	1	0	0	0	0
3	NC	1	0	0	0	0
3	OA	1	0	0	0	0
4	JA	4	0	6	0	0
5	HC	1	0	0	0	0
5	OA	1	0	0	0	0
5	OB	1	0	0	0	0
All	All	176522	0	171133	2813	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (2813) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NA:65:THR:HG21	1:NA:526:THR:H	1.25	1.01
1:GA:65:THR:HG21	1:GA:526:THR:H	1.25	1.01
1:AA:65:THR:HG21	1:AA:526:THR:H	1.23	1.00
1:MA:65:THR:HG21	1:MA:526:THR:H	1.28	0.98
1:CA:65:THR:HG21	1:CA:526:THR:H	1.30	0.96
1:OA:65:THR:HG21	1:OA:526:THR:H	1.30	0.96
1:FA:65:THR:HG21	1:FA:526:THR:H	1.27	0.96
1:BA:65:THR:HG21	1:BA:526:THR:H	1.32	0.95
1:HA:65:THR:HG21	1:HA:526:THR:H	1.29	0.95
1:KA:65:THR:HG21	1:KA:526:THR:H	1.32	0.95
1:LA:65:THR:HG21	1:LA:526:THR:H	1.32	0.93
1:DA:65:THR:HG21	1:DA:526:THR:H	1.32	0.93
1:JA:65:THR:HG21	1:JA:526:THR:H	1.30	0.93
1:EA:65:THR:HG21	1:EA:526:THR:H	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FA:120:ILE:HG12	1:FA:145:ILE:HG12	1.56	0.88
1:KC:267:THR:HG22	1:KC:271:VAL:H	1.39	0.87
1:CA:46:ASN:ND2	1:CA:213:ILE:O	2.07	0.87
1:EC:94:ARG:HD2	1:EC:219:THR:HG22	1.57	0.86
1:AA:46:ASN:ND2	1:AA:213:ILE:O	2.10	0.84
1:DC:94:ARG:HD2	1:DC:219:THR:HG22	1.59	0.83
1:DA:120:ILE:HG12	1:DA:145:ILE:HG12	1.58	0.82
1:HB:137:GLN:HA	1:HB:140:MET:HE3	1.61	0.82
1:CB:223:ARG:HA	1:CB:467:PRO:HG3	1.62	0.82
1:HC:371:THR:HG22	1:HC:373:ASN:H	1.42	0.82
1:FB:120:ILE:HG12	1:FB:145:ILE:HG12	1.62	0.80
1:JB:267:THR:HG22	1:JB:271:VAL:H	1.47	0.80
1:GC:371:THR:HG22	1:GC:373:ASN:H	1.47	0.80
1:LC:371:THR:HG22	1:LC:373:ASN:H	1.47	0.79
1:EB:12:ASP:OD1	1:GB:17:ASN:ND2	2.13	0.79
1:OB:137:GLN:HA	1:OB:140:MET:HE3	1.64	0.79
1:IC:94:ARG:HD2	1:IC:219:THR:HG22	1.63	0.79
1:MC:486:LEU:HD11	1:MC:510:PRO:HD2	1.63	0.79
1:NA:306:GLN:NE2	1:NA:321:LEU:O	2.16	0.79
1:FB:439:PRO:HB3	1:GA:335:THR:HG21	1.65	0.78
1:IB:265:ARG:NH2	1:IB:420:PRO:O	2.17	0.78
1:OC:382:LYS:NZ	1:OC:384:THR:OG1	2.17	0.78
1:GB:277:GLN:HE22	1:GB:279:SER:HB3	1.49	0.78
1:MB:286:PHE:HB3	1:MB:301:MET:HE1	1.64	0.78
1:DB:15:THR:HG21	1:DB:151:LEU:HD11	1.66	0.78
1:MB:267:THR:HG22	1:MB:271:VAL:H	1.48	0.78
1:GC:46:ASN:ND2	1:GC:213:ILE:O	2.17	0.78
1:BC:268:THR:HG21	1:BC:520:TRP:HH2	1.49	0.77
1:GC:233:THR:HB	1:GC:236:GLU:HG3	1.65	0.77
1:EA:120:ILE:HG12	1:EA:145:ILE:HG12	1.66	0.77
1:NC:267:THR:HG22	1:NC:271:VAL:H	1.50	0.77
1:CC:371:THR:HG22	1:CC:373:ASN:H	1.48	0.77
1:AA:144:ILE:HD12	1:AA:156:ILE:HG12	1.64	0.77
1:DB:120:ILE:HG12	1:DB:145:ILE:HG12	1.66	0.77
1:NB:15:THR:HG22	1:OC:149:ARG:HE	1.47	0.77
1:DB:286:PHE:HB3	1:DB:301:MET:HE1	1.66	0.77
1:IB:121:PHE:HB2	1:IB:144:ILE:HG22	1.64	0.77
1:HB:15:THR:HG21	1:HB:151:LEU:HD11	1.66	0.76
1:JA:265:ARG:NH2	1:JA:420:PRO:O	2.17	0.76
1:LC:94:ARG:HD2	1:LC:219:THR:HG22	1.67	0.76
1:GB:248:LYS:HE3	1:GB:435:ARG:HD2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IA:65:THR:HG21	1:IA:526:THR:HB	1.68	0.76
1:EC:359:THR:HG22	1:EC:410:GLY:HA3	1.68	0.76
1:IC:267:THR:HG22	1:IC:271:VAL:H	1.50	0.76
1:GC:268:THR:HG21	1:GC:520:TRP:HH2	1.51	0.76
1:EA:265:ARG:NH2	1:EA:420:PRO:O	2.19	0.75
1:DC:268:THR:HG21	1:DC:520:TRP:HH2	1.49	0.75
1:JC:233:THR:HB	1:JC:236:GLU:HG3	1.68	0.75
1:DB:439:PRO:HB3	1:EA:335:THR:HG21	1.68	0.75
1:BA:140:MET:HE1	1:BB:218:PRO:HD3	1.69	0.75
1:DA:120:ILE:HG13	1:DA:183:TYR:HB2	1.68	0.75
1:KA:484:ARG:NH2	1:OA:69:ARG:O	2.20	0.75
1:BC:94:ARG:HD2	1:BC:219:THR:HG22	1.68	0.74
1:MC:371:THR:HG22	1:MC:373:ASN:H	1.52	0.74
1:NC:94:ARG:HD2	1:NC:219:THR:HG22	1.66	0.74
1:KB:223:ARG:HA	1:KB:467:PRO:HG3	1.69	0.74
1:DC:267:THR:HG22	1:DC:271:VAL:H	1.51	0.74
1:AC:476:ARG:HD3	1:AC:488:GLU:HB3	1.67	0.74
1:DB:267:THR:HG22	1:DB:271:VAL:H	1.51	0.74
1:IB:248:LYS:HE3	1:IB:435:ARG:HD2	1.68	0.74
1:FB:135:PRO:HA	1:FB:181:MET:HE1	1.68	0.74
1:MA:149:ARG:NH1	1:NA:111:GLY:O	2.20	0.74
1:AC:268:THR:HG21	1:AC:520:TRP:HH2	1.52	0.74
1:EA:120:ILE:HG13	1:EA:183:TYR:HB2	1.70	0.74
1:NA:265:ARG:NH2	1:NA:420:PRO:O	2.19	0.74
1:KC:46:ASN:ND2	1:KC:213:ILE:O	2.19	0.74
1:HB:267:THR:HG22	1:HB:271:VAL:H	1.53	0.73
1:EB:120:ILE:HG12	1:EB:145:ILE:HG12	1.70	0.73
1:KB:265:ARG:NH2	1:KB:420:PRO:O	2.21	0.73
1:AC:359:THR:HG22	1:AC:410:GLY:H	1.54	0.73
1:CB:267:THR:HG22	1:CB:271:VAL:H	1.52	0.73
1:JC:371:THR:HG22	1:JC:373:ASN:H	1.53	0.73
1:LB:248:LYS:HE3	1:LB:435:ARG:HD2	1.71	0.73
1:OB:15:THR:HG21	1:OB:151:LEU:HD11	1.69	0.73
1:AC:267:THR:HG22	1:AC:271:VAL:H	1.54	0.73
1:EA:303:LEU:HD11	1:EA:365:VAL:HG22	1.71	0.73
1:FA:120:ILE:HG13	1:FA:183:TYR:HB2	1.70	0.73
1:GB:15:THR:HG21	1:GB:151:LEU:HD11	1.69	0.73
1:AC:371:THR:HG22	1:AC:373:ASN:H	1.52	0.73
1:EA:144:ILE:HD12	1:EA:156:ILE:HG12	1.70	0.73
1:FC:33:VAL:HG11	1:FC:37:ILE:HG13	1.70	0.73
1:IC:46:ASN:ND2	1:IC:213:ILE:O	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HA:282:ASN:OD1	1:HA:287:ARG:NH2	2.22	0.73
1:LC:268:THR:HG21	1:LC:520:TRP:HH2	1.52	0.73
1:AB:267:THR:HG22	1:AB:271:VAL:H	1.52	0.72
1:NC:233:THR:HB	1:NC:236:GLU:HG3	1.71	0.72
1:BB:267:THR:HG22	1:BB:271:VAL:H	1.54	0.72
1:EC:233:THR:HB	1:EC:236:GLU:HG3	1.71	0.72
1:EC:334:LEU:HD22	1:EC:381:THR:HG22	1.71	0.72
1:BB:345:ARG:NH2	1:BB:376:GLU:OE1	2.23	0.72
1:HA:233:THR:HG22	1:HA:235:GLU:H	1.54	0.72
1:HC:268:THR:HG21	1:HC:520:TRP:HH2	1.53	0.72
1:HA:251:THR:HG22	1:HA:430:GLN:HE21	1.54	0.72
1:IC:268:THR:HG21	1:IC:520:TRP:HH2	1.53	0.72
1:JA:338:THR:OG1	1:JA:345:ARG:NH2	2.17	0.72
1:HC:233:THR:HB	1:HC:236:GLU:HG3	1.70	0.72
1:FC:267:THR:HG22	1:FC:271:VAL:H	1.55	0.72
1:JB:317:ILE:HG13	1:JB:318:PRO:HD2	1.71	0.72
1:JC:268:THR:HG21	1:JC:520:TRP:HH2	1.55	0.72
1:AB:120:ILE:HG12	1:AB:145:ILE:HG12	1.71	0.72
1:EC:316:GLU:OE1	1:EC:417:HIS:NE2	2.22	0.72
1:KC:268:THR:HG21	1:KC:520:TRP:HH2	1.55	0.72
1:LC:390:GLN:HG2	1:LC:399:GLU:HG2	1.72	0.72
1:BA:144:ILE:HD12	1:BA:156:ILE:HG12	1.72	0.71
1:EC:46:ASN:ND2	1:EC:213:ILE:O	2.21	0.71
1:CB:439:PRO:HB3	1:DA:335:THR:HG21	1.70	0.71
1:KB:170:GLN:NE2	1:KB:222:SER:O	2.22	0.71
1:FA:312:ASP:HB3	1:FA:315:GLU:HG3	1.72	0.71
1:GB:135:PRO:HA	1:GB:181:MET:HE1	1.72	0.71
1:IA:69:ARG:O	1:JA:484:ARG:NH2	2.24	0.71
1:MA:265:ARG:NH2	1:MA:420:PRO:O	2.24	0.71
1:FA:338:THR:OG1	1:FA:345:ARG:NH2	2.22	0.71
1:LC:267:THR:HG22	1:LC:271:VAL:H	1.55	0.71
1:FA:335:THR:HG21	1:JB:439:PRO:HB3	1.72	0.71
1:IB:94:ARG:HG2	1:IB:224:THR:HG23	1.73	0.71
1:LA:233:THR:HG22	1:LA:235:GLU:H	1.54	0.71
1:AC:233:THR:HB	1:AC:236:GLU:HG3	1.72	0.71
1:IB:411:ARG:NH1	1:IB:412:THR:OG1	2.24	0.71
1:FB:15:THR:HG21	1:FB:151:LEU:HD11	1.73	0.71
1:OC:268:THR:HG21	1:OC:520:TRP:HH2	1.55	0.71
1:IC:44:GLN:NE2	1:IC:215:LEU:H	1.89	0.70
1:MC:336:GLN:HE21	1:MC:379:GLN:HB2	1.55	0.70
1:JB:135:PRO:HA	1:JB:181:MET:HE1	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:476:ARG:HD3	1:EA:485:VAL:HG11	1.73	0.70
1:OB:265:ARG:NH2	1:OB:420:PRO:O	2.24	0.70
1:IB:225:LYS:HE3	1:IB:464:GLU:HG3	1.72	0.70
1:KC:338:THR:OG1	1:KC:345:ARG:NH2	2.24	0.70
1:HB:439:PRO:HB3	1:IA:335:THR:HG21	1.72	0.70
1:FA:216:VAL:HG22	1:FA:217:PRO:HD2	1.74	0.70
1:FC:97:ASN:ND2	1:FC:221:GLU:OE2	2.25	0.70
1:DA:73:GLY:H	1:DA:181:MET:HE3	1.57	0.70
1:MB:223:ARG:HA	1:MB:467:PRO:HG3	1.74	0.70
1:OB:248:LYS:HE3	1:OB:435:ARG:HD2	1.74	0.70
1:AA:265:ARG:NH2	1:AA:420:PRO:O	2.25	0.69
1:GA:476:ARG:HD3	1:GA:485:VAL:HG11	1.74	0.69
1:CC:233:THR:HB	1:CC:236:GLU:HG3	1.73	0.69
1:FC:66:VAL:HG21	1:FC:119:ILE:HD11	1.74	0.69
1:KB:267:THR:HG22	1:KB:271:VAL:H	1.57	0.69
1:MA:338:THR:OG1	1:MA:345:ARG:NH2	2.25	0.69
1:MB:439:PRO:HB3	1:NA:335:THR:HG21	1.75	0.69
1:IB:439:PRO:HB3	1:JA:335:THR:HG21	1.73	0.69
1:KC:66:VAL:HG21	1:KC:119:ILE:HD11	1.73	0.69
1:BB:137:GLN:HA	1:BB:140:MET:HE3	1.75	0.69
1:FC:439:PRO:HB3	1:LC:335:THR:HG21	1.73	0.69
1:HA:147:ASP:OD1	1:HA:149:ARG:HG2	1.92	0.69
1:OB:275:THR:HG23	1:OB:318:PRO:HG2	1.72	0.69
1:BC:33:VAL:HG11	1:BC:37:ILE:HG13	1.75	0.69
1:DB:244:ILE:HD11	1:DB:439:PRO:HD3	1.74	0.69
1:KA:149:ARG:NH2	1:LA:149:ARG:O	2.26	0.69
1:KB:23:ASN:HD22	1:KB:144:ILE:HD11	1.55	0.69
1:OA:140:MET:HB2	1:OB:217:PRO:HG3	1.75	0.69
1:CB:197:THR:O	1:DC:187:ARG:NH1	2.25	0.69
1:GB:275:THR:HG23	1:GB:318:PRO:HG2	1.74	0.69
1:NC:438:MET:HE2	1:NC:449:LEU:HB2	1.75	0.69
1:DC:33:VAL:HG11	1:DC:37:ILE:HG13	1.73	0.69
1:JB:265:ARG:NH2	1:JB:420:PRO:O	2.26	0.68
1:AA:216:VAL:HG22	1:AA:217:PRO:HD2	1.76	0.68
1:BC:233:THR:HB	1:BC:236:GLU:HG3	1.74	0.68
1:KA:335:THR:HG21	1:OB:439:PRO:HB3	1.74	0.68
1:MA:69:ARG:HH21	1:MA:427:PRO:HB2	1.58	0.68
1:BB:439:PRO:HB3	1:CA:335:THR:HG21	1.76	0.68
1:AA:140:MET:HB2	1:AB:217:PRO:HG3	1.76	0.68
1:MC:66:VAL:HG21	1:MC:119:ILE:HD11	1.75	0.68
1:BC:66:VAL:HG21	1:BC:119:ILE:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OC:391:ASP:H	1:OC:399:GLU:HG3	1.58	0.68
1:AA:335:THR:HG21	1:EB:439:PRO:HB3	1.75	0.68
1:FB:33:VAL:HG21	1:FB:37:ILE:HG13	1.76	0.68
1:IC:233:THR:HB	1:IC:236:GLU:HG3	1.74	0.68
1:KB:197:THR:HB	1:LC:187:ARG:HH11	1.59	0.68
1:NC:44:GLN:NE2	1:NC:215:LEU:H	1.92	0.68
1:CC:267:THR:HG22	1:CC:271:VAL:H	1.57	0.68
1:FA:149:ARG:O	1:JA:149:ARG:NH2	2.27	0.68
1:HC:267:THR:HG22	1:HC:271:VAL:H	1.59	0.68
1:LC:66:VAL:HG21	1:LC:119:ILE:HD11	1.74	0.68
1:MC:233:THR:HB	1:MC:236:GLU:HG3	1.76	0.68
1:GB:121:PHE:HB2	1:GB:144:ILE:HG22	1.76	0.68
1:HC:66:VAL:HG21	1:HC:119:ILE:HD11	1.74	0.68
1:JC:66:VAL:HG21	1:JC:119:ILE:HD11	1.75	0.68
1:CA:73:GLY:H	1:CA:181:MET:HE3	1.59	0.67
1:CA:216:VAL:HG22	1:CA:217:PRO:HD2	1.75	0.67
1:FB:62:GLY:HA2	1:FB:202:VAL:HB	1.76	0.67
1:IC:66:VAL:HG21	1:IC:119:ILE:HD11	1.75	0.67
1:KB:275:THR:HG23	1:KB:318:PRO:HG2	1.76	0.67
1:HB:23:ASN:ND2	1:HB:144:ILE:HD11	2.09	0.67
1:AC:439:PRO:HB3	1:GC:335:THR:HG21	1.76	0.67
1:BA:424:PRO:HD3	1:BA:431:LEU:HD13	1.76	0.67
1:GC:24:ASN:CG	1:GC:25:GLU:H	2.03	0.67
1:IB:94:ARG:HD3	1:IB:226:PRO:HD3	1.75	0.67
1:JA:73:GLY:H	1:JA:181:MET:HE3	1.59	0.67
1:DC:390:GLN:HB2	1:DC:445:PRO:HB3	1.76	0.67
1:AB:439:PRO:HB3	1:BA:335:THR:HG21	1.77	0.67
1:EA:105:VAL:HG13	1:EA:156:ILE:HB	1.74	0.67
1:HB:265:ARG:NH2	1:HB:420:PRO:O	2.26	0.67
1:FB:231:ILE:HD11	1:GA:220:VAL:HG11	1.75	0.67
1:FC:371:THR:HG21	1:FC:374:ASP:HB2	1.77	0.67
1:MB:15:THR:HG21	1:MB:151:LEU:HD11	1.77	0.67
1:MC:267:THR:HG22	1:MC:271:VAL:H	1.59	0.67
1:BC:335:THR:HG21	1:KC:439:PRO:HB3	1.76	0.67
1:CC:46:ASN:ND2	1:CC:213:ILE:O	2.27	0.67
1:DC:66:VAL:HG21	1:DC:119:ILE:HD11	1.76	0.67
1:NB:439:PRO:HB3	1:OA:335:THR:HG21	1.77	0.67
1:NC:223:ARG:HA	1:NC:467:PRO:HG2	1.76	0.67
1:DA:476:ARG:HD3	1:DA:485:VAL:HG11	1.77	0.67
1:MA:140:MET:HE1	1:MB:218:PRO:HD3	1.77	0.67
1:IA:353:THR:HG22	1:IA:406:PRO:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:371:THR:HG22	1:LA:373:ASN:H	1.61	0.66
1:LB:265:ARG:NH2	1:LB:420:PRO:O	2.28	0.66
1:CC:66:VAL:HG21	1:CC:119:ILE:HD11	1.77	0.66
1:CC:268:THR:HG21	1:CC:520:TRP:HH2	1.60	0.66
1:FA:144:ILE:HD12	1:FA:156:ILE:HG12	1.76	0.66
1:GB:439:PRO:HB3	1:HA:335:THR:HG21	1.76	0.66
1:GC:44:GLN:NE2	1:GC:215:LEU:H	1.94	0.66
1:NC:268:THR:HG21	1:NC:520:TRP:HH2	1.60	0.66
1:OA:490:LYS:HB2	1:OA:498:THR:HG22	1.78	0.66
1:GB:233:THR:HB	1:GB:236:GLU:HG3	1.78	0.66
1:GC:66:VAL:HG21	1:GC:119:ILE:HD11	1.75	0.66
1:LC:433:PHE:HB3	1:LC:450:ASP:HB3	1.78	0.66
1:DA:251:THR:HG22	1:DA:430:GLN:HE21	1.60	0.66
1:IB:15:THR:HG21	1:IB:151:LEU:HD11	1.77	0.66
1:JB:15:THR:HG21	1:JB:151:LEU:HD11	1.78	0.66
1:KA:317:ILE:HG13	1:KA:318:PRO:HD2	1.77	0.66
1:EC:120:ILE:HG12	1:EC:145:ILE:HG12	1.78	0.66
1:GB:338:THR:OG1	1:GB:345:ARG:NH2	2.28	0.66
1:IC:120:ILE:HG12	1:IC:145:ILE:HG12	1.78	0.66
1:KC:233:THR:HB	1:KC:236:GLU:HG3	1.77	0.66
1:LB:215:LEU:HD21	1:MA:52:ILE:HD13	1.78	0.66
1:MB:135:PRO:HA	1:MB:181:MET:HE1	1.78	0.66
1:AA:490:LYS:HB2	1:AA:498:THR:HG22	1.78	0.66
1:HB:471:ASP:HA	1:HB:493:LYS:HD2	1.78	0.66
1:LB:267:THR:HG22	1:LB:271:VAL:H	1.61	0.66
1:CA:33:VAL:HG11	1:CA:37:ILE:HG13	1.78	0.66
1:AB:33:VAL:HG21	1:AB:37:ILE:HG13	1.79	0.65
1:BB:15:THR:HG21	1:BB:151:LEU:HD11	1.77	0.65
1:GC:120:ILE:HG12	1:GC:145:ILE:HG12	1.78	0.65
1:GC:390:GLN:HG2	1:GC:399:GLU:HG3	1.78	0.65
1:IA:233:THR:HG22	1:IA:235:GLU:H	1.61	0.65
1:BB:24:ASN:ND2	1:KC:152:GLU:OE2	2.28	0.65
1:EA:73:GLY:H	1:EA:181:MET:HE3	1.62	0.65
1:JA:69:ARG:HH21	1:JA:427:PRO:HB2	1.60	0.65
1:KB:15:THR:HG21	1:KB:151:LEU:HD11	1.77	0.65
1:KC:390:GLN:HB2	1:KC:445:PRO:HB3	1.77	0.65
1:LC:120:ILE:HG12	1:LC:145:ILE:HG12	1.79	0.65
1:OB:135:PRO:HA	1:OB:181:MET:HE1	1.78	0.65
1:CA:120:ILE:HD11	1:CA:183:TYR:CD1	2.31	0.65
1:NA:490:LYS:HB2	1:NA:498:THR:HG22	1.79	0.65
1:KA:140:MET:HE1	1:KB:218:PRO:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:140:MET:HB2	1:LB:217:PRO:HG3	1.78	0.65
1:LB:135:PRO:HA	1:LB:181:MET:HE1	1.79	0.65
1:BB:306:GLN:NE2	1:BB:321:LEU:O	2.30	0.65
1:BB:307:ASN:ND2	1:BB:309:ASN:OD1	2.30	0.65
1:DC:233:THR:HB	1:DC:236:GLU:HG3	1.77	0.65
1:EB:135:PRO:HA	1:EB:181:MET:HE1	1.79	0.65
1:HA:69:ARG:HH21	1:HA:427:PRO:HB2	1.60	0.65
1:JC:44:GLN:NE2	1:JC:215:LEU:H	1.94	0.65
1:LA:149:ARG:NH2	1:MA:149:ARG:O	2.30	0.65
1:KA:306:GLN:NE2	1:KA:321:LEU:O	2.30	0.65
1:LA:216:VAL:HG22	1:LA:217:PRO:HD2	1.78	0.65
1:AA:65:THR:HG21	1:AA:526:THR:N	2.05	0.65
1:BA:66:VAL:HG12	1:BA:186:LEU:HD22	1.79	0.65
1:IB:222:SER:HB3	1:IB:467:PRO:HD3	1.77	0.65
1:OB:233:THR:HB	1:OB:236:GLU:HG3	1.79	0.65
1:BA:490:LYS:HB2	1:BA:498:THR:HG22	1.77	0.65
1:FB:267:THR:HG22	1:FB:271:VAL:H	1.62	0.65
1:LC:438:MET:HE2	1:LC:449:LEU:HB2	1.78	0.65
1:AC:66:VAL:HG21	1:AC:119:ILE:HD11	1.77	0.64
1:GA:216:VAL:HG22	1:GA:217:PRO:HD2	1.78	0.64
1:LB:439:PRO:HB3	1:MA:335:THR:HG21	1.79	0.64
1:CB:306:GLN:NE2	1:CB:321:LEU:O	2.30	0.64
1:DB:248:LYS:HE3	1:DB:435:ARG:HD2	1.78	0.64
1:EB:33:VAL:HG21	1:EB:37:ILE:HG13	1.79	0.64
1:EB:265:ARG:NH2	1:EB:420:PRO:O	2.30	0.64
1:LC:121:PHE:HB2	1:LC:144:ILE:HG22	1.80	0.64
1:BA:149:ARG:NH2	1:CA:149:ARG:O	2.31	0.64
1:FC:476:ARG:HD3	1:FC:488:GLU:HB3	1.79	0.64
1:CB:15:THR:HG21	1:CB:151:LEU:HD11	1.80	0.64
1:CC:33:VAL:HG11	1:CC:37:ILE:HG13	1.79	0.64
1:CC:476:ARG:HD3	1:CC:488:GLU:HB3	1.80	0.64
1:FA:389:VAL:HG12	1:FA:441:CYS:HB2	1.79	0.64
1:IB:217:PRO:HB2	1:IB:219:THR:HG22	1.80	0.64
1:NC:46:ASN:ND2	1:NC:213:ILE:O	2.28	0.64
1:BB:94:ARG:HG3	1:BB:224:THR:HG23	1.78	0.64
1:BC:97:ASN:ND2	1:BC:221:GLU:OE2	2.30	0.64
1:EA:353:THR:HG22	1:EA:406:PRO:HB3	1.80	0.64
1:HB:197:THR:O	1:IC:187:ARG:NH1	2.31	0.64
1:OA:490:LYS:HG3	1:OA:527:LEU:HD11	1.78	0.64
1:AA:147:ASP:OD1	1:AA:149:ARG:HG2	1.97	0.64
1:BC:267:THR:HG22	1:BC:271:VAL:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CB:265:ARG:NH2	1:CB:420:PRO:O	2.30	0.64
1:FA:476:ARG:HD3	1:FA:485:VAL:HG11	1.78	0.64
1:IA:476:ARG:HD3	1:IA:485:VAL:HG11	1.78	0.64
1:AB:248:LYS:HE3	1:AB:435:ARG:HD2	1.80	0.64
1:AC:187:ARG:HH22	1:EB:197:THR:HB	1.63	0.64
1:FA:66:VAL:HG21	1:FA:119:ILE:HD11	1.78	0.64
1:JA:66:VAL:HG12	1:JA:186:LEU:HD22	1.78	0.64
1:KA:233:THR:HG22	1:KA:235:GLU:H	1.62	0.64
1:KB:439:PRO:HB3	1:LA:335:THR:HG21	1.79	0.64
1:KC:120:ILE:HG12	1:KC:145:ILE:HG12	1.79	0.64
1:OC:66:VAL:HG21	1:OC:119:ILE:HD11	1.80	0.64
1:CA:140:MET:HB2	1:CB:217:PRO:HG3	1.80	0.64
1:FB:286:PHE:HB3	1:FB:301:MET:HE1	1.79	0.64
1:AC:184:THR:HG23	1:EB:199:SER:HB2	1.80	0.64
1:FA:424:PRO:HD3	1:FA:431:LEU:HD13	1.79	0.64
1:NA:476:ARG:HD3	1:NA:485:VAL:HG11	1.80	0.64
1:AB:265:ARG:NH2	1:AB:420:PRO:O	2.32	0.63
1:DA:140:MET:HB2	1:DB:217:PRO:HG3	1.80	0.63
1:IC:359:THR:HG22	1:IC:410:GLY:HA3	1.80	0.63
1:NA:65:THR:HG21	1:NA:526:THR:N	2.07	0.63
1:EA:66:VAL:HG21	1:EA:119:ILE:HD11	1.80	0.63
1:GC:373:ASN:OD1	1:GC:374:ASP:N	2.31	0.63
1:HB:395:ALA:HB3	1:HB:398:ASN:ND2	2.14	0.63
1:MA:233:THR:HG22	1:MA:235:GLU:H	1.62	0.63
1:BA:144:ILE:HG21	1:BA:154:VAL:HG11	1.78	0.63
1:CA:120:ILE:HG13	1:CA:183:TYR:HB2	1.79	0.63
1:CB:130:THR:HG23	1:CB:179:ILE:HD11	1.80	0.63
1:EB:130:THR:HG23	1:EB:179:ILE:HD11	1.79	0.63
1:AA:304:ALA:O	1:AA:311:TYR:HB2	1.98	0.63
1:BA:490:LYS:HG3	1:BA:527:LEU:HD11	1.80	0.63
1:CA:233:THR:HG22	1:CA:235:GLU:H	1.64	0.63
1:CB:33:VAL:HG21	1:CB:37:ILE:HG13	1.78	0.63
1:CB:75:ILE:O	1:CB:522:ASN:ND2	2.32	0.63
1:JA:233:THR:HG22	1:JA:235:GLU:H	1.64	0.63
1:MC:476:ARG:HD3	1:MC:488:GLU:HB3	1.80	0.63
1:BB:46:ASN:ND2	1:BB:213:ILE:O	2.30	0.63
1:GB:471:ASP:HA	1:GB:493:LYS:HD2	1.79	0.63
1:JC:472:VAL:HG11	1:JC:490:LYS:HD2	1.79	0.63
1:KC:371:THR:HG22	1:KC:373:ASN:H	1.63	0.63
1:OA:233:THR:HG22	1:OA:235:GLU:H	1.61	0.63
1:EB:471:ASP:HA	1:EB:493:LYS:HD2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:184:THR:HG23	1:LC:199:SER:HB2	1.81	0.63
1:GA:353:THR:HG22	1:GA:406:PRO:HB3	1.79	0.63
1:LC:233:THR:HB	1:LC:236:GLU:HG3	1.79	0.63
1:MB:275:THR:HG23	1:MB:318:PRO:HG2	1.81	0.63
1:NA:424:PRO:HD3	1:NA:431:LEU:HD13	1.80	0.63
1:CA:144:ILE:HD12	1:CA:156:ILE:HG13	1.80	0.63
1:CC:120:ILE:HG12	1:CC:145:ILE:HG12	1.80	0.63
1:DA:37:ILE:HD11	1:DB:40:PRO:HB2	1.79	0.63
1:LA:147:ASP:OD1	1:LA:149:ARG:HG2	1.99	0.62
1:NB:275:THR:HG23	1:NB:318:PRO:HG2	1.81	0.62
1:KA:69:ARG:HH21	1:KA:427:PRO:HB2	1.65	0.62
1:AC:120:ILE:HG12	1:AC:145:ILE:HG12	1.81	0.62
1:BC:390:GLN:HB2	1:BC:445:PRO:HB3	1.81	0.62
1:DC:223:ARG:HA	1:DC:467:PRO:HG2	1.81	0.62
1:DC:286:PHE:HB3	1:DC:303:LEU:HD21	1.82	0.62
1:GA:233:THR:HG22	1:GA:235:GLU:H	1.63	0.62
1:KA:490:LYS:HB2	1:KA:498:THR:HG22	1.81	0.62
1:OC:371:THR:HG22	1:OC:373:ASN:H	1.64	0.62
1:DA:66:VAL:HG21	1:DA:119:ILE:HD11	1.80	0.62
1:EA:490:LYS:HG3	1:EA:527:LEU:HD11	1.80	0.62
1:GC:267:THR:HG22	1:GC:271:VAL:H	1.65	0.62
1:MA:66:VAL:HG12	1:MA:186:LEU:HD22	1.82	0.62
1:AC:335:THR:HG21	1:GC:439:PRO:HB3	1.82	0.62
1:BC:390:GLN:HG2	1:BC:399:GLU:HG3	1.81	0.62
1:EA:490:LYS:HB2	1:EA:498:THR:HG22	1.81	0.62
1:FC:233:THR:HB	1:FC:236:GLU:HG3	1.81	0.62
1:AB:135:PRO:HA	1:AB:181:MET:HE1	1.81	0.62
1:CC:44:GLN:NE2	1:CC:215:LEU:H	1.97	0.62
1:EA:233:THR:HG22	1:EA:235:GLU:H	1.65	0.62
1:JB:306:GLN:NE2	1:JB:321:LEU:O	2.33	0.62
1:KC:486:LEU:HD11	1:KC:510:PRO:HD2	1.82	0.62
1:BB:464:GLU:O	1:BB:464:GLU:HG3	2.00	0.62
1:CA:147:ASP:OD1	1:CA:149:ARG:HG2	2.00	0.62
1:FA:147:ASP:OD1	1:FA:149:ARG:HG2	1.99	0.62
1:HC:261:PRO:HG3	1:HC:403:TRP:HZ3	1.65	0.62
1:DA:69:ARG:HH21	1:DA:427:PRO:HB2	1.65	0.62
1:KA:65:THR:HG21	1:KA:526:THR:N	2.12	0.62
1:NC:261:PRO:HG3	1:NC:403:TRP:HZ3	1.64	0.62
1:OA:424:PRO:HD3	1:OA:431:LEU:HD13	1.81	0.62
1:OC:233:THR:HB	1:OC:236:GLU:HG3	1.82	0.62
1:DC:120:ILE:HG12	1:DC:145:ILE:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JA:490:LYS:HB2	1:JA:498:THR:HG22	1.81	0.61
1:LC:223:ARG:HA	1:LC:467:PRO:HG2	1.80	0.61
1:LC:500:ALA:HB2	1:LC:527:LEU:HG	1.82	0.61
1:AA:66:VAL:HG21	1:AA:119:ILE:HD11	1.81	0.61
1:BC:433:PHE:HB3	1:BC:450:ASP:HB3	1.81	0.61
1:FA:248:LYS:HE2	1:FA:435:ARG:HD2	1.81	0.61
1:OA:476:ARG:HD3	1:OA:485:VAL:HG11	1.82	0.61
1:FA:147:ASP:OD2	1:FA:149:ARG:NH1	2.33	0.61
1:HC:120:ILE:HG12	1:HC:145:ILE:HG12	1.83	0.61
1:JC:400:PRO:HG2	1:JC:446:ASN:HB3	1.82	0.61
1:BC:46:ASN:ND2	1:BC:213:ILE:O	2.32	0.61
1:DB:135:PRO:HA	1:DB:181:MET:HE1	1.82	0.61
1:JA:490:LYS:HG3	1:JA:527:LEU:HD11	1.83	0.61
1:NA:282:ASN:OD1	1:NA:287:ARG:NH2	2.33	0.61
1:BC:439:PRO:HB3	1:KC:335:THR:HG21	1.82	0.61
1:FC:268:THR:HG21	1:FC:520:TRP:HH2	1.66	0.61
1:FC:390:GLN:HG2	1:FC:399:GLU:HG3	1.82	0.61
1:JA:105:VAL:HG13	1:JA:156:ILE:HB	1.81	0.61
1:LA:490:LYS:HG3	1:LA:527:LEU:HD11	1.83	0.61
1:BA:147:ASP:OD1	1:BA:149:ARG:HG2	2.01	0.61
1:FA:140:MET:HB2	1:FB:217:PRO:HG3	1.83	0.61
1:JA:371:THR:HG22	1:JA:373:ASN:H	1.66	0.61
1:MC:44:GLN:NE2	1:MC:215:LEU:H	1.99	0.61
1:AA:73:GLY:H	1:AA:181:MET:HE3	1.66	0.61
1:BB:33:VAL:HG21	1:BB:37:ILE:HG13	1.82	0.61
1:KA:239:ASN:ND2	1:KA:436:SER:OG	2.34	0.61
1:BC:120:ILE:HG12	1:BC:145:ILE:HG12	1.81	0.61
1:JB:94:ARG:HB3	1:JB:218:PRO:O	2.01	0.61
1:JB:275:THR:HG23	1:JB:318:PRO:HG2	1.83	0.61
1:MB:23:ASN:ND2	1:MB:144:ILE:HD11	2.15	0.61
1:CB:135:PRO:HA	1:CB:181:MET:HE1	1.82	0.61
1:NA:140:MET:HB2	1:NB:217:PRO:HG3	1.82	0.61
1:OC:415:ASN:HB3	1:OC:418:LEU:HD11	1.82	0.61
1:DC:81:LEU:HD12	1:DC:158:LEU:HG	1.84	0.60
1:JB:301:MET:HE2	1:JB:303:LEU:HD23	1.82	0.60
1:LA:338:THR:OG1	1:LA:345:ARG:NH2	2.26	0.60
1:MA:147:ASP:OD1	1:MA:149:ARG:HG2	2.01	0.60
1:MA:316:GLU:OE1	1:MA:417:HIS:NE2	2.33	0.60
1:OC:33:VAL:HG11	1:OC:37:ILE:HB	1.82	0.60
1:MC:158:LEU:HD13	1:MC:178:LEU:HG	1.82	0.60
1:NC:66:VAL:HG21	1:NC:119:ILE:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:389:VAL:HG12	1:BB:441:CYS:HB2	1.84	0.60
1:EA:422:VAL:HG12	1:EA:431:LEU:HD21	1.84	0.60
1:FA:161:VAL:HB	1:FA:176:ILE:HD11	1.84	0.60
1:AB:197:THR:O	1:BC:187:ARG:NH1	2.34	0.60
1:CB:469:GLN:OE1	1:CB:520:TRP:NE1	2.34	0.60
1:DA:233:THR:HG22	1:DA:235:GLU:H	1.65	0.60
1:DC:254:SER:HA	1:DC:257:PHE:CE1	2.36	0.60
1:GC:261:PRO:HG3	1:GC:403:TRP:HZ3	1.67	0.60
1:HC:472:VAL:HG11	1:HC:490:LYS:HD2	1.84	0.60
1:IB:233:THR:HB	1:IB:236:GLU:HG3	1.83	0.60
1:KC:476:ARG:HD3	1:KC:488:GLU:HB3	1.82	0.60
1:BA:69:ARG:HH21	1:BA:427:PRO:HB2	1.66	0.60
1:FC:46:ASN:ND2	1:FC:213:ILE:O	2.31	0.60
1:GB:267:THR:HG22	1:GB:271:VAL:H	1.66	0.60
1:IC:97:ASN:ND2	1:IC:221:GLU:OE2	2.34	0.60
1:KA:490:LYS:HG3	1:KA:527:LEU:HD11	1.81	0.60
1:JB:471:ASP:HA	1:JB:493:LYS:HD2	1.83	0.60
1:HC:121:PHE:HB2	1:HC:144:ILE:HG22	1.84	0.60
1:KB:15:THR:HG22	1:LC:149:ARG:HE	1.66	0.60
1:OA:280:PRO:HB3	1:OA:455:GLN:HG2	1.82	0.60
1:DA:159:PRO:O	1:DA:176:ILE:HD12	2.02	0.60
1:BB:433:PHE:HB3	1:BB:450:ASP:HB3	1.84	0.60
1:FB:275:THR:HG23	1:FB:318:PRO:HG2	1.83	0.60
1:IA:490:LYS:HG3	1:IA:527:LEU:HD11	1.83	0.60
1:NA:144:ILE:HD12	1:NA:154:VAL:HG11	1.84	0.60
1:BB:135:PRO:HA	1:BB:181:MET:HE1	1.83	0.59
1:DC:109:LEU:HD13	1:DC:200:CYS:SG	2.42	0.59
1:JC:46:ASN:ND2	1:JC:213:ILE:O	2.35	0.59
1:JC:120:ILE:HG12	1:JC:145:ILE:HG12	1.83	0.59
1:AA:233:THR:HG22	1:AA:235:GLU:H	1.66	0.59
1:DA:490:LYS:HB2	1:DA:498:THR:HG22	1.82	0.59
1:HC:33:VAL:HG11	1:HC:37:ILE:HB	1.84	0.59
1:KC:223:ARG:HA	1:KC:467:PRO:HG2	1.83	0.59
1:GA:65:THR:HG21	1:GA:526:THR:N	2.06	0.59
1:DA:216:VAL:HG22	1:DA:217:PRO:HD2	1.84	0.59
1:EB:267:THR:HG22	1:EB:271:VAL:H	1.66	0.59
1:FA:159:PRO:O	1:FA:176:ILE:HD12	2.02	0.59
1:FA:233:THR:HG22	1:FA:235:GLU:H	1.66	0.59
1:KA:147:ASP:OD2	1:KA:149:ARG:NH1	2.36	0.59
1:LB:94:ARG:O	1:LB:218:PRO:HA	2.03	0.59
1:NA:225:LYS:HD3	1:NA:464:GLU:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:66:VAL:HG21	1:BA:119:ILE:HD11	1.85	0.59
1:BC:51:TRP:CG	1:KC:44:GLN:HE21	2.21	0.59
1:HB:135:PRO:HA	1:HB:181:MET:HE1	1.83	0.59
1:AA:159:PRO:O	1:AA:176:ILE:HD12	2.03	0.59
1:DA:275:THR:HG23	1:DA:318:PRO:HG2	1.83	0.59
1:IC:472:VAL:HG11	1:IC:490:LYS:HD2	1.85	0.59
1:NA:105:VAL:HG13	1:NA:156:ILE:HB	1.85	0.59
1:NC:338:THR:OG1	1:NC:345:ARG:NH2	2.35	0.59
1:AA:220:VAL:HG11	1:EB:231:ILE:HD11	1.85	0.59
1:DB:197:THR:O	1:EC:187:ARG:NH1	2.36	0.59
1:EC:343:SER:OG	1:EC:345:ARG:NH1	2.36	0.59
1:HA:147:ASP:OD2	1:HA:149:ARG:NH1	2.36	0.59
1:IC:246:LEU:HA	1:IC:436:SER:HB3	1.85	0.59
1:LB:507:LEU:HD21	1:LB:530:MET:HE1	1.85	0.59
1:NC:120:ILE:HG12	1:NC:145:ILE:HG12	1.84	0.59
1:NA:147:ASP:OD1	1:NA:149:ARG:HG2	2.02	0.59
1:NA:275:THR:HG23	1:NA:318:PRO:HG2	1.85	0.59
1:GA:317:ILE:HG22	1:GA:318:PRO:HD2	1.83	0.59
1:MB:121:PHE:HB2	1:MB:144:ILE:HG22	1.84	0.59
1:BB:286:PHE:HB3	1:BB:301:MET:HE1	1.84	0.59
1:FA:490:LYS:HB2	1:FA:498:THR:HG22	1.85	0.59
1:NA:353:THR:HG22	1:NA:406:PRO:HB3	1.85	0.59
1:AA:149:ARG:NH2	1:BA:149:ARG:O	2.36	0.58
1:AC:189:ASN:HD21	1:EB:190:ASN:HB2	1.68	0.58
1:EC:476:ARG:HD3	1:EC:488:GLU:HB3	1.83	0.58
1:HA:371:THR:HG22	1:HA:373:ASN:H	1.67	0.58
1:IB:94:ARG:HH22	1:JA:94:ARG:HH12	1.49	0.58
1:NC:371:THR:HG22	1:NC:373:ASN:H	1.68	0.58
1:CB:471:ASP:HA	1:CB:493:LYS:HD2	1.85	0.58
1:DB:101:GLY:HA3	1:DB:210:PHE:HA	1.85	0.58
1:HA:490:LYS:HG3	1:HA:527:LEU:HD11	1.85	0.58
1:KB:14:SER:O	1:KB:16:ALA:N	2.36	0.58
1:OC:120:ILE:HG12	1:OC:145:ILE:HG12	1.85	0.58
1:AA:105:VAL:HG13	1:AA:156:ILE:HB	1.84	0.58
1:BA:476:ARG:HD3	1:BA:485:VAL:HG11	1.85	0.58
1:OA:147:ASP:OD1	1:OA:149:ARG:HG2	2.03	0.58
1:CA:37:ILE:HD11	1:CB:40:PRO:HB2	1.84	0.58
1:CC:470:SER:OG	1:CC:521:VAL:O	2.21	0.58
1:EA:216:VAL:HG22	1:EA:217:PRO:HD2	1.85	0.58
1:LC:338:THR:HB	1:LC:343:SER:HB3	1.85	0.58
1:LC:472:VAL:HG11	1:LC:490:LYS:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:261:PRO:HG3	1:AC:403:TRP:HZ3	1.68	0.58
1:AC:338:THR:OG1	1:AC:345:ARG:NH2	2.35	0.58
1:FB:433:PHE:HB3	1:FB:450:ASP:HB3	1.86	0.58
1:MA:216:VAL:HG22	1:MA:217:PRO:HD2	1.85	0.58
1:MC:472:VAL:HG11	1:MC:490:LYS:HD2	1.85	0.58
1:BB:277:GLN:OE1	1:BB:279:SER:N	2.34	0.58
1:FA:37:ILE:HD11	1:FB:40:PRO:HB2	1.85	0.58
1:KB:471:ASP:HA	1:KB:493:LYS:HD2	1.85	0.58
1:KC:261:PRO:HG3	1:KC:403:TRP:HZ3	1.67	0.58
1:CA:338:THR:OG1	1:CA:345:ARG:NH2	2.30	0.58
1:CB:389:VAL:HG12	1:CB:441:CYS:HB2	1.86	0.58
1:DC:390:GLN:HG2	1:DC:399:GLU:HG3	1.86	0.58
1:HC:249:LEU:HB3	1:HC:507:LEU:HD12	1.86	0.58
1:IB:488:GLU:HG3	1:IB:527:LEU:HD22	1.85	0.58
1:EC:44:GLN:NE2	1:EC:215:LEU:H	2.02	0.58
1:HC:470:SER:OG	1:HC:521:VAL:O	2.13	0.58
1:LB:233:THR:HB	1:LB:236:GLU:HG3	1.85	0.58
1:OC:434:PHE:CE2	1:OC:454:PRO:HD3	2.39	0.58
1:DA:225:LYS:HD3	1:DA:464:GLU:HG3	1.85	0.58
1:FC:227:PHE:CE1	1:FC:268:THR:HG23	2.39	0.58
1:HB:482:THR:HG21	1:IC:427:PRO:HD3	1.86	0.58
1:JB:69:ARG:NH1	1:JB:428:GLY:HA3	2.18	0.58
1:JC:284:CYS:HB2	1:JC:324:PRO:HG3	1.85	0.58
1:MB:109:LEU:HD23	1:MB:200:CYS:SG	2.44	0.58
1:OC:476:ARG:HD3	1:OC:488:GLU:HB3	1.86	0.58
1:AC:199:SER:HB2	1:GB:184:THR:HG23	1.86	0.58
1:KA:105:VAL:HG13	1:KA:156:ILE:HB	1.86	0.58
1:AA:490:LYS:HG3	1:AA:527:LEU:HD11	1.85	0.57
1:BB:275:THR:HG23	1:BB:318:PRO:HG2	1.84	0.57
1:FA:73:GLY:H	1:FA:181:MET:HE3	1.68	0.57
1:GC:438:MET:HE2	1:GC:449:LEU:HB2	1.86	0.57
1:NA:216:VAL:HG22	1:NA:217:PRO:HD2	1.85	0.57
1:AC:227:PHE:CE1	1:AC:268:THR:HG23	2.38	0.57
1:CA:490:LYS:HB2	1:CA:498:THR:HG22	1.85	0.57
1:EC:66:VAL:HG21	1:EC:119:ILE:HD11	1.86	0.57
1:GA:306:GLN:NE2	1:GA:321:LEU:O	2.37	0.57
1:HA:275:THR:HG23	1:HA:318:PRO:HG2	1.86	0.57
1:KB:395:ALA:HB3	1:KB:398:ASN:ND2	2.17	0.57
1:OA:353:THR:HG22	1:OA:406:PRO:HB3	1.86	0.57
1:AA:140:MET:HE1	1:AB:218:PRO:HD2	1.86	0.57
1:CB:94:ARG:O	1:CB:218:PRO:HA	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IA:149:ARG:NH2	1:JA:149:ARG:O	2.37	0.57
1:LC:239:ASN:ND2	1:LC:436:SER:OG	2.35	0.57
1:MC:371:THR:HG21	1:MC:374:ASP:HB2	1.86	0.57
1:DC:261:PRO:HG3	1:DC:403:TRP:HZ3	1.69	0.57
1:IC:121:PHE:HB2	1:IC:144:ILE:HG22	1.86	0.57
1:LC:398:ASN:ND2	1:LC:398:ASN:O	2.38	0.57
1:MA:319:ALA:HB1	1:MA:320:PRO:HD2	1.85	0.57
1:NA:144:ILE:HD13	1:NA:156:ILE:HG12	1.87	0.57
1:AC:390:GLN:HG2	1:AC:399:GLU:HG3	1.86	0.57
1:CB:120:ILE:HG12	1:CB:145:ILE:HG12	1.86	0.57
1:DA:105:VAL:HG13	1:DA:156:ILE:HB	1.86	0.57
1:EA:424:PRO:HD3	1:EA:431:LEU:HD13	1.85	0.57
1:FA:490:LYS:HG3	1:FA:527:LEU:HD11	1.86	0.57
1:FB:233:THR:HB	1:FB:236:GLU:HG3	1.85	0.57
1:IA:216:VAL:HG22	1:IA:217:PRO:HD2	1.87	0.57
1:LC:227:PHE:CE1	1:LC:268:THR:HG23	2.39	0.57
1:EB:30:GLU:HG3	1:EC:44:GLN:HA	1.84	0.57
1:LA:476:ARG:HD3	1:LA:485:VAL:HG11	1.87	0.57
1:LB:137:GLN:HA	1:LB:140:MET:HE3	1.86	0.57
1:CB:286:PHE:HB3	1:CB:301:MET:HE1	1.84	0.57
1:CB:437:THR:HG23	1:CB:447:MET:HB3	1.86	0.57
1:HA:73:GLY:H	1:HA:181:MET:HE3	1.70	0.57
1:JA:216:VAL:HG22	1:JA:217:PRO:HD2	1.87	0.57
1:BB:109:LEU:HD23	1:BB:200:CYS:SG	2.45	0.57
1:FC:120:ILE:HG12	1:FC:145:ILE:HG12	1.86	0.57
1:GB:306:GLN:NE2	1:GB:321:LEU:O	2.38	0.57
1:HC:46:ASN:ND2	1:HC:213:ILE:O	2.37	0.57
1:IA:105:VAL:HG13	1:IA:156:ILE:HB	1.86	0.57
1:LB:464:GLU:HG3	1:LB:464:GLU:O	2.05	0.57
1:NC:371:THR:HG21	1:NC:374:ASP:HB2	1.86	0.57
1:OC:46:ASN:ND2	1:OC:213:ILE:O	2.34	0.57
1:CA:490:LYS:HG3	1:CA:527:LEU:HD11	1.87	0.57
1:IA:53:ARG:HB3	1:IA:206:PRO:HG2	1.87	0.57
1:LA:147:ASP:OD2	1:LA:149:ARG:NH1	2.38	0.57
1:MA:328:GLY:H	1:MA:353:THR:HB	1.68	0.57
1:MB:23:ASN:HD22	1:MB:144:ILE:HD11	1.70	0.57
1:MC:109:LEU:HD13	1:MC:200:CYS:SG	2.44	0.57
1:MC:434:PHE:CE2	1:MC:454:PRO:HD3	2.40	0.57
1:OB:471:ASP:HA	1:OB:493:LYS:HD2	1.87	0.57
1:AA:87:PRO:HG2	1:EA:140:MET:HE3	1.87	0.57
1:GC:254:SER:HA	1:GC:257:PHE:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IB:246:LEU:HD11	1:IB:454:PRO:HB3	1.87	0.57
1:LA:73:GLY:H	1:LA:181:MET:HE3	1.68	0.57
1:MC:268:THR:HG21	1:MC:520:TRP:HH2	1.68	0.57
1:EB:118:LYS:H	1:EB:184:THR:HB	1.70	0.56
1:EC:159:PRO:O	1:EC:176:ILE:HD12	2.05	0.56
1:FA:306:GLN:H	1:FA:306:GLN:CD	2.13	0.56
1:HC:227:PHE:CE1	1:HC:268:THR:HG23	2.40	0.56
1:LA:69:ARG:HH21	1:LA:427:PRO:HB2	1.70	0.56
1:LB:197:THR:O	1:MC:187:ARG:NH1	2.38	0.56
1:OC:267:THR:HG22	1:OC:271:VAL:H	1.69	0.56
1:MC:94:ARG:HD2	1:MC:219:THR:HG22	1.86	0.56
1:AC:33:VAL:HG11	1:AC:37:ILE:HB	1.87	0.56
1:BC:268:THR:HG21	1:BC:520:TRP:CH2	2.36	0.56
1:FB:227:PHE:CE1	1:FB:268:THR:HG23	2.40	0.56
1:FC:335:THR:HG21	1:LC:439:PRO:HB3	1.86	0.56
1:IA:73:GLY:H	1:IA:181:MET:HE3	1.70	0.56
1:JB:227:PHE:CE1	1:JB:268:THR:HG23	2.40	0.56
1:KC:390:GLN:HG2	1:KC:399:GLU:HG3	1.86	0.56
1:MA:490:LYS:HB2	1:MA:498:THR:HG22	1.87	0.56
1:MB:123:ALA:HB1	1:MB:176:ILE:HD11	1.86	0.56
1:MC:120:ILE:HG12	1:MC:145:ILE:HG12	1.87	0.56
1:AB:94:ARG:O	1:AB:218:PRO:HA	2.05	0.56
1:BC:199:SER:HB2	1:KB:184:THR:HG23	1.86	0.56
1:DA:144:ILE:HD12	1:DA:156:ILE:HG12	1.88	0.56
1:FB:471:ASP:HA	1:FB:493:LYS:HD2	1.87	0.56
1:HC:476:ARG:HD3	1:HC:488:GLU:HB3	1.86	0.56
1:OB:248:LYS:NZ	1:OB:506:ASP:OD2	2.32	0.56
1:DA:149:ARG:NH2	1:EA:149:ARG:O	2.38	0.56
1:FC:199:SER:HB2	1:LB:184:THR:HG23	1.88	0.56
1:IC:227:PHE:CE1	1:IC:268:THR:HG23	2.41	0.56
1:BB:30:GLU:HG3	1:BC:44:GLN:HA	1.87	0.56
1:JB:477:PHE:CE2	1:JB:509:ILE:HD12	2.41	0.56
1:KB:248:LYS:HE3	1:KB:435:ARG:HD2	1.86	0.56
1:LB:75:ILE:O	1:LB:522:ASN:ND2	2.39	0.56
1:OA:73:GLY:H	1:OA:181:MET:HE3	1.71	0.56
1:AB:88:TYR:HD1	1:BA:95:MET:HE3	1.71	0.56
1:DB:359:THR:HG22	1:DB:410:GLY:HA3	1.87	0.56
1:DC:46:ASN:ND2	1:DC:213:ILE:O	2.39	0.56
1:EB:19:VAL:HG23	1:EB:149:ARG:HB3	1.88	0.56
1:FC:44:GLN:HE21	1:LC:51:TRP:CG	2.24	0.56
1:GA:144:ILE:HD13	1:GA:156:ILE:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GB:287:ARG:HD2	1:GB:306:GLN:HA	1.88	0.56
1:GC:233:THR:HG22	1:GC:235:GLU:H	1.71	0.56
1:HA:149:ARG:NH2	1:IA:149:ARG:O	2.38	0.56
1:IB:267:THR:HG22	1:IB:271:VAL:H	1.71	0.56
1:JB:286:PHE:HB3	1:JB:301:MET:HE1	1.87	0.56
1:NA:73:GLY:H	1:NA:181:MET:HE3	1.70	0.56
1:DC:148:VAL:HG13	1:DC:198:VAL:HG21	1.88	0.56
1:IA:490:LYS:HB2	1:IA:498:THR:HG22	1.87	0.56
1:JC:415:ASN:HB3	1:JC:418:LEU:HD21	1.86	0.56
1:KA:149:ARG:O	1:OA:149:ARG:NH2	2.39	0.56
1:AB:338:THR:OG1	1:AB:345:ARG:NH2	2.38	0.56
1:MB:58:GLN:H	1:NC:139:THR:HG21	1.71	0.56
1:NB:30:GLU:HG3	1:NC:44:GLN:HA	1.87	0.56
1:NB:227:PHE:CE1	1:NB:268:THR:HG23	2.41	0.56
1:NB:301:MET:HE2	1:NB:303:LEU:HD23	1.88	0.56
1:AC:46:ASN:ND2	1:AC:213:ILE:O	2.38	0.56
1:CA:476:ARG:HD3	1:CA:485:VAL:HG11	1.88	0.56
1:CB:30:GLU:HG3	1:CC:44:GLN:HA	1.88	0.56
1:DB:244:ILE:CD1	1:DB:439:PRO:HD3	2.36	0.56
1:KC:476:ARG:HG3	1:KC:518:ASP:OD2	2.05	0.56
1:NB:135:PRO:HA	1:NB:181:MET:HE1	1.86	0.56
1:OB:267:THR:HG22	1:OB:271:VAL:H	1.71	0.56
1:JB:267:THR:CG2	1:JB:271:VAL:H	2.19	0.55
1:OA:319:ALA:HB1	1:OA:320:PRO:HD2	1.87	0.55
1:OC:472:VAL:HG11	1:OC:490:LYS:HD2	1.87	0.55
1:CB:120:ILE:HG13	1:CB:183:TYR:HB2	1.89	0.55
1:MB:454:PRO:HG2	1:MB:457:TRP:CG	2.41	0.55
1:AA:147:ASP:OD2	1:AA:149:ARG:NH1	2.40	0.55
1:LB:19:VAL:HG23	1:LB:149:ARG:HB3	1.88	0.55
1:FB:464:GLU:HG3	1:FB:464:GLU:O	2.07	0.55
1:HA:490:LYS:HB2	1:HA:498:THR:HG22	1.88	0.55
1:HB:454:PRO:HG2	1:HB:457:TRP:CG	2.41	0.55
1:HC:306:GLN:NE2	1:HC:321:LEU:O	2.40	0.55
1:IA:147:ASP:OD2	1:IA:149:ARG:NH1	2.40	0.55
1:JC:527:LEU:HD23	1:JC:527:LEU:H	1.72	0.55
1:NA:422:VAL:HG12	1:NA:431:LEU:HD21	1.89	0.55
1:AA:476:ARG:HD3	1:AA:485:VAL:HG11	1.88	0.55
1:DB:137:GLN:HA	1:DB:140:MET:HE3	1.89	0.55
1:DB:265:ARG:NH2	1:DB:420:PRO:O	2.38	0.55
1:GB:109:LEU:HD23	1:GB:200:CYS:SG	2.47	0.55
1:HC:390:GLN:HB2	1:HC:445:PRO:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IC:395:ALA:HB3	1:IC:398:ASN:HD22	1.72	0.55
1:EB:248:LYS:HD2	1:EB:435:ARG:HD2	1.89	0.55
1:KA:216:VAL:HG22	1:KA:217:PRO:HD2	1.88	0.55
1:EA:40:PRO:HB2	1:EC:37:ILE:HD11	1.88	0.55
1:EA:128:PHE:CZ	1:EB:220:VAL:HG11	2.42	0.55
1:EA:371:THR:HG22	1:EA:373:ASN:H	1.72	0.55
1:IB:482:THR:HG22	1:JC:426:PHE:HD1	1.70	0.55
1:KA:251:THR:HG22	1:KA:430:GLN:HE21	1.71	0.55
1:LC:109:LEU:HD13	1:LC:200:CYS:SG	2.46	0.55
1:MC:527:LEU:HD23	1:MC:527:LEU:H	1.72	0.55
1:NA:338:THR:OG1	1:NA:345:ARG:NH2	2.39	0.55
1:BB:118:LYS:H	1:BB:184:THR:HB	1.72	0.55
1:BC:159:PRO:O	1:BC:176:ILE:HD12	2.06	0.55
1:DA:147:ASP:OD1	1:DA:149:ARG:HG2	2.07	0.55
1:EB:275:THR:HG23	1:EB:318:PRO:HG2	1.88	0.55
1:HA:476:ARG:HD3	1:HA:485:VAL:HG11	1.89	0.55
1:KA:147:ASP:OD1	1:KA:149:ARG:HG2	2.07	0.55
1:LA:422:VAL:HG12	1:LA:431:LEU:HD21	1.89	0.55
1:NC:390:GLN:HG2	1:NC:399:GLU:HG3	1.88	0.55
1:OA:312:ASP:HB3	1:OA:315:GLU:HG3	1.89	0.55
1:DA:329:LYS:HE2	1:DA:352:SER:HB2	1.89	0.55
1:HC:389:VAL:HG23	1:HC:442:SER:HB3	1.88	0.55
1:IB:109:LEU:HD23	1:IB:200:CYS:SG	2.47	0.55
1:IB:135:PRO:HA	1:IB:181:MET:HE1	1.88	0.55
1:JB:78:SER:HB2	1:JB:179:ILE:HD13	1.89	0.55
1:KC:527:LEU:HD23	1:KC:527:LEU:H	1.72	0.55
1:LC:46:ASN:ND2	1:LC:213:ILE:O	2.37	0.55
1:EB:144:ILE:HG22	1:EB:146:VAL:HG23	1.87	0.55
1:EB:233:THR:HB	1:EB:236:GLU:HG3	1.89	0.55
1:MC:233:THR:HG22	1:MC:235:GLU:H	1.70	0.55
1:MC:305:SER:HB2	1:MC:307:ASN:OD1	2.06	0.55
1:NA:233:THR:HG22	1:NA:235:GLU:H	1.72	0.55
1:OC:94:ARG:NH1	1:OC:226:PRO:HD3	2.22	0.55
1:BC:447:MET:HE1	1:KC:337:THR:HG21	1.89	0.54
1:DB:130:THR:HG23	1:DB:179:ILE:HD11	1.89	0.54
1:EB:15:THR:HG21	1:EB:151:LEU:HD11	1.89	0.54
1:FA:149:ARG:NH2	1:GA:149:ARG:O	2.40	0.54
1:HB:121:PHE:HB2	1:HB:144:ILE:HG22	1.89	0.54
1:AB:267:THR:CG2	1:AB:271:VAL:H	2.18	0.54
1:AC:148:VAL:HG13	1:AC:198:VAL:HG21	1.88	0.54
1:DB:159:PRO:O	1:DB:176:ILE:HD12	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HA:66:VAL:HG12	1:HA:186:LEU:HD22	1.90	0.54
1:IB:275:THR:HG23	1:IB:318:PRO:HG2	1.89	0.54
1:AA:149:ARG:O	1:EA:149:ARG:NH2	2.39	0.54
1:AB:159:PRO:O	1:AB:176:ILE:HD12	2.07	0.54
1:CC:390:GLN:HB2	1:CC:445:PRO:HB3	1.88	0.54
1:FB:389:VAL:HG12	1:FB:441:CYS:HB2	1.89	0.54
1:JA:430:GLN:HE22	1:JA:503:GLY:H	1.54	0.54
1:MB:471:ASP:HA	1:MB:493:LYS:HD2	1.89	0.54
1:MC:148:VAL:HG13	1:MC:198:VAL:HG21	1.90	0.54
1:BC:389:VAL:HG23	1:BC:442:SER:HB3	1.89	0.54
1:FC:244:ILE:HG22	1:FC:245:PRO:HD2	1.89	0.54
1:HB:277:GLN:OE1	1:HB:279:SER:N	2.37	0.54
1:HC:477:PHE:HD1	1:HC:486:LEU:HD12	1.72	0.54
1:KB:399:GLU:HB3	1:KB:400:PRO:HD3	1.88	0.54
1:NC:338:THR:HB	1:NC:343:SER:HB3	1.89	0.54
1:OB:170:GLN:NE2	1:OB:222:SER:O	2.40	0.54
1:FA:33:VAL:HG11	1:FA:37:ILE:HG13	1.89	0.54
1:FA:87:PRO:HG2	1:JA:140:MET:HE3	1.90	0.54
1:FC:23:ASN:HD22	1:JB:153:PRO:HG3	1.72	0.54
1:GB:196:PHE:HA	1:HC:187:ARG:HD2	1.90	0.54
1:IC:158:LEU:HD13	1:IC:178:LEU:HG	1.90	0.54
1:NB:94:ARG:O	1:NB:218:PRO:HA	2.08	0.54
1:NC:233:THR:HG22	1:NC:235:GLU:H	1.71	0.54
1:DC:527:LEU:HD23	1:DC:527:LEU:H	1.73	0.54
1:GA:140:MET:HE3	1:HA:87:PRO:HG2	1.89	0.54
1:GA:490:LYS:HG3	1:GA:527:LEU:HD11	1.88	0.54
1:LA:140:MET:HE1	1:LB:218:PRO:HD2	1.88	0.54
1:AA:161:VAL:HB	1:AA:176:ILE:HD11	1.89	0.54
1:DC:472:VAL:HG11	1:DC:490:LYS:HD2	1.90	0.54
1:IC:433:PHE:HB3	1:IC:450:ASP:HB3	1.89	0.54
1:LC:403:TRP:CZ2	1:LC:450:ASP:HB2	2.42	0.54
1:BB:190:ASN:HB2	1:CC:189:ASN:HD21	1.73	0.54
1:EA:53:ARG:HB3	1:EA:206:PRO:HG2	1.90	0.54
1:EC:472:VAL:HG11	1:EC:490:LYS:HD2	1.90	0.54
1:IC:223:ARG:HA	1:IC:467:PRO:HG2	1.90	0.54
1:JC:227:PHE:CE1	1:JC:268:THR:HG23	2.42	0.54
1:LB:227:PHE:CE1	1:LB:268:THR:HG23	2.43	0.54
1:CC:56:PHE:HB3	1:CC:203:LEU:HB3	1.90	0.54
1:GA:424:PRO:HD3	1:GA:431:LEU:HD13	1.89	0.54
1:LA:275:THR:HG23	1:LA:318:PRO:HG2	1.89	0.54
1:OC:254:SER:HA	1:OC:257:PHE:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:33:VAL:HG11	1:AA:37:ILE:HB	1.90	0.54
1:AB:184:THR:HG23	1:GC:199:SER:HB2	1.88	0.54
1:BB:227:PHE:CE1	1:BB:268:THR:HG23	2.43	0.54
1:EC:243:PRO:HG3	1:EC:283:ILE:HB	1.89	0.54
1:IB:454:PRO:HG2	1:IB:457:TRP:CG	2.43	0.54
1:LA:430:GLN:HE22	1:LA:503:GLY:H	1.56	0.54
1:OC:227:PHE:CE1	1:OC:268:THR:HG23	2.43	0.54
1:OC:343:SER:OG	1:OC:345:ARG:NH1	2.41	0.54
1:AC:191:ALA:HB1	1:GB:194:ASP:HB3	1.90	0.53
1:BC:109:LEU:HD13	1:BC:200:CYS:SG	2.48	0.53
1:BC:472:VAL:HG11	1:BC:490:LYS:HD2	1.89	0.53
1:FB:34:GLY:HA3	1:FB:209:ASP:HB2	1.91	0.53
1:FC:46:ASN:HD21	1:FC:213:ILE:C	2.15	0.53
1:JA:435:ARG:NH1	1:JA:448:ASN:HB3	2.23	0.53
1:KB:121:PHE:HB2	1:KB:144:ILE:HG22	1.90	0.53
1:MA:140:MET:HG2	1:NA:57:VAL:HG21	1.90	0.53
1:MA:399:GLU:HB3	1:MA:400:PRO:HD3	1.90	0.53
1:NB:233:THR:HG21	1:NB:511:PRO:O	2.08	0.53
1:OA:338:THR:OG1	1:OA:345:ARG:NH2	2.33	0.53
1:DC:227:PHE:CE1	1:DC:268:THR:HG23	2.44	0.53
1:HB:84:ASP:HB3	1:HB:469:GLN:OE1	2.09	0.53
1:MA:73:GLY:H	1:MA:181:MET:HE3	1.72	0.53
1:NA:430:GLN:HE22	1:NA:503:GLY:H	1.54	0.53
1:AA:430:GLN:HE22	1:AA:503:GLY:H	1.56	0.53
1:AC:305:SER:HB2	1:AC:307:ASN:OD1	2.07	0.53
1:BB:184:THR:HG23	1:KC:199:SER:HB2	1.90	0.53
1:FC:233:THR:HG22	1:FC:235:GLU:H	1.74	0.53
1:FC:249:LEU:HB2	1:FC:509:ILE:HD11	1.90	0.53
1:IC:390:GLN:HA	1:IC:399:GLU:OE1	2.07	0.53
1:KA:215:LEU:HD12	1:OB:51:TRP:HB3	1.89	0.53
1:BC:77:TRP:HZ3	1:BC:178:LEU:HD22	1.73	0.53
1:CB:45:GLN:O	1:DA:51:TRP:NE1	2.42	0.53
1:CC:261:PRO:HG3	1:CC:403:TRP:HZ3	1.72	0.53
1:FA:65:THR:HG21	1:FA:526:THR:N	2.10	0.53
1:GC:109:LEU:HD13	1:GC:200:CYS:SG	2.48	0.53
1:IC:312:ASP:HB3	1:IC:313:PRO:HD2	1.90	0.53
1:KA:73:GLY:H	1:KA:181:MET:HE3	1.74	0.53
1:LB:471:ASP:HA	1:LB:493:LYS:HG3	1.89	0.53
1:NC:268:THR:HG21	1:NC:520:TRP:CH2	2.43	0.53
1:AA:353:THR:HG22	1:AA:406:PRO:HB3	1.90	0.53
1:GA:490:LYS:HB2	1:GA:498:THR:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MB:227:PHE:CE1	1:MB:268:THR:HG23	2.44	0.53
1:MC:25:GLU:OE1	1:MC:25:GLU:N	2.41	0.53
1:MC:227:PHE:CE1	1:MC:268:THR:HG23	2.44	0.53
1:NB:248:LYS:HD2	1:NB:435:ARG:HD2	1.90	0.53
1:BC:308:TRP:CZ3	1:BC:380:ASN:HB3	2.44	0.53
1:DB:32:VAL:HB	1:DB:159:PRO:HB2	1.90	0.53
1:EA:147:ASP:OD2	1:EA:149:ARG:NH1	2.42	0.53
1:EC:268:THR:HG21	1:EC:520:TRP:HH2	1.74	0.53
1:FC:527:LEU:HD23	1:FC:527:LEU:H	1.73	0.53
1:HC:433:PHE:HB3	1:HC:450:ASP:HB3	1.89	0.53
1:IB:57:VAL:HA	1:JC:139:THR:HG22	1.89	0.53
1:CB:199:SER:HB2	1:DC:184:THR:HG23	1.91	0.53
1:IC:239:ASN:ND2	1:IC:436:SER:OG	2.35	0.53
1:LB:66:VAL:HG21	1:LB:119:ILE:HD11	1.91	0.53
1:LB:267:THR:CG2	1:LB:271:VAL:H	2.22	0.53
1:AB:94:ARG:HG2	1:AB:224:THR:HB	1.90	0.53
1:CC:109:LEU:HD13	1:CC:200:CYS:SG	2.49	0.53
1:CC:472:VAL:HG11	1:CC:490:LYS:HD2	1.90	0.53
1:HC:338:THR:OG1	1:HC:345:ARG:NH2	2.20	0.53
1:IA:147:ASP:OD1	1:IA:149:ARG:HG2	2.09	0.53
1:KC:472:VAL:HG11	1:KC:490:LYS:HD2	1.90	0.53
1:MC:390:GLN:HB2	1:MC:445:PRO:HB3	1.91	0.53
1:CB:109:LEU:HD23	1:CB:200:CYS:SG	2.49	0.53
1:GA:101:GLY:HA3	1:GA:210:PHE:HA	1.91	0.53
1:KC:433:PHE:HB3	1:KC:450:ASP:HB3	1.91	0.53
1:NC:239:ASN:ND2	1:NC:436:SER:OG	2.39	0.53
1:BB:57:VAL:HA	1:CC:139:THR:HG22	1.91	0.53
1:BB:249:LEU:HB2	1:BB:509:ILE:HD11	1.91	0.53
1:GA:105:VAL:HG13	1:GA:156:ILE:HB	1.90	0.53
1:GA:319:ALA:HB1	1:GA:320:PRO:HD2	1.90	0.53
1:GC:338:THR:HB	1:GC:341:ASP:OD1	2.09	0.53
1:HB:501:HIS:ND1	1:HB:531:GLY:HA3	2.23	0.53
1:HC:223:ARG:HA	1:HC:467:PRO:HG2	1.91	0.53
1:KA:311:TYR:CE1	1:KA:320:PRO:HG3	2.44	0.53
1:KC:308:TRP:CZ3	1:KC:380:ASN:HB3	2.44	0.53
1:NB:286:PHE:HB3	1:NB:301:MET:HE1	1.91	0.53
1:BC:267:THR:CG2	1:BC:271:VAL:H	2.22	0.52
1:DC:268:THR:HG21	1:DC:520:TRP:CH2	2.38	0.52
1:EA:433:PHE:HB3	1:EA:450:ASP:HB3	1.91	0.52
1:JA:223:ARG:NH2	1:JA:269:ASP:HB2	2.24	0.52
1:JC:359:THR:HG22	1:JC:410:GLY:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:245:PRO:O	1:BB:436:SER:OG	2.19	0.52
1:EA:159:PRO:O	1:EA:176:ILE:HD12	2.09	0.52
1:EB:359:THR:HG22	1:EB:410:GLY:HA3	1.90	0.52
1:FC:37:ILE:HG22	1:FC:165:PHE:HD1	1.74	0.52
1:FC:159:PRO:O	1:FC:176:ILE:HD12	2.07	0.52
1:FC:486:LEU:HD11	1:FC:510:PRO:CD	2.40	0.52
1:GA:144:ILE:HD12	1:GA:154:VAL:HG11	1.92	0.52
1:AB:15:THR:HG21	1:AB:151:LEU:HD11	1.90	0.52
1:EB:94:ARG:HD3	1:EB:226:PRO:HD3	1.91	0.52
1:EB:159:PRO:O	1:EB:176:ILE:HD12	2.09	0.52
1:GB:30:GLU:HG3	1:GC:44:GLN:HA	1.91	0.52
1:HB:14:SER:HA	1:IC:149:ARG:O	2.08	0.52
1:IC:338:THR:OG1	1:IC:345:ARG:NH2	2.38	0.52
1:JA:328:GLY:H	1:JA:353:THR:HB	1.74	0.52
1:JB:338:THR:OG1	1:JB:345:ARG:NH2	2.41	0.52
1:JC:434:PHE:CE2	1:JC:454:PRO:HD3	2.44	0.52
1:LC:338:THR:OG1	1:LC:345:ARG:NH2	2.40	0.52
1:MB:338:THR:OG1	1:MB:345:ARG:NH2	2.31	0.52
1:OA:105:VAL:HG13	1:OA:156:ILE:HB	1.90	0.52
1:OB:94:ARG:O	1:OB:218:PRO:HA	2.09	0.52
1:OB:124:VAL:HG22	1:OB:177:LYS:HB2	1.91	0.52
1:OC:247:GLU:CD	1:OC:437:THR:H	2.17	0.52
1:AA:422:VAL:HG12	1:AA:431:LEU:HD21	1.92	0.52
1:CA:147:ASP:OD2	1:CA:149:ARG:NH1	2.41	0.52
1:CB:159:PRO:O	1:CB:176:ILE:HD12	2.09	0.52
1:DB:482:THR:HG22	1:EC:426:PHE:HD1	1.72	0.52
1:EB:94:ARG:O	1:EB:218:PRO:HA	2.10	0.52
1:EB:233:THR:HG22	1:EB:235:GLU:H	1.75	0.52
1:EB:464:GLU:HG3	1:EB:464:GLU:O	2.09	0.52
1:FA:105:VAL:HG13	1:FA:156:ILE:HB	1.90	0.52
1:FB:338:THR:OG1	1:FB:345:ARG:NH2	2.35	0.52
1:IA:275:THR:HG23	1:IA:318:PRO:HG2	1.90	0.52
1:LB:306:GLN:CD	1:LB:306:GLN:H	2.18	0.52
1:AC:472:VAL:HG11	1:AC:490:LYS:HD2	1.92	0.52
1:BA:216:VAL:HG22	1:BA:217:PRO:HD2	1.92	0.52
1:CC:527:LEU:HD23	1:CC:527:LEU:H	1.75	0.52
1:GB:57:VAL:HA	1:HC:139:THR:HG22	1.91	0.52
1:GC:227:PHE:CE1	1:GC:268:THR:HG23	2.44	0.52
1:JA:147:ASP:OD2	1:JA:149:ARG:NH1	2.41	0.52
1:LC:33:VAL:HG11	1:LC:37:ILE:HB	1.91	0.52
1:OC:527:LEU:HD23	1:OC:527:LEU:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:433:PHE:HB3	1:AA:450:ASP:HB3	1.90	0.52
1:AB:120:ILE:HG13	1:AB:183:TYR:HB2	1.91	0.52
1:AB:433:PHE:HB3	1:AB:450:ASP:HB3	1.89	0.52
1:FC:249:LEU:HB3	1:FC:507:LEU:HD12	1.92	0.52
1:GC:472:VAL:HG11	1:GC:490:LYS:HD2	1.92	0.52
1:HB:94:ARG:HG2	1:HB:224:THR:HB	1.92	0.52
1:KC:434:PHE:CE2	1:KC:454:PRO:HD3	2.45	0.52
1:MB:197:THR:HB	1:NC:187:ARG:HH12	1.75	0.52
1:NB:45:GLN:O	1:OA:51:TRP:NE1	2.42	0.52
1:NC:33:VAL:HG11	1:NC:37:ILE:HB	1.91	0.52
1:NC:227:PHE:CE1	1:NC:268:THR:HG23	2.44	0.52
1:BA:328:GLY:H	1:BA:353:THR:HB	1.74	0.52
1:EB:227:PHE:CE1	1:EB:268:THR:HG23	2.44	0.52
1:FB:301:MET:HE2	1:FB:303:LEU:HD23	1.90	0.52
1:GA:53:ARG:HB3	1:GA:206:PRO:HG2	1.92	0.52
1:HC:319:ALA:HB1	1:HC:320:PRO:HD2	1.91	0.52
1:KB:454:PRO:HG2	1:KB:457:TRP:CG	2.44	0.52
1:LC:389:VAL:HG23	1:LC:442:SER:HB3	1.91	0.52
1:NB:101:GLY:HA3	1:NB:210:PHE:HA	1.92	0.52
1:NB:197:THR:HB	1:OC:187:ARG:HH11	1.74	0.52
1:NB:424:PRO:HD3	1:NB:431:LEU:HG	1.91	0.52
1:OB:225:LYS:HD2	1:OB:226:PRO:HD2	1.91	0.52
1:OC:46:ASN:HD21	1:OC:213:ILE:C	2.18	0.52
1:AB:233:THR:HB	1:AB:236:GLU:HG3	1.91	0.52
1:AC:267:THR:CG2	1:AC:271:VAL:H	2.21	0.52
1:IB:81:LEU:HD11	1:IB:102:GLY:HA2	1.90	0.52
1:MA:225:LYS:HD2	1:MA:464:GLU:HG3	1.92	0.52
1:NC:347:HIS:CE1	1:NC:374:ASP:HB3	2.45	0.52
1:CA:424:PRO:HD3	1:CA:431:LEU:HD13	1.91	0.52
1:EB:81:LEU:HD11	1:EB:102:GLY:HA2	1.91	0.52
1:EC:33:VAL:HG11	1:EC:37:ILE:HG13	1.91	0.52
1:HA:318:PRO:HB3	1:HA:418:LEU:HD23	1.92	0.52
1:HA:326:PHE:O	1:HA:353:THR:HG21	2.10	0.52
1:JB:464:GLU:O	1:JB:464:GLU:HG3	2.10	0.52
1:KC:305:SER:HB2	1:KC:309:ASN:H	1.74	0.52
1:LA:53:ARG:HB3	1:LA:206:PRO:HG2	1.92	0.52
1:LA:233:THR:HG22	1:LA:235:GLU:N	2.23	0.52
1:MA:140:MET:HG2	1:NA:57:VAL:CG2	2.40	0.52
1:MB:267:THR:CG2	1:MB:271:VAL:H	2.22	0.52
1:MC:46:ASN:ND2	1:MC:213:ILE:O	2.42	0.52
1:MC:456:GLU:OE1	1:MC:456:GLU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:65:THR:HG21	1:CA:526:THR:N	2.12	0.52
1:CC:267:THR:CG2	1:CC:271:VAL:H	2.23	0.52
1:HB:267:THR:CG2	1:HB:271:VAL:H	2.22	0.52
1:IA:144:ILE:HD12	1:IA:154:VAL:HG11	1.91	0.52
1:LC:233:THR:HG22	1:LC:235:GLU:H	1.74	0.52
1:AB:244:ILE:HA	1:BA:281:VAL:HG11	1.91	0.51
1:BC:478:VAL:HG22	1:BC:485:VAL:HG22	1.92	0.51
1:CA:109:LEU:HD22	1:CA:200:CYS:SG	2.50	0.51
1:EC:391:ASP:H	1:EC:399:GLU:HG3	1.74	0.51
1:FA:328:GLY:H	1:FA:353:THR:HB	1.74	0.51
1:FC:44:GLN:NE2	1:FC:215:LEU:HD23	2.25	0.51
1:GB:286:PHE:HB3	1:GB:301:MET:HE1	1.92	0.51
1:JA:476:ARG:HD3	1:JA:485:VAL:HG11	1.92	0.51
1:JB:282:ASN:OD1	1:JB:287:ARG:NH2	2.42	0.51
1:MB:115:THR:O	1:MB:149:ARG:HD3	2.11	0.51
1:NA:53:ARG:O	1:NA:205:ARG:HD2	2.10	0.51
1:AB:471:ASP:HA	1:AB:493:LYS:CD	2.40	0.51
1:BB:359:THR:HG22	1:BB:410:GLY:HA3	1.93	0.51
1:FA:101:GLY:HA3	1:FA:210:PHE:HA	1.92	0.51
1:FA:117:GLY:O	1:FA:148:VAL:HG22	2.10	0.51
1:GC:416:VAL:HG12	1:GC:417:HIS:CD2	2.45	0.51
1:KA:424:PRO:HD3	1:KA:431:LEU:HD13	1.93	0.51
1:MB:306:GLN:H	1:MB:306:GLN:CD	2.18	0.51
1:NA:490:LYS:HG3	1:NA:527:LEU:HD11	1.91	0.51
1:BA:248:LYS:HE2	1:BA:435:ARG:HD2	1.91	0.51
1:BC:335:THR:HG23	1:KC:440:GLY:O	2.10	0.51
1:CB:101:GLY:HA3	1:CB:210:PHE:HA	1.92	0.51
1:FB:94:ARG:HD3	1:FB:226:PRO:HD3	1.92	0.51
1:FB:94:ARG:O	1:FB:218:PRO:HA	2.10	0.51
1:GA:77:TRP:HB3	1:GA:180:ALA:HB3	1.93	0.51
1:HC:233:THR:HG22	1:HC:235:GLU:H	1.75	0.51
1:JB:454:PRO:HG2	1:JB:457:TRP:CG	2.45	0.51
1:LB:81:LEU:HD11	1:LB:102:GLY:HA2	1.91	0.51
1:OB:501:HIS:CE1	1:OB:531:GLY:HA3	2.46	0.51
1:AB:249:LEU:HB2	1:AB:509:ILE:HD11	1.91	0.51
1:CC:37:ILE:HG22	1:CC:165:PHE:HD1	1.76	0.51
1:DC:433:PHE:HB3	1:DC:450:ASP:HB3	1.91	0.51
1:IA:30:GLU:HG3	1:JA:51:TRP:CZ2	2.45	0.51
1:IB:244:ILE:HA	1:JA:281:VAL:HG11	1.92	0.51
1:JB:343:SER:OG	1:JB:345:ARG:NH2	2.42	0.51
1:LB:15:THR:HG21	1:LB:151:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MB:197:THR:HB	1:NC:187:ARG:NH1	2.25	0.51
1:CA:140:MET:HE1	1:CB:218:PRO:HD2	1.92	0.51
1:FA:422:VAL:HG12	1:FA:431:LEU:HD21	1.92	0.51
1:FA:484:ARG:NH2	1:JA:69:ARG:O	2.40	0.51
1:FB:57:VAL:HA	1:GC:139:THR:HG22	1.91	0.51
1:FB:69:ARG:HD3	1:FB:427:PRO:HB2	1.91	0.51
1:GA:389:VAL:HG12	1:GA:441:CYS:HB2	1.93	0.51
1:GC:94:ARG:NH1	1:GC:226:PRO:HD3	2.25	0.51
1:HA:105:VAL:HG13	1:HA:156:ILE:HB	1.91	0.51
1:IA:306:GLN:OE1	1:IA:306:GLN:N	2.41	0.51
1:KA:233:THR:HG22	1:KA:235:GLU:N	2.26	0.51
1:KB:389:VAL:HG12	1:KB:441:CYS:HB2	1.93	0.51
1:MC:56:PHE:HB3	1:MC:203:LEU:HB3	1.91	0.51
1:OA:216:VAL:HG22	1:OA:217:PRO:HD2	1.92	0.51
1:AC:56:PHE:HB3	1:AC:203:LEU:HB3	1.92	0.51
1:BA:138:VAL:HG21	1:BA:181:MET:SD	2.50	0.51
1:FB:32:VAL:HB	1:FB:159:PRO:HB2	1.93	0.51
1:FC:434:PHE:CE2	1:FC:454:PRO:HD3	2.46	0.51
1:HA:353:THR:CG2	1:HA:406:PRO:HB3	2.40	0.51
1:HB:19:VAL:HG23	1:HB:149:ARG:HB3	1.92	0.51
1:IC:233:THR:HG22	1:IC:235:GLU:H	1.74	0.51
1:KB:115:THR:O	1:KB:149:ARG:HD3	2.11	0.51
1:MB:30:GLU:HG3	1:MC:44:GLN:HA	1.93	0.51
1:MB:233:THR:HG22	1:MB:235:GLU:HG2	1.91	0.51
1:NA:241:ARG:NE	1:NA:325:ASP:OD2	2.44	0.51
1:NC:148:VAL:HG13	1:NC:198:VAL:HG21	1.92	0.51
1:NC:389:VAL:HG23	1:NC:442:SER:HB3	1.92	0.51
1:AA:51:TRP:CH2	1:EA:30:GLU:HG3	2.45	0.51
1:AA:117:GLY:O	1:AA:148:VAL:HG22	2.10	0.51
1:AB:227:PHE:CE1	1:AB:268:THR:HG23	2.46	0.51
1:DA:140:MET:HE1	1:DB:218:PRO:HD2	1.93	0.51
1:FC:56:PHE:HB3	1:FC:203:LEU:HB3	1.93	0.51
1:GC:267:THR:CG2	1:GC:271:VAL:H	2.24	0.51
1:HC:107:VAL:CG1	1:HC:154:VAL:HB	2.41	0.51
1:HC:434:PHE:CE2	1:HC:454:PRO:HD3	2.46	0.51
1:AC:390:GLN:HB2	1:AC:445:PRO:HB3	1.92	0.51
1:DB:88:TYR:HD1	1:EA:95:MET:HE3	1.76	0.51
1:LA:490:LYS:HB2	1:LA:498:THR:HG22	1.93	0.51
1:LC:527:LEU:HD23	1:LC:527:LEU:H	1.75	0.51
1:MA:117:GLY:O	1:MA:148:VAL:HG22	2.11	0.51
1:MA:430:GLN:HE22	1:MA:503:GLY:H	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NC:46:ASN:HD21	1:NC:213:ILE:C	2.18	0.51
1:BB:301:MET:HE2	1:BB:303:LEU:HD23	1.92	0.51
1:EC:227:PHE:CE1	1:EC:268:THR:HG23	2.46	0.51
1:GB:267:THR:CG2	1:GB:271:VAL:H	2.24	0.51
1:HB:230:PRO:HG2	1:HB:457:TRP:CD1	2.46	0.51
1:HB:275:THR:HG23	1:HB:318:PRO:HG2	1.93	0.51
1:IB:30:GLU:HG3	1:IC:44:GLN:HA	1.93	0.51
1:JC:56:PHE:HB3	1:JC:203:LEU:HB3	1.93	0.51
1:KA:95:MET:HE3	1:OB:88:TYR:CD1	2.46	0.51
1:KB:135:PRO:HA	1:KB:181:MET:HE1	1.93	0.51
1:KC:189:ASN:HD21	1:OB:190:ASN:HB2	1.75	0.51
1:LB:57:VAL:HA	1:MC:139:THR:HG22	1.92	0.51
1:NB:66:VAL:HG12	1:NB:186:LEU:HB2	1.93	0.51
1:NB:471:ASP:HA	1:NB:493:LYS:CD	2.41	0.51
1:NC:267:THR:CG2	1:NC:271:VAL:H	2.22	0.51
1:BA:147:ASP:OD2	1:BA:149:ARG:NH1	2.44	0.51
1:BC:51:TRP:CG	1:KC:44:GLN:NE2	2.79	0.51
1:DB:94:ARG:O	1:DB:218:PRO:HA	2.10	0.51
1:IA:65:THR:HG23	1:IA:197:THR:HG23	1.93	0.51
1:JA:225:LYS:HE3	1:JA:464:GLU:HG3	1.92	0.51
1:MC:336:GLN:NE2	1:MC:379:GLN:HB2	2.24	0.51
1:CA:105:VAL:HG13	1:CA:156:ILE:HB	1.93	0.50
1:FB:267:THR:CG2	1:FB:271:VAL:H	2.24	0.50
1:GB:301:MET:HE2	1:GB:303:LEU:HD23	1.92	0.50
1:GC:481:ASP:OD1	1:GC:512:ASN:ND2	2.39	0.50
1:IA:140:MET:HE1	1:IB:218:PRO:HD3	1.92	0.50
1:IC:109:LEU:HD13	1:IC:200:CYS:SG	2.51	0.50
1:JB:359:THR:HG22	1:JB:410:GLY:HA3	1.92	0.50
1:MA:101:GLY:HA3	1:MA:210:PHE:HA	1.93	0.50
1:NA:53:ARG:HB3	1:NA:206:PRO:HG2	1.93	0.50
1:NB:134:SER:OG	1:NB:137:GLN:HG3	2.11	0.50
1:AC:57:VAL:HA	1:GB:139:THR:HG22	1.93	0.50
1:BA:125:PRO:HG3	1:BB:214:PHE:CD1	2.46	0.50
1:EA:62:GLY:HA2	1:EA:202:VAL:HB	1.92	0.50
1:EB:267:THR:CG2	1:EB:271:VAL:H	2.24	0.50
1:IB:338:THR:OG1	1:IB:345:ARG:NH2	2.45	0.50
1:JB:501:HIS:ND1	1:JB:531:GLY:HA3	2.26	0.50
1:MB:101:GLY:HA3	1:MB:210:PHE:HA	1.92	0.50
1:NB:84:ASP:HB3	1:NB:469:GLN:OE1	2.11	0.50
1:NB:267:THR:HG22	1:NB:271:VAL:H	1.76	0.50
1:OB:228:THR:OG1	1:OB:464:GLU:OE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:118:LYS:H	1:FB:184:THR:HB	1.76	0.50
1:GA:233:THR:HG22	1:GA:235:GLU:N	2.26	0.50
1:GC:434:PHE:CE2	1:GC:454:PRO:HD3	2.47	0.50
1:HC:267:THR:CG2	1:HC:271:VAL:H	2.23	0.50
1:JB:399:GLU:HB3	1:JB:400:PRO:HD3	1.93	0.50
1:KC:233:THR:HG22	1:KC:235:GLU:H	1.76	0.50
1:LC:286:PHE:HB3	1:LC:303:LEU:HD21	1.93	0.50
1:MA:490:LYS:HG3	1:MA:527:LEU:HD11	1.92	0.50
1:MC:399:GLU:HB3	1:MC:400:PRO:HD3	1.93	0.50
1:NC:472:VAL:HG11	1:NC:490:LYS:HD2	1.93	0.50
1:AA:138:VAL:HG21	1:AA:181:MET:SD	2.50	0.50
1:BA:438:MET:O	1:BA:447:MET:HG2	2.11	0.50
1:DC:389:VAL:HG23	1:DC:442:SER:HB3	1.94	0.50
1:EC:37:ILE:HG22	1:EC:165:PHE:HD1	1.76	0.50
1:EC:527:LEU:HD23	1:EC:527:LEU:H	1.76	0.50
1:FC:101:GLY:HA3	1:FC:210:PHE:HA	1.93	0.50
1:IB:94:ARG:O	1:IB:218:PRO:HA	2.11	0.50
1:JA:390:GLN:HG2	1:JA:399:GLU:HB2	1.93	0.50
1:JC:109:LEU:HD13	1:JC:200:CYS:SG	2.51	0.50
1:MA:490:LYS:HE3	1:MA:527:LEU:HG	1.93	0.50
1:NB:115:THR:O	1:NB:149:ARG:HD3	2.11	0.50
1:AB:275:THR:HG23	1:AB:318:PRO:HG2	1.94	0.50
1:BB:265:ARG:HE	1:BB:419:ALA:HB1	1.76	0.50
1:BC:227:PHE:CE1	1:BC:268:THR:HG23	2.46	0.50
1:CB:57:VAL:HA	1:DC:139:THR:HG22	1.93	0.50
1:CC:227:PHE:CE1	1:CC:268:THR:HG23	2.47	0.50
1:DB:233:THR:HB	1:DB:236:GLU:HG3	1.92	0.50
1:EC:434:PHE:CE2	1:EC:454:PRO:HD3	2.47	0.50
1:FA:53:ARG:HB3	1:FA:206:PRO:HG2	1.94	0.50
1:HB:115:THR:O	1:HB:149:ARG:HD3	2.12	0.50
1:JA:53:ARG:HB3	1:JA:206:PRO:HG2	1.92	0.50
1:JC:244:ILE:HD13	1:JC:438:MET:HA	1.93	0.50
1:KB:227:PHE:CE1	1:KB:268:THR:HG23	2.46	0.50
1:KC:109:LEU:HD13	1:KC:200:CYS:SG	2.52	0.50
1:LA:353:THR:CG2	1:LA:406:PRO:HB3	2.42	0.50
1:MB:233:THR:HB	1:MB:236:GLU:HG3	1.93	0.50
1:NB:15:THR:HG22	1:OC:149:ARG:NE	2.23	0.50
1:AB:190:ASN:HB2	1:BC:189:ASN:HD21	1.76	0.50
1:BB:277:GLN:HB3	1:BB:321:LEU:HB3	1.92	0.50
1:DB:118:LYS:H	1:DB:184:THR:HB	1.77	0.50
1:JB:233:THR:HB	1:JB:236:GLU:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KC:81:LEU:HD12	1:KC:158:LEU:HG	1.94	0.50
1:LC:416:VAL:HG12	1:LC:417:HIS:ND1	2.26	0.50
1:MA:353:THR:HG22	1:MA:406:PRO:HB3	1.94	0.50
1:AC:463:GLN:HA	1:GC:231:ILE:HD11	1.94	0.50
1:BB:233:THR:HB	1:BB:236:GLU:HG3	1.94	0.50
1:CA:159:PRO:O	1:CA:176:ILE:HD12	2.11	0.50
1:CA:280:PRO:HB3	1:CA:455:GLN:HG2	1.94	0.50
1:EB:249:LEU:HB2	1:EB:509:ILE:HD11	1.93	0.50
1:GA:30:GLU:HG3	1:HA:51:TRP:CH2	2.47	0.50
1:GC:33:VAL:HG11	1:GC:37:ILE:HB	1.92	0.50
1:HC:527:LEU:HD23	1:HC:527:LEU:H	1.77	0.50
1:LC:265:ARG:HD3	1:LC:452:LEU:HD12	1.94	0.50
1:MB:197:THR:O	1:NC:187:ARG:NH1	2.44	0.50
1:NB:128:PHE:HE1	1:NB:133:LEU:HD21	1.77	0.50
1:OA:499:VAL:HG21	1:OA:530:MET:HE3	1.93	0.50
1:HA:280:PRO:HB3	1:HA:455:GLN:HG2	1.94	0.50
1:IA:422:VAL:HG12	1:IA:431:LEU:HD21	1.93	0.50
1:IB:94:ARG:HG2	1:IB:224:THR:CG2	2.42	0.50
1:IB:124:VAL:HG22	1:IB:177:LYS:HB2	1.94	0.50
1:JA:105:VAL:CG1	1:JA:156:ILE:HB	2.42	0.50
1:JB:245:PRO:O	1:JB:436:SER:OG	2.19	0.50
1:JC:185:PRO:HG2	1:JC:187:ARG:HE	1.77	0.50
1:MB:440:GLY:O	1:NA:335:THR:HG23	2.12	0.50
1:NB:310:ASN:OD1	1:NB:311:TYR:N	2.45	0.50
1:OA:317:ILE:HG22	1:OA:318:PRO:HD2	1.94	0.50
1:OB:400:PRO:HG2	1:OB:446:ASN:HB3	1.94	0.50
1:AC:123:ALA:HB1	1:AC:176:ILE:HD11	1.93	0.50
1:AC:527:LEU:H	1:AC:527:LEU:HD23	1.77	0.50
1:BA:371:THR:HG22	1:BA:373:ASN:H	1.77	0.50
1:CA:40:PRO:HB2	1:CC:37:ILE:HD11	1.94	0.50
1:CA:319:ALA:HB1	1:CA:320:PRO:HD2	1.93	0.50
1:FA:353:THR:CG2	1:FA:406:PRO:HB3	2.42	0.50
1:FA:435:ARG:NH1	1:FA:448:ASN:HB3	2.26	0.50
1:FC:265:ARG:HD3	1:FC:452:LEU:HD12	1.93	0.50
1:GA:69:ARG:HH21	1:GA:427:PRO:HB2	1.76	0.50
1:GA:248:LYS:HE2	1:GA:435:ARG:HD2	1.94	0.50
1:HC:469:GLN:HB2	1:HC:520:TRP:CG	2.46	0.50
1:IA:101:GLY:HA3	1:IA:210:PHE:HA	1.94	0.50
1:IA:144:ILE:HD13	1:IA:156:ILE:HG12	1.94	0.50
1:IA:225:LYS:HD3	1:IA:464:GLU:HG3	1.94	0.50
1:LA:347:HIS:HE2	1:LA:374:ASP:HB3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OC:243:PRO:HG3	1:OC:283:ILE:HB	1.93	0.50
1:AC:109:LEU:HD13	1:AC:200:CYS:SG	2.51	0.49
1:BA:96:TYR:CG	1:BA:212:PHE:HB3	2.47	0.49
1:BA:433:PHE:HB3	1:BA:450:ASP:HB3	1.94	0.49
1:BC:37:ILE:HG22	1:BC:165:PHE:HD1	1.77	0.49
1:BC:124:VAL:HG21	1:BC:179:ILE:HD12	1.94	0.49
1:CC:148:VAL:HG13	1:CC:198:VAL:HG21	1.94	0.49
1:EC:249:LEU:HB3	1:EC:507:LEU:HD12	1.93	0.49
1:FB:24:ASN:ND2	1:LC:152:GLU:OE2	2.44	0.49
1:FB:399:GLU:HB3	1:FB:400:PRO:HD3	1.94	0.49
1:IA:424:PRO:HD3	1:IA:431:LEU:HD13	1.94	0.49
1:MA:158:LEU:HD13	1:MA:178:LEU:HD13	1.93	0.49
1:NB:34:GLY:HA3	1:NB:209:ASP:HB2	1.94	0.49
1:OA:96:TYR:CG	1:OA:212:PHE:HB3	2.46	0.49
1:CC:94:ARG:NH1	1:CC:226:PRO:HD3	2.26	0.49
1:DB:33:VAL:HG21	1:DB:37:ILE:CD1	2.41	0.49
1:EA:65:THR:CG2	1:EA:526:THR:H	2.19	0.49
1:EA:69:ARG:HH21	1:EA:427:PRO:HB2	1.77	0.49
1:FA:75:ILE:HG23	1:FA:179:ILE:HG23	1.94	0.49
1:FC:336:GLN:NE2	1:FC:379:GLN:HB2	2.27	0.49
1:HA:399:GLU:HB3	1:HA:400:PRO:HD3	1.94	0.49
1:KA:265:ARG:NH2	1:KA:420:PRO:O	2.40	0.49
1:LA:353:THR:HG22	1:LA:406:PRO:HB3	1.94	0.49
1:LC:123:ALA:HB1	1:LC:176:ILE:HD11	1.94	0.49
1:OC:148:VAL:HG13	1:OC:198:VAL:HG21	1.94	0.49
1:AB:337:THR:HG21	1:BA:447:MET:HE1	1.92	0.49
1:BA:233:THR:HG21	1:BA:511:PRO:O	2.12	0.49
1:BB:32:VAL:HB	1:BB:159:PRO:HB2	1.94	0.49
1:FC:486:LEU:HD11	1:FC:510:PRO:HD2	1.93	0.49
1:IB:501:HIS:CE1	1:IB:531:GLY:HA3	2.47	0.49
1:JA:399:GLU:HB3	1:JA:400:PRO:HD3	1.95	0.49
1:JA:424:PRO:HD3	1:JA:431:LEU:HD13	1.93	0.49
1:KB:233:THR:HB	1:KB:236:GLU:HG3	1.94	0.49
1:NB:106:GLN:HE22	1:OC:23:ASN:N	2.10	0.49
1:NB:433:PHE:HB3	1:NB:450:ASP:HB3	1.95	0.49
1:OA:140:MET:HE1	1:OB:218:PRO:HD2	1.95	0.49
1:DA:109:LEU:HD22	1:DA:200:CYS:SG	2.51	0.49
1:DA:353:THR:CG2	1:DA:406:PRO:HB3	2.42	0.49
1:DB:199:SER:HB2	1:EC:184:THR:HG23	1.95	0.49
1:FA:215:LEU:HD12	1:JB:51:TRP:HB3	1.93	0.49
1:GA:109:LEU:HD22	1:GA:200:CYS:SG	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IC:389:VAL:HG23	1:IC:442:SER:HB3	1.94	0.49
1:KA:422:VAL:HG12	1:KA:431:LEU:HD21	1.93	0.49
1:MA:233:THR:HG22	1:MA:235:GLU:N	2.27	0.49
1:MB:389:VAL:HG12	1:MB:441:CYS:HB2	1.95	0.49
1:AB:30:GLU:HG3	1:AC:44:GLN:HA	1.93	0.49
1:AC:94:ARG:NH1	1:AC:226:PRO:HD3	2.27	0.49
1:BA:140:MET:CE	1:BB:218:PRO:HD3	2.41	0.49
1:BA:326:PHE:CZ	1:BA:438:MET:HE1	2.48	0.49
1:BC:527:LEU:HD23	1:BC:527:LEU:H	1.77	0.49
1:DB:267:THR:CG2	1:DB:271:VAL:H	2.24	0.49
1:HA:435:ARG:NH1	1:HA:448:ASN:HB3	2.28	0.49
1:HB:301:MET:HE2	1:HB:303:LEU:HD23	1.94	0.49
1:IB:137:GLN:HA	1:IB:140:MET:HE2	1.93	0.49
1:JA:144:ILE:HD11	1:JA:156:ILE:HD11	1.95	0.49
1:JB:267:THR:HG22	1:JB:271:VAL:N	2.22	0.49
1:LC:148:VAL:HG13	1:LC:198:VAL:HG21	1.95	0.49
1:AA:125:PRO:HG3	1:AB:214:PHE:CD1	2.48	0.49
1:AB:81:LEU:HD11	1:AB:102:GLY:HA2	1.95	0.49
1:BC:434:PHE:CE2	1:BC:454:PRO:HD3	2.48	0.49
1:DA:319:ALA:HB1	1:DA:320:PRO:HD2	1.94	0.49
1:EB:101:GLY:HA3	1:EB:210:PHE:HA	1.94	0.49
1:FC:44:GLN:NE2	1:LC:51:TRP:CG	2.81	0.49
1:GC:377:THR:HG22	1:GC:378:GLY:H	1.77	0.49
1:GC:433:PHE:HB3	1:GC:450:ASP:HB3	1.93	0.49
1:JC:30:GLU:HG3	1:JC:31:PRO:HD2	1.94	0.49
1:KA:95:MET:HE3	1:OB:88:TYR:HD1	1.77	0.49
1:KA:247:GLU:OE1	1:KA:437:THR:HG22	2.11	0.49
1:LB:233:THR:HG22	1:LB:235:GLU:H	1.77	0.49
1:BB:115:THR:O	1:BB:149:ARG:HD3	2.12	0.49
1:DB:57:VAL:HA	1:EC:139:THR:HG22	1.94	0.49
1:GB:75:ILE:HD13	1:GB:179:ILE:HD12	1.95	0.49
1:GB:359:THR:HG22	1:GB:410:GLY:HA3	1.95	0.49
1:GB:471:ASP:HA	1:GB:493:LYS:CD	2.40	0.49
1:KC:33:VAL:HG11	1:KC:37:ILE:HB	1.95	0.49
1:NB:239:ASN:HD22	1:NB:436:SER:HB3	1.77	0.49
1:OC:118:LYS:H	1:OC:184:THR:HB	1.78	0.49
1:BB:159:PRO:O	1:BB:176:ILE:HD12	2.13	0.49
1:BC:261:PRO:HG3	1:BC:403:TRP:HZ3	1.78	0.49
1:DB:227:PHE:CE1	1:DB:268:THR:HG23	2.47	0.49
1:DB:501:HIS:CE1	1:DB:531:GLY:HA3	2.48	0.49
1:FB:265:ARG:NH2	1:FB:420:PRO:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FC:33:VAL:CG1	1:FC:37:ILE:HG13	2.42	0.49
1:GC:107:VAL:CG1	1:GC:154:VAL:HB	2.43	0.49
1:GC:476:ARG:HG3	1:GC:516:ARG:HH21	1.78	0.49
1:HB:286:PHE:HB3	1:HB:301:MET:HE1	1.95	0.49
1:IB:115:THR:O	1:IB:149:ARG:HD3	2.13	0.49
1:JA:65:THR:HG21	1:JA:526:THR:N	2.12	0.49
1:JA:147:ASP:OD1	1:JA:149:ARG:HG2	2.13	0.49
1:JA:233:THR:HG22	1:JA:235:GLU:N	2.28	0.49
1:MA:48:ILE:HD12	1:MA:211:ASP:HA	1.95	0.49
1:BB:14:SER:O	1:BB:15:THR:OG1	2.24	0.49
1:DB:88:TYR:CD1	1:EA:95:MET:HE3	2.48	0.49
1:EB:403:TRP:CZ2	1:EB:450:ASP:HB2	2.48	0.49
1:GA:499:VAL:HG21	1:GA:530:MET:HE3	1.95	0.49
1:HC:390:GLN:HG2	1:HC:399:GLU:HG3	1.94	0.49
1:IB:389:VAL:HG12	1:IB:441:CYS:HB2	1.95	0.49
1:KC:389:VAL:HG23	1:KC:442:SER:HB3	1.94	0.49
1:MA:71:ALA:HB3	1:NA:484:ARG:HG3	1.95	0.49
1:MC:46:ASN:HD21	1:MC:213:ILE:C	2.20	0.49
1:MC:336:GLN:NE2	1:MC:376:GLU:O	2.40	0.49
1:AC:434:PHE:CE2	1:AC:454:PRO:HD3	2.47	0.49
1:AC:476:ARG:HG3	1:AC:518:ASP:OD2	2.12	0.49
1:FB:195:VAL:HG13	1:FB:196:PHE:N	2.27	0.49
1:GA:422:VAL:HG12	1:GA:431:LEU:HD21	1.95	0.49
1:JB:310:ASN:OD1	1:JB:311:TYR:N	2.46	0.49
1:MB:131:GLU:N	1:MB:131:GLU:OE1	2.46	0.49
1:CB:499:VAL:HB	1:CB:530:MET:HE3	1.95	0.48
1:CC:317:ILE:HG13	1:CC:318:PRO:HD2	1.95	0.48
1:EC:358:PHE:HD1	1:EC:365:VAL:HG13	1.78	0.48
1:FC:424:PRO:HD3	1:FC:431:LEU:HG	1.93	0.48
1:HB:32:VAL:HG13	1:HC:41:VAL:HA	1.95	0.48
1:IB:118:LYS:H	1:IB:184:THR:HB	1.78	0.48
1:JA:223:ARG:HH22	1:JA:269:ASP:HB2	1.76	0.48
1:MA:343:SER:HB3	1:MA:345:ARG:HH12	1.78	0.48
1:AB:137:GLN:HA	1:AB:140:MET:HE3	1.94	0.48
1:CB:424:PRO:HD3	1:CB:431:LEU:HG	1.95	0.48
1:EC:434:PHE:CD2	1:EC:454:PRO:HD3	2.48	0.48
1:FB:125:PRO:HG3	1:FC:214:PHE:CD1	2.49	0.48
1:IA:105:VAL:CG1	1:IA:156:ILE:HB	2.42	0.48
1:IA:140:MET:HB2	1:IB:217:PRO:HG3	1.96	0.48
1:IA:145:ILE:HD13	1:IA:183:TYR:CE2	2.48	0.48
1:IA:326:PHE:CZ	1:IA:438:MET:HE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IA:430:GLN:HE22	1:IA:503:GLY:H	1.60	0.48
1:IB:456:GLU:OE1	1:IB:456:GLU:N	2.45	0.48
1:IC:277:GLN:HB3	1:IC:321:LEU:HB3	1.94	0.48
1:KA:399:GLU:HB3	1:KA:400:PRO:HD3	1.95	0.48
1:KC:187:ARG:HD2	1:OB:196:PHE:HA	1.95	0.48
1:LA:105:VAL:HG13	1:LA:156:ILE:HB	1.95	0.48
1:LC:158:LEU:HD13	1:LC:178:LEU:HG	1.95	0.48
1:AB:286:PHE:HB3	1:AB:301:MET:HE1	1.95	0.48
1:BA:422:VAL:HG12	1:BA:431:LEU:HD21	1.94	0.48
1:CA:433:PHE:HB3	1:CA:450:ASP:HB3	1.95	0.48
1:DB:439:PRO:CB	1:EA:335:THR:HG21	2.40	0.48
1:DB:454:PRO:HG2	1:DB:457:TRP:CG	2.48	0.48
1:EC:182:LEU:HD21	1:EC:185:PRO:HA	1.94	0.48
1:FB:115:THR:O	1:FB:149:ARG:HD3	2.13	0.48
1:HB:238:THR:HA	1:HB:245:PRO:HA	1.95	0.48
1:IC:426:PHE:CD1	1:IC:427:PRO:HD2	2.49	0.48
1:JB:239:ASN:HD22	1:JB:436:SER:HB3	1.77	0.48
1:KA:57:VAL:HG21	1:OA:140:MET:HG2	1.95	0.48
1:KB:267:THR:CG2	1:KB:271:VAL:H	2.23	0.48
1:LC:267:THR:CG2	1:LC:271:VAL:H	2.24	0.48
1:BA:101:GLY:HA3	1:BA:210:PHE:HA	1.95	0.48
1:BB:388:VAL:HG21	1:BB:400:PRO:HB3	1.95	0.48
1:BC:233:THR:HG22	1:BC:235:GLU:H	1.79	0.48
1:CA:53:ARG:HB3	1:CA:206:PRO:HG2	1.94	0.48
1:CA:371:THR:HG22	1:CA:373:ASN:H	1.77	0.48
1:EA:459:LEU:O	1:EA:463:GLN:HG3	2.14	0.48
1:EC:107:VAL:CG1	1:EC:154:VAL:HB	2.44	0.48
1:EC:336:GLN:NE2	1:EC:379:GLN:HB2	2.29	0.48
1:FB:402:GLN:HE21	1:FB:403:TRP:NE1	2.11	0.48
1:HB:109:LEU:HD23	1:HB:200:CYS:SG	2.52	0.48
1:IA:143:HIS:HE1	1:JA:56:PHE:O	1.96	0.48
1:IA:347:HIS:NE2	1:IA:374:ASP:HB3	2.27	0.48
1:KA:51:TRP:CH2	1:OA:30:GLU:HG3	2.49	0.48
1:KB:116:ALA:N	1:KB:187:ARG:O	2.38	0.48
1:LA:71:ALA:HB3	1:MA:484:ARG:HG3	1.94	0.48
1:MA:275:THR:HG23	1:MA:318:PRO:HG2	1.94	0.48
1:NC:527:LEU:HD23	1:NC:527:LEU:H	1.78	0.48
1:OB:19:VAL:HG13	1:OB:149:ARG:O	2.12	0.48
1:OB:359:THR:HG22	1:OB:410:GLY:HA3	1.94	0.48
1:BA:40:PRO:HB2	1:BC:37:ILE:HD11	1.95	0.48
1:BB:317:ILE:HD13	1:BB:321:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:353:THR:HG22	1:DA:406:PRO:HB3	1.95	0.48
1:DC:319:ALA:HB1	1:DC:320:PRO:HD2	1.95	0.48
1:EA:140:MET:HE1	1:EB:218:PRO:HD2	1.95	0.48
1:EA:434:PHE:CE1	1:EA:454:PRO:HD3	2.49	0.48
1:GA:338:THR:OG1	1:GA:345:ARG:NH2	2.40	0.48
1:JC:358:PHE:HD1	1:JC:365:VAL:HG13	1.78	0.48
1:MB:32:VAL:HB	1:MB:159:PRO:HB2	1.95	0.48
1:MC:34:GLY:HA3	1:MC:209:ASP:HB2	1.96	0.48
1:NA:81:LEU:HD11	1:NA:102:GLY:HA2	1.95	0.48
1:NA:326:PHE:CZ	1:NA:438:MET:HE1	2.49	0.48
1:AB:34:GLY:HA3	1:AB:209:ASP:HB2	1.96	0.48
1:AC:139:THR:HG22	1:EB:57:VAL:HA	1.94	0.48
1:BC:46:ASN:HD21	1:BC:213:ILE:C	2.20	0.48
1:DA:140:MET:HG2	1:EA:57:VAL:HG21	1.94	0.48
1:DA:490:LYS:HG3	1:DA:527:LEU:HD11	1.95	0.48
1:DB:115:THR:O	1:DB:149:ARG:HD3	2.13	0.48
1:EC:290:VAL:HG21	1:EC:375:LEU:HD13	1.94	0.48
1:GC:341:ASP:OD1	1:GC:342:GLY:N	2.47	0.48
1:IB:78:SER:HB2	1:IB:179:ILE:HD13	1.94	0.48
1:IB:432:LEU:HB2	1:IB:499:VAL:HG13	1.95	0.48
1:JB:115:THR:O	1:JB:149:ARG:HD3	2.13	0.48
1:KC:94:ARG:NH1	1:KC:226:PRO:HD3	2.29	0.48
1:KC:139:THR:HG22	1:OB:57:VAL:HA	1.96	0.48
1:LC:434:PHE:CE2	1:LC:454:PRO:HD3	2.48	0.48
1:MA:422:VAL:HG12	1:MA:431:LEU:HD21	1.96	0.48
1:NA:96:TYR:CG	1:NA:212:PHE:HB3	2.49	0.48
1:NB:57:VAL:HA	1:OC:139:THR:HG22	1.96	0.48
1:NC:109:LEU:HD13	1:NC:200:CYS:SG	2.54	0.48
1:CB:137:GLN:HA	1:CB:140:MET:HE2	1.94	0.48
1:DB:94:ARG:HD3	1:DB:226:PRO:HD3	1.96	0.48
1:EB:84:ASP:HB3	1:EB:469:GLN:OE1	2.14	0.48
1:EB:286:PHE:HB3	1:EB:301:MET:HE1	1.94	0.48
1:FA:43:GLY:HA3	1:FA:214:PHE:HE1	1.78	0.48
1:FB:306:GLN:CD	1:FB:306:GLN:H	2.22	0.48
1:FC:109:LEU:HD13	1:FC:200:CYS:SG	2.53	0.48
1:FC:390:GLN:HB2	1:FC:445:PRO:HB3	1.96	0.48
1:GB:454:PRO:HG2	1:GB:457:TRP:CG	2.48	0.48
1:IA:233:THR:HG22	1:IA:235:GLU:N	2.26	0.48
1:IC:377:THR:HG22	1:IC:378:GLY:H	1.79	0.48
1:LB:280:PRO:HB3	1:LB:455:GLN:HG2	1.96	0.48
1:LC:359:THR:HG22	1:LC:410:GLY:HA3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MB:230:PRO:HD3	1:MB:460:HIS:CD2	2.48	0.48
1:OC:290:VAL:HG11	1:OC:375:LEU:HD13	1.96	0.48
1:AA:27:MET:HE3	1:BA:205:ARG:HH12	1.78	0.48
1:AA:118:LYS:HE2	1:BA:110:ALA:HA	1.96	0.48
1:AA:326:PHE:CZ	1:AA:438:MET:HE1	2.48	0.48
1:AA:424:PRO:HD3	1:AA:431:LEU:HD13	1.93	0.48
1:FC:336:GLN:HE21	1:FC:379:GLN:HB2	1.79	0.48
1:JC:469:GLN:HB2	1:JC:520:TRP:CD1	2.49	0.48
1:NB:244:ILE:HA	1:OA:281:VAL:HG11	1.95	0.48
1:AA:215:LEU:HD12	1:EB:51:TRP:HB3	1.95	0.48
1:AA:216:VAL:CG2	1:AA:217:PRO:HD2	2.44	0.48
1:AB:130:THR:HG23	1:AB:179:ILE:HD11	1.94	0.48
1:BB:128:PHE:HE1	1:BB:133:LEU:HD21	1.79	0.48
1:EA:147:ASP:OD1	1:EA:149:ARG:HG2	2.13	0.48
1:GA:138:VAL:HG21	1:GA:181:MET:SD	2.53	0.48
1:GC:24:ASN:CG	1:GC:25:GLU:N	2.70	0.48
1:HB:230:PRO:HD3	1:HB:460:HIS:ND1	2.28	0.48
1:IB:530:MET:HG3	1:IB:531:GLY:N	2.28	0.48
1:LA:328:GLY:H	1:LA:353:THR:HB	1.78	0.48
1:MC:377:THR:HG22	1:MC:378:GLY:H	1.78	0.48
1:NA:233:THR:HB	1:NA:236:GLU:HG2	1.96	0.48
1:NB:484:ARG:HG3	1:OC:74:GLU:OE2	2.13	0.48
1:OA:305:SER:OG	1:OA:306:GLN:N	2.45	0.48
1:BA:353:THR:CG2	1:BA:406:PRO:HB3	2.44	0.48
1:CB:267:THR:HG22	1:CB:271:VAL:N	2.27	0.48
1:FA:140:MET:HE3	1:GA:87:PRO:HG2	1.95	0.48
1:LA:315:GLU:HB3	1:LA:317:ILE:HG13	1.94	0.48
1:AB:88:TYR:CD1	1:BA:95:MET:HE3	2.49	0.47
1:BA:430:GLN:HE22	1:BA:503:GLY:H	1.62	0.47
1:BB:124:VAL:HG22	1:BB:177:LYS:HB2	1.95	0.47
1:BC:463:GLN:HA	1:KC:231:ILE:HD11	1.94	0.47
1:CB:454:PRO:HG2	1:CB:457:TRP:CG	2.49	0.47
1:EC:429:GLU:OE2	1:EC:490:LYS:HE2	2.13	0.47
1:FC:472:VAL:HG11	1:FC:490:LYS:HD2	1.96	0.47
1:GA:96:TYR:CG	1:GA:212:PHE:HB3	2.48	0.47
1:HA:43:GLY:HA3	1:HA:214:PHE:HE1	1.79	0.47
1:HA:433:PHE:HB3	1:HA:450:ASP:HB3	1.96	0.47
1:HB:471:ASP:HA	1:HB:493:LYS:CD	2.43	0.47
1:JB:69:ARG:HH12	1:JB:428:GLY:HA3	1.78	0.47
1:KB:471:ASP:HA	1:KB:493:LYS:CD	2.43	0.47
1:LC:443:GLY:O	1:LC:444:TYR:HD1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MC:285:THR:HG22	1:MC:385:PRO:HD2	1.96	0.47
1:NB:66:VAL:HG21	1:NB:119:ILE:HD11	1.95	0.47
1:NC:259:VAL:HG13	1:NC:403:TRP:CZ3	2.49	0.47
1:AA:319:ALA:HB1	1:AA:320:PRO:HD2	1.96	0.47
1:AC:107:VAL:CG1	1:AC:154:VAL:HB	2.44	0.47
1:BB:34:GLY:HA3	1:BB:209:ASP:HB2	1.95	0.47
1:DB:343:SER:OG	1:DB:345:ARG:NH2	2.48	0.47
1:DC:336:GLN:OE1	1:DC:379:GLN:HB2	2.13	0.47
1:FA:343:SER:HB3	1:FA:345:ARG:HH12	1.78	0.47
1:GA:147:ASP:OD1	1:GA:149:ARG:HG2	2.14	0.47
1:GB:81:LEU:HD11	1:GB:102:GLY:HA2	1.95	0.47
1:KC:121:PHE:HB2	1:KC:144:ILE:HG22	1.96	0.47
1:KC:227:PHE:CE1	1:KC:268:THR:HG23	2.49	0.47
1:LA:317:ILE:HG22	1:LA:318:PRO:HD2	1.96	0.47
1:LB:265:ARG:HH22	1:LB:422:VAL:HG23	1.79	0.47
1:NB:51:TRP:HB3	1:OA:215:LEU:HD12	1.96	0.47
1:OB:286:PHE:HB3	1:OB:301:MET:HE1	1.96	0.47
1:OB:459:LEU:O	1:OB:463:GLN:HG3	2.15	0.47
1:DA:33:VAL:HG11	1:DA:37:ILE:HG13	1.96	0.47
1:DB:432:LEU:HB2	1:DB:499:VAL:HG13	1.96	0.47
1:DC:301:MET:HE3	1:DC:367:PHE:CE1	2.49	0.47
1:GB:477:PHE:CE2	1:GB:509:ILE:HD12	2.50	0.47
1:GC:123:ALA:HB1	1:GC:176:ILE:HD11	1.97	0.47
1:KA:87:PRO:HG2	1:OA:140:MET:HE3	1.97	0.47
1:KA:371:THR:HG22	1:KA:373:ASN:H	1.79	0.47
1:KB:14:SER:O	1:KB:15:THR:OG1	2.26	0.47
1:LB:501:HIS:ND1	1:LB:531:GLY:HA3	2.30	0.47
1:LC:107:VAL:HG13	1:LC:154:VAL:HB	1.96	0.47
1:MC:459:LEU:O	1:MC:463:GLN:HG3	2.14	0.47
1:OC:265:ARG:HD3	1:OC:452:LEU:HD12	1.96	0.47
1:AA:338:THR:HB	1:AA:343:SER:HB2	1.97	0.47
1:AB:115:THR:O	1:AB:149:ARG:HD3	2.14	0.47
1:CA:353:THR:HG22	1:CA:406:PRO:HB3	1.97	0.47
1:CC:159:PRO:O	1:CC:176:ILE:HD12	2.14	0.47
1:EA:105:VAL:CG1	1:EA:156:ILE:HB	2.42	0.47
1:EA:359:THR:HG22	1:EA:410:GLY:HA3	1.96	0.47
1:EB:109:LEU:HD23	1:EB:200:CYS:SG	2.55	0.47
1:FB:238:THR:HG21	1:GA:280:PRO:HD2	1.95	0.47
1:GA:149:ARG:NH2	1:HA:149:ARG:O	2.47	0.47
1:GC:148:VAL:HG13	1:GC:198:VAL:HG21	1.97	0.47
1:HB:75:ILE:O	1:HB:522:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KA:66:VAL:HG12	1:KA:186:LEU:HD22	1.95	0.47
1:KA:433:PHE:HB3	1:KA:450:ASP:HB3	1.95	0.47
1:KA:438:MET:O	1:KA:447:MET:HG2	2.14	0.47
1:KB:81:LEU:HD11	1:KB:102:GLY:HA2	1.96	0.47
1:KB:482:THR:HG21	1:LC:427:PRO:HD3	1.97	0.47
1:KC:44:GLN:HE22	1:KC:215:LEU:HD23	1.78	0.47
1:KC:358:PHE:HD1	1:KC:365:VAL:HG13	1.78	0.47
1:LA:424:PRO:HD3	1:LA:431:LEU:HD13	1.96	0.47
1:MA:52:ILE:HD12	1:MA:88:TYR:HB3	1.94	0.47
1:MA:89:LEU:HD11	1:MA:206:PRO:HB3	1.96	0.47
1:MA:476:ARG:HD3	1:MA:485:VAL:HG11	1.94	0.47
1:MB:75:ILE:HD13	1:MB:179:ILE:HD12	1.96	0.47
1:NC:308:TRP:CH2	1:NC:380:ASN:HB3	2.49	0.47
1:OB:267:THR:CG2	1:OB:271:VAL:H	2.26	0.47
1:AB:15:THR:HG22	1:BC:149:ARG:HE	1.80	0.47
1:BB:432:LEU:HB2	1:BB:499:VAL:HG13	1.96	0.47
1:DC:25:GLU:O	1:DC:25:GLU:HG3	2.14	0.47
1:DC:37:ILE:HG22	1:DC:165:PHE:HD1	1.78	0.47
1:EA:318:PRO:HD3	1:EA:417:HIS:O	2.14	0.47
1:EC:477:PHE:HD2	1:EC:515:PHE:CE1	2.33	0.47
1:HC:94:ARG:NH1	1:HC:225:LYS:HA	2.29	0.47
1:JC:254:SER:HA	1:JC:257:PHE:CE1	2.49	0.47
1:KC:311:TYR:CZ	1:KC:320:PRO:HD3	2.48	0.47
1:LA:140:MET:HG2	1:MA:57:VAL:HG21	1.96	0.47
1:MA:140:MET:CE	1:MB:218:PRO:HD3	2.41	0.47
1:NA:319:ALA:HB1	1:NA:320:PRO:HD2	1.96	0.47
1:BB:440:GLY:O	1:CA:335:THR:HG23	2.15	0.47
1:DB:84:ASP:HB3	1:DB:469:GLN:OE1	2.14	0.47
1:FC:148:VAL:HG13	1:FC:198:VAL:HG21	1.95	0.47
1:GC:527:LEU:HD23	1:GC:527:LEU:H	1.80	0.47
1:HA:265:ARG:NH2	1:HA:420:PRO:O	2.37	0.47
1:HA:326:PHE:CZ	1:HA:438:MET:HE1	2.49	0.47
1:JC:148:VAL:HG13	1:JC:198:VAL:HG21	1.95	0.47
1:KA:138:VAL:HG21	1:KA:181:MET:SD	2.54	0.47
1:KC:107:VAL:HG13	1:KC:154:VAL:HB	1.97	0.47
1:MB:318:PRO:HD3	1:MB:417:HIS:O	2.14	0.47
1:NC:107:VAL:CG1	1:NC:154:VAL:HB	2.44	0.47
1:OC:424:PRO:HD3	1:OC:431:LEU:HG	1.96	0.47
1:AB:66:VAL:HG12	1:AB:186:LEU:HB2	1.97	0.47
1:AC:233:THR:HG22	1:AC:235:GLU:H	1.79	0.47
1:BB:454:PRO:HG2	1:BB:457:TRP:CG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:107:VAL:CG1	1:BC:154:VAL:HB	2.45	0.47
1:CA:73:GLY:H	1:CA:181:MET:CE	2.26	0.47
1:CA:422:VAL:HG12	1:CA:431:LEU:HD21	1.95	0.47
1:CC:318:PRO:HG3	1:CC:417:HIS:O	2.14	0.47
1:DC:135:PRO:HA	1:DC:181:MET:HE1	1.97	0.47
1:DC:443:GLY:C	1:DC:444:TYR:HD1	2.23	0.47
1:FC:389:VAL:HG23	1:FC:442:SER:HB3	1.96	0.47
1:GC:390:GLN:HB2	1:GC:445:PRO:HB3	1.97	0.47
1:HB:94:ARG:O	1:HB:218:PRO:HA	2.15	0.47
1:IA:338:THR:OG1	1:IA:345:ARG:NH2	2.37	0.47
1:IB:230:PRO:HD3	1:IB:460:HIS:CD2	2.50	0.47
1:IB:471:ASP:OD1	1:IB:522:ASN:HA	2.15	0.47
1:JC:46:ASN:HD21	1:JC:213:ILE:C	2.21	0.47
1:KA:115:THR:HG22	1:KA:148:VAL:HG21	1.97	0.47
1:KA:140:MET:HG2	1:LA:57:VAL:HG21	1.96	0.47
1:LA:347:HIS:NE2	1:LA:374:ASP:HB3	2.29	0.47
1:LC:107:VAL:CG1	1:LC:154:VAL:HB	2.44	0.47
1:MA:424:PRO:HD3	1:MA:431:LEU:HD13	1.95	0.47
1:MB:46:ASN:ND2	1:MB:213:ILE:O	2.39	0.47
1:MB:78:SER:HB2	1:MB:179:ILE:HD13	1.96	0.47
1:MB:265:ARG:NH2	1:MB:420:PRO:O	2.40	0.47
1:NA:105:VAL:CG1	1:NA:156:ILE:HB	2.44	0.47
1:OA:341:ASP:OD2	1:OA:343:SER:OG	2.28	0.47
1:BA:371:THR:CG2	1:BA:374:ASP:H	2.27	0.47
1:BB:144:ILE:HG22	1:BB:146:VAL:HG23	1.97	0.47
1:CB:115:THR:O	1:CB:149:ARG:HD3	2.14	0.47
1:CB:227:PHE:CE1	1:CB:268:THR:HG23	2.50	0.47
1:DB:75:ILE:O	1:DB:522:ASN:ND2	2.48	0.47
1:DB:230:PRO:HD3	1:DB:460:HIS:CD2	2.50	0.47
1:DB:389:VAL:HG12	1:DB:441:CYS:HB2	1.97	0.47
1:EC:109:LEU:HD22	1:EC:200:CYS:SG	2.54	0.47
1:FB:471:ASP:OD1	1:FB:522:ASN:HA	2.14	0.47
1:GB:433:PHE:HB3	1:GB:450:ASP:HB3	1.97	0.47
1:GC:277:GLN:HB3	1:GC:321:LEU:HB3	1.97	0.47
1:IC:480:PRO:HD3	1:IC:513:GLY:HA2	1.97	0.47
1:KB:34:GLY:HA3	1:KB:209:ASP:HB2	1.96	0.47
1:LA:48:ILE:HD12	1:LA:211:ASP:HA	1.97	0.47
1:LA:318:PRO:HD3	1:LA:417:HIS:O	2.15	0.47
1:MC:277:GLN:HE21	1:MC:283:ILE:HD13	1.80	0.47
1:OB:81:LEU:HD11	1:OB:102:GLY:HA2	1.96	0.47
1:OC:120:ILE:HG13	1:OC:183:TYR:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FA:275:THR:HG23	1:FA:318:PRO:HG2	1.96	0.47
1:FB:454:PRO:HG2	1:FB:457:TRP:CG	2.50	0.47
1:HA:353:THR:HG23	1:HA:406:PRO:HB3	1.97	0.47
1:HB:305:SER:HB3	1:HB:309:ASN:HB2	1.97	0.47
1:IB:471:ASP:HA	1:IB:493:LYS:CD	2.45	0.47
1:KB:94:ARG:HB3	1:KB:218:PRO:O	2.15	0.47
1:KB:471:ASP:OD1	1:KB:522:ASN:HA	2.14	0.47
1:LB:326:PHE:CZ	1:LB:438:MET:HE1	2.49	0.47
1:MC:107:VAL:CG1	1:MC:154:VAL:HB	2.44	0.47
1:OB:32:VAL:HG13	1:OC:41:VAL:HA	1.95	0.47
1:OB:227:PHE:CE1	1:OB:268:THR:HG23	2.50	0.47
1:AA:30:GLU:HG3	1:BA:51:TRP:CZ2	2.50	0.47
1:AA:51:TRP:NE1	1:EB:45:GLN:O	2.47	0.47
1:AA:247:GLU:OE1	1:AA:437:THR:HG22	2.15	0.47
1:AC:249:LEU:HD21	1:AC:515:PHE:HZ	1.80	0.47
1:AC:389:VAL:HG23	1:AC:442:SER:HB3	1.97	0.47
1:CA:125:PRO:HA	1:CA:176:ILE:HG12	1.97	0.47
1:EB:230:PRO:HD3	1:EB:460:HIS:ND1	2.30	0.47
1:GA:135:PRO:HG3	1:GA:181:MET:HE2	1.97	0.47
1:GC:249:LEU:HB3	1:GC:507:LEU:HD12	1.96	0.47
1:HA:422:VAL:HG12	1:HA:431:LEU:HD21	1.97	0.47
1:IB:75:ILE:HD13	1:IB:179:ILE:HD12	1.97	0.47
1:KA:140:MET:CE	1:KB:218:PRO:HD3	2.42	0.47
1:LA:399:GLU:HB3	1:LA:400:PRO:HD3	1.97	0.47
1:LB:424:PRO:HD3	1:LB:431:LEU:HG	1.96	0.47
1:OC:56:PHE:HB3	1:OC:203:LEU:HB3	1.97	0.47
1:AA:140:MET:CE	1:AB:218:PRO:HD2	2.44	0.46
1:AA:318:PRO:HD3	1:AA:417:HIS:O	2.16	0.46
1:EB:230:PRO:HG2	1:EB:457:TRP:CD1	2.50	0.46
1:EB:280:PRO:HB3	1:EB:455:GLN:HG2	1.97	0.46
1:FB:45:GLN:O	1:GA:51:TRP:NE1	2.48	0.46
1:GA:275:THR:HG23	1:GA:318:PRO:HG2	1.97	0.46
1:GB:51:TRP:HB3	1:HA:215:LEU:HD12	1.97	0.46
1:GC:223:ARG:HA	1:GC:467:PRO:HG2	1.96	0.46
1:HA:118:LYS:HE2	1:IA:110:ALA:HA	1.96	0.46
1:JC:476:ARG:HD3	1:JC:488:GLU:HB3	1.98	0.46
1:LA:223:ARG:NH2	1:LA:269:ASP:HB2	2.30	0.46
1:LB:144:ILE:HG22	1:LB:146:VAL:HG23	1.97	0.46
1:MB:45:GLN:O	1:NA:51:TRP:NE1	2.47	0.46
1:NA:353:THR:CG2	1:NA:406:PRO:HB3	2.45	0.46
1:AA:46:ASN:HB3	1:EB:49:ASP:OD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:434:PHE:CE1	1:AA:454:PRO:HD3	2.50	0.46
1:DA:117:GLY:O	1:DA:148:VAL:HG22	2.16	0.46
1:DA:338:THR:OG1	1:DA:345:ARG:NH2	2.46	0.46
1:DC:233:THR:HG22	1:DC:235:GLU:H	1.81	0.46
1:DC:305:SER:HB2	1:DC:309:ASN:H	1.81	0.46
1:FB:244:ILE:HD13	1:FB:438:MET:HA	1.98	0.46
1:GB:399:GLU:HB3	1:GB:400:PRO:HD3	1.96	0.46
1:HB:233:THR:CG2	1:HB:235:GLU:HG2	2.46	0.46
1:IB:32:VAL:HB	1:IB:159:PRO:HB2	1.96	0.46
1:LA:308:TRP:CD1	1:LA:380:ASN:HD22	2.33	0.46
1:LC:225:LYS:HE3	1:LC:464:GLU:HB3	1.97	0.46
1:NC:433:PHE:HB3	1:NC:450:ASP:HB3	1.97	0.46
1:OC:107:VAL:CG1	1:OC:154:VAL:HB	2.45	0.46
1:BA:30:GLU:HG3	1:CA:51:TRP:CZ2	2.49	0.46
1:CA:233:THR:HG22	1:CA:235:GLU:N	2.29	0.46
1:CC:469:GLN:HB2	1:CC:520:TRP:CG	2.50	0.46
1:EA:96:TYR:CG	1:EA:212:PHE:HB3	2.51	0.46
1:EA:109:LEU:HD22	1:EA:200:CYS:SG	2.56	0.46
1:FA:219:THR:HG22	1:FA:222:SER:OG	2.16	0.46
1:FC:46:ASN:ND2	1:FC:213:ILE:C	2.73	0.46
1:FC:139:THR:HG22	1:JB:57:VAL:HA	1.97	0.46
1:HA:326:PHE:HB2	1:HA:402:GLN:HA	1.98	0.46
1:KB:306:GLN:CD	1:KB:306:GLN:H	2.23	0.46
1:LB:399:GLU:HB3	1:LB:400:PRO:HD3	1.97	0.46
1:MB:267:THR:HG22	1:MB:271:VAL:N	2.22	0.46
1:NB:78:SER:HB2	1:NB:179:ILE:HD13	1.96	0.46
1:OB:424:PRO:HD3	1:OB:431:LEU:HG	1.97	0.46
1:AC:267:THR:HG22	1:AC:271:VAL:N	2.28	0.46
1:CB:81:LEU:HD11	1:CB:102:GLY:HA2	1.98	0.46
1:DA:65:THR:CG2	1:DA:526:THR:H	2.16	0.46
1:DC:239:ASN:ND2	1:DC:436:SER:OG	2.47	0.46
1:EB:433:PHE:HB3	1:EB:450:ASP:HB3	1.97	0.46
1:EB:471:ASP:HA	1:EB:493:LYS:CD	2.43	0.46
1:EB:471:ASP:OD1	1:EB:522:ASN:HA	2.16	0.46
1:FA:282:ASN:OD1	1:FA:287:ARG:NH2	2.48	0.46
1:FA:371:THR:HG22	1:FA:373:ASN:H	1.80	0.46
1:FA:430:GLN:HE22	1:FA:503:GLY:H	1.62	0.46
1:GB:199:SER:HB2	1:HC:184:THR:HG23	1.98	0.46
1:HB:15:THR:HG22	1:IC:149:ARG:HE	1.81	0.46
1:KA:51:TRP:NE1	1:OB:45:GLN:O	2.48	0.46
1:LA:434:PHE:CE1	1:LA:454:PRO:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LC:268:THR:HG21	1:LC:520:TRP:CH2	2.42	0.46
1:NC:135:PRO:HA	1:NC:181:MET:HE1	1.95	0.46
1:BB:230:PRO:HD3	1:BB:460:HIS:ND1	2.31	0.46
1:BC:305:SER:HB2	1:BC:309:ASN:H	1.81	0.46
1:DC:424:PRO:HD3	1:DC:431:LEU:HG	1.98	0.46
1:EC:299:TYR:CE2	1:EC:375:LEU:HB2	2.50	0.46
1:FC:223:ARG:HA	1:FC:467:PRO:HG2	1.97	0.46
1:GC:115:THR:O	1:GC:149:ARG:HD3	2.15	0.46
1:HB:78:SER:HB2	1:HB:179:ILE:HD13	1.98	0.46
1:HC:78:SER:HB2	1:HC:179:ILE:HD13	1.97	0.46
1:JC:248:LYS:HE3	1:JC:435:ARG:HD3	1.98	0.46
1:KB:19:VAL:HG13	1:KB:149:ARG:O	2.16	0.46
1:KB:501:HIS:ND1	1:KB:531:GLY:HA3	2.30	0.46
1:KC:500:ALA:HB2	1:KC:527:LEU:HG	1.97	0.46
1:LB:501:HIS:CE1	1:LB:531:GLY:HA3	2.51	0.46
1:MC:225:LYS:NZ	2:MC:602:CL:CL	2.85	0.46
1:NC:479:ASN:ND2	1:NC:510:PRO:HG3	2.31	0.46
1:OA:147:ASP:OD2	1:OA:149:ARG:NH1	2.49	0.46
1:OC:267:THR:CG2	1:OC:271:VAL:H	2.26	0.46
1:BA:187:ARG:NH2	1:CA:197:THR:O	2.49	0.46
1:BC:278:LEU:HD22	1:BC:459:LEU:HD23	1.96	0.46
1:CC:429:GLU:OE2	1:CC:490:LYS:HE2	2.16	0.46
1:DB:246:LEU:HD11	1:DB:454:PRO:HB3	1.96	0.46
1:FA:96:TYR:CG	1:FA:212:PHE:HB3	2.51	0.46
1:FC:267:THR:CG2	1:FC:271:VAL:H	2.26	0.46
1:GA:125:PRO:HG3	1:GB:214:PHE:CD1	2.51	0.46
1:IB:51:TRP:HB3	1:JA:215:LEU:HD12	1.96	0.46
1:JB:501:HIS:CE1	1:JB:531:GLY:HA3	2.51	0.46
1:KB:51:TRP:HB3	1:LA:215:LEU:HD12	1.98	0.46
1:KB:78:SER:HB2	1:KB:179:ILE:HD13	1.97	0.46
1:KB:94:ARG:NH2	1:LA:91:HIS:HE1	2.12	0.46
1:LB:115:THR:O	1:LB:149:ARG:HD3	2.15	0.46
1:LB:197:THR:HB	1:MC:187:ARG:NH1	2.31	0.46
1:NB:267:THR:CG2	1:NB:271:VAL:H	2.28	0.46
1:NB:372:ASN:OD1	1:NB:372:ASN:N	2.48	0.46
1:OC:359:THR:HG22	1:OC:410:GLY:H	1.80	0.46
1:AA:110:ALA:HA	1:EA:118:LYS:HE2	1.97	0.46
1:AB:101:GLY:HA3	1:AB:210:PHE:HA	1.98	0.46
1:AB:267:THR:HG22	1:AB:271:VAL:N	2.26	0.46
1:BC:101:GLY:HA3	1:BC:210:PHE:HA	1.96	0.46
1:BC:249:LEU:HB2	1:BC:509:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:318:PRO:HD3	1:CA:417:HIS:O	2.15	0.46
1:CB:233:THR:HG21	1:CB:511:PRO:O	2.16	0.46
1:FA:78:SER:HA	1:FA:178:LEU:O	2.16	0.46
1:FC:265:ARG:NH2	1:FC:420:PRO:O	2.39	0.46
1:GA:219:THR:HG22	1:GA:222:SER:OG	2.16	0.46
1:GB:471:ASP:OD1	1:GB:522:ASN:HA	2.16	0.46
1:HB:81:LEU:HD11	1:HB:102:GLY:HA2	1.97	0.46
1:MC:389:VAL:HG23	1:MC:442:SER:HB3	1.98	0.46
1:OC:330:ILE:HG12	1:OC:388:VAL:HG12	1.96	0.46
1:AC:182:LEU:HD21	1:AC:185:PRO:HA	1.98	0.46
1:CA:140:MET:HG2	1:DA:57:VAL:HG21	1.97	0.46
1:CA:434:PHE:CE1	1:CA:454:PRO:HD3	2.51	0.46
1:EB:454:PRO:HG2	1:EB:457:TRP:CG	2.50	0.46
1:FA:57:VAL:HG21	1:JA:140:MET:HG2	1.97	0.46
1:FB:319:ALA:HB1	1:FB:320:PRO:HD2	1.98	0.46
1:HA:138:VAL:HG21	1:HA:181:MET:SD	2.56	0.46
1:JA:459:LEU:O	1:JA:463:GLN:HG3	2.16	0.46
1:LA:53:ARG:O	1:LA:205:ARG:HD2	2.16	0.46
1:LA:76:LEU:C	1:LA:522:ASN:HD21	2.24	0.46
1:MB:317:ILE:HD13	1:MB:321:LEU:HD21	1.98	0.46
1:MC:241:ARG:HB2	1:MC:449:LEU:HD21	1.97	0.46
1:OB:464:GLU:O	1:OB:464:GLU:HG3	2.15	0.46
1:AA:51:TRP:CZ2	1:EA:30:GLU:HG3	2.51	0.46
1:AC:144:ILE:HG22	1:AC:146:VAL:HG23	1.97	0.46
1:BA:73:GLY:H	1:BA:181:MET:HE3	1.80	0.46
1:CA:96:TYR:CG	1:CA:212:PHE:HB3	2.51	0.46
1:CB:301:MET:HE2	1:CB:303:LEU:HD23	1.97	0.46
1:CC:158:LEU:HD13	1:CC:178:LEU:HG	1.96	0.46
1:DA:216:VAL:CG2	1:DA:217:PRO:HD2	2.46	0.46
1:DA:233:THR:HG22	1:DA:235:GLU:N	2.31	0.46
1:DA:318:PRO:HD3	1:DA:417:HIS:O	2.15	0.46
1:DA:399:GLU:HB3	1:DA:400:PRO:HD3	1.97	0.46
1:DB:81:LEU:HD11	1:DB:102:GLY:HA2	1.98	0.46
1:DC:267:THR:CG2	1:DC:271:VAL:H	2.24	0.46
1:DC:434:PHE:CE2	1:DC:454:PRO:HD3	2.51	0.46
1:EC:409:SER:HB2	1:EC:412:THR:O	2.16	0.46
1:FA:56:PHE:O	1:JA:143:HIS:HE1	1.99	0.46
1:FB:215:LEU:HD21	1:GA:52:ILE:HG12	1.98	0.46
1:FB:402:GLN:OE1	1:FB:449:LEU:HA	2.16	0.46
1:GA:400:PRO:HG2	1:GA:446:ASN:O	2.15	0.46
1:GB:233:THR:HG21	1:GB:511:PRO:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GB:432:LEU:HB2	1:GB:499:VAL:HG13	1.97	0.46
1:HB:471:ASP:OD1	1:HB:471:ASP:N	2.43	0.46
1:JB:217:PRO:HA	1:JB:218:PRO:HD3	1.62	0.46
1:JB:471:ASP:HA	1:JB:493:LYS:CD	2.46	0.46
1:JC:44:GLN:HE22	1:JC:215:LEU:HB2	1.81	0.46
1:JC:241:ARG:NE	1:JC:325:ASP:OD2	2.49	0.46
1:JC:244:ILE:HD11	1:JC:439:PRO:HD3	1.98	0.46
1:KC:44:GLN:NE2	1:KC:215:LEU:HD23	2.31	0.46
1:KC:336:GLN:OE1	1:KC:379:GLN:HB2	2.16	0.46
1:DA:96:TYR:CG	1:DA:212:PHE:HB3	2.51	0.46
1:FB:316:GLU:OE1	1:FB:417:HIS:NE2	2.49	0.46
1:HB:75:ILE:HD13	1:HB:179:ILE:HD12	1.97	0.46
1:IB:227:PHE:CE1	1:IB:268:THR:HG23	2.51	0.46
1:JB:19:VAL:HG13	1:JB:149:ARG:O	2.15	0.46
1:JB:280:PRO:HB3	1:JB:455:GLN:HG2	1.97	0.46
1:JC:390:GLN:HB2	1:JC:445:PRO:HB3	1.97	0.46
1:KC:470:SER:OG	1:KC:521:VAL:O	2.20	0.46
1:LC:46:ASN:HD21	1:LC:213:ILE:C	2.23	0.46
1:MB:94:ARG:NH2	1:NA:91:HIS:HE1	2.14	0.46
1:NA:149:ARG:NH2	1:OA:149:ARG:O	2.48	0.46
1:OC:25:GLU:CD	1:OC:25:GLU:H	2.23	0.46
1:CB:275:THR:HG23	1:CB:318:PRO:HG2	1.98	0.45
1:EC:217:PRO:HA	1:EC:218:PRO:HD3	1.85	0.45
1:EC:426:PHE:HD2	1:EC:429:GLU:OE2	2.00	0.45
1:FA:318:PRO:HD3	1:FA:417:HIS:O	2.16	0.45
1:FB:432:LEU:HB2	1:FB:499:VAL:HG13	1.98	0.45
1:GA:338:THR:HG23	1:GA:379:GLN:NE2	2.31	0.45
1:HB:233:THR:HG22	1:HB:235:GLU:HG2	1.97	0.45
1:HB:327:VAL:HA	1:HB:353:THR:OG1	2.15	0.45
1:IA:140:MET:HG2	1:JA:57:VAL:HG21	1.97	0.45
1:IB:267:THR:CG2	1:IB:271:VAL:H	2.29	0.45
1:JA:353:THR:CG2	1:JA:406:PRO:HB3	2.46	0.45
1:KA:135:PRO:HG3	1:KA:181:MET:HE2	1.98	0.45
1:KA:280:PRO:HB3	1:KA:455:GLN:HG2	1.97	0.45
1:MB:118:LYS:H	1:MB:184:THR:HB	1.80	0.45
1:MC:267:THR:CG2	1:MC:271:VAL:H	2.26	0.45
1:NA:219:THR:HG22	1:NA:222:SER:OG	2.15	0.45
1:NB:345:ARG:NE	1:NB:376:GLU:OE1	2.49	0.45
1:NB:469:GLN:HG3	1:NB:520:TRP:NE1	2.31	0.45
1:NC:121:PHE:HA	1:NC:179:ILE:O	2.16	0.45
1:NC:299:TYR:CE2	1:NC:375:LEU:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NC:456:GLU:OE1	1:NC:456:GLU:N	2.48	0.45
1:NC:476:ARG:HG3	1:NC:516:ARG:HH21	1.81	0.45
1:OC:242:PHE:O	1:OC:244:ILE:N	2.49	0.45
1:CB:88:TYR:CD1	1:DA:95:MET:HE3	2.51	0.45
1:DA:125:PRO:HG3	1:DB:214:PHE:CD1	2.52	0.45
1:FC:242:PHE:HD2	1:FC:244:ILE:HD11	1.81	0.45
1:GB:94:ARG:HB3	1:GB:218:PRO:O	2.16	0.45
1:GC:107:VAL:HG13	1:GC:154:VAL:HB	1.99	0.45
1:HA:140:MET:HE3	1:IA:87:PRO:HG2	1.98	0.45
1:MA:266:CYS:HB2	1:MA:458:VAL:HG13	1.99	0.45
1:NB:46:ASN:ND2	1:NB:213:ILE:O	2.49	0.45
1:NC:431:LEU:HD23	1:NC:498:THR:HG22	1.98	0.45
1:AB:84:ASP:HB3	1:AB:469:GLN:OE1	2.16	0.45
1:AB:471:ASP:HA	1:AB:493:LYS:HD2	1.97	0.45
1:CA:118:LYS:HE2	1:DA:110:ALA:HA	1.99	0.45
1:CB:267:THR:CG2	1:CB:271:VAL:H	2.25	0.45
1:CC:30:GLU:HG3	1:CC:31:PRO:HD2	1.99	0.45
1:CC:46:ASN:HD21	1:CC:213:ILE:C	2.20	0.45
1:DB:471:ASP:OD1	1:DB:471:ASP:N	2.49	0.45
1:DC:107:VAL:CG1	1:DC:154:VAL:HB	2.46	0.45
1:EB:105:VAL:HG22	1:EB:156:ILE:HB	1.98	0.45
1:FB:280:PRO:HB3	1:FB:455:GLN:HG2	1.99	0.45
1:GA:347:HIS:NE2	1:GA:374:ASP:HB3	2.31	0.45
1:IA:219:THR:HG22	1:IA:222:SER:OG	2.16	0.45
1:IC:377:THR:HG22	1:IC:378:GLY:N	2.31	0.45
1:KB:45:GLN:O	1:LA:51:TRP:NE1	2.47	0.45
1:MA:65:THR:HG21	1:MA:526:THR:N	2.12	0.45
1:NC:319:ALA:HB1	1:NC:320:PRO:HD2	1.99	0.45
1:AC:193:ASP:OD1	1:AC:193:ASP:N	2.42	0.45
1:AC:489:CYS:HB3	1:AC:499:VAL:HG12	1.97	0.45
1:BA:434:PHE:CE1	1:BA:454:PRO:HD3	2.51	0.45
1:BC:338:THR:HG1	1:BC:345:ARG:HH22	1.63	0.45
1:CA:105:VAL:CG1	1:CA:156:ILE:HB	2.46	0.45
1:CC:225:LYS:NZ	2:CC:601:CL:CL	2.86	0.45
1:DB:109:LEU:HD23	1:DB:200:CYS:SG	2.57	0.45
1:DC:148:VAL:CG1	1:DC:198:VAL:HG21	2.47	0.45
1:DC:308:TRP:CZ3	1:DC:380:ASN:HB3	2.52	0.45
1:GA:490:LYS:HE3	1:GA:527:LEU:HG	1.99	0.45
1:GC:268:THR:HG21	1:GC:520:TRP:CH2	2.42	0.45
1:HB:227:PHE:CE1	1:HB:268:THR:HG23	2.51	0.45
1:IB:19:VAL:HG13	1:IB:149:ARG:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JB:105:VAL:HG22	1:JB:156:ILE:HB	1.99	0.45
1:LA:280:PRO:HA	1:LA:283:ILE:HD11	1.99	0.45
1:LB:124:VAL:HG22	1:LB:177:LYS:HB2	1.98	0.45
1:LC:118:LYS:H	1:LC:184:THR:HB	1.80	0.45
1:LC:459:LEU:O	1:LC:463:GLN:HG3	2.17	0.45
1:MA:216:VAL:CG2	1:MA:217:PRO:HD2	2.47	0.45
1:AA:44:GLN:HA	1:AC:30:GLU:HG2	1.98	0.45
1:AB:477:PHE:CE2	1:AB:509:ILE:HG23	2.52	0.45
1:BA:221:GLU:OE1	1:BA:221:GLU:N	2.49	0.45
1:BB:403:TRP:CZ2	1:BB:450:ASP:HB2	2.52	0.45
1:CA:219:THR:HG22	1:CA:222:SER:OG	2.17	0.45
1:DA:338:THR:HB	1:DA:343:SER:HB2	1.98	0.45
1:DB:507:LEU:HD21	1:DB:530:MET:HE1	1.98	0.45
1:EC:372:ASN:OD1	1:EC:372:ASN:N	2.49	0.45
1:JC:336:GLN:NE2	1:JC:379:GLN:HB2	2.32	0.45
1:JC:389:VAL:HG23	1:JC:442:SER:HB3	1.98	0.45
1:LB:471:ASP:HA	1:LB:493:LYS:HE2	1.97	0.45
1:LB:490:LYS:HG3	1:LB:527:LEU:HD21	1.96	0.45
1:NA:115:THR:HG22	1:NA:148:VAL:HG21	1.99	0.45
1:OA:105:VAL:CG1	1:OA:156:ILE:HB	2.45	0.45
1:OA:433:PHE:HB3	1:OA:450:ASP:HB3	1.97	0.45
1:OC:456:GLU:OE1	1:OC:456:GLU:N	2.49	0.45
1:BB:81:LEU:HD11	1:BB:102:GLY:HA2	1.98	0.45
1:BB:130:THR:HG23	1:BB:179:ILE:HD11	1.99	0.45
1:CC:389:VAL:HG23	1:CC:442:SER:HB3	1.98	0.45
1:DA:424:PRO:HD3	1:DA:431:LEU:HD13	1.98	0.45
1:DC:267:THR:HG22	1:DC:271:VAL:N	2.26	0.45
1:EA:233:THR:HG22	1:EA:235:GLU:N	2.29	0.45
1:EB:218:PRO:O	1:EB:219:THR:HG22	2.17	0.45
1:FA:223:ARG:HH21	1:FA:269:ASP:HB2	1.82	0.45
1:HA:109:LEU:HD22	1:HA:200:CYS:SG	2.57	0.45
1:HC:477:PHE:CD1	1:HC:486:LEU:HD12	2.51	0.45
1:IA:434:PHE:CE1	1:IA:454:PRO:HD3	2.51	0.45
1:IC:267:THR:CG2	1:IC:271:VAL:H	2.26	0.45
1:JC:118:LYS:H	1:JC:184:THR:HB	1.81	0.45
1:JC:249:LEU:HD23	1:JC:432:LEU:HD21	1.97	0.45
1:KA:476:ARG:HD3	1:KA:485:VAL:HG11	1.97	0.45
1:LC:390:GLN:HB2	1:LC:445:PRO:HB3	1.98	0.45
1:MC:416:VAL:HG12	1:MC:417:HIS:N	2.32	0.45
1:OB:115:THR:O	1:OB:149:ARG:HD3	2.17	0.45
1:OB:230:PRO:HD3	1:OB:460:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OC:358:PHE:HD1	1:OC:365:VAL:HG13	1.81	0.45
1:AB:57:VAL:HG23	1:AB:87:PRO:HD2	1.98	0.45
1:CB:121:PHE:HA	1:CB:179:ILE:O	2.17	0.45
1:DA:75:ILE:HG23	1:DA:179:ILE:HG23	1.99	0.45
1:DA:161:VAL:HB	1:DA:176:ILE:HD11	1.98	0.45
1:DB:280:PRO:HA	1:DB:283:ILE:HD11	1.98	0.45
1:FC:217:PRO:HA	1:FC:218:PRO:HD3	1.85	0.45
1:GA:105:VAL:CG1	1:GA:156:ILE:HB	2.46	0.45
1:GB:306:GLN:H	1:GB:306:GLN:CD	2.24	0.45
1:HB:34:GLY:HA3	1:HB:209:ASP:HB2	1.97	0.45
1:HB:440:GLY:O	1:IA:335:THR:HG23	2.16	0.45
1:IC:527:LEU:H	1:IC:527:LEU:HD23	1.82	0.45
1:JC:347:HIS:NE2	1:JC:374:ASP:HB3	2.31	0.45
1:KA:371:THR:HG21	1:KA:374:ASP:HB2	1.99	0.45
1:MA:173:ASP:OD1	1:MA:174:PRO:HD2	2.16	0.45
1:MB:60:PRO:HD3	1:MB:87:PRO:HD3	1.99	0.45
1:NB:230:PRO:HD3	1:NB:460:HIS:CD2	2.52	0.45
1:OB:34:GLY:HA3	1:OB:209:ASP:HB2	1.97	0.45
1:AB:454:PRO:HG2	1:AB:457:TRP:CG	2.52	0.45
1:CA:120:ILE:CG1	1:CA:183:TYR:HB2	2.47	0.45
1:CA:140:MET:HE3	1:DA:87:PRO:HG2	1.99	0.45
1:CB:32:VAL:HB	1:CB:159:PRO:HB2	1.98	0.45
1:CC:107:VAL:CG1	1:CC:154:VAL:HB	2.47	0.45
1:FA:223:ARG:NH2	1:FA:269:ASP:HB2	2.32	0.45
1:GB:115:THR:O	1:GB:149:ARG:HD3	2.17	0.45
1:HB:233:THR:HB	1:HB:236:GLU:HG3	1.99	0.45
1:JA:101:GLY:HA3	1:JA:210:PHE:HA	1.98	0.45
1:KB:57:VAL:HA	1:LC:139:THR:HG22	1.98	0.45
1:KC:107:VAL:CG1	1:KC:154:VAL:HB	2.47	0.45
1:LC:241:ARG:NE	1:LC:325:ASP:OD2	2.45	0.45
1:NB:265:ARG:NH2	1:NB:420:PRO:O	2.44	0.45
1:OB:403:TRP:CZ2	1:OB:450:ASP:HB2	2.52	0.45
1:OC:148:VAL:CG1	1:OC:198:VAL:HG21	2.47	0.45
1:OC:233:THR:HG22	1:OC:235:GLU:H	1.81	0.45
1:AA:438:MET:HE3	1:AA:449:LEU:HD22	1.99	0.45
1:AB:109:LEU:HD23	1:AB:200:CYS:SG	2.56	0.45
1:AB:424:PRO:HD3	1:AB:431:LEU:HG	1.98	0.45
1:AC:124:VAL:HG21	1:AC:179:ILE:HD12	1.99	0.45
1:BA:326:PHE:O	1:BA:353:THR:HG21	2.17	0.45
1:BB:24:ASN:OD1	1:BB:25:GLU:N	2.49	0.45
1:BB:482:THR:HG22	1:CC:426:PHE:HD1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:347:HIS:NE2	1:DA:374:ASP:HB3	2.32	0.45
1:DA:371:THR:HG22	1:DA:373:ASN:H	1.82	0.45
1:DC:130:THR:HG23	1:DC:179:ILE:HD11	1.98	0.45
1:FB:199:SER:HB2	1:GC:184:THR:HG23	1.99	0.45
1:FC:118:LYS:H	1:FC:184:THR:HB	1.80	0.45
1:HA:306:GLN:H	1:HA:306:GLN:CD	2.25	0.45
1:IC:371:THR:CG2	1:IC:374:ASP:H	2.30	0.45
1:KB:395:ALA:HB3	1:KB:398:ASN:HD22	1.81	0.45
1:LB:51:TRP:HB3	1:MA:215:LEU:HD12	1.98	0.45
1:LC:148:VAL:CG1	1:LC:198:VAL:HG21	2.47	0.45
1:NA:318:PRO:HD3	1:NA:417:HIS:O	2.17	0.45
1:OA:371:THR:HG22	1:OA:373:ASN:H	1.81	0.45
1:OB:233:THR:CG2	1:OB:235:GLU:HG2	2.46	0.45
1:AC:46:ASN:HD21	1:AC:213:ILE:C	2.24	0.45
1:BA:116:ALA:O	1:BA:186:LEU:HD12	2.17	0.45
1:CA:161:VAL:HB	1:CA:176:ILE:HD11	1.99	0.45
1:CA:399:GLU:HB3	1:CA:400:PRO:HD3	1.98	0.45
1:CC:267:THR:HG22	1:CC:271:VAL:N	2.30	0.45
1:DB:121:PHE:HA	1:DB:179:ILE:O	2.17	0.45
1:DB:197:THR:HB	1:EC:187:ARG:NH1	2.31	0.45
1:DB:316:GLU:OE1	1:DB:417:HIS:NE2	2.50	0.45
1:DC:426:PHE:CD1	1:DC:427:PRO:HD2	2.51	0.45
1:FC:107:VAL:CG1	1:FC:154:VAL:HB	2.47	0.45
1:GA:108:ILE:HG12	1:GA:153:PRO:HB3	1.98	0.45
1:HA:43:GLY:HA3	1:HA:214:PHE:CE1	2.52	0.45
1:HA:267:THR:HG23	1:HA:493:LYS:O	2.17	0.45
1:HB:51:TRP:HB3	1:IA:215:LEU:HD12	1.99	0.45
1:KC:312:ASP:HB3	1:KC:315:GLU:HG3	1.99	0.45
1:LA:435:ARG:HG3	1:LA:450:ASP:OD1	2.17	0.45
1:LB:118:LYS:H	1:LB:184:THR:HB	1.82	0.45
1:MB:215:LEU:HD21	1:NA:52:ILE:HG12	2.00	0.45
1:NB:454:PRO:HG2	1:NB:457:TRP:CD1	2.52	0.45
1:OB:30:GLU:HG3	1:OC:44:GLN:HA	1.97	0.45
1:AC:249:LEU:HB2	1:AC:509:ILE:HD11	1.99	0.44
1:CA:140:MET:HG2	1:DA:57:VAL:CG2	2.47	0.44
1:CC:130:THR:O	1:CC:133:LEU:HD23	2.17	0.44
1:CC:338:THR:OG1	1:CC:345:ARG:NH2	2.41	0.44
1:DB:482:THR:HG22	1:EC:426:PHE:CD1	2.52	0.44
1:EB:32:VAL:HB	1:EB:159:PRO:HB2	1.99	0.44
1:GA:216:VAL:CG2	1:GA:217:PRO:HD2	2.45	0.44
1:GA:399:GLU:HB3	1:GA:400:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GB:447:MET:HE1	1:HA:337:THR:HG21	1.99	0.44
1:HA:219:THR:HG22	1:HA:222:SER:OG	2.17	0.44
1:JA:389:VAL:HG12	1:JA:441:CYS:HB2	1.98	0.44
1:JB:30:GLU:HG3	1:JC:44:GLN:HA	1.98	0.44
1:KA:248:LYS:HE2	1:KA:435:ARG:HD2	1.99	0.44
1:KC:118:LYS:H	1:KC:184:THR:HB	1.82	0.44
1:LA:118:LYS:HE2	1:MA:110:ALA:HA	2.00	0.44
1:LC:424:PRO:HD3	1:LC:431:LEU:HG	1.99	0.44
1:LC:443:GLY:C	1:LC:444:TYR:HD1	2.26	0.44
1:OB:222:SER:O	1:OB:223:ARG:HB2	2.18	0.44
1:OB:325:ASP:OD1	1:OB:325:ASP:N	2.50	0.44
1:CA:105:VAL:HG11	1:CA:178:LEU:HD22	2.00	0.44
1:EC:25:GLU:HG3	1:EC:25:GLU:O	2.17	0.44
1:FB:195:VAL:HG13	1:FB:197:THR:H	1.82	0.44
1:FB:471:ASP:HA	1:FB:493:LYS:CD	2.46	0.44
1:FC:303:LEU:HD11	1:FC:365:VAL:HG23	1.98	0.44
1:HA:125:PRO:HG3	1:HB:214:PHE:CD1	2.53	0.44
1:KA:30:GLU:HG3	1:LA:51:TRP:CH2	2.51	0.44
1:LC:477:PHE:HD2	1:LC:515:PHE:CE1	2.35	0.44
1:NA:30:GLU:HG3	1:OA:51:TRP:CH2	2.52	0.44
1:OC:182:LEU:HD21	1:OC:185:PRO:HA	1.99	0.44
1:AB:338:THR:HG22	1:AB:340:GLY:H	1.82	0.44
1:BC:44:GLN:HE21	1:BC:215:LEU:HD23	1.83	0.44
1:CA:115:THR:HG22	1:CA:148:VAL:CG2	2.48	0.44
1:CA:275:THR:HG23	1:CA:318:PRO:HG2	1.99	0.44
1:CB:134:SER:OG	1:CB:137:GLN:HG3	2.18	0.44
1:FA:317:ILE:HD13	1:FA:321:LEU:HD21	2.00	0.44
1:GB:124:VAL:HG22	1:GB:177:LYS:HB2	1.99	0.44
1:GB:343:SER:OG	1:GB:345:ARG:NH2	2.50	0.44
1:GB:456:GLU:OE1	1:GB:456:GLU:N	2.46	0.44
1:IA:247:GLU:OE1	1:IA:437:THR:HG22	2.16	0.44
1:KA:499:VAL:HG21	1:KA:530:MET:HE3	1.99	0.44
1:KB:424:PRO:HD3	1:KB:431:LEU:HG	1.99	0.44
1:MA:326:PHE:CZ	1:MA:438:MET:HE1	2.51	0.44
1:AA:140:MET:HE3	1:BA:87:PRO:HG2	2.00	0.44
1:AB:144:ILE:HG22	1:AB:146:VAL:HG23	2.00	0.44
1:CA:251:THR:HG23	1:CA:431:LEU:O	2.17	0.44
1:CB:489:CYS:HB3	1:CB:499:VAL:HG12	1.99	0.44
1:DB:219:THR:HG22	1:DB:219:THR:O	2.18	0.44
1:DB:249:LEU:HB2	1:DB:509:ILE:HD11	1.99	0.44
1:DC:434:PHE:CD2	1:DC:454:PRO:HD3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EC:130:THR:O	1:EC:133:LEU:HD23	2.17	0.44
1:FB:196:PHE:HA	1:GC:187:ARG:HD2	2.00	0.44
1:FC:158:LEU:HD13	1:FC:178:LEU:HG	1.98	0.44
1:GC:416:VAL:HG12	1:GC:417:HIS:CG	2.53	0.44
1:HA:216:VAL:HG22	1:HA:217:PRO:HD2	2.00	0.44
1:HA:233:THR:HG22	1:HA:235:GLU:N	2.29	0.44
1:IC:434:PHE:CE2	1:IC:454:PRO:HD3	2.52	0.44
1:JB:233:THR:HG21	1:JB:511:PRO:O	2.16	0.44
1:JB:429:GLU:HB3	1:JB:498:THR:CG2	2.47	0.44
1:KA:281:VAL:HG11	1:OB:244:ILE:HA	1.99	0.44
1:MA:53:ARG:HB3	1:MA:206:PRO:HG2	2.00	0.44
1:OA:216:VAL:HG21	1:OC:128:PHE:CD1	2.52	0.44
1:OB:233:THR:HG22	1:OB:235:GLU:HG2	1.99	0.44
1:BC:319:ALA:HB1	1:BC:320:PRO:HD2	1.99	0.44
1:DB:37:ILE:HG22	1:DB:165:PHE:CD1	2.53	0.44
1:EA:430:GLN:HE22	1:EA:503:GLY:H	1.65	0.44
1:EB:345:ARG:NE	1:EB:376:GLU:OE1	2.51	0.44
1:EC:66:VAL:HB	1:EC:198:VAL:HB	2.00	0.44
1:GB:34:GLY:HA3	1:GB:209:ASP:HB2	2.00	0.44
1:GC:217:PRO:HA	1:GC:218:PRO:HD3	1.63	0.44
1:JC:426:PHE:HD2	1:JC:429:GLU:OE2	1.99	0.44
1:JC:429:GLU:OE2	1:JC:490:LYS:HE2	2.17	0.44
1:LA:66:VAL:HG12	1:LA:186:LEU:HD22	1.99	0.44
1:LA:341:ASP:OD1	1:LA:341:ASP:N	2.51	0.44
1:LB:219:THR:HG22	1:LB:219:THR:O	2.17	0.44
1:LC:278:LEU:HD22	1:LC:459:LEU:HD23	2.00	0.44
1:NA:372:ASN:OD1	1:NA:372:ASN:N	2.51	0.44
1:NC:269:ASP:OD1	1:NC:269:ASP:N	2.47	0.44
1:OC:241:ARG:NE	1:OC:325:ASP:OD2	2.47	0.44
1:BB:464:GLU:O	1:BB:466:ALA:N	2.49	0.44
1:BC:57:VAL:HA	1:KB:139:THR:HG22	2.00	0.44
1:CA:66:VAL:HG21	1:CA:119:ILE:HD11	2.00	0.44
1:DC:269:ASP:OD1	1:DC:269:ASP:N	2.51	0.44
1:EA:231:ILE:HD12	1:EA:231:ILE:H	1.83	0.44
1:FC:227:PHE:HD1	1:FC:466:ALA:HB1	1.82	0.44
1:GA:117:GLY:O	1:GA:148:VAL:HG22	2.17	0.44
1:IC:459:LEU:O	1:IC:463:GLN:HG3	2.18	0.44
1:KA:96:TYR:HA	1:KA:214:PHE:O	2.17	0.44
1:KA:108:ILE:HG12	1:KA:153:PRO:HB3	2.00	0.44
1:LA:140:MET:HE3	1:MA:87:PRO:HG2	1.99	0.44
1:LA:326:PHE:CZ	1:LA:438:MET:HE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LC:102:GLY:C	1:LC:103:PHE:HD1	2.26	0.44
1:LC:241:ARG:NH1	1:LC:450:ASP:O	2.43	0.44
1:NA:312:ASP:O	1:NA:315:GLU:HG3	2.18	0.44
1:OB:477:PHE:CE2	1:OB:509:ILE:HD12	2.52	0.44
1:AA:96:TYR:CG	1:AA:212:PHE:HB3	2.53	0.44
1:BB:278:LEU:HD22	1:BB:459:LEU:HD23	1.98	0.44
1:CB:118:LYS:H	1:CB:184:THR:HB	1.82	0.44
1:CB:247:GLU:OE2	1:CB:437:THR:N	2.51	0.44
1:EA:399:GLU:HB3	1:EA:400:PRO:HD3	2.00	0.44
1:EB:121:PHE:HA	1:EB:179:ILE:O	2.17	0.44
1:EC:57:VAL:HG11	1:EC:87:PRO:HD2	2.00	0.44
1:FC:459:LEU:O	1:FC:463:GLN:HG3	2.18	0.44
1:IA:318:PRO:HD3	1:IA:417:HIS:O	2.18	0.44
1:IC:319:ALA:HB1	1:IC:320:PRO:HD2	1.99	0.44
1:JB:32:VAL:HB	1:JB:159:PRO:HB2	1.98	0.44
1:JC:469:GLN:HB2	1:JC:520:TRP:CG	2.52	0.44
1:KA:386:VAL:HG11	1:OB:333:VAL:HB	1.99	0.44
1:LB:282:ASN:HD22	1:LB:306:GLN:HB3	1.81	0.44
1:MA:239:ASN:ND2	1:MA:436:SER:OG	2.49	0.44
1:MC:135:PRO:HA	1:MC:181:MET:HE1	1.99	0.44
1:CC:46:ASN:ND2	1:CC:213:ILE:C	2.75	0.44
1:DC:159:PRO:O	1:DC:176:ILE:HD12	2.18	0.44
1:FA:66:VAL:HG12	1:FA:186:LEU:HD22	2.00	0.44
1:FA:468:ALA:HA	1:FA:520:TRP:CH2	2.53	0.44
1:FC:327:VAL:HG23	1:FC:404:VAL:O	2.17	0.44
1:HA:76:LEU:C	1:HA:522:ASN:HD21	2.26	0.44
1:HA:338:THR:HG1	1:HA:345:ARG:HH22	1.60	0.44
1:HC:489:CYS:HB3	1:HC:499:VAL:HG12	2.00	0.44
1:IB:34:GLY:HA3	1:IB:209:ASP:HB2	2.00	0.44
1:IB:230:PRO:HG2	1:IB:457:TRP:CD1	2.53	0.44
1:OB:230:PRO:HG2	1:OB:457:TRP:CD1	2.53	0.44
1:OC:319:ALA:HB1	1:OC:320:PRO:HD2	1.99	0.44
1:AB:317:ILE:HD13	1:AB:321:LEU:HD21	1.99	0.44
1:BC:135:PRO:HA	1:BC:181:MET:HE1	2.00	0.44
1:CA:341:ASP:OD1	1:CA:341:ASP:N	2.46	0.44
1:CC:81:LEU:HD12	1:CC:158:LEU:HG	1.99	0.44
1:DA:158:LEU:HD13	1:DA:178:LEU:HD13	2.00	0.44
1:DA:390:GLN:O	1:DA:443:GLY:HA3	2.18	0.44
1:DC:424:PRO:HG3	1:DC:430:GLN:HA	2.00	0.44
1:EA:219:THR:HG22	1:EA:222:SER:OG	2.17	0.44
1:FA:51:TRP:CH2	1:JA:30:GLU:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:121:PHE:HA	1:FB:179:ILE:O	2.18	0.44
1:FC:148:VAL:CG1	1:FC:198:VAL:HG21	2.47	0.44
1:HA:105:VAL:CG1	1:HA:156:ILE:HB	2.48	0.44
1:HB:361:LYS:HD2	1:HB:409:SER:OG	2.18	0.44
1:HC:116:ALA:HB3	1:HC:187:ARG:HB2	2.00	0.44
1:IC:107:VAL:CG1	1:IC:154:VAL:HB	2.48	0.44
1:JA:306:GLN:H	1:JA:306:GLN:CD	2.24	0.44
1:JC:53:ARG:NH2	1:JC:210:PHE:O	2.37	0.44
1:KC:347:HIS:NE2	1:KC:374:ASP:HB3	2.32	0.44
1:MB:51:TRP:HB3	1:NA:215:LEU:HD12	2.00	0.44
1:MB:233:THR:CG2	1:MB:235:GLU:HG2	2.48	0.44
1:NB:124:VAL:HG22	1:NB:177:LYS:HB2	1.99	0.44
1:OA:33:VAL:HG11	1:OA:37:ILE:HB	1.99	0.44
1:OA:304:ALA:O	1:OA:311:TYR:HB2	2.18	0.44
1:OB:345:ARG:NH2	1:OB:376:GLU:OE2	2.48	0.44
1:AB:19:VAL:HG13	1:AB:149:ARG:O	2.17	0.43
1:BA:64:PHE:CG	1:BA:77:TRP:HB2	2.53	0.43
1:BC:107:VAL:HG13	1:BC:154:VAL:HB	1.98	0.43
1:CA:299:TYR:CE2	1:CA:375:LEU:HB2	2.53	0.43
1:CB:471:ASP:HA	1:CB:493:LYS:CD	2.47	0.43
1:DC:403:TRP:CZ2	1:DC:450:ASP:HB2	2.53	0.43
1:EC:25:GLU:OE1	1:EC:154:VAL:HG13	2.17	0.43
1:EC:106:GLN:HB3	1:EC:203:LEU:HB2	1.99	0.43
1:EC:469:GLN:HB2	1:EC:520:TRP:CG	2.53	0.43
1:EC:500:ALA:HB3	1:EC:529:PRO:HA	1.99	0.43
1:GC:58:GLN:HA	1:GC:203:LEU:HD13	2.00	0.43
1:HA:372:ASN:OD1	1:HA:372:ASN:N	2.49	0.43
1:HB:23:ASN:HD21	1:HB:144:ILE:HD11	1.83	0.43
1:HC:259:VAL:HG13	1:HC:403:TRP:CZ3	2.53	0.43
1:JC:334:LEU:HD22	1:JC:381:THR:HG22	1.99	0.43
1:KC:319:ALA:HB1	1:KC:320:PRO:HD2	1.99	0.43
1:LA:326:PHE:O	1:LA:353:THR:HG21	2.17	0.43
1:MB:248:LYS:HD2	1:MB:435:ARG:HD2	2.00	0.43
1:MC:25:GLU:HA	1:MC:144:ILE:HG23	2.00	0.43
1:NC:484:ARG:HH11	1:NC:486:LEU:HD23	1.83	0.43
1:OA:347:HIS:NE2	1:OA:374:ASP:HB3	2.32	0.43
1:AA:390:GLN:O	1:AA:443:GLY:HA3	2.17	0.43
1:BC:523:GLN:HG3	1:BC:523:GLN:O	2.17	0.43
1:DC:259:VAL:HG13	1:DC:403:TRP:CZ3	2.53	0.43
1:EC:124:VAL:HG21	1:EC:179:ILE:HD12	1.99	0.43
1:FA:140:MET:HG2	1:GA:57:VAL:CG2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FC:232:LEU:HD11	1:LC:459:LEU:HD22	2.00	0.43
1:IB:343:SER:OG	1:IB:345:ARG:NH2	2.51	0.43
1:JA:311:TYR:OH	1:JA:320:PRO:HD3	2.18	0.43
1:JA:317:ILE:HG21	1:JA:321:LEU:HD21	2.00	0.43
1:JC:330:ILE:HG12	1:JC:388:VAL:HG12	2.00	0.43
1:KA:105:VAL:CG1	1:KA:156:ILE:HB	2.48	0.43
1:KB:228:THR:OG1	1:KB:464:GLU:OE2	2.36	0.43
1:KB:400:PRO:HD2	1:KB:446:ASN:H	1.81	0.43
1:KB:433:PHE:HB3	1:KB:450:ASP:HB3	2.00	0.43
1:MB:88:TYR:CD1	1:NA:95:MET:HE3	2.53	0.43
1:MB:280:PRO:HB3	1:MB:455:GLN:HG2	2.00	0.43
1:NA:138:VAL:HG21	1:NA:181:MET:SD	2.58	0.43
1:BC:232:LEU:HB2	1:BC:237:MET:HE2	2.00	0.43
1:DB:125:PRO:HG3	1:DC:214:PHE:CD1	2.52	0.43
1:DB:161:VAL:HB	1:DB:176:ILE:HD11	2.01	0.43
1:EC:260:GLN:N	1:EC:261:PRO:HD3	2.34	0.43
1:FA:216:VAL:CG2	1:FA:217:PRO:HD2	2.45	0.43
1:FB:440:GLY:O	1:GA:335:THR:HG23	2.18	0.43
1:GB:230:PRO:HG2	1:GB:457:TRP:CD1	2.53	0.43
1:IA:48:ILE:HD11	1:IA:89:LEU:CD2	2.48	0.43
1:IC:130:THR:O	1:IC:133:LEU:HD23	2.18	0.43
1:KC:121:PHE:HA	1:KC:179:ILE:O	2.18	0.43
1:MA:53:ARG:O	1:MA:205:ARG:HD2	2.17	0.43
1:MA:377:THR:OG1	1:MA:378:GLY:N	2.52	0.43
1:MB:14:SER:O	1:MB:16:ALA:N	2.43	0.43
1:MB:125:PRO:HG3	1:MC:214:PHE:CD1	2.53	0.43
1:NC:479:ASN:HD22	1:NC:510:PRO:HG3	1.82	0.43
1:OA:117:GLY:O	1:OA:148:VAL:HG22	2.17	0.43
1:CA:435:ARG:HG3	1:CA:450:ASP:OD1	2.18	0.43
1:CB:124:VAL:HG22	1:CB:177:LYS:HB2	2.00	0.43
1:DA:367:PHE:HE2	1:DA:383:PHE:CG	2.36	0.43
1:DB:230:PRO:HG2	1:DB:457:TRP:CD1	2.53	0.43
1:GB:437:THR:HG23	1:GB:447:MET:HB3	2.00	0.43
1:GC:377:THR:HG22	1:GC:378:GLY:N	2.33	0.43
1:IB:359:THR:HG22	1:IB:410:GLY:HA3	1.99	0.43
1:JC:107:VAL:CG1	1:JC:154:VAL:HB	2.49	0.43
1:JC:359:THR:HG22	1:JC:410:GLY:N	2.33	0.43
1:LB:57:VAL:HG23	1:LB:87:PRO:HD2	2.00	0.43
1:OB:109:LEU:HD23	1:OB:200:CYS:SG	2.58	0.43
1:AB:306:GLN:CD	1:AB:306:GLN:H	2.26	0.43
1:AB:488:GLU:HG3	1:AB:527:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:120:ILE:HG13	1:AC:183:TYR:HB2	2.01	0.43
1:BC:241:ARG:NE	1:BC:325:ASP:OD2	2.50	0.43
1:BC:260:GLN:N	1:BC:261:PRO:HD3	2.33	0.43
1:CA:216:VAL:CG2	1:CA:217:PRO:HD2	2.47	0.43
1:CB:57:VAL:HG23	1:CB:87:PRO:HD2	2.01	0.43
1:CC:72:PRO:HA	1:CC:182:LEU:O	2.18	0.43
1:CC:148:VAL:CG1	1:CC:198:VAL:HG21	2.47	0.43
1:DA:500:ALA:HB2	1:DA:527:LEU:HB2	2.00	0.43
1:DC:257:PHE:H	1:DC:257:PHE:HD1	1.65	0.43
1:EB:424:PRO:HD3	1:EB:431:LEU:HG	2.00	0.43
1:FA:30:GLU:HG3	1:GA:51:TRP:CZ2	2.53	0.43
1:FB:280:PRO:HA	1:FB:283:ILE:HD11	1.99	0.43
1:GB:124:VAL:CG2	1:GB:177:LYS:HB2	2.48	0.43
1:HA:328:GLY:H	1:HA:353:THR:HB	1.83	0.43
1:HC:268:THR:HG21	1:HC:520:TRP:CH2	2.43	0.43
1:IB:454:PRO:HG2	1:IB:457:TRP:CD1	2.53	0.43
1:IC:234:VAL:O	1:IC:246:LEU:HB2	2.18	0.43
1:JA:246:LEU:HA	1:JA:436:SER:HB3	2.00	0.43
1:JA:319:ALA:HB1	1:JA:320:PRO:HD2	2.00	0.43
1:JB:124:VAL:CG2	1:JB:177:LYS:HB2	2.47	0.43
1:JC:433:PHE:HB3	1:JC:450:ASP:HB3	2.01	0.43
1:KA:116:ALA:O	1:KA:186:LEU:HD12	2.18	0.43
1:KC:265:ARG:NH2	1:KC:420:PRO:O	2.26	0.43
1:LB:109:LEU:HD23	1:LB:200:CYS:SG	2.58	0.43
1:LB:484:ARG:HH21	1:MC:526:THR:HG21	1.83	0.43
1:MA:33:VAL:HG11	1:MA:37:ILE:HB	2.00	0.43
1:MB:14:SER:C	1:MB:15:THR:HG1	2.26	0.43
1:MB:66:VAL:HG12	1:MB:186:LEU:HB2	2.01	0.43
1:MC:308:TRP:CH2	1:MC:380:ASN:HB3	2.53	0.43
1:NC:148:VAL:CG1	1:NC:198:VAL:HG21	2.48	0.43
1:AA:372:ASN:OD1	1:AA:372:ASN:N	2.52	0.43
1:AC:433:PHE:HB3	1:AC:450:ASP:HB3	1.99	0.43
1:BA:140:MET:HG2	1:CA:57:VAL:CG2	2.49	0.43
1:DA:101:GLY:HA3	1:DA:210:PHE:HA	2.00	0.43
1:DA:433:PHE:HB3	1:DA:450:ASP:HB3	2.00	0.43
1:DB:249:LEU:HD12	1:DB:509:ILE:HD11	2.01	0.43
1:DC:101:GLY:HA3	1:DC:210:PHE:HA	2.01	0.43
1:DC:326:PHE:HB2	1:DC:402:GLN:HA	2.00	0.43
1:EA:60:PRO:HD2	1:EA:84:ASP:O	2.18	0.43
1:EC:390:GLN:HG2	1:EC:399:GLU:HG3	2.01	0.43
1:GA:29:LEU:HA	1:GA:29:LEU:HD23	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GB:265:ARG:NH2	1:GB:420:PRO:O	2.49	0.43
1:GC:27:MET:HE3	1:GC:144:ILE:HG13	2.00	0.43
1:IA:108:ILE:HG12	1:IA:153:PRO:HB3	1.99	0.43
1:IC:390:GLN:HB2	1:IC:445:PRO:HB3	2.00	0.43
1:JB:97:ASN:HB3	1:JB:214:PHE:HB3	2.00	0.43
1:KA:76:LEU:C	1:KA:522:ASN:HD21	2.26	0.43
1:KA:144:ILE:HD12	1:KA:154:VAL:HG11	2.01	0.43
1:KA:145:ILE:HG21	1:LA:108:ILE:HD13	2.00	0.43
1:LA:216:VAL:HG21	1:LC:128:PHE:CD1	2.54	0.43
1:MA:326:PHE:O	1:MA:353:THR:HG21	2.18	0.43
1:NC:120:ILE:HG13	1:NC:183:TYR:HB2	2.00	0.43
1:NC:336:GLN:HE22	1:NC:375:LEU:HA	1.83	0.43
1:OA:326:PHE:CZ	1:OA:438:MET:HE1	2.54	0.43
1:OB:432:LEU:HB2	1:OB:499:VAL:HG13	2.00	0.43
1:DC:481:ASP:CG	1:DC:512:ASN:HD21	2.27	0.43
1:HA:394:SER:OG	1:HA:398:ASN:ND2	2.42	0.43
1:HB:507:LEU:CD2	1:HB:530:MET:HE1	2.48	0.43
1:IA:29:LEU:HD23	1:IA:29:LEU:HA	1.81	0.43
1:IA:216:VAL:CG2	1:IA:217:PRO:HD2	2.48	0.43
1:IC:182:LEU:HD21	1:IC:185:PRO:HA	2.00	0.43
1:IC:233:THR:HG21	1:IC:511:PRO:O	2.19	0.43
1:JC:148:VAL:CG1	1:JC:198:VAL:HG21	2.48	0.43
1:KA:434:PHE:CE1	1:KA:454:PRO:HD3	2.53	0.43
1:MC:106:GLN:HB3	1:MC:203:LEU:HB2	1.99	0.43
1:MC:416:VAL:HG12	1:MC:417:HIS:H	1.83	0.43
1:OB:336:GLN:NE2	1:OB:379:GLN:HB2	2.34	0.43
1:AC:371:THR:HG21	1:AC:374:ASP:HB2	1.99	0.43
1:DB:24:ASN:OD1	1:DB:24:ASN:N	2.51	0.43
1:DB:267:THR:HG22	1:DB:271:VAL:N	2.27	0.43
1:FA:105:VAL:CG1	1:FA:156:ILE:HB	2.49	0.43
1:FB:327:VAL:HA	1:FB:353:THR:OG1	2.18	0.43
1:GB:96:TYR:CG	1:GB:212:PHE:HB3	2.54	0.43
1:IA:96:TYR:CG	1:IA:212:PHE:HB3	2.54	0.43
1:IA:242:PHE:O	1:IA:244:ILE:N	2.51	0.43
1:IC:449:LEU:HD12	1:IC:449:LEU:HA	1.91	0.43
1:JB:66:VAL:HG21	1:JB:119:ILE:HD11	2.01	0.43
1:JC:94:ARG:NH1	1:JC:226:PRO:HD3	2.32	0.43
1:KB:101:GLY:HA3	1:KB:210:PHE:HA	1.99	0.43
1:LC:57:VAL:HG11	1:LC:87:PRO:HD2	2.00	0.43
1:LC:317:ILE:HD12	1:LC:319:ALA:O	2.18	0.43
1:MB:280:PRO:HA	1:MB:283:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NA:328:GLY:H	1:NA:353:THR:HB	1.84	0.43
1:NB:121:PHE:HA	1:NB:179:ILE:O	2.18	0.43
1:NB:454:PRO:HG2	1:NB:457:TRP:CG	2.54	0.43
1:NC:81:LEU:HD11	1:NC:102:GLY:HA2	2.01	0.43
1:AB:57:VAL:HA	1:BC:139:THR:HG22	2.00	0.43
1:BA:341:ASP:OD2	1:BA:341:ASP:N	2.51	0.43
1:CA:134:SER:OG	1:CA:137:GLN:HG3	2.18	0.43
1:CA:249:LEU:HD12	1:CA:509:ILE:HD11	2.01	0.43
1:CB:131:GLU:OE1	1:CB:131:GLU:N	2.52	0.43
1:CB:259:VAL:HG13	1:CB:403:TRP:CZ3	2.54	0.43
1:DA:73:GLY:N	1:DA:181:MET:HE3	2.31	0.43
1:DA:219:THR:HG22	1:DA:222:SER:OG	2.19	0.43
1:EA:138:VAL:HG21	1:EA:181:MET:SD	2.59	0.43
1:EB:403:TRP:HZ2	1:EB:450:ASP:HB2	1.83	0.43
1:FA:43:GLY:HA3	1:FA:214:PHE:CE1	2.54	0.43
1:FC:280:PRO:HA	1:FC:283:ILE:HD11	2.01	0.43
1:GB:66:VAL:HG21	1:GB:119:ILE:HD11	2.01	0.43
1:GB:101:GLY:HA3	1:GB:210:PHE:HA	2.01	0.43
1:GB:471:ASP:OD1	1:GB:471:ASP:N	2.52	0.43
1:GC:233:THR:HG22	1:GC:235:GLU:N	2.34	0.43
1:GC:259:VAL:HG13	1:GC:403:TRP:CZ3	2.54	0.43
1:HB:23:ASN:HB3	1:HB:150:GLN:OE1	2.19	0.43
1:HC:46:ASN:HD21	1:HC:213:ILE:C	2.27	0.43
1:IB:435:ARG:NH1	1:IB:448:ASN:HB3	2.34	0.43
1:MA:144:ILE:O	1:MA:144:ILE:HG13	2.19	0.43
1:MB:230:PRO:HG2	1:MB:457:TRP:CD1	2.54	0.43
1:MB:301:MET:HE2	1:MB:303:LEU:HD23	2.01	0.43
1:NA:140:MET:HG2	1:OA:57:VAL:HG21	2.00	0.43
1:OA:53:ARG:O	1:OA:205:ARG:HD2	2.19	0.43
1:OA:81:LEU:HD11	1:OA:102:GLY:HA2	2.00	0.43
1:OA:422:VAL:HG12	1:OA:431:LEU:HD21	2.01	0.43
1:AA:280:PRO:HA	1:AA:283:ILE:HD11	2.00	0.43
1:DA:78:SER:HA	1:DA:178:LEU:O	2.18	0.43
1:EB:195:VAL:O	1:EB:195:VAL:HG12	2.19	0.43
1:EC:118:LYS:H	1:EC:184:THR:HB	1.82	0.43
1:FA:96:TYR:HA	1:FA:214:PHE:O	2.19	0.43
1:FA:307:ASN:O	1:FA:309:ASN:N	2.52	0.43
1:FA:319:ALA:HB1	1:FA:320:PRO:HD2	2.00	0.43
1:HC:134:SER:OG	1:HC:137:GLN:HG3	2.19	0.43
1:HC:311:TYR:CZ	1:HC:320:PRO:HD3	2.54	0.43
1:HC:469:GLN:HB2	1:HC:520:TRP:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IB:317:ILE:CG2	1:IB:318:PRO:HD2	2.49	0.43
1:IC:317:ILE:HD12	1:IC:319:ALA:O	2.19	0.43
1:JA:216:VAL:CG2	1:JA:217:PRO:HD2	2.48	0.43
1:JC:399:GLU:HB2	1:JC:400:PRO:HD3	2.01	0.43
1:JC:434:PHE:CD2	1:JC:454:PRO:HD3	2.54	0.43
1:LA:265:ARG:HG3	1:LA:273:LEU:HD12	2.01	0.43
1:LB:374:ASP:O	1:LB:375:LEU:HD23	2.19	0.43
1:LC:403:TRP:HZ2	1:LC:450:ASP:HB2	1.83	0.43
1:MB:146:VAL:HG11	1:MB:154:VAL:HG21	2.01	0.43
1:NB:57:VAL:HG23	1:NB:87:PRO:HD2	2.01	0.43
1:NB:440:GLY:O	1:OA:335:THR:HG23	2.18	0.43
1:OB:471:ASP:OD1	1:OB:471:ASP:N	2.49	0.43
1:AC:57:VAL:HA	1:GB:139:THR:CG2	2.49	0.42
1:AC:94:ARG:NH1	1:AC:225:LYS:HA	2.34	0.42
1:CA:64:PHE:HB3	1:CA:77:TRP:CD1	2.53	0.42
1:DA:434:PHE:CE1	1:DA:454:PRO:HD3	2.53	0.42
1:DB:245:PRO:O	1:DB:436:SER:OG	2.30	0.42
1:FA:44:GLN:HE22	1:FA:215:LEU:HB2	1.83	0.42
1:FA:57:VAL:CG2	1:JA:140:MET:HG2	2.49	0.42
1:FA:233:THR:HG22	1:FA:235:GLU:N	2.32	0.42
1:FB:344:THR:O	1:GA:442:SER:HA	2.19	0.42
1:IB:61:GLY:HA2	1:IB:520:TRP:O	2.19	0.42
1:KA:219:THR:HG22	1:KA:222:SER:OG	2.19	0.42
1:KB:317:ILE:HD13	1:KB:321:LEU:HD21	2.01	0.42
1:KB:327:VAL:HA	1:KB:353:THR:OG1	2.19	0.42
1:KC:217:PRO:HA	1:KC:218:PRO:HD3	1.64	0.42
1:MA:216:VAL:HG21	1:MC:128:PHE:CD2	2.54	0.42
1:MC:148:VAL:CG1	1:MC:198:VAL:HG21	2.49	0.42
1:NA:145:ILE:HD13	1:NA:183:TYR:CE2	2.54	0.42
1:OA:34:GLY:HA3	1:OA:209:ASP:O	2.19	0.42
1:OA:318:PRO:HD3	1:OA:417:HIS:O	2.18	0.42
1:OB:307:ASN:O	1:OB:308:TRP:HB2	2.19	0.42
1:BA:109:LEU:HD22	1:BA:200:CYS:SG	2.60	0.42
1:BC:44:GLN:NE2	1:BC:215:LEU:HD23	2.34	0.42
1:CA:301:MET:HE2	1:CA:381:THR:HB	2.01	0.42
1:CC:182:LEU:HD21	1:CC:185:PRO:HA	2.01	0.42
1:DA:247:GLU:HG2	1:DA:248:LYS:HE3	2.01	0.42
1:DA:422:VAL:HG12	1:DA:431:LEU:HD21	2.01	0.42
1:EC:265:ARG:NH2	1:EC:420:PRO:O	2.48	0.42
1:EC:473:ALA:HB2	1:EC:520:TRP:CZ3	2.54	0.42
1:FA:125:PRO:HG3	1:FB:214:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:61:GLY:HA2	1:FB:520:TRP:O	2.19	0.42
1:FB:109:LEU:HD23	1:FB:200:CYS:SG	2.58	0.42
1:FB:246:LEU:HD11	1:FB:454:PRO:HB3	2.01	0.42
1:HA:456:GLU:OE1	1:HA:456:GLU:N	2.51	0.42
1:HB:476:ARG:HD3	1:HB:485:VAL:HG11	2.02	0.42
1:HC:135:PRO:HA	1:HC:181:MET:HE1	2.01	0.42
1:HC:280:PRO:HB3	1:HC:455:GLN:HG2	2.00	0.42
1:IB:311:TYR:OH	1:IB:320:PRO:HD3	2.19	0.42
1:JA:374:ASP:O	1:JA:375:LEU:HD23	2.19	0.42
1:KA:267:THR:HG23	1:KA:493:LYS:O	2.19	0.42
1:MB:372:ASN:OD1	1:MB:372:ASN:N	2.52	0.42
1:MC:260:GLN:N	1:MC:261:PRO:HD3	2.34	0.42
1:NB:230:PRO:HG2	1:NB:457:TRP:CD1	2.54	0.42
1:NC:130:THR:O	1:NC:133:LEU:HD23	2.19	0.42
1:NC:217:PRO:HA	1:NC:218:PRO:HD3	1.87	0.42
1:AB:121:PHE:HA	1:AB:179:ILE:O	2.20	0.42
1:AC:329:LYS:HA	1:AC:351:VAL:O	2.18	0.42
1:AC:440:GLY:O	1:GC:335:THR:HG23	2.19	0.42
1:BC:434:PHE:CD2	1:BC:454:PRO:HD3	2.54	0.42
1:BC:481:ASP:OD1	1:BC:512:ASN:ND2	2.51	0.42
1:DA:234:VAL:HA	1:DA:237:MET:HE3	2.01	0.42
1:DA:328:GLY:H	1:DA:353:THR:HB	1.83	0.42
1:DB:34:GLY:HA3	1:DB:209:ASP:HB2	2.01	0.42
1:DB:509:ILE:HG22	1:DB:510:PRO:O	2.20	0.42
1:EA:81:LEU:HD11	1:EA:102:GLY:HA2	2.00	0.42
1:EB:290:VAL:HG22	1:EB:299:TYR:HB3	2.01	0.42
1:EB:488:GLU:HG3	1:EB:527:LEU:HD22	2.02	0.42
1:EC:101:GLY:HA3	1:EC:210:PHE:HA	2.00	0.42
1:FA:65:THR:HG22	1:FA:525:TYR:HA	2.02	0.42
1:GB:440:GLY:O	1:HA:335:THR:HG23	2.18	0.42
1:GC:225:LYS:HA	1:GC:226:PRO:HD3	1.93	0.42
1:HA:143:HIS:HE1	1:IA:56:PHE:O	2.02	0.42
1:HC:94:ARG:NH1	1:HC:226:PRO:HD3	2.34	0.42
1:JB:223:ARG:HA	1:JB:467:PRO:HG3	2.01	0.42
1:JC:265:ARG:NH2	1:JC:420:PRO:O	2.48	0.42
1:KA:144:ILE:HD13	1:KA:156:ILE:HG12	2.00	0.42
1:LC:27:MET:HE3	1:LC:156:ILE:HG23	2.02	0.42
1:NC:123:ALA:HB1	1:NC:176:ILE:HD11	2.01	0.42
1:OB:97:ASN:HB3	1:OB:214:PHE:HB3	2.02	0.42
1:OB:223:ARG:HA	1:OB:467:PRO:HG3	2.00	0.42
1:BC:326:PHE:CZ	1:BC:330:ILE:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CB:319:ALA:HB1	1:CB:320:PRO:HD2	2.01	0.42
1:CC:313:PRO:HB3	1:CC:361:LYS:O	2.19	0.42
1:DB:19:VAL:HG13	1:DB:149:ARG:O	2.20	0.42
1:DC:121:PHE:HA	1:DC:179:ILE:O	2.20	0.42
1:DC:257:PHE:CD2	1:DC:403:TRP:CD1	3.08	0.42
1:FA:120:ILE:HD11	1:FA:183:TYR:CD1	2.53	0.42
1:JC:33:VAL:HG11	1:JC:37:ILE:HB	2.01	0.42
1:KC:416:VAL:HG12	1:KC:417:HIS:N	2.34	0.42
1:MA:69:ARG:O	1:NA:484:ARG:NH2	2.45	0.42
1:MA:337:THR:HA	1:MA:343:SER:O	2.19	0.42
1:MA:353:THR:CG2	1:MA:406:PRO:HB3	2.49	0.42
1:MB:66:VAL:HG21	1:MB:119:ILE:HD11	2.00	0.42
1:MC:434:PHE:CD2	1:MC:454:PRO:HD3	2.53	0.42
1:NA:109:LEU:HD22	1:NA:200:CYS:SG	2.60	0.42
1:NA:371:THR:HG22	1:NA:373:ASN:H	1.84	0.42
1:OB:429:GLU:HB3	1:OB:498:THR:CG2	2.49	0.42
1:OC:338:THR:OG1	1:OC:345:ARG:NH2	2.41	0.42
1:AC:311:TYR:CZ	1:AC:320:PRO:HD3	2.54	0.42
1:BA:115:THR:HG22	1:BA:148:VAL:CG2	2.50	0.42
1:DA:325:ASP:OD1	1:DA:325:ASP:N	2.52	0.42
1:DC:329:LYS:HA	1:DC:351:VAL:O	2.20	0.42
1:FB:51:TRP:HB3	1:GA:215:LEU:HD12	2.02	0.42
1:FC:144:ILE:HG22	1:FC:146:VAL:HG23	2.00	0.42
1:GA:140:MET:HG2	1:HA:57:VAL:HG21	2.00	0.42
1:GC:319:ALA:HB1	1:GC:320:PRO:HD2	2.01	0.42
1:HB:501:HIS:CE1	1:HB:531:GLY:HA3	2.54	0.42
1:HC:148:VAL:HG13	1:HC:198:VAL:HG21	2.00	0.42
1:JA:313:PRO:O	1:JA:361:LYS:NZ	2.48	0.42
1:JB:124:VAL:HG22	1:JB:177:LYS:HB2	2.00	0.42
1:JC:246:LEU:HA	1:JC:436:SER:HB3	2.00	0.42
1:KA:435:ARG:HH12	1:KA:448:ASN:HB3	1.85	0.42
1:KB:222:SER:OG	1:KB:223:ARG:N	2.52	0.42
1:LA:30:GLU:HG3	1:MA:51:TRP:CZ2	2.55	0.42
1:LA:216:VAL:CG2	1:LA:217:PRO:HD2	2.46	0.42
1:MB:476:ARG:HD3	1:MB:485:VAL:HG11	2.01	0.42
1:NB:282:ASN:OD1	1:NB:287:ARG:NH2	2.49	0.42
1:NB:336:GLN:NE2	1:NB:379:GLN:HB2	2.34	0.42
1:NC:267:THR:HG22	1:NC:271:VAL:N	2.26	0.42
1:OA:282:ASN:OD1	1:OA:287:ARG:NH2	2.50	0.42
1:OC:158:LEU:HD12	1:OC:158:LEU:HA	1.88	0.42
1:BB:471:ASP:N	1:BB:471:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:267:THR:HG22	1:BC:271:VAL:N	2.33	0.42
1:CA:64:PHE:HB3	1:CA:77:TRP:HD1	1.85	0.42
1:CA:459:LEU:O	1:CA:463:GLN:HG3	2.19	0.42
1:CB:390:GLN:HA	1:CB:399:GLU:OE1	2.20	0.42
1:DA:241:ARG:HG3	1:DA:451:CYS:HB3	2.02	0.42
1:FC:261:PRO:HG3	1:FC:403:TRP:HZ3	1.85	0.42
1:GA:73:GLY:H	1:GA:181:MET:HE3	1.82	0.42
1:GC:389:VAL:HG23	1:GC:442:SER:HB3	2.02	0.42
1:HA:233:THR:HG21	1:HA:511:PRO:O	2.19	0.42
1:IC:246:LEU:HD13	1:IC:434:PHE:HB3	2.00	0.42
1:JB:14:SER:O	1:JB:15:THR:OG1	2.31	0.42
1:JB:403:TRP:CZ2	1:JB:450:ASP:HB2	2.55	0.42
1:JC:260:GLN:N	1:JC:261:PRO:HD3	2.35	0.42
1:LA:223:ARG:HH22	1:LA:269:ASP:HB2	1.85	0.42
1:LB:61:GLY:HA2	1:LB:520:TRP:O	2.19	0.42
1:MA:30:GLU:HG3	1:NA:51:TRP:CZ2	2.54	0.42
1:AB:105:VAL:CG2	1:AB:156:ILE:HB	2.49	0.42
1:AB:403:TRP:CZ2	1:AB:450:ASP:HB2	2.55	0.42
1:BA:219:THR:HG22	1:BA:222:SER:OG	2.19	0.42
1:BC:197:THR:O	1:KB:187:ARG:HG2	2.20	0.42
1:EB:106:GLN:HG3	1:EB:153:PRO:HB3	2.01	0.42
1:EB:181:MET:HE2	1:EB:181:MET:HB3	1.88	0.42
1:FB:190:ASN:HB2	1:GC:189:ASN:HD21	1.85	0.42
1:GA:341:ASP:OD1	1:GA:341:ASP:N	2.44	0.42
1:HB:66:VAL:HG21	1:HB:119:ILE:HD11	2.02	0.42
1:LB:437:THR:HG23	1:LB:447:MET:HB3	2.01	0.42
1:LC:267:THR:HG22	1:LC:271:VAL:N	2.29	0.42
1:LC:377:THR:HG22	1:LC:378:GLY:N	2.35	0.42
1:MC:46:ASN:ND2	1:MC:213:ILE:C	2.78	0.42
1:NB:105:VAL:CG2	1:NB:156:ILE:HB	2.50	0.42
1:OA:144:ILE:O	1:OA:144:ILE:HG13	2.19	0.42
1:OB:94:ARG:HD3	1:OB:226:PRO:HD3	2.01	0.42
1:OC:72:PRO:HA	1:OC:182:LEU:O	2.20	0.42
1:OC:109:LEU:HD13	1:OC:200:CYS:SG	2.59	0.42
1:CA:149:ARG:NH2	1:DA:149:ARG:O	2.46	0.42
1:CC:279:SER:HB3	1:CC:282:ASN:HB2	2.01	0.42
1:DA:143:HIS:HE1	1:EA:56:PHE:O	2.02	0.42
1:DC:308:TRP:CH2	1:DC:380:ASN:HB3	2.54	0.42
1:GB:267:THR:HG22	1:GB:271:VAL:N	2.34	0.42
1:IB:440:GLY:O	1:JA:335:THR:HG23	2.20	0.42
1:IB:482:THR:HG22	1:JC:426:PHE:CD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IC:326:PHE:CZ	1:IC:330:ILE:HD11	2.55	0.42
1:IC:359:THR:HB	1:IC:362:LEU:HD12	2.02	0.42
1:JA:371:THR:HG21	1:JA:374:ASP:HB2	2.01	0.42
1:JC:34:GLY:HA3	1:JC:209:ASP:HB2	2.02	0.42
1:KB:403:TRP:CZ2	1:KB:450:ASP:HB2	2.55	0.42
1:MA:280:PRO:HB3	1:MA:455:GLN:HG2	2.01	0.42
1:NC:390:GLN:HG2	1:NC:399:GLU:CG	2.49	0.42
1:OA:339:ARG:H	1:OA:339:ARG:HG2	1.70	0.42
1:OB:118:LYS:H	1:OB:184:THR:HB	1.84	0.42
1:OC:260:GLN:N	1:OC:261:PRO:HD3	2.34	0.42
1:OC:268:THR:HG21	1:OC:520:TRP:CH2	2.44	0.42
1:BA:29:LEU:HD23	1:BA:29:LEU:HA	1.81	0.42
1:BC:148:VAL:CG1	1:BC:198:VAL:HG21	2.50	0.42
1:CB:66:VAL:HG12	1:CB:186:LEU:HB2	2.01	0.42
1:DB:95:MET:HE3	1:DB:215:LEU:HD11	2.02	0.42
1:DB:244:ILE:HD13	1:DB:244:ILE:HG21	1.84	0.42
1:FC:242:PHE:CD2	1:FC:244:ILE:HD11	2.55	0.42
1:GA:430:GLN:HG3	1:GA:501:HIS:O	2.20	0.42
1:HA:134:SER:OG	1:HA:137:GLN:HG3	2.19	0.42
1:HB:124:VAL:HG12	1:HB:141:PHE:CD2	2.55	0.42
1:HB:298:ASP:OD1	1:HB:368:THR:HG22	2.20	0.42
1:HC:120:ILE:HG13	1:HC:183:TYR:HB2	2.01	0.42
1:HC:267:THR:HG22	1:HC:271:VAL:N	2.32	0.42
1:IC:241:ARG:NH1	1:IC:450:ASP:O	2.48	0.42
1:JC:46:ASN:ND2	1:JC:213:ILE:C	2.77	0.42
1:JC:347:HIS:CE1	1:JC:374:ASP:HB3	2.55	0.42
1:KB:230:PRO:HG2	1:KB:457:TRP:CD1	2.54	0.42
1:LA:337:THR:HA	1:LA:343:SER:O	2.19	0.42
1:LA:435:ARG:NH1	1:LA:448:ASN:HB3	2.35	0.42
1:LC:70:ASN:HB3	1:LC:182:LEU:HD22	2.02	0.42
1:MC:325:ASP:OD1	1:MC:325:ASP:N	2.53	0.42
1:MC:469:GLN:HB2	1:MC:520:TRP:CG	2.55	0.42
1:AC:121:PHE:HA	1:AC:179:ILE:O	2.20	0.42
1:AC:148:VAL:CG1	1:AC:198:VAL:HG21	2.50	0.42
1:CB:432:LEU:HB2	1:CB:499:VAL:HG13	2.01	0.42
1:CC:480:PRO:HG3	1:CC:514:TYR:CD1	2.54	0.42
1:EA:233:THR:HG21	1:EA:511:PRO:O	2.20	0.42
1:EC:24:ASN:O	1:EC:25:GLU:HB3	2.20	0.42
1:EC:150:GLN:NE2	1:EC:154:VAL:HG22	2.35	0.42
1:EC:486:LEU:HD11	1:EC:510:PRO:HG3	2.02	0.42
1:FC:71:ALA:HB3	1:JB:485:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GA:373:ASN:OD1	1:GA:373:ASN:N	2.51	0.42
1:GB:32:VAL:HB	1:GB:159:PRO:HB2	2.02	0.42
1:GB:217:PRO:HA	1:GB:218:PRO:HD3	1.73	0.42
1:HA:144:ILE:O	1:HA:144:ILE:HG13	2.20	0.42
1:HB:402:GLN:HE21	1:HB:403:TRP:NE1	2.18	0.42
1:IB:305:SER:HB3	1:IB:309:ASN:H	1.84	0.42
1:IB:326:PHE:CZ	1:IB:438:MET:HE1	2.55	0.42
1:IB:433:PHE:HB3	1:IB:450:ASP:HB3	2.02	0.42
1:KB:58:GLN:H	1:LC:139:THR:HG21	1.85	0.42
1:KB:280:PRO:HB3	1:KB:455:GLN:HG2	2.02	0.42
1:MB:94:ARG:O	1:MB:218:PRO:HA	2.20	0.42
1:OB:42:ALA:HB1	1:OB:213:ILE:HG23	2.02	0.42
1:OB:233:THR:HG22	1:OB:235:GLU:H	1.85	0.42
1:OB:259:VAL:HG13	1:OB:403:TRP:CZ3	2.55	0.42
1:AA:233:THR:HG22	1:AA:235:GLU:N	2.34	0.41
1:AA:325:ASP:OD1	1:AA:325:ASP:N	2.54	0.41
1:BB:231:ILE:HD11	1:CA:220:VAL:HG11	2.02	0.41
1:CA:116:ALA:O	1:CA:186:LEU:HD12	2.20	0.41
1:CC:426:PHE:HD2	1:CC:429:GLU:OE2	2.02	0.41
1:DA:326:PHE:CZ	1:DA:438:MET:HE1	2.54	0.41
1:GA:318:PRO:HD3	1:GA:417:HIS:O	2.20	0.41
1:GB:501:HIS:CE1	1:GB:531:GLY:HA3	2.55	0.41
1:HA:301:MET:O	1:HA:364:SER:HA	2.20	0.41
1:IB:399:GLU:HB3	1:IB:400:PRO:HD3	2.02	0.41
1:JA:219:THR:HG22	1:JA:222:SER:OG	2.20	0.41
1:JA:326:PHE:O	1:JA:353:THR:HG21	2.20	0.41
1:JB:57:VAL:HG23	1:JB:87:PRO:HD2	2.01	0.41
1:KB:454:PRO:HG2	1:KB:457:TRP:CD1	2.55	0.41
1:LC:120:ILE:HG13	1:LC:183:TYR:HB2	2.02	0.41
1:NB:359:THR:HG22	1:NB:410:GLY:HA3	2.01	0.41
1:AA:317:ILE:HG22	1:AA:318:PRO:HD2	2.02	0.41
1:BC:134:SER:OG	1:BC:137:GLN:HG3	2.20	0.41
1:BC:443:GLY:C	1:BC:444:TYR:HD1	2.28	0.41
1:BC:469:GLN:HB2	1:BC:520:TRP:CG	2.55	0.41
1:CB:124:VAL:CG2	1:CB:177:LYS:HB2	2.50	0.41
1:DA:242:PHE:CZ	1:DA:385:PRO:HB2	2.55	0.41
1:DC:287:ARG:HB3	1:DC:308:TRP:CH2	2.55	0.41
1:EC:32:VAL:HB	1:EC:159:PRO:HB2	2.02	0.41
1:EC:241:ARG:HH12	1:EC:402:GLN:HG3	1.85	0.41
1:EC:318:PRO:HG3	1:EC:417:HIS:O	2.19	0.41
1:FB:57:VAL:HG23	1:FB:87:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:261:PRO:HG2	1:FB:265:ARG:HD3	2.02	0.41
1:GB:318:PRO:HB3	1:GB:418:LEU:HD23	2.02	0.41
1:HA:434:PHE:CE1	1:HA:454:PRO:HD3	2.55	0.41
1:JC:213:ILE:HG23	1:JC:214:PHE:N	2.36	0.41
1:LB:230:PRO:HD3	1:LB:460:HIS:CD2	2.55	0.41
1:MA:305:SER:HB3	1:MA:309:ASN:H	1.84	0.41
1:NC:329:LYS:HA	1:NC:351:VAL:O	2.19	0.41
1:OA:119:ILE:HD13	1:OA:182:LEU:HD23	2.01	0.41
1:OA:219:THR:HG22	1:OA:222:SER:OG	2.20	0.41
1:OB:24:ASN:OD1	1:OB:25:GLU:N	2.53	0.41
1:AB:223:ARG:HA	1:AB:467:PRO:HG3	2.02	0.41
1:AB:435:ARG:NH1	1:AB:450:ASP:OD1	2.54	0.41
1:AC:319:ALA:HB1	1:AC:320:PRO:HD2	2.01	0.41
1:BA:301:MET:O	1:BA:364:SER:HA	2.19	0.41
1:BB:191:ALA:HB3	1:OB:191:ALA:HB3	2.02	0.41
1:BC:121:PHE:HA	1:BC:179:ILE:O	2.21	0.41
1:DA:284:CYS:SG	1:DA:324:PRO:HG3	2.60	0.41
1:FB:231:ILE:CD1	1:GA:220:VAL:HG11	2.48	0.41
1:FC:470:SER:OG	1:FC:521:VAL:O	2.33	0.41
1:GA:435:ARG:HH12	1:GA:448:ASN:HB3	1.85	0.41
1:IC:148:VAL:CG1	1:IC:198:VAL:HG21	2.51	0.41
1:JC:144:ILE:HG22	1:JC:146:VAL:HG23	2.01	0.41
1:JC:249:LEU:HD21	1:JC:515:PHE:HZ	1.84	0.41
1:KA:96:TYR:CG	1:KA:212:PHE:HB3	2.55	0.41
1:KA:185:PRO:HB2	1:KA:187:ARG:NH1	2.35	0.41
1:KA:266:CYS:HB2	1:KA:458:VAL:HG13	2.01	0.41
1:KB:14:SER:C	1:KB:15:THR:HG1	2.27	0.41
1:KB:482:THR:HG21	1:LC:427:PRO:CD	2.51	0.41
1:LA:117:GLY:O	1:LA:148:VAL:HG22	2.20	0.41
1:LB:267:THR:HG22	1:LB:271:VAL:N	2.32	0.41
1:LC:179:ILE:HA	1:LC:179:ILE:HD13	1.81	0.41
1:LC:489:CYS:HB3	1:LC:499:VAL:HG12	2.02	0.41
1:MB:124:VAL:HG22	1:MB:177:LYS:HB2	2.01	0.41
1:MC:33:VAL:HG11	1:MC:37:ILE:HB	2.01	0.41
1:OA:115:THR:HG22	1:OA:148:VAL:CG2	2.50	0.41
1:OA:435:ARG:NH1	1:OA:448:ASN:HB3	2.36	0.41
1:OB:327:VAL:HA	1:OB:353:THR:OG1	2.21	0.41
1:AA:76:LEU:C	1:AA:522:ASN:HD21	2.29	0.41
1:AC:46:ASN:ND2	1:AC:213:ILE:C	2.78	0.41
1:BA:242:PHE:O	1:BA:244:ILE:N	2.52	0.41
1:BA:275:THR:HG23	1:BA:318:PRO:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:335:THR:O	1:BC:381:THR:HA	2.20	0.41
1:CC:217:PRO:HA	1:CC:218:PRO:HD3	1.86	0.41
1:DA:233:THR:HG21	1:DA:511:PRO:O	2.20	0.41
1:DB:390:GLN:HB2	1:DB:445:PRO:HB3	2.02	0.41
1:DC:327:VAL:HA	1:DC:353:THR:OG1	2.20	0.41
1:EA:328:GLY:H	1:EA:353:THR:HB	1.86	0.41
1:EB:105:VAL:CG2	1:EB:156:ILE:HB	2.51	0.41
1:FC:135:PRO:HA	1:FC:181:MET:HE1	2.02	0.41
1:GB:293:ILE:HD13	1:GB:293:ILE:HA	1.92	0.41
1:HA:216:VAL:HG23	1:HC:141:PHE:CE1	2.55	0.41
1:HA:438:MET:O	1:HA:447:MET:HG2	2.20	0.41
1:HB:267:THR:HG22	1:HB:271:VAL:N	2.27	0.41
1:IB:66:VAL:HG12	1:IB:186:LEU:HB2	2.02	0.41
1:IB:217:PRO:HA	1:IB:218:PRO:HD3	1.96	0.41
1:IC:434:PHE:HE1	1:IC:515:PHE:HE2	1.67	0.41
1:JA:239:ASN:ND2	1:JA:436:SER:OG	2.40	0.41
1:JC:267:THR:HG22	1:JC:271:VAL:H	1.84	0.41
1:LA:144:ILE:O	1:LA:144:ILE:HG13	2.20	0.41
1:LB:454:PRO:HG2	1:LB:457:TRP:CG	2.55	0.41
1:MA:149:ARG:NH2	1:NA:149:ARG:O	2.51	0.41
1:MA:318:PRO:HD3	1:MA:417:HIS:O	2.20	0.41
1:MB:58:GLN:N	1:NC:139:THR:HG21	2.35	0.41
1:MB:403:TRP:CZ2	1:MB:450:ASP:HB2	2.56	0.41
1:MB:471:ASP:HA	1:MB:493:LYS:CD	2.50	0.41
1:NA:167:HIS:ND1	1:NA:173:ASP:OD2	2.49	0.41
1:OA:43:GLY:HA3	1:OA:214:PHE:CE1	2.56	0.41
1:OA:64:PHE:CG	1:OA:77:TRP:HB2	2.55	0.41
1:OA:216:VAL:CG2	1:OA:217:PRO:HD2	2.51	0.41
1:OB:32:VAL:HB	1:OB:159:PRO:HB2	2.02	0.41
1:OB:402:GLN:OE1	1:OB:449:LEU:HA	2.21	0.41
1:BA:53:ARG:HB3	1:BA:206:PRO:HG2	2.01	0.41
1:BA:216:VAL:CG2	1:BA:217:PRO:HD2	2.50	0.41
1:BB:403:TRP:HZ2	1:BB:450:ASP:HB2	1.85	0.41
1:BC:431:LEU:HD23	1:BC:498:THR:HG22	2.03	0.41
1:CB:167:HIS:ND1	1:CB:173:ASP:OD2	2.48	0.41
1:CB:509:ILE:HG22	1:CB:510:PRO:O	2.21	0.41
1:DA:96:TYR:HA	1:DA:214:PHE:O	2.20	0.41
1:DA:244:ILE:HD13	1:DA:438:MET:HA	2.03	0.41
1:EB:34:GLY:HA3	1:EB:209:ASP:HB2	2.03	0.41
1:EC:158:LEU:HD13	1:EC:178:LEU:HG	2.02	0.41
1:EC:305:SER:HB2	1:EC:307:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FC:37:ILE:HG22	1:FC:165:PHE:CD1	2.54	0.41
1:GA:307:ASN:O	1:GA:308:TRP:HB2	2.20	0.41
1:GB:134:SER:OG	1:GB:137:GLN:HG3	2.21	0.41
1:GB:146:VAL:HG11	1:GB:154:VAL:HG21	2.03	0.41
1:GB:402:GLN:OE1	1:GB:449:LEU:HA	2.21	0.41
1:GC:257:PHE:CE2	1:GC:403:TRP:CD1	3.08	0.41
1:HB:507:LEU:HD21	1:HB:530:MET:HE1	2.03	0.41
1:IB:403:TRP:CZ2	1:IB:450:ASP:HB2	2.55	0.41
1:JA:144:ILE:O	1:JA:144:ILE:HG13	2.21	0.41
1:JC:130:THR:O	1:JC:133:LEU:HD23	2.20	0.41
1:KB:65:THR:HG23	1:KB:525:TYR:CE1	2.56	0.41
1:LA:96:TYR:CG	1:LA:212:PHE:HB3	2.55	0.41
1:MA:64:PHE:CG	1:MA:77:TRP:HB2	2.55	0.41
1:MA:434:PHE:CE1	1:MA:454:PRO:HD3	2.55	0.41
1:NA:343:SER:HB3	1:NA:345:ARG:HH12	1.86	0.41
1:NC:46:ASN:ND2	1:NC:213:ILE:C	2.77	0.41
1:OB:170:GLN:HE21	1:OB:221:GLU:HB3	1.85	0.41
1:AB:60:PRO:HD3	1:AB:87:PRO:HD3	2.03	0.41
1:AB:139:THR:HG22	1:GC:57:VAL:HA	2.02	0.41
1:CA:145:ILE:HD13	1:CA:183:TYR:CE2	2.56	0.41
1:DA:40:PRO:HB2	1:DC:37:ILE:HD11	2.02	0.41
1:DA:53:ARG:HB3	1:DA:206:PRO:HG2	2.01	0.41
1:DA:140:MET:HE3	1:EA:87:PRO:HG2	2.02	0.41
1:DC:443:GLY:O	1:DC:444:TYR:HD1	2.02	0.41
1:EA:326:PHE:CZ	1:EA:438:MET:HE1	2.55	0.41
1:FA:390:GLN:HB3	1:FA:444:TYR:H	1.86	0.41
1:GC:308:TRP:CH2	1:GC:380:ASN:HB3	2.56	0.41
1:HB:124:VAL:HG22	1:HB:177:LYS:HB2	2.02	0.41
1:HC:391:ASP:H	1:HC:399:GLU:HG3	1.86	0.41
1:IC:181:MET:HE2	1:IC:181:MET:HB3	1.95	0.41
1:IC:395:ALA:HB3	1:IC:398:ASN:ND2	2.35	0.41
1:JB:403:TRP:HZ2	1:JB:450:ASP:HB2	1.85	0.41
1:KA:57:VAL:CG2	1:OA:140:MET:HG2	2.50	0.41
1:LB:254:SER:HA	1:LB:257:PHE:CE1	2.55	0.41
1:LB:477:PHE:CE2	1:LB:509:ILE:HD12	2.55	0.41
1:LC:325:ASP:N	1:LC:325:ASP:OD1	2.52	0.41
1:MA:105:VAL:CG1	1:MA:156:ILE:HB	2.51	0.41
1:NB:32:VAL:HG13	1:NC:41:VAL:HA	2.03	0.41
1:NC:277:GLN:HB3	1:NC:321:LEU:HB3	2.03	0.41
1:NC:426:PHE:HZ	1:NC:523:GLN:O	2.03	0.41
1:OC:134:SER:OG	1:OC:137:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:238:THR:HA	1:AB:245:PRO:HA	2.02	0.41
1:BB:66:VAL:HG21	1:BB:119:ILE:HD11	2.01	0.41
1:BB:490:LYS:HG3	1:BB:527:LEU:HD21	2.02	0.41
1:BC:249:LEU:HB3	1:BC:507:LEU:HD12	2.03	0.41
1:CB:359:THR:HG22	1:CB:410:GLY:HA3	2.03	0.41
1:DA:108:ILE:HG12	1:DA:153:PRO:HB3	2.02	0.41
1:DA:456:GLU:OE1	1:DA:456:GLU:N	2.52	0.41
1:DB:403:TRP:CZ2	1:DB:450:ASP:HB2	2.56	0.41
1:EA:140:MET:HB2	1:EB:217:PRO:HG3	2.02	0.41
1:EB:94:ARG:HG2	1:EB:224:THR:HB	2.03	0.41
1:EC:371:THR:HG22	1:EC:373:ASN:H	1.85	0.41
1:FA:371:THR:CG2	1:FA:374:ASP:H	2.34	0.41
1:FB:449:LEU:HA	1:FB:449:LEU:HD12	1.89	0.41
1:GB:454:PRO:HG2	1:GB:457:TRP:CD1	2.55	0.41
1:HB:84:ASP:CG	1:HB:469:GLN:HE22	2.29	0.41
1:JC:98:GLY:N	1:JC:213:ILE:HG22	2.36	0.41
1:JC:217:PRO:HA	1:JC:218:PRO:HD3	1.85	0.41
1:KB:317:ILE:HG22	1:KB:318:PRO:HD2	2.02	0.41
1:KC:135:PRO:HA	1:KC:181:MET:HE1	2.02	0.41
1:KC:259:VAL:HG13	1:KC:403:TRP:CZ3	2.56	0.41
1:LB:395:ALA:HB3	1:LB:398:ASN:HD22	1.85	0.41
1:LB:440:GLY:O	1:MA:335:THR:HG23	2.21	0.41
1:NA:433:PHE:HB3	1:NA:450:ASP:HB3	2.01	0.41
1:NB:233:THR:HB	1:NB:236:GLU:HG3	2.03	0.41
1:NC:403:TRP:CZ2	1:NC:450:ASP:HB2	2.56	0.41
1:OB:134:SER:OG	1:OB:137:GLN:HG3	2.21	0.41
1:OB:471:ASP:HA	1:OB:493:LYS:CD	2.49	0.41
1:AB:181:MET:HB3	1:AB:181:MET:HE2	1.79	0.41
1:AC:484:ARG:HH11	1:AC:486:LEU:HD23	1.86	0.41
1:CB:116:ALA:N	1:CB:187:ARG:O	2.49	0.41
1:DC:509:ILE:HG22	1:DC:510:PRO:O	2.20	0.41
1:EA:64:PHE:CG	1:EA:77:TRP:HB2	2.56	0.41
1:EA:315:GLU:HB3	1:EA:317:ILE:HG13	2.02	0.41
1:FB:242:PHE:HD1	1:FB:284:CYS:HG	1.64	0.41
1:GA:69:ARG:O	1:HA:484:ARG:NH2	2.50	0.41
1:GB:121:PHE:HA	1:GB:179:ILE:O	2.19	0.41
1:HB:118:LYS:H	1:HB:184:THR:HB	1.86	0.41
1:IA:399:GLU:HB3	1:IA:400:PRO:HD3	2.02	0.41
1:IC:371:THR:HG21	1:IC:374:ASP:HB3	2.03	0.41
1:JA:64:PHE:CG	1:JA:77:TRP:HB2	2.56	0.41
1:JA:266:CYS:HB2	1:JA:458:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JA:299:TYR:CE2	1:JA:375:LEU:HB2	2.55	0.41
1:JB:96:TYR:CG	1:JB:212:PHE:HB3	2.56	0.41
1:KB:267:THR:HG22	1:KB:271:VAL:N	2.29	0.41
1:LA:247:GLU:OE1	1:LA:437:THR:HG22	2.21	0.41
1:NA:216:VAL:CG2	1:NA:217:PRO:HD2	2.48	0.41
1:OA:43:GLY:HA3	1:OA:214:PHE:HE1	1.85	0.41
1:AB:471:ASP:OD1	1:AB:522:ASN:HA	2.21	0.41
1:BA:399:GLU:HB3	1:BA:400:PRO:HD3	2.02	0.41
1:BB:105:VAL:CG2	1:BB:156:ILE:HB	2.51	0.41
1:BB:121:PHE:HA	1:BB:179:ILE:O	2.20	0.41
1:CB:51:TRP:HB3	1:DA:215:LEU:HD12	2.02	0.41
1:CB:501:HIS:CE1	1:CB:531:GLY:HA3	2.56	0.41
1:CC:178:LEU:HD23	1:CC:178:LEU:HA	1.87	0.41
1:DA:280:PRO:HA	1:DA:283:ILE:HD11	2.03	0.41
1:DB:329:LYS:HE2	1:DB:352:SER:HB2	2.03	0.41
1:DC:182:LEU:HD21	1:DC:185:PRO:HA	2.02	0.41
1:EB:125:PRO:HG3	1:EC:214:PHE:CD1	2.56	0.41
1:EC:78:SER:HA	1:EC:178:LEU:O	2.21	0.41
1:EC:406:PRO:HG2	1:EC:408:TYR:CE1	2.56	0.41
1:EC:414:HIS:O	1:EC:416:VAL:HG23	2.21	0.41
1:FA:115:THR:HG22	1:FA:148:VAL:CG2	2.51	0.41
1:FA:335:THR:HG23	1:JB:440:GLY:O	2.21	0.41
1:FB:19:VAL:HG13	1:FB:149:ARG:O	2.20	0.41
1:FB:267:THR:HG22	1:FB:271:VAL:N	2.34	0.41
1:GA:242:PHE:O	1:GA:244:ILE:N	2.53	0.41
1:GB:94:ARG:HG2	1:GB:224:THR:HB	2.03	0.41
1:GB:250:PHE:CD2	1:GB:435:ARG:NH2	2.89	0.41
1:GC:121:PHE:HA	1:GC:179:ILE:O	2.20	0.41
1:HA:117:GLY:O	1:HA:148:VAL:HG22	2.21	0.41
1:HA:280:PRO:HA	1:HA:283:ILE:HD11	2.03	0.41
1:HB:287:ARG:C	1:HB:301:MET:HE3	2.46	0.41
1:HB:344:THR:HG21	1:IA:440:GLY:HA3	2.02	0.41
1:IA:319:ALA:HB1	1:IA:320:PRO:HD2	2.03	0.41
1:IB:306:GLN:CD	1:IB:306:GLN:H	2.28	0.41
1:IC:121:PHE:HA	1:IC:179:ILE:O	2.20	0.41
1:JA:422:VAL:HG12	1:JA:431:LEU:HD21	2.02	0.41
1:JB:81:LEU:HD11	1:JB:102:GLY:HA2	2.03	0.41
1:KA:326:PHE:CZ	1:KA:438:MET:HE1	2.56	0.41
1:KA:459:LEU:O	1:KA:463:GLN:HG3	2.21	0.41
1:KB:77:TRP:HB3	1:KB:180:ALA:HB3	2.03	0.41
1:KB:456:GLU:OE1	1:KB:456:GLU:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:105:VAL:CG1	1:LA:156:ILE:HB	2.50	0.41
1:LB:293:ILE:HD13	1:LB:293:ILE:HA	1.94	0.41
1:LB:317:ILE:HG22	1:LB:318:PRO:HD2	2.03	0.41
1:LC:443:GLY:C	1:LC:444:TYR:CD1	2.99	0.41
1:MA:400:PRO:HG2	1:MA:446:ASN:O	2.21	0.41
1:MB:121:PHE:HB2	1:MB:144:ILE:CG2	2.50	0.41
1:NA:134:SER:OG	1:NA:137:GLN:HG3	2.20	0.41
1:NB:89:LEU:HD11	1:NB:206:PRO:HB3	2.03	0.41
1:OA:120:ILE:HD13	1:OA:138:VAL:HG12	2.02	0.41
1:OB:181:MET:HE2	1:OB:181:MET:HB3	1.90	0.41
1:OC:358:PHE:CZ	1:OC:360:PRO:HG3	2.56	0.41
1:AA:280:PRO:HB3	1:AA:455:GLN:HG2	2.03	0.41
1:AA:459:LEU:O	1:AA:463:GLN:HG3	2.21	0.41
1:AC:390:GLN:HG2	1:AC:399:GLU:CG	2.50	0.41
1:BA:318:PRO:HD3	1:BA:417:HIS:O	2.21	0.41
1:BB:435:ARG:NH1	1:BB:448:ASN:HB3	2.36	0.41
1:CA:242:PHE:O	1:CA:244:ILE:N	2.54	0.41
1:CC:233:THR:HG22	1:CC:235:GLU:H	1.86	0.41
1:DB:30:GLU:HG3	1:DC:44:GLN:HA	2.03	0.41
1:EC:148:VAL:CG1	1:EC:198:VAL:HG21	2.52	0.41
1:FB:248:LYS:HD2	1:FB:435:ARG:HD2	2.02	0.41
1:FB:439:PRO:CB	1:GA:335:THR:HG21	2.44	0.41
1:GB:244:ILE:HA	1:HA:281:VAL:HG11	2.03	0.41
1:GB:326:PHE:CZ	1:GB:438:MET:HE1	2.56	0.41
1:HB:372:ASN:OD1	1:HB:372:ASN:N	2.53	0.41
1:HC:121:PHE:HA	1:HC:179:ILE:O	2.21	0.41
1:IC:434:PHE:CD2	1:IC:454:PRO:HD3	2.57	0.41
1:IC:477:PHE:HD2	1:IC:487:PHE:CE1	2.38	0.41
1:JA:341:ASP:OD1	1:JA:341:ASP:N	2.53	0.41
1:JC:331:GLN:HG2	1:JC:350:THR:OG1	2.21	0.41
1:KA:353:THR:CG2	1:KA:406:PRO:HB3	2.51	0.41
1:KA:353:THR:HG22	1:KA:406:PRO:HB3	2.03	0.41
1:KB:402:GLN:OE1	1:KB:449:LEU:HA	2.20	0.41
1:LA:109:LEU:HD22	1:LA:200:CYS:SG	2.61	0.41
1:LC:311:TYR:HE1	1:LC:320:PRO:HB3	1.86	0.41
1:LC:480:PRO:HG3	1:LC:514:TYR:CE1	2.55	0.41
1:MC:101:GLY:HA3	1:MC:210:PHE:HA	2.02	0.41
1:AA:187:ARG:NH2	1:BA:197:THR:O	2.54	0.40
1:AB:75:ILE:O	1:AB:522:ASN:ND2	2.54	0.40
1:AC:347:HIS:NE2	1:AC:374:ASP:HB3	2.36	0.40
1:BA:282:ASN:OD1	1:BA:287:ARG:NH2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:209:ASP:OD1	1:CA:209:ASP:N	2.53	0.40
1:CB:120:ILE:HD11	1:CB:183:TYR:CD1	2.55	0.40
1:CB:403:TRP:CZ2	1:CB:450:ASP:HB2	2.55	0.40
1:CC:259:VAL:HG13	1:CC:403:TRP:CZ3	2.56	0.40
1:DA:48:ILE:HD12	1:DA:211:ASP:HA	2.03	0.40
1:EC:46:ASN:ND2	1:EC:213:ILE:C	2.78	0.40
1:FA:120:ILE:HD13	1:FA:120:ILE:HG21	1.79	0.40
1:FA:244:ILE:HD13	1:FA:438:MET:HA	2.03	0.40
1:FC:49:ASP:OD2	1:LC:46:ASN:HB3	2.20	0.40
1:GA:216:VAL:HG21	1:GC:128:PHE:CD1	2.56	0.40
1:GA:251:THR:HG22	1:GA:430:GLN:HE21	1.86	0.40
1:GB:227:PHE:CE1	1:GB:268:THR:HG23	2.56	0.40
1:HB:433:PHE:HB3	1:HB:450:ASP:HB3	2.02	0.40
1:IB:121:PHE:HA	1:IB:179:ILE:O	2.21	0.40
1:IB:233:THR:HG21	1:IB:511:PRO:O	2.21	0.40
1:JA:41:VAL:HA	1:JC:32:VAL:HG13	2.02	0.40
1:JB:454:PRO:HG2	1:JB:457:TRP:CD1	2.55	0.40
1:MB:124:VAL:CG2	1:MB:177:LYS:HB2	2.50	0.40
1:NA:89:LEU:HD12	1:NA:103:PHE:HE2	1.85	0.40
1:OA:341:ASP:N	1:OA:341:ASP:OD1	2.55	0.40
1:OA:400:PRO:HG2	1:OA:446:ASN:HB3	2.03	0.40
1:OB:66:VAL:HG21	1:OB:119:ILE:HD11	2.03	0.40
1:AA:225:LYS:HD3	1:AA:464:GLU:HG3	2.03	0.40
1:BC:440:GLY:O	1:KC:335:THR:HG23	2.20	0.40
1:CA:117:GLY:O	1:CA:148:VAL:HG22	2.21	0.40
1:CA:124:VAL:HG23	1:CA:141:PHE:CE1	2.57	0.40
1:DB:51:TRP:HB3	1:EA:215:LEU:HD12	2.02	0.40
1:DB:440:GLY:O	1:EA:335:THR:HG23	2.21	0.40
1:DC:241:ARG:NE	1:DC:325:ASP:OD2	2.52	0.40
1:EA:216:VAL:CG2	1:EA:217:PRO:HD2	2.49	0.40
1:EC:242:PHE:O	1:EC:244:ILE:N	2.52	0.40
1:EC:395:ALA:HB3	1:EC:398:ASN:HD22	1.85	0.40
1:FA:433:PHE:HB3	1:FA:450:ASP:HB3	2.03	0.40
1:FB:282:ASN:OD1	1:FB:287:ARG:NH2	2.53	0.40
1:GA:144:ILE:CD1	1:GA:156:ILE:HG12	2.51	0.40
1:GC:146:VAL:HG13	1:GC:150:GLN:OE1	2.21	0.40
1:HB:233:THR:HG22	1:HB:235:GLU:H	1.85	0.40
1:HC:449:LEU:HD12	1:HC:449:LEU:HA	1.93	0.40
1:IA:435:ARG:HG3	1:IA:450:ASP:OD1	2.20	0.40
1:JA:353:THR:HG22	1:JA:406:PRO:HB3	2.03	0.40
1:KB:124:VAL:HG22	1:KB:177:LYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LB:23:ASN:HB3	1:LB:150:GLN:NE2	2.36	0.40
1:MA:293:ILE:HD13	1:MA:293:ILE:HA	1.93	0.40
1:NA:399:GLU:HB3	1:NA:400:PRO:HD3	2.02	0.40
1:OB:96:TYR:CG	1:OB:212:PHE:HB3	2.56	0.40
1:AA:219:THR:HG22	1:AA:222:SER:OG	2.21	0.40
1:AB:432:LEU:HB2	1:AB:499:VAL:HG13	2.03	0.40
1:BB:244:ILE:HA	1:CA:281:VAL:HG11	2.04	0.40
1:CA:216:VAL:HG21	1:CC:128:PHE:CD1	2.56	0.40
1:CB:233:THR:HG22	1:CB:234:VAL:N	2.36	0.40
1:DA:65:THR:OG1	1:DA:197:THR:HG23	2.22	0.40
1:DA:371:THR:CG2	1:DA:374:ASP:H	2.35	0.40
1:DB:94:ARG:HH11	1:DB:94:ARG:HD2	1.78	0.40
1:DB:469:GLN:HG3	1:DB:520:TRP:NE1	2.36	0.40
1:DC:56:PHE:HB3	1:DC:203:LEU:HB3	2.03	0.40
1:DC:242:PHE:CD2	1:DC:243:PRO:HD2	2.57	0.40
1:EA:89:LEU:HD11	1:EA:206:PRO:HB3	2.03	0.40
1:FA:403:TRP:CZ2	1:FA:450:ASP:HB2	2.56	0.40
1:FB:191:ALA:CB	1:KB:191:ALA:HB3	2.51	0.40
1:FC:358:PHE:CZ	1:FC:360:PRO:HG3	2.56	0.40
1:GA:326:PHE:CZ	1:GA:438:MET:HE1	2.56	0.40
1:GB:66:VAL:HG12	1:GB:186:LEU:HB2	2.04	0.40
1:GB:230:PRO:HD3	1:GB:460:HIS:CD2	2.57	0.40
1:GC:265:ARG:HA	1:GC:265:ARG:HD2	1.94	0.40
1:HA:124:VAL:HG13	1:HA:177:LYS:HB3	2.03	0.40
1:HA:216:VAL:CG2	1:HA:217:PRO:HD2	2.52	0.40
1:HB:398:ASN:OD1	1:HB:398:ASN:C	2.65	0.40
1:HC:178:LEU:HD23	1:HC:178:LEU:HA	1.88	0.40
1:IA:490:LYS:HE3	1:IA:527:LEU:HG	2.02	0.40
1:IB:179:ILE:HD13	1:IB:179:ILE:HA	1.97	0.40
1:JB:118:LYS:HD3	1:JB:147:ASP:HA	2.03	0.40
1:KB:201:ARG:HG3	1:LC:183:TYR:CE2	2.56	0.40
1:KC:179:ILE:HD13	1:KC:179:ILE:HA	1.83	0.40
1:KC:249:LEU:HD21	1:KC:515:PHE:HZ	1.87	0.40
1:LC:217:PRO:HA	1:LC:218:PRO:HD3	1.89	0.40
1:MC:57:VAL:HG11	1:MC:87:PRO:HD2	2.02	0.40
1:NA:65:THR:HG22	1:NA:525:TYR:HA	2.02	0.40
1:OC:336:GLN:NE2	1:OC:379:GLN:HB2	2.36	0.40
1:BA:403:TRP:CZ2	1:BA:450:ASP:HB2	2.56	0.40
1:BB:411:ARG:H	1:BB:411:ARG:HG2	1.72	0.40
1:BC:437:THR:HG23	1:BC:447:MET:HB3	2.03	0.40
1:CB:215:LEU:HD21	1:DA:52:ILE:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CC:319:ALA:HB1	1:CC:320:PRO:HD2	2.03	0.40
1:CC:459:LEU:O	1:CC:463:GLN:HG3	2.22	0.40
1:DA:118:LYS:HE2	1:EA:110:ALA:HA	2.03	0.40
1:DA:128:PHE:CE1	1:DA:141:PHE:HZ	2.39	0.40
1:DB:161:VAL:CG2	1:DB:176:ILE:HD11	2.51	0.40
1:FA:115:THR:HG23	1:FA:186:LEU:HD11	2.03	0.40
1:FB:94:ARG:HH11	1:FB:94:ARG:HD2	1.77	0.40
1:FC:38:ALA:O	1:FC:42:ALA:N	2.52	0.40
1:HA:424:PRO:HD3	1:HA:431:LEU:CD1	2.51	0.40
1:HB:490:LYS:HG3	1:HB:527:LEU:HD11	2.04	0.40
1:IA:170:GLN:HG3	1:IC:127:ASN:O	2.22	0.40
1:IB:269:ASP:HB3	1:IB:467:PRO:HA	2.03	0.40
1:IC:148:VAL:HG13	1:IC:198:VAL:HG21	2.03	0.40
1:JB:433:PHE:HB3	1:JB:450:ASP:HB3	2.04	0.40
1:JC:53:ARG:O	1:JC:205:ARG:HD2	2.21	0.40
1:JC:390:GLN:HG2	1:JC:399:GLU:HG3	2.03	0.40
1:KA:48:ILE:HD11	1:KA:212:PHE:CD2	2.56	0.40
1:KA:51:TRP:CZ2	1:OA:30:GLU:HG3	2.57	0.40
1:KA:124:VAL:HG23	1:KA:141:PHE:CE1	2.56	0.40
1:KA:403:TRP:CZ2	1:KA:450:ASP:HB2	2.56	0.40
1:KB:432:LEU:HB2	1:KB:499:VAL:HG13	2.04	0.40
1:LB:395:ALA:HB3	1:LB:398:ASN:ND2	2.37	0.40
1:MA:96:TYR:CG	1:MA:212:PHE:HB3	2.56	0.40
1:MA:306:GLN:H	1:MA:306:GLN:CD	2.30	0.40
1:MB:259:VAL:HG13	1:MB:403:TRP:CZ3	2.57	0.40
1:NA:29:LEU:HD23	1:NA:29:LEU:HA	1.78	0.40
1:NB:118:LYS:HD3	1:NB:147:ASP:HA	2.03	0.40
1:NB:471:ASP:OD1	1:NB:522:ASN:HA	2.22	0.40
1:OA:101:GLY:HA3	1:OA:210:PHE:HA	2.03	0.40
1:OB:101:GLY:HA3	1:OB:210:PHE:HA	2.02	0.40
1:AA:65:THR:HG22	1:AA:525:TYR:HA	2.02	0.40
1:AA:135:PRO:HG3	1:AA:181:MET:HE2	2.04	0.40
1:AB:444:TYR:HE2	1:BA:341:ASP:HB2	1.87	0.40
1:BB:307:ASN:ND2	1:CA:235:GLU:OE2	2.55	0.40
1:CA:78:SER:HA	1:CA:178:LEU:O	2.21	0.40
1:DA:115:THR:HG22	1:DA:148:VAL:CG2	2.51	0.40
1:DB:334:LEU:HD22	1:DB:381:THR:HG22	2.03	0.40
1:GA:500:ALA:HB2	1:GA:527:LEU:HB2	2.02	0.40
1:HB:293:ILE:HD13	1:HB:293:ILE:HA	1.91	0.40
1:HB:454:PRO:HG2	1:HB:457:TRP:CD1	2.57	0.40
1:HC:358:PHE:HD1	1:HC:365:VAL:HG13	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HC:390:GLN:HG2	1:HC:399:GLU:CG	2.51	0.40
1:IB:468:ALA:HA	1:IB:520:TRP:CH2	2.57	0.40
1:JC:261:PRO:HG3	1:JC:403:TRP:HZ3	1.87	0.40
1:KA:216:VAL:CG2	1:KA:217:PRO:HD2	2.50	0.40
1:LA:144:ILE:HD13	1:LA:156:ILE:HG12	2.03	0.40
1:LC:434:PHE:CD2	1:LC:454:PRO:HD3	2.57	0.40
1:MA:449:LEU:HD12	1:MA:449:LEU:HA	1.87	0.40
1:MB:88:TYR:CE1	1:NC:140:MET:HE2	2.57	0.40
1:OB:66:VAL:HG12	1:OB:186:LEU:HB2	2.03	0.40
1:OC:107:VAL:HG13	1:OC:154:VAL:HB	2.04	0.40
1:OC:277:GLN:NE2	1:OC:283:ILE:HD13	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	496/540 (92%)	482 (97%)	14 (3%)	0	100	100
1	AB	521/540 (96%)	505 (97%)	16 (3%)	0	100	100
1	AC	506/540 (94%)	489 (97%)	17 (3%)	0	100	100
1	BA	495/540 (92%)	480 (97%)	15 (3%)	0	100	100
1	BB	521/540 (96%)	502 (96%)	19 (4%)	0	100	100
1	BC	505/540 (94%)	488 (97%)	17 (3%)	0	100	100
1	CA	495/540 (92%)	481 (97%)	14 (3%)	0	100	100
1	CB	521/540 (96%)	501 (96%)	20 (4%)	0	100	100
1	CC	505/540 (94%)	488 (97%)	17 (3%)	0	100	100
1	DA	494/540 (92%)	480 (97%)	14 (3%)	0	100	100
1	DB	521/540 (96%)	501 (96%)	20 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DC	504/540 (93%)	489 (97%)	15 (3%)	0	100	100
1	EA	495/540 (92%)	484 (98%)	11 (2%)	0	100	100
1	EB	521/540 (96%)	505 (97%)	16 (3%)	0	100	100
1	EC	489/540 (91%)	475 (97%)	14 (3%)	0	100	100
1	FA	495/540 (92%)	473 (96%)	22 (4%)	0	100	100
1	FB	521/540 (96%)	502 (96%)	19 (4%)	0	100	100
1	FC	507/540 (94%)	491 (97%)	16 (3%)	0	100	100
1	GA	495/540 (92%)	478 (97%)	17 (3%)	0	100	100
1	GB	521/540 (96%)	500 (96%)	21 (4%)	0	100	100
1	GC	505/540 (94%)	488 (97%)	17 (3%)	0	100	100
1	HA	495/540 (92%)	481 (97%)	14 (3%)	0	100	100
1	HB	521/540 (96%)	499 (96%)	22 (4%)	0	100	100
1	HC	505/540 (94%)	491 (97%)	14 (3%)	0	100	100
1	IA	495/540 (92%)	481 (97%)	14 (3%)	0	100	100
1	IB	521/540 (96%)	497 (95%)	24 (5%)	0	100	100
1	IC	499/540 (92%)	485 (97%)	14 (3%)	0	100	100
1	JA	495/540 (92%)	479 (97%)	16 (3%)	0	100	100
1	JB	521/540 (96%)	501 (96%)	20 (4%)	0	100	100
1	JC	504/540 (93%)	487 (97%)	17 (3%)	0	100	100
1	KA	495/540 (92%)	479 (97%)	16 (3%)	0	100	100
1	KB	521/540 (96%)	505 (97%)	16 (3%)	0	100	100
1	KC	505/540 (94%)	491 (97%)	14 (3%)	0	100	100
1	LA	495/540 (92%)	477 (96%)	18 (4%)	0	100	100
1	LB	521/540 (96%)	503 (96%)	18 (4%)	0	100	100
1	LC	498/540 (92%)	480 (96%)	18 (4%)	0	100	100
1	MA	495/540 (92%)	483 (98%)	12 (2%)	0	100	100
1	MB	521/540 (96%)	506 (97%)	15 (3%)	0	100	100
1	MC	504/540 (93%)	490 (97%)	14 (3%)	0	100	100
1	NA	495/540 (92%)	480 (97%)	15 (3%)	0	100	100
1	NB	521/540 (96%)	505 (97%)	16 (3%)	0	100	100
1	NC	504/540 (93%)	486 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	OA	495/540 (92%)	482 (97%)	13 (3%)	0	100	100
1	OB	521/540 (96%)	502 (96%)	19 (4%)	0	100	100
1	OC	494/540 (92%)	476 (96%)	18 (4%)	0	100	100
All	All	22774/24300 (94%)	22028 (97%)	746 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	427/457 (93%)	427 (100%)	0	100	100
1	AB	444/457 (97%)	444 (100%)	0	100	100
1	AC	434/457 (95%)	434 (100%)	0	100	100
1	BA	426/457 (93%)	426 (100%)	0	100	100
1	BB	445/457 (97%)	445 (100%)	0	100	100
1	BC	433/457 (95%)	433 (100%)	0	100	100
1	CA	426/457 (93%)	426 (100%)	0	100	100
1	CB	444/457 (97%)	444 (100%)	0	100	100
1	CC	433/457 (95%)	433 (100%)	0	100	100
1	DA	425/457 (93%)	425 (100%)	0	100	100
1	DB	444/457 (97%)	444 (100%)	0	100	100
1	DC	432/457 (94%)	432 (100%)	0	100	100
1	EA	426/457 (93%)	426 (100%)	0	100	100
1	EB	444/457 (97%)	444 (100%)	0	100	100
1	EC	421/457 (92%)	421 (100%)	0	100	100
1	FA	426/457 (93%)	426 (100%)	0	100	100
1	FB	445/457 (97%)	445 (100%)	0	100	100
1	FC	435/457 (95%)	435 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GA	426/457 (93%)	426 (100%)	0	100	100
1	GB	444/457 (97%)	444 (100%)	0	100	100
1	GC	433/457 (95%)	433 (100%)	0	100	100
1	HA	426/457 (93%)	426 (100%)	0	100	100
1	HB	444/457 (97%)	444 (100%)	0	100	100
1	HC	433/457 (95%)	433 (100%)	0	100	100
1	IA	426/457 (93%)	426 (100%)	0	100	100
1	IB	445/457 (97%)	445 (100%)	0	100	100
1	IC	430/457 (94%)	430 (100%)	0	100	100
1	JA	426/457 (93%)	426 (100%)	0	100	100
1	JB	442/457 (97%)	442 (100%)	0	100	100
1	JC	432/457 (94%)	432 (100%)	0	100	100
1	KA	426/457 (93%)	426 (100%)	0	100	100
1	KB	443/457 (97%)	443 (100%)	0	100	100
1	KC	433/457 (95%)	433 (100%)	0	100	100
1	LA	426/457 (93%)	426 (100%)	0	100	100
1	LB	441/457 (96%)	441 (100%)	0	100	100
1	LC	427/457 (93%)	427 (100%)	0	100	100
1	MA	426/457 (93%)	426 (100%)	0	100	100
1	MB	443/457 (97%)	443 (100%)	0	100	100
1	MC	432/457 (94%)	432 (100%)	0	100	100
1	NA	426/457 (93%)	426 (100%)	0	100	100
1	NB	444/457 (97%)	444 (100%)	0	100	100
1	NC	430/457 (94%)	430 (100%)	0	100	100
1	OA	426/457 (93%)	426 (100%)	0	100	100
1	OB	444/457 (97%)	444 (100%)	0	100	100
1	OC	426/457 (93%)	426 (100%)	0	100	100
All	All	19510/20565 (95%)	19510 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (198) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	45	GLN
1	AA	106	GLN
1	AA	331	GLN
1	AA	366	GLN
1	AA	417	HIS
1	AB	58	GLN
1	AB	366	GLN
1	AB	401	GLN
1	AC	45	GLN
1	AC	55	ASN
1	AC	127	ASN
1	AC	373	ASN
1	AC	522	ASN
1	BA	45	GLN
1	BA	380	ASN
1	BB	54	ASN
1	BB	91	HIS
1	BB	190	ASN
1	BB	366	GLN
1	BB	380	ASN
1	BB	430	GLN
1	BB	492	HIS
1	BC	44	GLN
1	BC	45	GLN
1	BC	127	ASN
1	BC	379	GLN
1	BC	492	HIS
1	CA	45	GLN
1	CA	106	GLN
1	CB	44	GLN
1	CB	45	GLN
1	CB	46	ASN
1	CB	58	GLN
1	CB	307	ASN
1	CB	331	GLN
1	CB	366	GLN
1	CB	414	HIS
1	CC	44	GLN
1	CC	189	ASN
1	CC	297	HIS
1	DA	167	HIS
1	DA	379	GLN
1	DA	469	GLN

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Mol	Chain	Res	Type
1	DB	302	ASN
1	DB	430	GLN
1	DC	58	GLN
1	DC	189	ASN
1	DC	297	HIS
1	DC	306	GLN
1	DC	357	HIS
1	DC	366	GLN
1	DC	379	GLN
1	DC	501	HIS
1	EA	45	GLN
1	EA	106	GLN
1	EA	331	GLN
1	EA	501	HIS
1	EB	44	GLN
1	EB	46	ASN
1	EB	137	GLN
1	EB	331	GLN
1	EC	44	GLN
1	EC	55	ASN
1	EC	150	GLN
1	EC	401	GLN
1	EC	469	GLN
1	EC	522	ASN
1	FA	44	GLN
1	FA	45	GLN
1	FA	58	GLN
1	FA	366	GLN
1	FB	17	ASN
1	FB	127	ASN
1	FB	170	GLN
1	FB	172	ASN
1	FB	307	ASN
1	FB	309	ASN
1	FB	366	GLN
1	FB	379	GLN
1	FC	23	ASN
1	FC	45	GLN
1	FC	297	HIS
1	GA	414	HIS
1	GA	505	HIS
1	GB	58	GLN

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Mol	Chain	Res	Type
1	GB	277	GLN
1	GB	347	HIS
1	GB	357	HIS
1	GB	417	HIS
1	GC	44	GLN
1	GC	45	GLN
1	GC	263	ASN
1	GC	309	ASN
1	GC	366	GLN
1	GC	417	HIS
1	GC	479	ASN
1	HA	357	HIS
1	HA	379	GLN
1	HA	430	GLN
1	HB	44	GLN
1	HB	58	GLN
1	HB	91	HIS
1	HB	366	GLN
1	HB	417	HIS
1	HB	430	GLN
1	HC	45	GLN
1	HC	190	ASN
1	HC	297	HIS
1	HC	306	GLN
1	HC	309	ASN
1	HC	336	GLN
1	HC	446	ASN
1	IA	45	GLN
1	IA	58	GLN
1	IA	366	GLN
1	IA	396	HIS
1	IB	45	GLN
1	IB	46	ASN
1	IB	414	HIS
1	IC	44	GLN
1	IC	55	ASN
1	IC	106	GLN
1	IC	189	ASN
1	IC	297	HIS
1	IC	366	GLN
1	IC	379	GLN
1	IC	398	ASN

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Mol	Chain	Res	Type
1	IC	417	HIS
1	JA	45	GLN
1	JA	307	ASN
1	JA	366	GLN
1	JA	414	HIS
1	JA	417	HIS
1	JA	463	GLN
1	JB	366	GLN
1	JB	492	HIS
1	JC	44	GLN
1	JC	46	ASN
1	JC	55	ASN
1	JC	106	GLN
1	JC	331	GLN
1	JC	357	HIS
1	KA	58	GLN
1	KA	127	ASN
1	KA	307	ASN
1	KA	331	GLN
1	KA	460	HIS
1	KB	44	GLN
1	KB	54	ASN
1	KB	306	GLN
1	KB	331	GLN
1	KB	357	HIS
1	KB	366	GLN
1	KB	414	HIS
1	KB	492	HIS
1	LA	91	HIS
1	LA	97	ASN
1	LA	106	GLN
1	LA	331	GLN
1	LA	417	HIS
1	LB	44	GLN
1	LB	46	ASN
1	LB	91	HIS
1	LB	347	HIS
1	LB	469	GLN
1	LC	91	HIS
1	LC	302	ASN
1	LC	347	HIS
1	LC	501	HIS

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Mol	Chain	Res	Type
1	MA	58	GLN
1	MA	407	ASN
1	MA	505	HIS
1	MB	309	ASN
1	MB	401	GLN
1	MC	44	GLN
1	MC	55	ASN
1	NA	58	GLN
1	NA	307	ASN
1	NA	417	HIS
1	NB	17	ASN
1	NB	366	GLN
1	NB	396	HIS
1	NB	401	GLN
1	NC	44	GLN
1	NC	55	ASN
1	NC	357	HIS
1	NC	379	GLN
1	NC	501	HIS
1	OA	460	HIS
1	OB	44	GLN
1	OB	46	ASN
1	OB	170	GLN
1	OC	127	ASN
1	OC	190	ASN
1	OC	306	GLN
1	OC	336	GLN
1	OC	357	HIS
1	OC	379	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 73 ligands modelled in this entry, 72 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	JA	601	-	3,3,3	0.46	0	2,2,2	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	JA	601	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	AA	500/540 (92%)	0.02	15 (3%)	52	30	34, 56, 104, 132	0
1	AB	523/540 (96%)	0.05	16 (3%)	51	30	34, 58, 105, 138	0
1	AC	508/540 (94%)	-0.04	14 (2%)	55	32	33, 58, 104, 143	0
1	BA	499/540 (92%)	0.05	17 (3%)	48	27	35, 56, 110, 140	0
1	BB	523/540 (96%)	0.10	23 (4%)	39	21	33, 57, 107, 140	0
1	BC	507/540 (93%)	0.36	35 (6%)	23	12	32, 68, 131, 159	0
1	CA	499/540 (92%)	0.05	14 (2%)	55	32	36, 57, 105, 131	0
1	CB	523/540 (96%)	0.05	17 (3%)	49	28	33, 57, 106, 141	0
1	CC	507/540 (93%)	0.03	12 (2%)	59	36	33, 59, 105, 152	0
1	DA	498/540 (92%)	0.06	15 (3%)	52	30	36, 57, 107, 152	0
1	DB	523/540 (96%)	0.12	20 (3%)	44	24	35, 58, 115, 148	0
1	DC	506/540 (93%)	0.35	25 (4%)	35	18	35, 69, 130, 168	0
1	EA	499/540 (92%)	0.20	20 (4%)	42	23	35, 58, 113, 139	0
1	EB	523/540 (96%)	0.02	14 (2%)	56	33	34, 56, 109, 148	0
1	EC	493/540 (91%)	0.83	105 (21%)	2	1	34, 81, 168, 194	0
1	FA	499/540 (92%)	0.11	15 (3%)	52	30	36, 59, 111, 137	0
1	FB	523/540 (96%)	-0.05	13 (2%)	58	35	32, 54, 101, 132	0
1	FC	509/540 (94%)	0.37	38 (7%)	20	10	34, 74, 127, 175	0
1	GA	499/540 (92%)	-0.04	15 (3%)	52	30	36, 53, 103, 138	0
1	GB	523/540 (96%)	0.10	17 (3%)	49	28	34, 55, 110, 139	0
1	GC	507/540 (93%)	0.04	18 (3%)	46	26	34, 59, 109, 148	0
1	HA	499/540 (92%)	0.07	18 (3%)	46	26	36, 57, 109, 138	0
1	HB	523/540 (96%)	0.04	17 (3%)	49	28	35, 56, 101, 145	0
1	HC	507/540 (93%)	0.19	19 (3%)	45	25	33, 67, 124, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	IA	499/540 (92%)	0.02	14 (2%) 55 32	35, 55, 104, 144	0
1	IB	523/540 (96%)	0.18	32 (6%) 27 14	34, 58, 119, 149	0
1	IC	503/540 (93%)	0.60	59 (11%) 9 5	34, 81, 142, 174	0
1	JA	499/540 (92%)	0.14	17 (3%) 48 27	35, 59, 117, 156	0
1	JB	523/540 (96%)	0.10	22 (4%) 40 22	36, 58, 113, 145	0
1	JC	506/540 (93%)	0.83	116 (22%) 2 1	34, 85, 178, 204	0
1	KA	499/540 (92%)	0.12	19 (3%) 44 24	36, 59, 111, 137	0
1	KB	523/540 (96%)	-0.03	19 (3%) 46 26	35, 55, 106, 144	0
1	KC	507/540 (93%)	0.17	11 (2%) 62 39	34, 67, 123, 145	0
1	LA	499/540 (92%)	0.00	16 (3%) 50 29	36, 56, 102, 151	0
1	LB	523/540 (96%)	0.11	19 (3%) 46 26	31, 58, 118, 142	0
1	LC	502/540 (92%)	0.60	55 (10%) 10 6	35, 81, 137, 167	0
1	MA	499/540 (92%)	0.12	14 (2%) 55 32	34, 59, 111, 143	0
1	MB	523/540 (96%)	-0.06	17 (3%) 49 28	35, 53, 98, 142	0
1	MC	506/540 (93%)	0.33	34 (6%) 24 12	33, 73, 128, 153	0
1	NA	499/540 (92%)	-0.03	15 (3%) 52 30	35, 53, 103, 144	0
1	NB	523/540 (96%)	0.13	22 (4%) 40 22	34, 58, 114, 145	0
1	NC	506/540 (93%)	0.02	14 (2%) 55 32	33, 60, 111, 171	0
1	OA	499/540 (92%)	0.17	25 (5%) 34 18	35, 59, 116, 141	0
1	OB	523/540 (96%)	0.14	24 (4%) 37 20	35, 58, 115, 147	0
1	OC	498/540 (92%)	0.84	108 (21%) 2 1	37, 83, 171, 191	0
All	All	22902/24300 (94%)	0.17	1204 (5%) 32 16	31, 59, 123, 204	0

All (1204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	KC	530	MET	8.7
1	FC	530	MET	8.3
1	EC	530	MET	7.2
1	IC	530	MET	7.2
1	LC	530	MET	7.1
1	HC	530	MET	6.7
1	GB	194	ASP	6.6
1	DA	28	ALA	6.3
1	OC	349	ALA	6.3

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Mol	Chain	Res	Type	RSRZ
1	EC	400	PRO	6.2
1	IB	222	SER	6.1
1	BC	530	MET	5.7
1	OC	332	GLY	5.6
1	OC	400	PRO	5.6
1	EC	349	ALA	5.5
1	LC	528	ALA	5.5
1	LB	308	TRP	5.4
1	JC	382	LYS	5.2
1	EC	347	HIS	5.1
1	HB	308	TRP	5.1
1	JC	349	ALA	5.0
1	OC	412	THR	5.0
1	JC	367	PHE	5.0
1	EC	367	PHE	5.0
1	JC	388	VAL	4.9
1	MA	114	PHE	4.9
1	IA	308	TRP	4.8
1	IC	311	TYR	4.8
1	HA	195	VAL	4.8
1	JC	295	GLY	4.7
1	MB	308	TRP	4.7
1	IB	308	TRP	4.7
1	EC	332	GLY	4.6
1	CC	530	MET	4.6
1	EC	371	THR	4.6
1	OA	114	PHE	4.6
1	GC	530	MET	4.6
1	DC	368	THR	4.5
1	OC	23	ASN	4.5
1	AC	530	MET	4.5
1	HB	219	THR	4.5
1	FC	508	VAL	4.4
1	KC	413	GLY	4.4
1	DA	195	VAL	4.4
1	FC	348	LYS	4.4
1	JC	414	HIS	4.4
1	JC	337	THR	4.4
1	NA	114	PHE	4.3
1	OB	308	TRP	4.3
1	JC	286	PHE	4.3
1	EC	388	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	MA	195	VAL	4.3
1	GC	528	ALA	4.2
1	MB	194	ASP	4.2
1	EC	387	GLY	4.2
1	JC	347	HIS	4.2
1	JC	445	PRO	4.2
1	JC	285	THR	4.2
1	JC	306	GLN	4.2
1	IC	526	THR	4.1
1	GA	195	VAL	4.1
1	NB	194	ASP	4.1
1	JC	440	GLY	4.1
1	JC	333	VAL	4.1
1	GC	306	GLN	4.1
1	IC	400	PRO	4.1
1	EB	194	ASP	4.1
1	KA	195	VAL	4.1
1	GA	399	GLU	4.1
1	HA	114	PHE	4.1
1	EC	294	ALA	4.1
1	EB	308	TRP	4.1
1	IA	114	PHE	4.1
1	FA	188	ALA	4.1
1	OC	508	VAL	4.0
1	EC	286	PHE	4.0
1	CA	195	VAL	4.0
1	KC	440	GLY	4.0
1	CB	195	VAL	4.0
1	JC	348	LYS	4.0
1	EA	188	ALA	4.0
1	IA	195	VAL	4.0
1	LA	306	GLN	4.0
1	AB	308	TRP	3.9
1	AA	114	PHE	3.9
1	JA	114	PHE	3.9
1	LC	348	LYS	3.9
1	NB	308	TRP	3.9
1	CA	399	GLU	3.9
1	HB	393	ASN	3.9
1	NC	311	TYR	3.9
1	NA	399	GLU	3.9
1	OC	291	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	OC	346	GLY	3.9
1	MC	348	LYS	3.9
1	OC	304	ALA	3.9
1	EC	295	GLY	3.9
1	FB	308	TRP	3.9
1	KB	308	TRP	3.9
1	BA	195	VAL	3.8
1	OC	389	VAL	3.8
1	BC	306	GLN	3.8
1	GA	114	PHE	3.8
1	MA	308	TRP	3.8
1	KA	399	GLU	3.8
1	CC	371	THR	3.8
1	IB	219	THR	3.8
1	JC	335	THR	3.8
1	EC	383	PHE	3.8
1	IC	528	ALA	3.8
1	HB	218	PRO	3.8
1	MA	531	GLY	3.8
1	OA	354	GLY	3.8
1	OC	334	LEU	3.8
1	OC	331	GLN	3.8
1	LC	349	ALA	3.8
1	NC	399	GLU	3.8
1	FA	114	PHE	3.8
1	JC	371	THR	3.8
1	NA	371	THR	3.8
1	EC	348	LYS	3.8
1	DA	308	TRP	3.8
1	GB	308	TRP	3.8
1	MB	222	SER	3.8
1	HC	400	PRO	3.8
1	FC	371	THR	3.8
1	JC	284	CYS	3.8
1	FC	23	ASN	3.7
1	JC	386	VAL	3.7
1	LA	195	VAL	3.7
1	JC	387	GLY	3.7
1	EA	114	PHE	3.7
1	JC	383	PHE	3.7
1	GA	28	ALA	3.7
1	KA	306	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	HA	531	GLY	3.7
1	LC	400	PRO	3.7
1	DA	188	ALA	3.7
1	NA	306	GLN	3.7
1	CA	114	PHE	3.7
1	AA	26	VAL	3.7
1	JC	439	PRO	3.7
1	NA	28	ALA	3.7
1	EC	368	THR	3.7
1	BB	94	ARG	3.7
1	EC	297	HIS	3.7
1	IC	407	ASN	3.7
1	GC	313	PRO	3.6
1	EA	195	VAL	3.6
1	FA	28	ALA	3.6
1	EC	330	ILE	3.6
1	OC	348	LYS	3.6
1	EC	414	HIS	3.6
1	OA	195	VAL	3.6
1	JA	399	GLU	3.6
1	OC	413	GLY	3.6
1	JC	351	VAL	3.6
1	JC	399	GLU	3.6
1	EC	435	ARG	3.6
1	JB	308	TRP	3.6
1	IC	529	PRO	3.6
1	AC	409	SER	3.6
1	EA	306	GLN	3.5
1	FA	308	TRP	3.5
1	FC	22	VAL	3.5
1	OC	362	LEU	3.5
1	OC	438	MET	3.5
1	HC	442	SER	3.5
1	EC	413	GLY	3.5
1	OC	347	HIS	3.5
1	FB	195	VAL	3.5
1	NC	313	PRO	3.5
1	JC	362	LEU	3.5
1	JC	438	MET	3.5
1	JC	377	THR	3.5
1	OC	242	PHE	3.5
1	OC	390	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	MC	340	GLY	3.5
1	OC	387	GLY	3.5
1	OC	351	VAL	3.5
1	JA	188	ALA	3.5
1	KB	218	PRO	3.5
1	DB	308	TRP	3.5
1	IC	414	HIS	3.5
1	JA	195	VAL	3.5
1	KA	531	GLY	3.5
1	LC	529	PRO	3.5
1	IB	220	VAL	3.5
1	OC	300	THR	3.5
1	JC	297	HIS	3.5
1	OC	414	HIS	3.5
1	OA	311	TYR	3.4
1	CA	188	ALA	3.4
1	OC	294	ALA	3.4
1	OC	321	LEU	3.4
1	NA	308	TRP	3.4
1	BA	114	PHE	3.4
1	JC	242	PHE	3.4
1	EC	334	LEU	3.4
1	IC	527	LEU	3.4
1	MC	413	GLY	3.4
1	JC	447	MET	3.4
1	NC	529	PRO	3.4
1	FB	399	GLU	3.4
1	KB	399	GLU	3.4
1	OC	367	PHE	3.4
1	NB	440	GLY	3.4
1	DB	532	ASN	3.4
1	NB	10	PRO	3.4
1	EC	351	VAL	3.4
1	JC	408	TYR	3.4
1	AC	495	GLY	3.4
1	FC	412	THR	3.4
1	CC	400	PRO	3.4
1	BA	308	TRP	3.4
1	KA	308	TRP	3.4
1	EC	364	SER	3.4
1	JC	441	CYS	3.4
1	EC	508	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	FC	413	GLY	3.4
1	DC	400	PRO	3.4
1	EB	10	PRO	3.4
1	OC	335	THR	3.4
1	JA	304	ALA	3.3
1	CC	373	ASN	3.3
1	HA	399	GLU	3.3
1	OC	364	SER	3.3
1	BC	440	GLY	3.3
1	EC	395	ALA	3.3
1	JC	294	ALA	3.3
1	OB	194	ASP	3.3
1	AA	414	HIS	3.3
1	BB	10	PRO	3.3
1	DB	10	PRO	3.3
1	EC	331	GLN	3.3
1	JC	526	THR	3.3
1	DA	114	PHE	3.3
1	BB	399	GLU	3.3
1	LA	399	GLU	3.3
1	HA	188	ALA	3.3
1	OB	173	ASP	3.3
1	JC	400	PRO	3.3
1	EC	300	THR	3.3
1	IC	368	THR	3.3
1	JC	331	GLN	3.3
1	MC	371	THR	3.3
1	LA	114	PHE	3.3
1	EC	365	VAL	3.3
1	EA	399	GLU	3.3
1	EC	319	ALA	3.3
1	MA	399	GLU	3.3
1	BA	440	GLY	3.3
1	BC	392	GLY	3.3
1	OC	529	PRO	3.3
1	EC	242	PHE	3.3
1	LC	335	THR	3.3
1	OC	526	THR	3.3
1	JC	508	VAL	3.3
1	LC	389	VAL	3.3
1	OC	373	ASN	3.3
1	AA	188	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	FA	399	GLU	3.3
1	IC	293	ILE	3.3
1	NB	411	ARG	3.2
1	EC	409	SER	3.2
1	OC	286	PHE	3.2
1	EC	293	ILE	3.2
1	MC	447	MET	3.2
1	JC	302	ASN	3.2
1	KA	28	ALA	3.2
1	JC	529	PRO	3.2
1	HC	414	HIS	3.2
1	LC	414	HIS	3.2
1	MC	414	HIS	3.2
1	FC	465	ALA	3.2
1	BC	399	GLU	3.2
1	IA	531	GLY	3.2
1	IA	399	GLU	3.2
1	DC	526	THR	3.2
1	IC	314	THR	3.2
1	LC	377	THR	3.2
1	JB	194	ASP	3.2
1	BC	395	ALA	3.2
1	BB	308	TRP	3.2
1	OC	382	LYS	3.2
1	LB	532	ASN	3.2
1	GB	400	PRO	3.2
1	JC	290	VAL	3.2
1	MC	508	VAL	3.2
1	OC	386	VAL	3.2
1	GA	306	GLN	3.2
1	NC	528	ALA	3.2
1	GA	531	GLY	3.1
1	JC	354	GLY	3.1
1	BC	400	PRO	3.1
1	OC	385	PRO	3.1
1	AA	28	ALA	3.1
1	AC	494	SER	3.1
1	EC	304	ALA	3.1
1	EC	412	THR	3.1
1	MC	349	ALA	3.1
1	KA	114	PHE	3.1
1	DC	529	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	EC	415	ASN	3.1
1	NC	393	ASN	3.1
1	OC	293	ILE	3.1
1	DC	396	HIS	3.1
1	DC	414	HIS	3.1
1	EC	384	THR	3.1
1	OA	308	TRP	3.1
1	CC	399	GLU	3.1
1	JC	385	PRO	3.1
1	AC	23	ASN	3.1
1	DA	306	GLN	3.1
1	EC	335	THR	3.1
1	JC	291	THR	3.1
1	LC	314	THR	3.1
1	OA	531	GLY	3.1
1	EC	327	VAL	3.1
1	IC	257	PHE	3.1
1	JB	399	GLU	3.1
1	MB	399	GLU	3.1
1	DB	441	CYS	3.1
1	NA	311	TYR	3.1
1	FC	373	ASN	3.1
1	AA	304	ALA	3.1
1	EA	28	ALA	3.1
1	JC	528	ALA	3.1
1	IB	306	GLN	3.1
1	LC	336	GLN	3.1
1	NB	306	GLN	3.1
1	EC	369	THR	3.1
1	KB	314	THR	3.1
1	OC	384	THR	3.1
1	LC	508	VAL	3.1
1	OC	290	VAL	3.1
1	IC	348	LYS	3.1
1	FC	400	PRO	3.1
1	IC	427	PRO	3.1
1	LC	526	THR	3.0
1	LB	195	VAL	3.0
1	LC	499	VAL	3.0
1	OC	326	PHE	3.0
1	BA	400	PRO	3.0
1	OB	313	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	MC	341	ASP	3.0
1	NB	173	ASP	3.0
1	GC	311	TYR	3.0
1	JB	311	TYR	3.0
1	BA	188	ALA	3.0
1	DA	304	ALA	3.0
1	IC	294	ALA	3.0
1	KC	373	ASN	3.0
1	EB	412	THR	3.0
1	EC	350	THR	3.0
1	OC	327	VAL	3.0
1	DB	399	GLU	3.0
1	EA	308	TRP	3.0
1	EC	235	GLU	3.0
1	EA	311	TYR	3.0
1	HA	311	TYR	3.0
1	MC	523	GLN	3.0
1	NA	531	GLY	3.0
1	OC	295	GLY	3.0
1	IC	290	VAL	3.0
1	EB	399	GLU	3.0
1	BC	445	PRO	3.0
1	MC	529	PRO	3.0
1	OC	439	PRO	3.0
1	NC	394	SER	3.0
1	NA	188	ALA	3.0
1	OA	304	ALA	3.0
1	LC	374	ASP	3.0
1	AC	414	HIS	3.0
1	AB	440	GLY	3.0
1	IA	306	GLN	3.0
1	HC	393	ASN	3.0
1	MC	373	ASN	3.0
1	JC	300	THR	3.0
1	OC	344	THR	3.0
1	OC	377	THR	3.0
1	LB	348	LYS	3.0
1	AA	195	VAL	3.0
1	DB	413	GLY	3.0
1	NC	306	GLN	3.0
1	AC	371	THR	3.0
1	OC	437	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	AA	308	TRP	2.9
1	AC	399	GLU	2.9
1	GC	304	ALA	2.9
1	KA	188	ALA	2.9
1	LC	319	ALA	2.9
1	MA	28	ALA	2.9
1	OA	188	ALA	2.9
1	LC	311	TYR	2.9
1	BA	354	GLY	2.9
1	BB	194	ASP	2.9
1	FC	410	GLY	2.9
1	JC	365	VAL	2.9
1	NB	414	HIS	2.9
1	OB	195	VAL	2.9
1	OC	388	VAL	2.9
1	JC	289	ASP	2.9
1	OC	401	GLN	2.9
1	OC	415	ASN	2.9
1	OC	287	ARG	2.9
1	GA	308	TRP	2.9
1	GB	10	PRO	2.9
1	JC	304	ALA	2.9
1	BC	444	TYR	2.9
1	FC	394	SER	2.9
1	DB	306	GLN	2.9
1	OB	306	GLN	2.9
1	DC	314	THR	2.9
1	OC	284	CYS	2.9
1	CA	28	ALA	2.9
1	GB	399	GLU	2.9
1	IC	426	PHE	2.9
1	LB	91	HIS	2.9
1	JA	293	ILE	2.9
1	DC	366	GLN	2.9
1	KB	306	GLN	2.9
1	DB	307	ASN	2.9
1	GC	314	THR	2.9
1	GC	529	PRO	2.9
1	JC	446	ASN	2.9
1	LC	395	ALA	2.9
1	OB	399	GLU	2.9
1	IC	508	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	IC	326	PHE	2.9
1	LC	257	PHE	2.9
1	OA	306	GLN	2.9
1	KB	313	PRO	2.9
1	OC	371	THR	2.9
1	EA	441	CYS	2.9
1	JC	389	VAL	2.9
1	BA	311	TYR	2.9
1	FC	340	GLY	2.9
1	IB	311	TYR	2.9
1	AB	348	LYS	2.9
1	IA	305	SER	2.8
1	BB	218	PRO	2.8
1	EB	314	THR	2.8
1	MC	400	PRO	2.8
1	BA	399	GLU	2.8
1	HB	221	GLU	2.8
1	AC	373	ASN	2.8
1	EC	373	ASN	2.8
1	OC	24	ASN	2.8
1	OB	311	TYR	2.8
1	BA	414	HIS	2.8
1	BB	91	HIS	2.8
1	IB	91	HIS	2.8
1	DC	442	SER	2.8
1	JB	331	GLN	2.8
1	MC	409	SER	2.8
1	OC	528	ALA	2.8
1	BA	313	PRO	2.8
1	NB	400	PRO	2.8
1	BB	224	THR	2.8
1	EC	377	THR	2.8
1	GC	308	TRP	2.8
1	EC	346	GLY	2.8
1	OA	257	PHE	2.8
1	OB	91	HIS	2.8
1	GB	306	GLN	2.8
1	CB	411	ARG	2.8
1	DA	399	GLU	2.8
1	EC	248	LYS	2.8
1	LC	399	GLU	2.8
1	MB	219	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	AA	531	GLY	2.8
1	BC	213	ILE	2.8
1	EC	386	VAL	2.8
1	BB	412	THR	2.8
1	LC	527	LEU	2.8
1	AC	213	ILE	2.8
1	CB	308	TRP	2.8
1	FA	173	ASP	2.8
1	NC	308	TRP	2.8
1	AC	413	GLY	2.8
1	MC	440	GLY	2.8
1	FB	532	ASN	2.8
1	JC	282	ASN	2.8
1	JC	484	ARG	2.8
1	EC	401	GLN	2.8
1	BB	313	PRO	2.8
1	JB	195	VAL	2.8
1	DB	412	THR	2.8
1	EA	27	MET	2.7
1	IA	354	GLY	2.7
1	OC	342	GLY	2.7
1	FB	91	HIS	2.7
1	BC	329	LYS	2.7
1	OB	329	LYS	2.7
1	OC	395	ALA	2.7
1	AA	306	GLN	2.7
1	EC	389	VAL	2.7
1	DB	219	THR	2.7
1	HB	399	GLU	2.7
1	KB	222	SER	2.7
1	OC	330	ILE	2.7
1	BB	531	GLY	2.7
1	LC	378	GLY	2.7
1	MC	387	GLY	2.7
1	AC	374	ASP	2.7
1	JC	370	ASP	2.7
1	AB	532	ASN	2.7
1	HB	532	ASN	2.7
1	LC	426	PHE	2.7
1	DC	399	GLU	2.7
1	DC	392	GLY	2.7
1	EA	340	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	OA	314	THR	2.7
1	DB	414	HIS	2.7
1	HC	307	ASN	2.7
1	JC	356	VAL	2.7
1	LC	290	VAL	2.7
1	OC	333	VAL	2.7
1	CB	400	PRO	2.7
1	JB	10	PRO	2.7
1	JC	401	GLN	2.7
1	KB	10	PRO	2.7
1	MA	306	GLN	2.7
1	CA	27	MET	2.7
1	AB	219	THR	2.7
1	FA	348	LYS	2.7
1	KA	305	SER	2.7
1	BC	311	TYR	2.7
1	OC	408	TYR	2.7
1	BC	414	HIS	2.7
1	EC	333	VAL	2.7
1	IC	334	LEU	2.7
1	NA	373	ASN	2.7
1	OC	375	LEU	2.7
1	BA	306	GLN	2.7
1	EC	283	ILE	2.7
1	EC	529	PRO	2.7
1	FC	523	GLN	2.7
1	JB	213	ILE	2.7
1	JB	306	GLN	2.7
1	JC	336	GLN	2.7
1	IB	464	GLU	2.7
1	LB	441	CYS	2.7
1	LC	255	GLY	2.7
1	OC	323	THR	2.7
1	DC	311	TYR	2.7
1	DB	194	ASP	2.7
1	IB	312	ASP	2.7
1	JC	213	ILE	2.6
1	JC	283	ILE	2.6
1	KA	213	ILE	2.6
1	OC	313	PRO	2.6
1	DC	426	PHE	2.6
1	IB	411	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	JC	257	PHE	2.6
1	IB	399	GLU	2.6
1	EC	234	VAL	2.6
1	EC	290	VAL	2.6
1	IC	389	VAL	2.6
1	JC	500	ALA	2.6
1	MB	311	TYR	2.6
1	EC	374	ASP	2.6
1	BC	257	PHE	2.6
1	DA	400	PRO	2.6
1	FC	24	ASN	2.6
1	FC	447	MET	2.6
1	LC	427	PRO	2.6
1	MB	10	PRO	2.6
1	NA	27	MET	2.6
1	OC	383	PHE	2.6
1	GB	413	GLY	2.6
1	OA	413	GLY	2.6
1	MC	399	GLU	2.6
1	EC	451	CYS	2.6
1	EB	191	ALA	2.6
1	IA	304	ALA	2.6
1	OC	303	LEU	2.6
1	JA	311	TYR	2.6
1	BB	411	ARG	2.6
1	JB	411	ARG	2.6
1	HB	400	PRO	2.6
1	OC	324	PRO	2.6
1	OC	306	GLN	2.6
1	JC	381	THR	2.6
1	LA	308	TRP	2.6
1	NB	219	THR	2.6
1	OC	350	THR	2.6
1	EC	329	LYS	2.6
1	BC	442	SER	2.6
1	IA	311	TYR	2.6
1	JC	299	TYR	2.6
1	JC	352	SER	2.6
1	AA	27	MET	2.6
1	OC	504	PRO	2.6
1	DC	306	GLN	2.6
1	DC	393	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	EA	531	GLY	2.6
1	FA	531	GLY	2.6
1	IC	340	GLY	2.6
1	OB	373	ASN	2.6
1	FA	195	VAL	2.6
1	LC	258	VAL	2.6
1	MC	290	VAL	2.6
1	IC	308	TRP	2.6
1	IC	476	ARG	2.6
1	KC	371	THR	2.6
1	JC	244	ILE	2.6
1	EC	311	TYR	2.6
1	EC	357	HIS	2.6
1	FC	347	HIS	2.6
1	OC	297	HIS	2.6
1	BC	529	PRO	2.6
1	OC	436	SER	2.6
1	CB	306	GLN	2.6
1	CC	398	ASN	2.6
1	HB	391	ASP	2.6
1	IC	375	LEU	2.6
1	LC	452	LEU	2.6
1	OC	405	LEU	2.6
1	BA	28	ALA	2.6
1	EC	382	LYS	2.6
1	IB	223	ARG	2.6
1	IC	333	VAL	2.6
1	JC	330	ILE	2.5
1	LC	396	HIS	2.5
1	EC	318	PRO	2.5
1	HA	400	PRO	2.5
1	LA	400	PRO	2.5
1	AA	340	GLY	2.5
1	EC	306	GLN	2.5
1	OC	410	GLY	2.5
1	EC	375	LEU	2.5
1	JC	334	LEU	2.5
1	HC	373	ASN	2.5
1	IB	24	ASN	2.5
1	IC	372	ASN	2.5
1	JA	348	LYS	2.5
1	JC	327	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	JC	516	ARG	2.5
1	IC	256	ALA	2.5
1	FA	283	ILE	2.5
1	JC	384	THR	2.5
1	OC	213	ILE	2.5
1	FB	400	PRO	2.5
1	EC	362	LEU	2.5
1	IC	416	VAL	2.5
1	JC	234	VAL	2.5
1	JC	416	VAL	2.5
1	CB	194	ASP	2.5
1	EB	307	ASN	2.5
1	IC	415	ASN	2.5
1	JC	415	ASN	2.5
1	LA	188	ALA	2.5
1	LA	307	ASN	2.5
1	OA	399	GLU	2.5
1	DA	314	THR	2.5
1	EC	296	THR	2.5
1	IB	530	MET	2.5
1	LB	314	THR	2.5
1	OC	368	THR	2.5
1	DA	311	TYR	2.5
1	OC	318	PRO	2.5
1	BC	378	GLY	2.5
1	JA	306	GLN	2.5
1	NB	11	SER	2.5
1	OC	485	VAL	2.5
1	FC	395	ALA	2.5
1	KC	399	GLU	2.5
1	EC	23	ASN	2.5
1	EC	302	ASN	2.5
1	GA	312	ASP	2.5
1	LA	283	ILE	2.5
1	NB	193	ASP	2.5
1	OB	302	ASN	2.5
1	BA	27	MET	2.5
1	DB	314	THR	2.5
1	JA	308	TRP	2.5
1	JC	323	THR	2.5
1	MC	412	THR	2.5
1	BB	400	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	LC	313	PRO	2.5
1	OC	329	LYS	2.5
1	JC	392	GLY	2.5
1	IC	283	ILE	2.5
1	EC	298	ASP	2.5
1	NC	312	ASP	2.5
1	IB	291	THR	2.5
1	MB	223	ARG	2.5
1	OB	223	ARG	2.5
1	DB	400	PRO	2.5
1	GB	218	PRO	2.5
1	HC	529	PRO	2.5
1	CA	414	HIS	2.5
1	OC	264	GLY	2.5
1	IC	258	VAL	2.5
1	EC	390	GLN	2.5
1	MC	306	GLN	2.5
1	KA	284	CYS	2.4
1	JC	247	GLU	2.4
1	FB	257	PHE	2.4
1	HA	391	ASP	2.4
1	JC	369	THR	2.4
1	KC	370	ASP	2.4
1	NB	373	ASN	2.4
1	IB	224	THR	2.4
1	OC	370	ASP	2.4
1	EC	324	PRO	2.4
1	NA	400	PRO	2.4
1	OB	400	PRO	2.4
1	GA	414	HIS	2.4
1	IC	356	VAL	2.4
1	OC	274	GLY	2.4
1	OC	319	ALA	2.4
1	LA	530	MET	2.4
1	FB	21	GLU	2.4
1	KB	394	SER	2.4
1	DC	412	THR	2.4
1	FA	314	THR	2.4
1	GB	219	THR	2.4
1	BC	297	HIS	2.4
1	KB	91	HIS	2.4
1	HC	306	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	IB	213	ILE	2.4
1	IC	402	GLN	2.4
1	JC	397	GLN	2.4
1	OA	530	MET	2.4
1	NB	329	LYS	2.4
1	GC	399	GLU	2.4
1	HC	399	GLU	2.4
1	OB	222	SER	2.4
1	EC	285	THR	2.4
1	FA	400	PRO	2.4
1	OC	296	THR	2.4
1	EC	289	ASP	2.4
1	GA	173	ASP	2.4
1	CA	531	GLY	2.4
1	DB	311	TYR	2.4
1	EC	328	GLY	2.4
1	GB	311	TYR	2.4
1	JC	332	GLY	2.4
1	KA	354	GLY	2.4
1	LC	346	GLY	2.4
1	LC	392	GLY	2.4
1	DC	294	ALA	2.4
1	EC	213	ILE	2.4
1	FC	283	ILE	2.4
1	HA	283	ILE	2.4
1	CB	469	GLN	2.4
1	EC	366	GLN	2.4
1	LA	27	MET	2.4
1	FC	257	PHE	2.4
1	CB	399	GLU	2.4
1	DB	464	GLU	2.4
1	GC	305	SER	2.4
1	CC	508	VAL	2.4
1	IB	400	PRO	2.4
1	IB	412	THR	2.4
1	IC	425	THR	2.4
1	MB	224	THR	2.4
1	MB	24	ASN	2.4
1	DC	370	ASP	2.4
1	IC	312	ASP	2.4
1	JB	193	ASP	2.4
1	JC	357	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	OA	357	HIS	2.4
1	OC	357	HIS	2.4
1	BC	528	ALA	2.4
1	AA	382	LYS	2.4
1	GA	187	ARG	2.4
1	JA	530	MET	2.4
1	JC	345	ARG	2.4
1	OA	27	MET	2.4
1	CC	523	GLN	2.4
1	CB	222	SER	2.4
1	HA	308	TRP	2.4
1	JC	324	PRO	2.4
1	OC	416	VAL	2.4
1	DA	531	GLY	2.3
1	HB	13	GLY	2.3
1	JB	219	THR	2.3
1	JB	412	THR	2.3
1	IB	294	ALA	2.3
1	MA	414	HIS	2.3
1	OC	325	ASP	2.3
1	EC	303	LEU	2.3
1	AB	10	PRO	2.3
1	BB	222	SER	2.3
1	CB	10	PRO	2.3
1	JA	400	PRO	2.3
1	NC	400	PRO	2.3
1	OC	243	PRO	2.3
1	BB	425	THR	2.3
1	CB	371	THR	2.3
1	EC	340	GLY	2.3
1	FA	342	GLY	2.3
1	GB	371	THR	2.3
1	JC	322	GLY	2.3
1	KA	340	GLY	2.3
1	EA	304	ALA	2.3
1	GB	284	CYS	2.3
1	HB	414	HIS	2.3
1	KB	393	ASN	2.3
1	LC	310	ASN	2.3
1	JC	375	LEU	2.3
1	LB	399	GLU	2.3
1	LB	464	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	NB	464	GLU	2.3
1	OC	399	GLU	2.3
1	EA	225	LYS	2.3
1	EA	354	GLY	2.3
1	BC	294	ALA	2.3
1	FC	442	SER	2.3
1	JC	410	GLY	2.3
1	JC	314	THR	2.3
1	NB	442	SER	2.3
1	CC	414	HIS	2.3
1	EA	414	HIS	2.3
1	FC	297	HIS	2.3
1	HA	27	MET	2.3
1	JC	301	MET	2.3
1	OA	414	HIS	2.3
1	OC	257	PHE	2.3
1	AB	193	ASP	2.3
1	CB	173	ASP	2.3
1	NB	298	ASP	2.3
1	OA	312	ASP	2.3
1	OC	374	ASP	2.3
1	EC	399	GLU	2.3
1	LC	247	GLU	2.3
1	EC	356	VAL	2.3
1	HB	348	LYS	2.3
1	JB	348	LYS	2.3
1	MA	348	LYS	2.3
1	AB	313	PRO	2.3
1	DC	313	PRO	2.3
1	EA	400	PRO	2.3
1	IB	10	PRO	2.3
1	JB	43	GLY	2.3
1	LB	295	GLY	2.3
1	MA	295	GLY	2.3
1	DC	395	ALA	2.3
1	LA	28	ALA	2.3
1	LC	291	THR	2.3
1	AB	414	HIS	2.3
1	OC	352	SER	2.3
1	IC	278	LEU	2.3
1	JC	246	LEU	2.3
1	OC	486	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	EC	299	TYR	2.3
1	IB	257	PHE	2.3
1	BB	532	ASN	2.3
1	EC	310	ASN	2.3
1	FC	302	ASN	2.3
1	FC	372	ASN	2.3
1	BA	225	LYS	2.3
1	LB	329	LYS	2.3
1	AB	399	GLU	2.3
1	LC	333	VAL	2.3
1	CA	400	PRO	2.3
1	EB	400	PRO	2.3
1	FB	10	PRO	2.3
1	FC	509	ILE	2.3
1	EC	392	GLY	2.3
1	EC	501	HIS	2.3
1	GA	371	THR	2.3
1	HC	371	THR	2.3
1	IC	291	THR	2.3
1	IC	335	THR	2.3
1	JC	412	THR	2.3
1	KA	412	THR	2.3
1	LB	219	THR	2.3
1	FB	494	SER	2.3
1	MB	257	PHE	2.3
1	OB	257	PHE	2.3
1	IB	532	ASN	2.3
1	BC	523	GLN	2.3
1	DA	225	LYS	2.3
1	EC	284	CYS	2.3
1	NB	372	ASN	2.3
1	EA	173	ASP	2.3
1	FC	193	ASP	2.3
1	GA	400	PRO	2.2
1	AA	530	MET	2.2
1	AC	392	GLY	2.2
1	AC	400	PRO	2.2
1	NA	313	PRO	2.2
1	GA	188	ALA	2.2
1	JC	395	ALA	2.2
1	BC	527	LEU	2.2
1	BA	314	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	FB	371	THR	2.2
1	IC	219	THR	2.2
1	IC	477	PHE	2.2
1	JC	326	PHE	2.2
1	LC	326	PHE	2.2
1	BC	348	LYS	2.2
1	EC	408	TYR	2.2
1	NC	305	SER	2.2
1	EC	516	ARG	2.2
1	CB	307	ASN	2.2
1	HA	306	GLN	2.2
1	IC	365	VAL	2.2
1	JC	373	ASN	2.2
1	OC	234	VAL	2.2
1	OC	302	ASN	2.2
1	IB	193	ASP	2.2
1	IC	370	ASP	2.2
1	KB	194	ASP	2.2
1	CA	213	ILE	2.2
1	OC	283	ILE	2.2
1	CA	354	GLY	2.2
1	DB	378	GLY	2.2
1	FC	346	GLY	2.2
1	FC	387	GLY	2.2
1	GB	304	ALA	2.2
1	HC	255	GLY	2.2
1	KC	400	PRO	2.2
1	LA	313	PRO	2.2
1	JC	308	TRP	2.2
1	CB	412	THR	2.2
1	EC	344	THR	2.2
1	EC	482	THR	2.2
1	FC	337	THR	2.2
1	GA	225	LYS	2.2
1	KA	414	HIS	2.2
1	MC	297	HIS	2.2
1	EC	287	ARG	2.2
1	LC	442	SER	2.2
1	BC	389	VAL	2.2
1	FC	258	VAL	2.2
1	HB	195	VAL	2.2
1	DC	523	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	IC	523	GLN	2.2
1	BC	398	ASN	2.2
1	EC	25	GLU	2.2
1	DC	427	PRO	2.2
1	EC	301	MET	2.2
1	FA	354	GLY	2.2
1	HA	530	MET	2.2
1	KA	27	MET	2.2
1	KB	391	ASP	2.2
1	IC	288	GLY	2.2
1	KA	400	PRO	2.2
1	LC	294	ALA	2.2
1	HC	329	LYS	2.2
1	HB	223	ARG	2.2
1	OC	411	ARG	2.2
1	BB	314	THR	2.2
1	BC	314	THR	2.2
1	FC	414	HIS	2.2
1	KB	311	TYR	2.2
1	CA	306	GLN	2.2
1	GC	523	GLN	2.2
1	JC	366	GLN	2.2
1	JC	523	GLN	2.2
1	LB	331	GLN	2.2
1	FC	330	ILE	2.2
1	KA	283	ILE	2.2
1	LA	213	ILE	2.2
1	CB	373	ASN	2.2
1	IC	446	ASN	2.2
1	JC	372	ASN	2.2
1	CC	178	LEU	2.2
1	OC	235	GLU	2.2
1	EC	342	GLY	2.2
1	OB	110	ALA	2.2
1	BC	370	ASP	2.2
1	MB	193	ASP	2.2
1	MC	329	LYS	2.2
1	OB	193	ASP	2.2
1	CC	426	PHE	2.2
1	OC	345	ARG	2.2
1	AB	412	THR	2.2
1	GC	371	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	JA	314	THR	2.2
1	JC	296	THR	2.2
1	MA	437	THR	2.2
1	MC	357	HIS	2.2
1	NB	297	HIS	2.2
1	OC	365	VAL	2.2
1	CC	394	SER	2.2
1	EA	283	ILE	2.2
1	LC	213	ILE	2.2
1	IC	303	LEU	2.2
1	JC	527	LEU	2.2
1	IA	530	MET	2.2
1	JB	329	LYS	2.2
1	LC	522	ASN	2.2
1	MC	24	ASN	2.2
1	AB	400	PRO	2.2
1	EC	274	GLY	2.2
1	GC	392	GLY	2.2
1	JB	400	PRO	2.2
1	OC	511	PRO	2.2
1	CB	94	ARG	2.2
1	BB	391	ASP	2.2
1	HB	284	CYS	2.2
1	NB	370	ASP	2.2
1	CA	308	TRP	2.2
1	MB	91	HIS	2.2
1	MB	195	VAL	2.1
1	NB	296	THR	2.1
1	JC	311	TYR	2.1
1	LA	311	TYR	2.1
1	MC	283	ILE	2.1
1	OA	293	ILE	2.1
1	AB	44	GLN	2.1
1	DC	527	LEU	2.1
1	EB	44	GLN	2.1
1	FC	362	LEU	2.1
1	IA	28	ALA	2.1
1	IC	399	GLU	2.1
1	EB	531	GLY	2.1
1	HA	392	GLY	2.1
1	LC	440	GLY	2.1
1	MA	354	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	DA	307	ASN	2.1
1	EC	398	ASN	2.1
1	FC	310	ASN	2.1
1	KB	373	ASN	2.1
1	HA	257	PHE	2.1
1	HC	524	PHE	2.1
1	JC	426	PHE	2.1
1	JC	391	ASP	2.1
1	OC	341	ASP	2.1
1	BC	396	HIS	2.1
1	IA	414	HIS	2.1
1	JA	414	HIS	2.1
1	EB	219	THR	2.1
1	KC	412	THR	2.1
1	NC	314	THR	2.1
1	OA	296	THR	2.1
1	OC	509	ILE	2.1
1	AB	329	LYS	2.1
1	HA	329	LYS	2.1
1	DB	277	GLN	2.1
1	CA	304	ALA	2.1
1	EC	339	ARG	2.1
1	MC	331	GLN	2.1
1	NA	150	GLN	2.1
1	BC	364	SER	2.1
1	EB	305	SER	2.1
1	FC	494	SER	2.1
1	JA	354	GLY	2.1
1	JC	364	SER	2.1
1	MB	221	GLU	2.1
1	MC	378	GLY	2.1
1	OB	392	GLY	2.1
1	OB	464	GLU	2.1
1	OC	360	PRO	2.1
1	DC	257	PHE	2.1
1	HB	257	PHE	2.1
1	IB	307	ASN	2.1
1	LC	286	PHE	2.1
1	LC	433	PHE	2.1
1	MB	532	ASN	2.1
1	BB	173	ASP	2.1
1	DC	391	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	HB	12	ASP	2.1
1	JC	325	ASP	2.1
1	OC	308	TRP	2.1
1	IB	297	HIS	2.1
1	LB	414	HIS	2.1
1	IC	377	THR	2.1
1	JC	338	THR	2.1
1	LC	321	LEU	2.1
1	JC	256	ALA	2.1
1	KC	304	ALA	2.1
1	FA	313	PRO	2.1
1	IC	513	GLY	2.1
1	JC	413	GLY	2.1
1	MC	445	PRO	2.1
1	NB	399	GLU	2.1
1	OC	322	GLY	2.1
1	OC	406	PRO	2.1
1	DB	257	PHE	2.1
1	IC	487	PHE	2.1
1	BC	446	ASN	2.1
1	HC	522	ASN	2.1
1	IA	307	ASN	2.1
1	KB	532	ASN	2.1
1	LC	415	ASN	2.1
1	OC	404	VAL	2.1
1	EC	405	LEU	2.1
1	FC	357	HIS	2.1
1	GB	193	ASP	2.1
1	JA	347	HIS	2.1
1	LC	391	ASP	2.1
1	MC	248	LYS	2.1
1	MC	347	HIS	2.1
1	AB	314	THR	2.1
1	BC	296	THR	2.1
1	EC	397	GLN	2.1
1	IC	264	GLY	2.1
1	OA	342	GLY	2.1
1	GB	464	GLU	2.1
1	IC	242	PHE	2.1
1	KC	257	PHE	2.1
1	JC	436	SER	2.1
1	MA	494	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	OB	305	SER	2.1
1	EB	195	VAL	2.1
1	FB	24	ASN	2.1
1	FC	329	LYS	2.1
1	GB	532	ASN	2.1
1	KB	307	ASN	2.1
1	LC	329	LYS	2.1
1	LC	393	ASN	2.1
1	MB	373	ASN	2.1
1	MC	307	ASN	2.1
1	OB	24	ASN	2.1
1	BC	505	HIS	2.1
1	EC	403	TRP	2.1
1	HA	414	HIS	2.1
1	IB	94	ARG	2.1
1	IC	292	HIS	2.1
1	IC	297	HIS	2.1
1	JA	357	HIS	2.1
1	JC	287	ARG	2.1
1	LB	265	ARG	2.1
1	MC	308	TRP	2.1
1	AB	173	ASP	2.1
1	BB	312	ASP	2.1
1	EC	370	ASP	2.1
1	HC	312	ASP	2.1
1	BC	526	THR	2.1
1	EC	291	THR	2.1
1	HC	441	CYS	2.1
1	LA	284	CYS	2.1
1	LB	291	THR	2.1
1	LC	482	THR	2.1
1	IB	304	ALA	2.1
1	BA	392	GLY	2.1
1	BB	306	GLN	2.1
1	DA	340	GLY	2.1
1	JC	288	GLY	2.1
1	JC	342	GLY	2.1
1	EA	313	PRO	2.1
1	EC	313	PRO	2.1
1	IC	324	PRO	2.1
1	IB	195	VAL	2.0
1	JC	329	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	JB	394	SER	2.0
1	LB	14	SER	2.0
1	BC	307	ASN	2.0
1	BC	411	ARG	2.0
1	GC	307	ASN	2.0
1	LC	263	ASN	2.0
1	DB	347	HIS	2.0
1	EC	417	HIS	2.0
1	GB	91	HIS	2.0
1	IB	414	HIS	2.0
1	FB	412	THR	2.0
1	IB	374	ASP	2.0
1	KB	219	THR	2.0
1	LC	256	ALA	2.0
1	MA	188	ALA	2.0
1	MC	370	ASP	2.0
1	NC	304	ALA	2.0
1	EC	495	GLY	2.0
1	IC	332	GLY	2.0
1	IC	401	GLN	2.0
1	GC	400	PRO	2.0
1	JC	60	PRO	2.0
1	LB	313	PRO	2.0
1	LB	400	PRO	2.0
1	OA	313	PRO	2.0
1	OA	400	PRO	2.0
1	OB	10	PRO	2.0
1	BB	464	GLU	2.0
1	OA	348	LYS	2.0
1	EC	321	LEU	2.0
1	JB	94	ARG	2.0
1	JC	321	LEU	2.0
1	KB	411	ARG	2.0
1	OC	484	ARG	2.0
1	HC	213	ILE	2.0
1	JC	409	SER	2.0
1	GC	24	ASN	2.0
1	EC	308	TRP	2.0
1	NA	530	MET	2.0
1	GC	377	THR	2.0
1	HC	304	ALA	2.0
1	JC	344	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	KA	335	THR	2.0
1	LC	304	ALA	2.0
1	MC	314	THR	2.0
1	OA	294	ALA	2.0
1	IB	194	ASP	2.0
1	LC	289	ASP	2.0
1	CB	413	GLY	2.0
1	EC	354	GLY	2.0
1	HA	354	GLY	2.0
1	JB	257	PHE	2.0
1	JC	255	GLY	2.0
1	JB	313	PRO	2.0
1	JB	21	GLU	2.0
1	JC	404	VAL	2.0
1	OB	287	ARG	2.0
1	OC	258	VAL	2.0
1	OC	464	GLU	2.0
1	AA	283	ILE	2.0
1	BB	213	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	JA	601	4/4	0.73	0.20	69,69,69,69	0
2	CL	JA	604	1/1	0.83	0.24	82,82,82,82	0
2	CL	KC	602	1/1	0.85	0.11	74,74,74,74	0
3	CD	GB	601	1/1	0.86	0.09	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	CC	602	1/1	0.87	0.27	95,95,95,95	0
3	CD	EA	601	1/1	0.88	0.10	144,144,144,144	0
2	CL	AA	603	1/1	0.88	0.17	77,77,77,77	0
2	CL	MA	604	1/1	0.88	0.18	76,76,76,76	0
3	CD	MB	601	1/1	0.89	0.08	140,140,140,140	0
3	CD	KA	601	1/1	0.90	0.08	142,142,142,142	0
3	CD	MA	601	1/1	0.91	0.09	138,138,138,138	0
2	CL	IA	603	1/1	0.92	0.16	78,78,78,78	0
2	CL	DC	601	1/1	0.92	0.23	56,56,56,56	0
3	CD	BA	601	1/1	0.92	0.08	142,142,142,142	0
3	CD	DA	601	1/1	0.93	0.10	136,136,136,136	0
3	CD	IA	601	1/1	0.93	0.07	135,135,135,135	0
2	CL	CC	601	1/1	0.93	0.16	56,56,56,56	0
2	CL	NC	602	1/1	0.94	0.10	68,68,68,68	0
2	CL	LC	601	1/1	0.94	0.18	59,59,59,59	0
3	CD	JA	602	1/1	0.94	0.11	136,136,136,136	0
2	CL	KA	603	1/1	0.94	0.21	76,76,76,76	0
2	CL	MC	601	1/1	0.94	0.23	54,54,54,54	0
3	CD	EB	601	1/1	0.94	0.06	133,133,133,133	0
3	CD	OA	601	1/1	0.94	0.08	139,139,139,139	0
3	CD	FA	601	1/1	0.94	0.07	134,134,134,134	0
2	CL	LA	601	1/1	0.95	0.13	49,49,49,49	0
2	CL	AC	602	1/1	0.95	0.11	76,76,76,76	0
2	CL	CC	603	1/1	0.95	0.15	79,79,79,79	0
2	CL	AB	601	1/1	0.95	0.09	67,67,67,67	0
2	CL	GC	601	1/1	0.95	0.26	63,63,63,63	0
3	CD	GA	601	1/1	0.95	0.05	127,127,127,127	0
3	CD	AC	601	1/1	0.95	0.06	121,121,121,121	0
3	CD	HC	601	1/1	0.96	0.06	127,127,127,127	0
2	CL	KA	602	1/1	0.96	0.20	48,48,48,48	0
2	CL	DB	601	1/1	0.96	0.07	65,65,65,65	0
2	CL	BC	602	1/1	0.96	0.21	55,55,55,55	0
3	CD	EC	601	1/1	0.96	0.19	195,195,195,195	0
2	CL	EA	603	1/1	0.96	0.28	80,80,80,80	0
3	CD	NC	601	1/1	0.96	0.06	128,128,128,128	0
2	CL	JA	605	1/1	0.96	0.17	44,44,44,44	0
3	CD	BC	601	1/1	0.96	0.04	127,127,127,127	0
2	CL	EA	604	1/1	0.97	0.17	46,46,46,46	0
2	CL	OA	603	1/1	0.97	0.16	47,47,47,47	0
3	CD	JC	601	1/1	0.97	0.14	176,176,176,176	0
2	CL	GC	602	1/1	0.97	0.19	46,46,46,46	0
3	CD	KB	601	1/1	0.97	0.04	138,138,138,138	0

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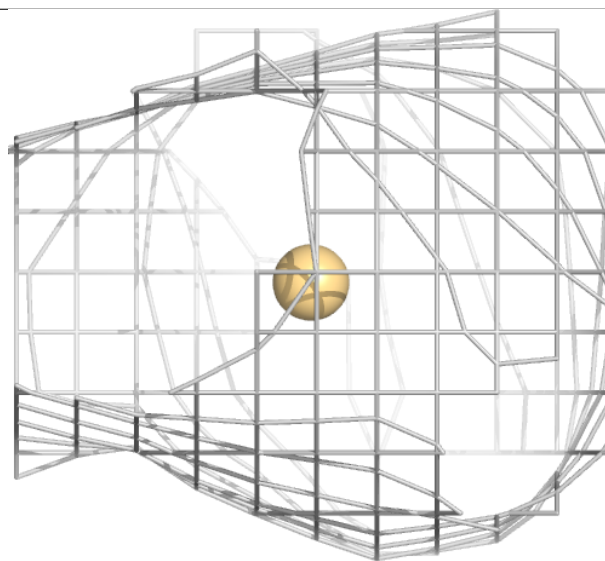
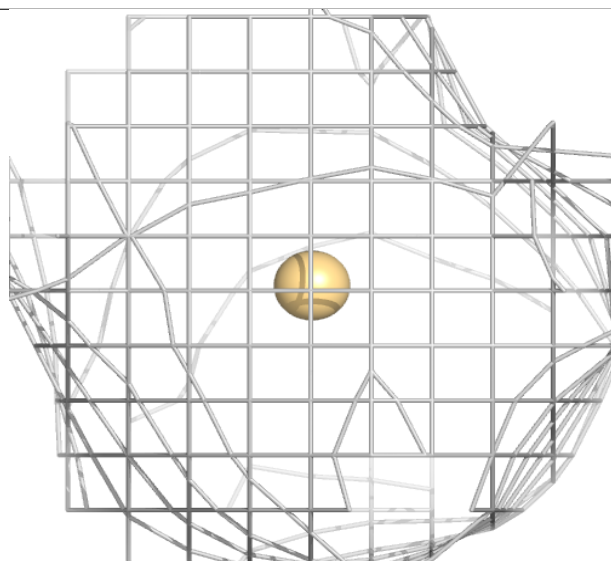
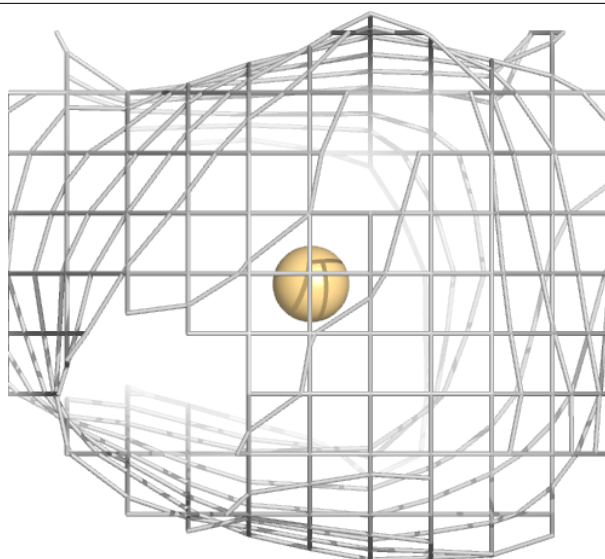
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	KC	601	1/1	0.97	0.12	42,42,42,42	0
3	CD	FC	601	1/1	0.97	0.04	127,127,127,127	0
2	CL	HA	601	1/1	0.97	0.21	48,48,48,48	0
3	CD	CA	601	1/1	0.97	0.08	136,136,136,136	0
2	CL	MC	602	1/1	0.97	0.17	58,58,58,58	0
2	CL	CA	602	1/1	0.98	0.15	42,42,42,42	0
2	CL	JA	603	1/1	0.98	0.18	51,51,51,51	0
2	CL	NA	601	1/1	0.98	0.14	37,37,37,37	0
2	CL	NA	602	1/1	0.98	0.19	42,42,42,42	0
2	CL	EA	602	1/1	0.98	0.15	50,50,50,50	0
2	CL	OA	602	1/1	0.98	0.22	50,50,50,50	0
2	CL	CA	603	1/1	0.98	0.16	44,44,44,44	0
2	CL	AA	601	1/1	0.98	0.21	49,49,49,49	0
2	CL	FA	603	1/1	0.98	0.16	47,47,47,47	0
2	CL	BA	602	1/1	0.98	0.19	45,45,45,45	0
2	CL	BA	603	1/1	0.98	0.16	48,48,48,48	0
2	CL	AA	602	1/1	0.98	0.13	43,43,43,43	0
2	CL	HC	602	1/1	0.98	0.18	45,45,45,45	0
2	CL	LC	602	1/1	0.98	0.13	40,40,40,40	0
2	CL	IA	602	1/1	0.98	0.19	47,47,47,47	0
2	CL	FA	602	1/1	0.99	0.15	42,42,42,42	0
2	CL	IA	604	1/1	0.99	0.15	41,41,41,41	0
2	CL	MA	602	1/1	0.99	0.14	41,41,41,41	0
2	CL	MA	603	1/1	0.99	0.18	50,50,50,50	0
2	CL	DC	602	1/1	0.99	0.15	44,44,44,44	0
2	CL	GA	602	1/1	0.99	0.22	41,41,41,41	0
2	CL	DA	602	1/1	0.99	0.21	48,48,48,48	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

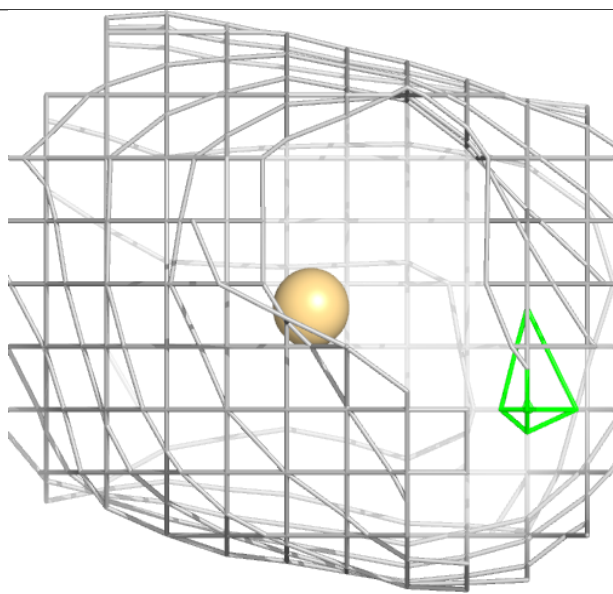
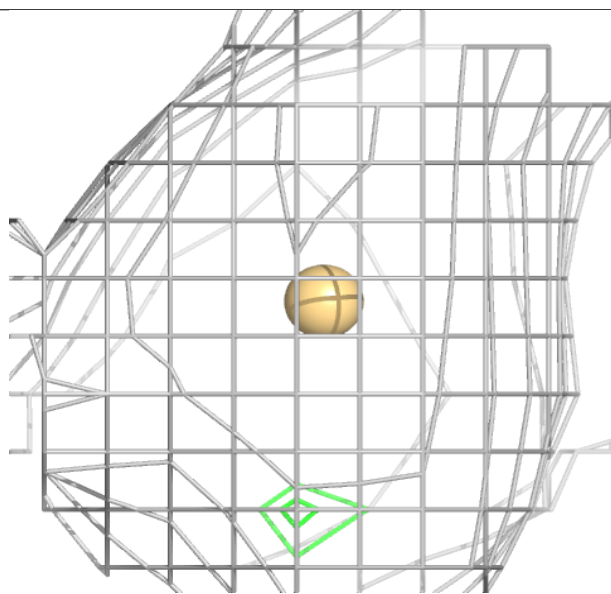
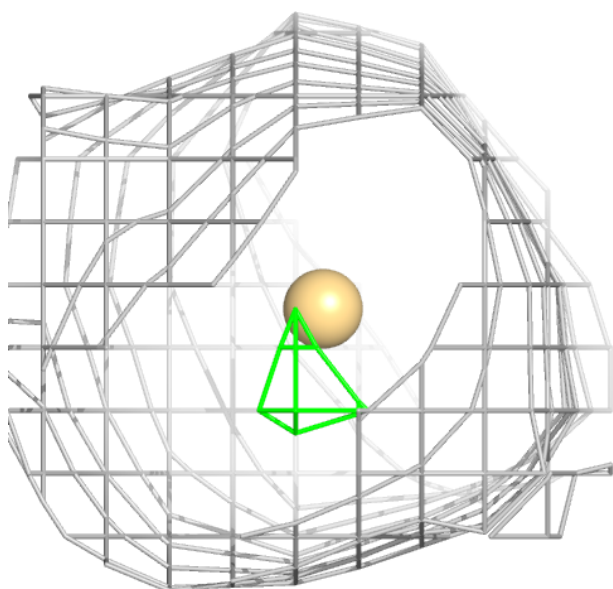
Electron density around CD GB 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



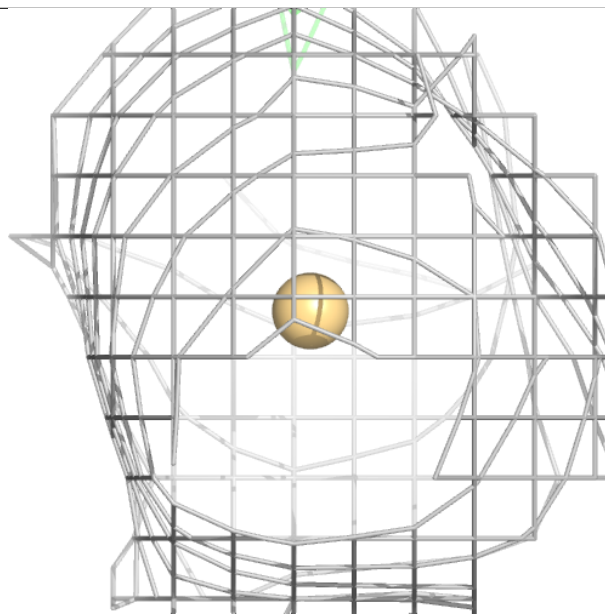
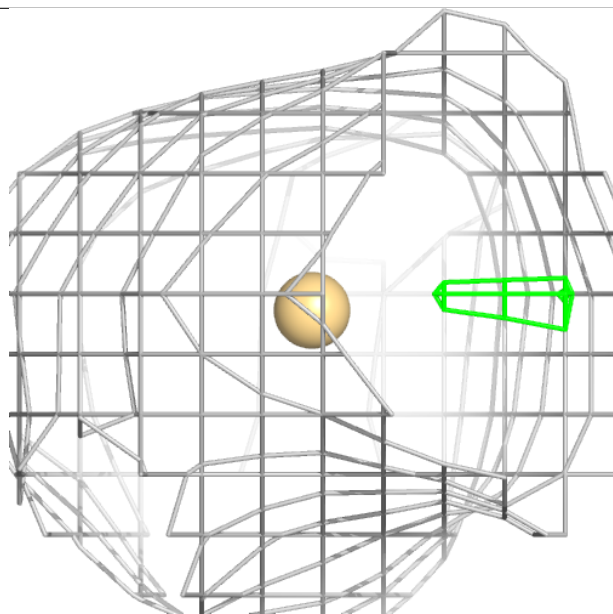
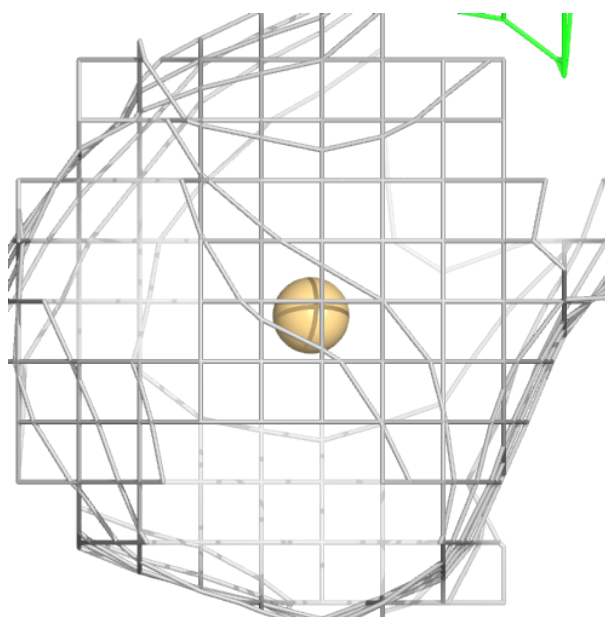
Electron density around CD EA 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



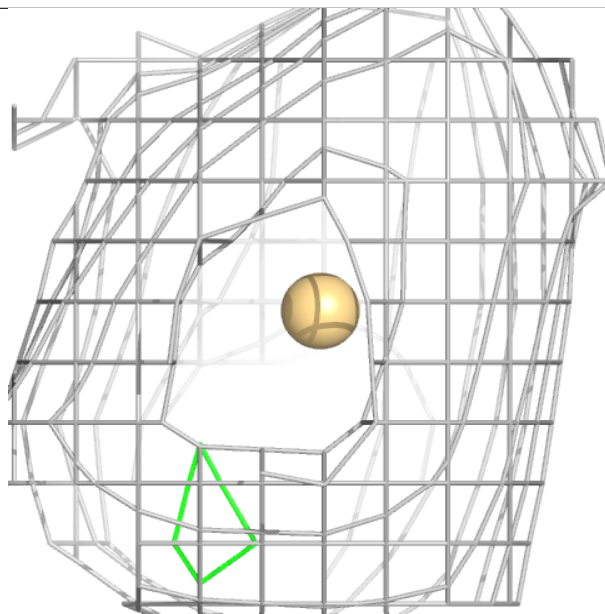
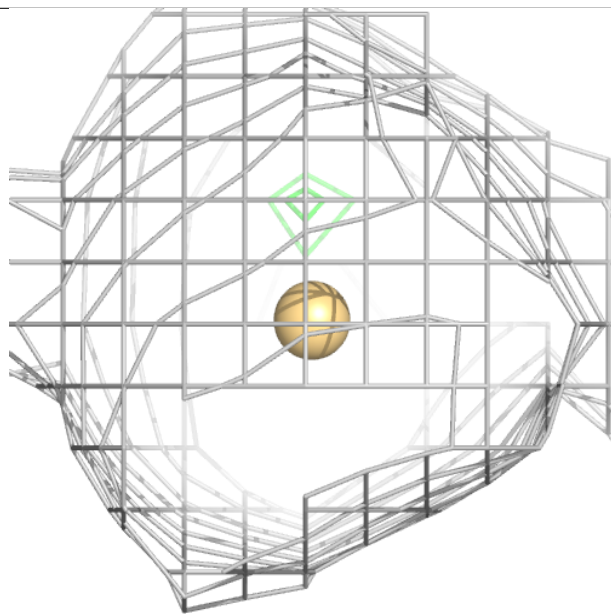
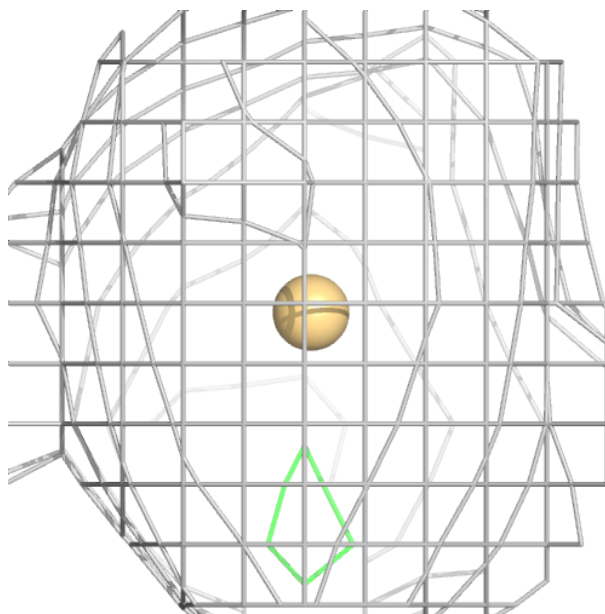
Electron density around CD MB 601:

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and green (positive)



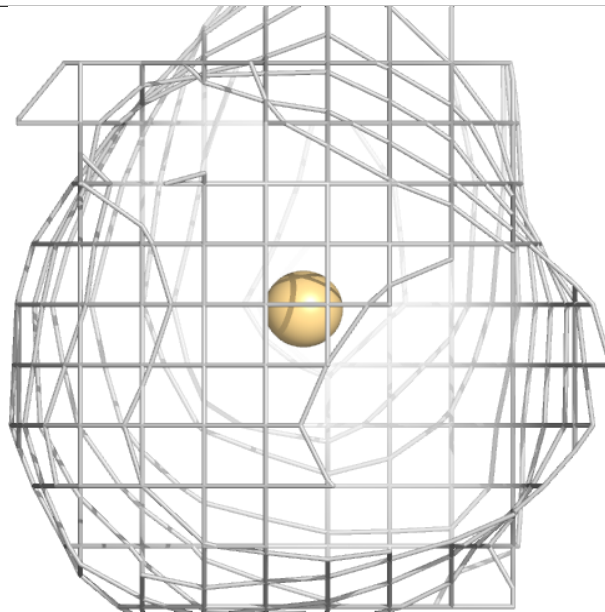
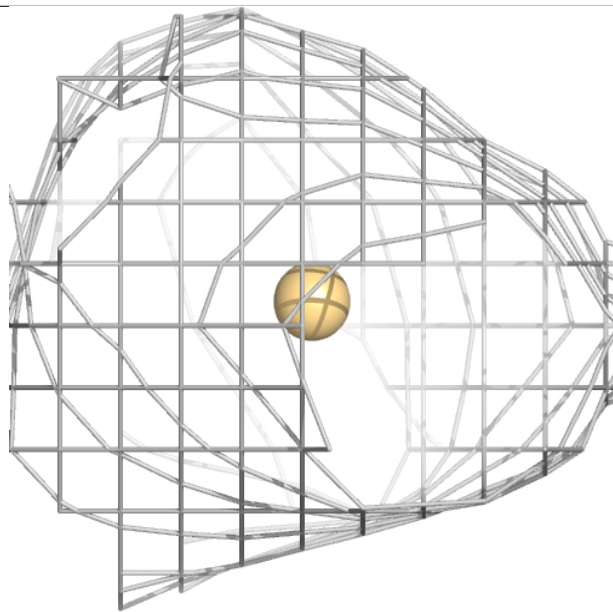
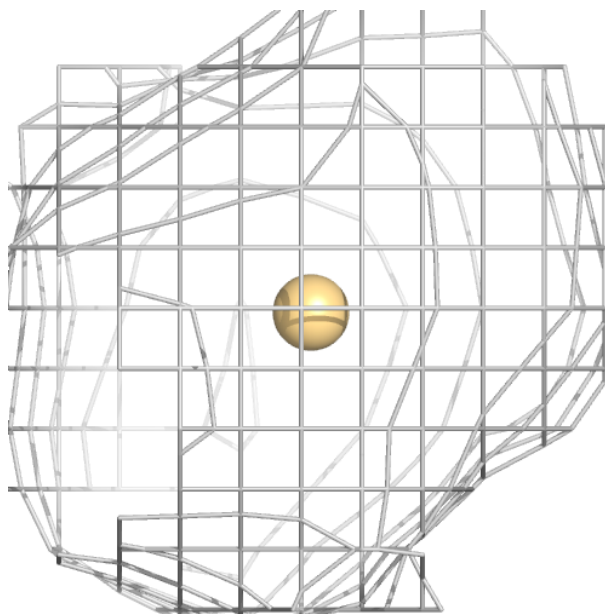
Electron density around CD KA 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



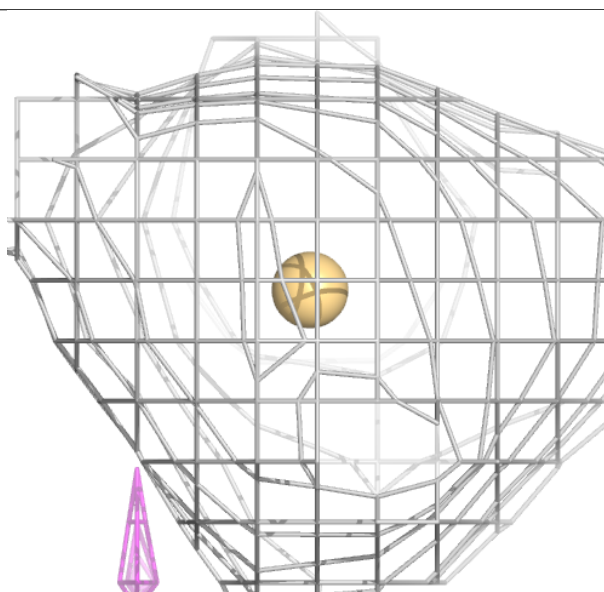
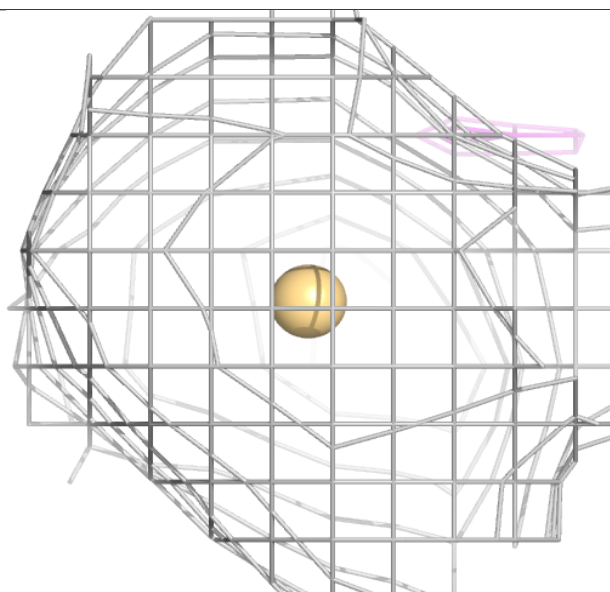
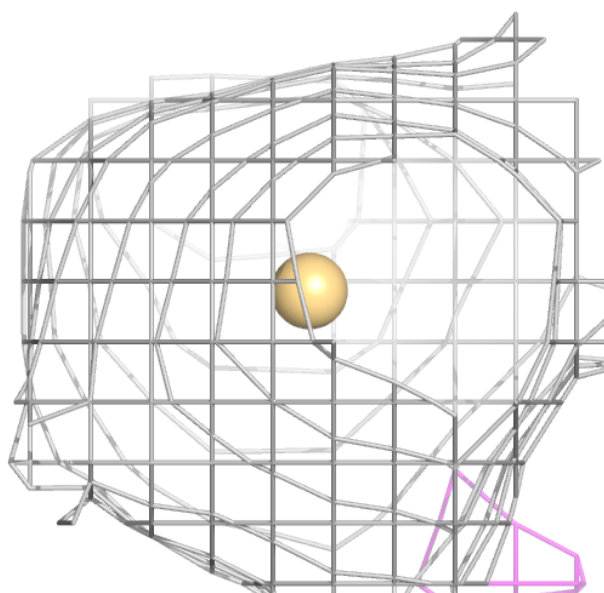
Electron density around CD MA 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



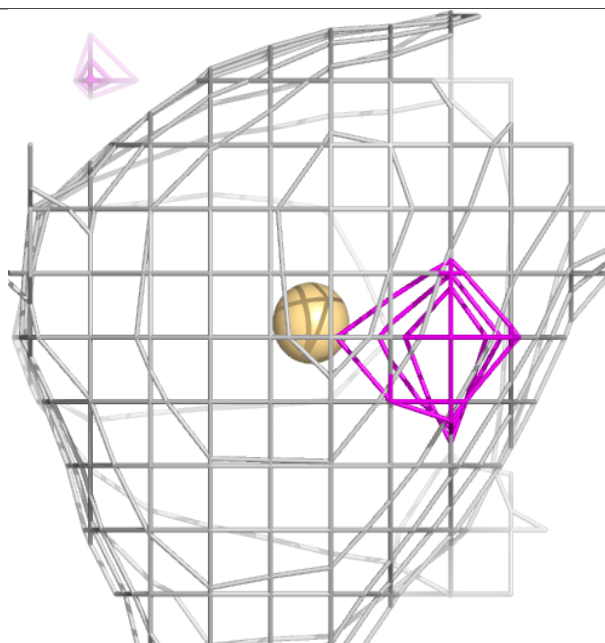
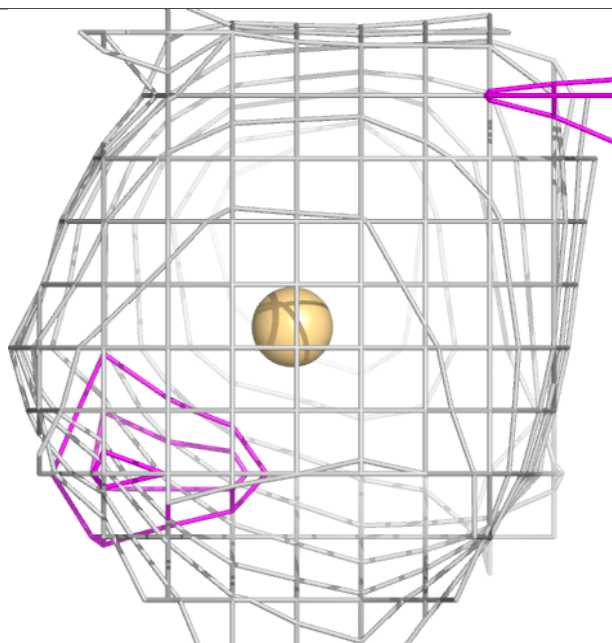
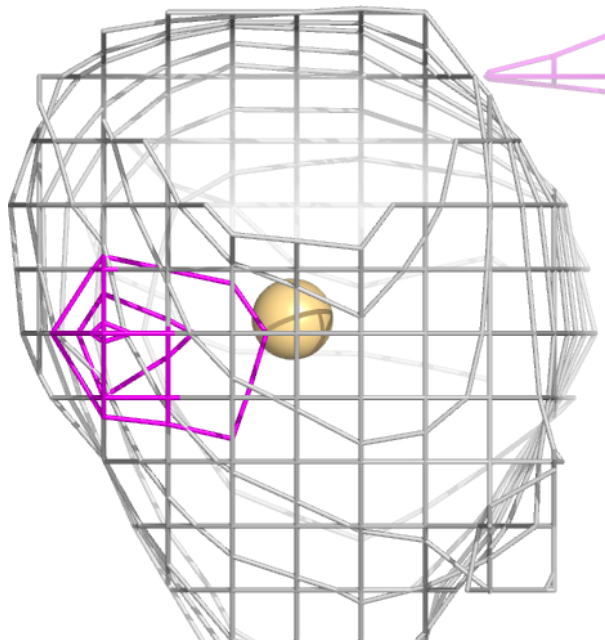
Electron density around CD BA 601:

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and green (positive)



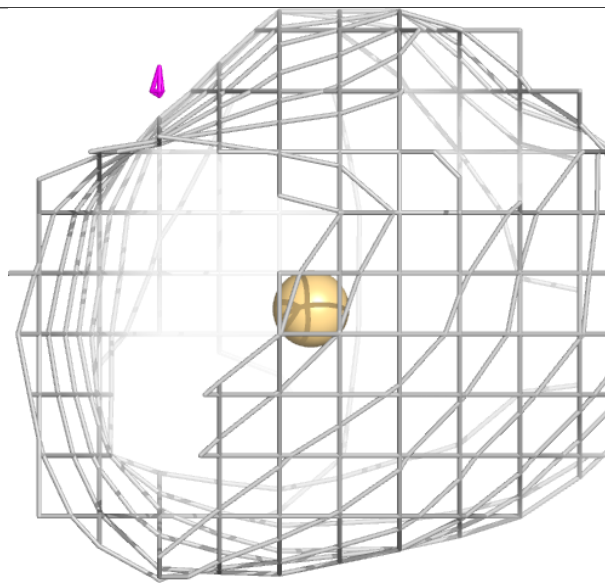
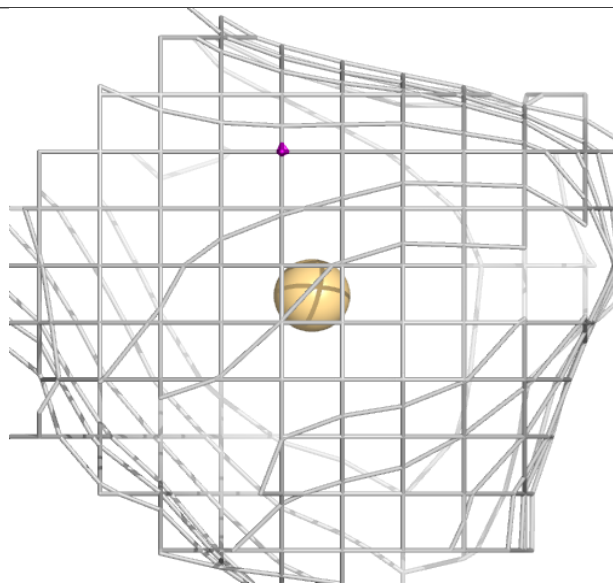
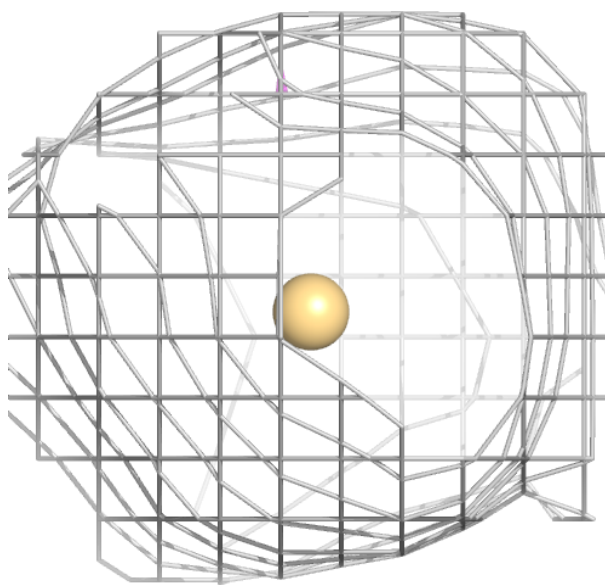
Electron density around CD DA 601:

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and green (positive)



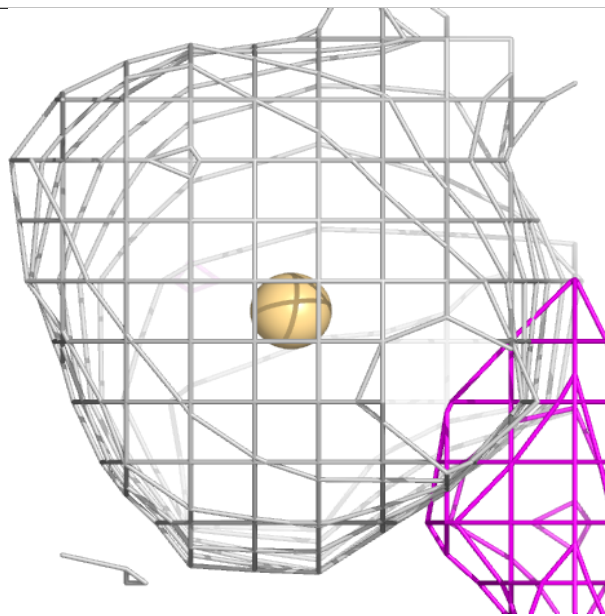
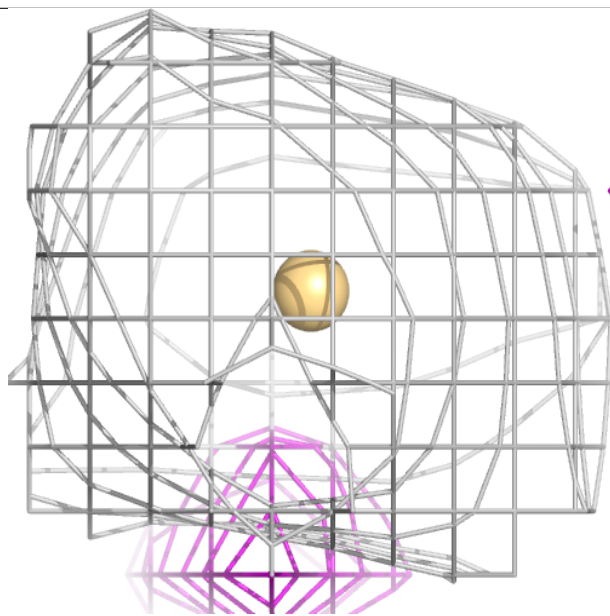
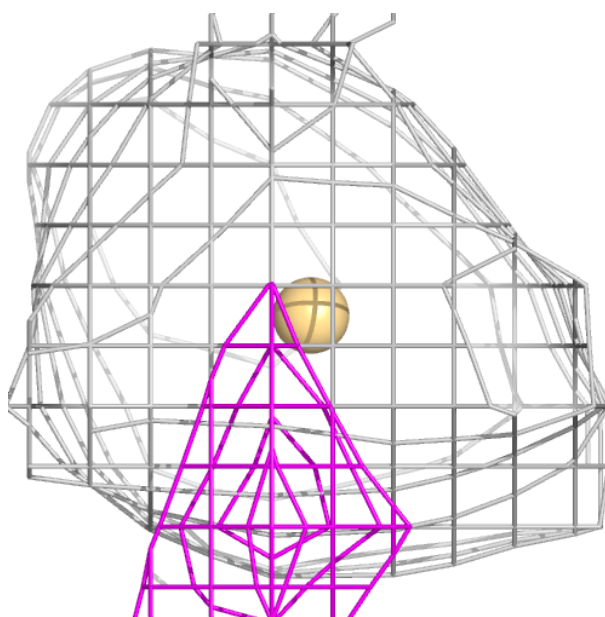
Electron density around CD IA 601:

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and green (positive)



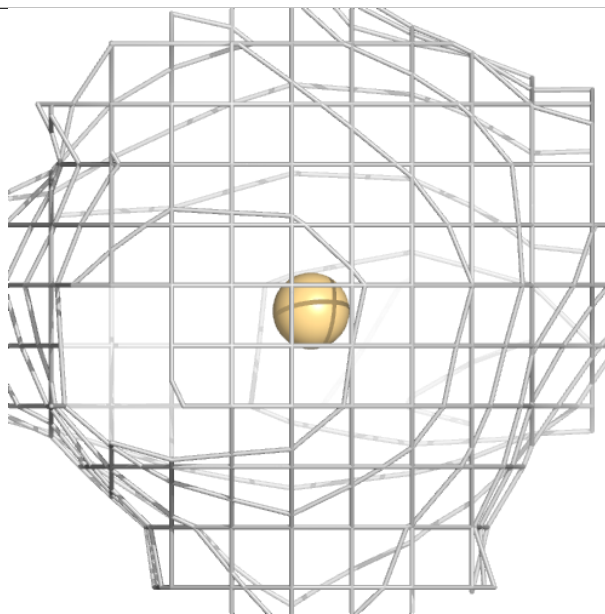
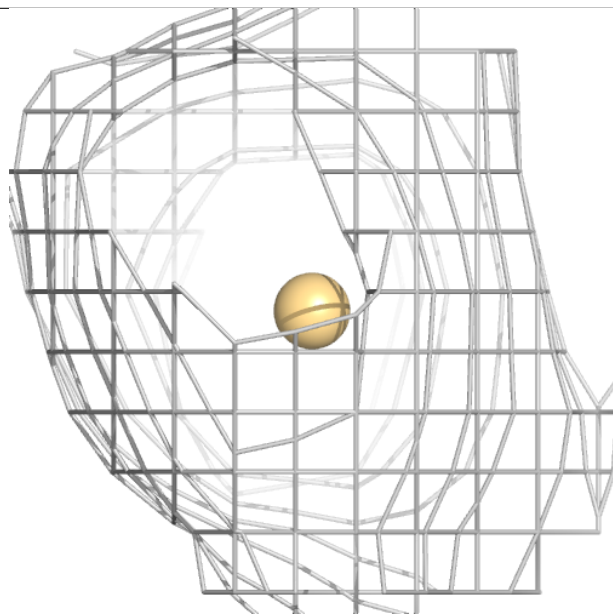
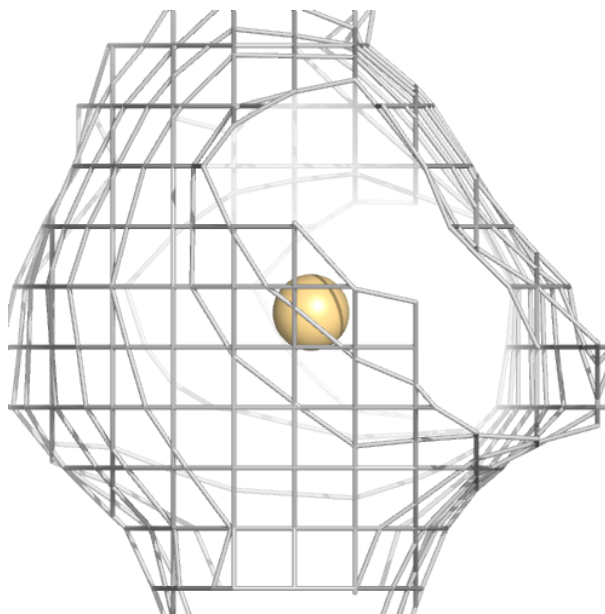
Electron density around CD JA 602:

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and green (positive)



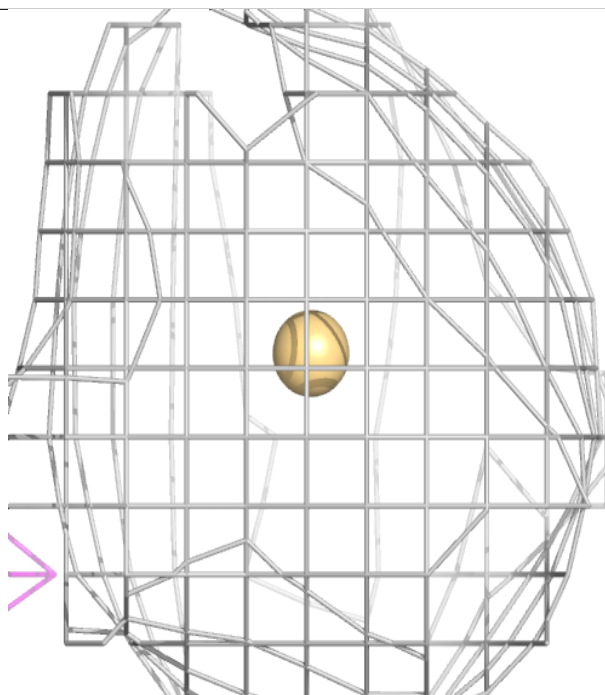
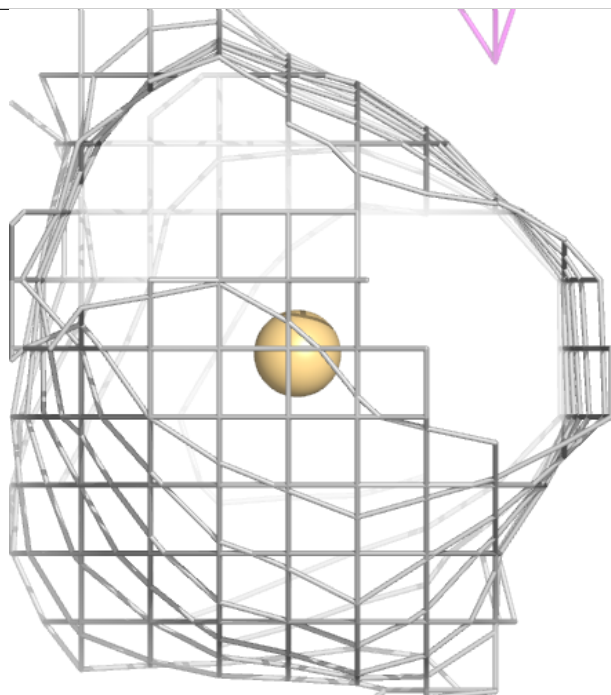
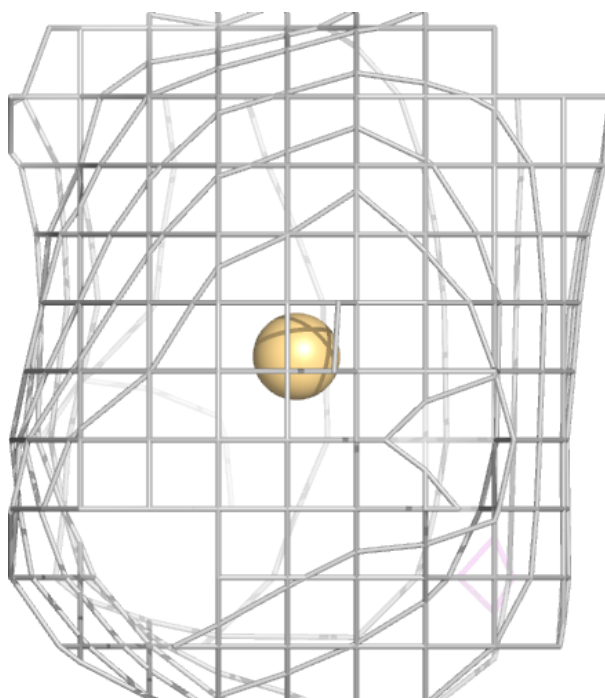
Electron density around CD EB 601:

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and green (positive)



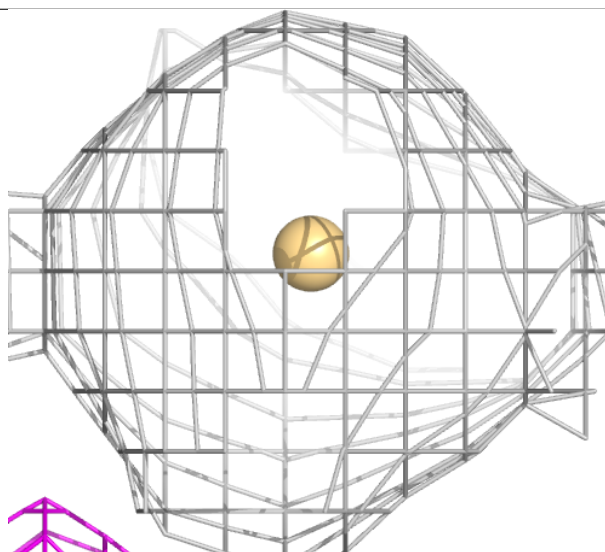
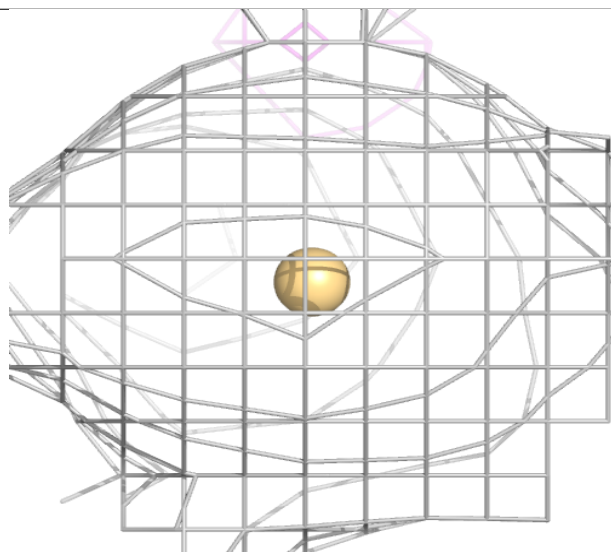
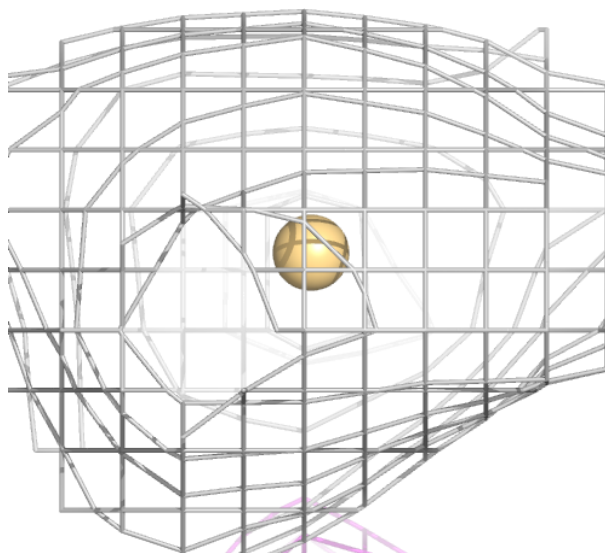
Electron density around CD OA 601:

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and green (positive)



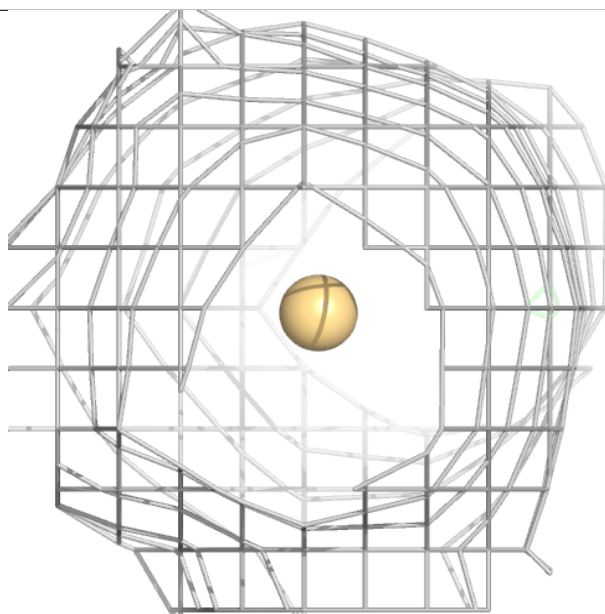
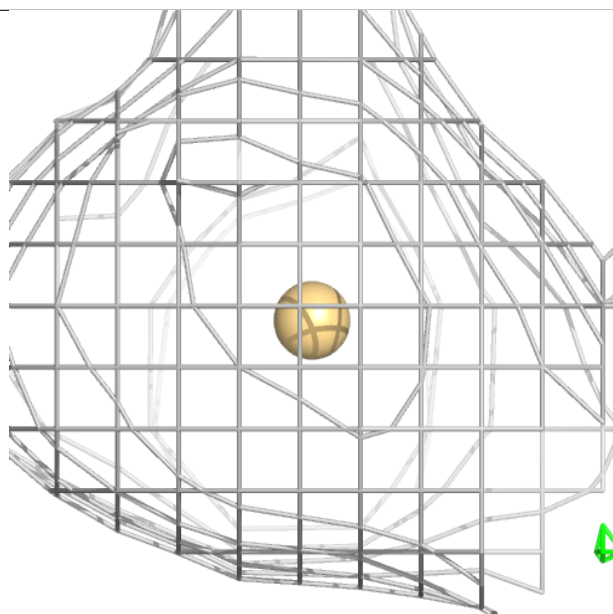
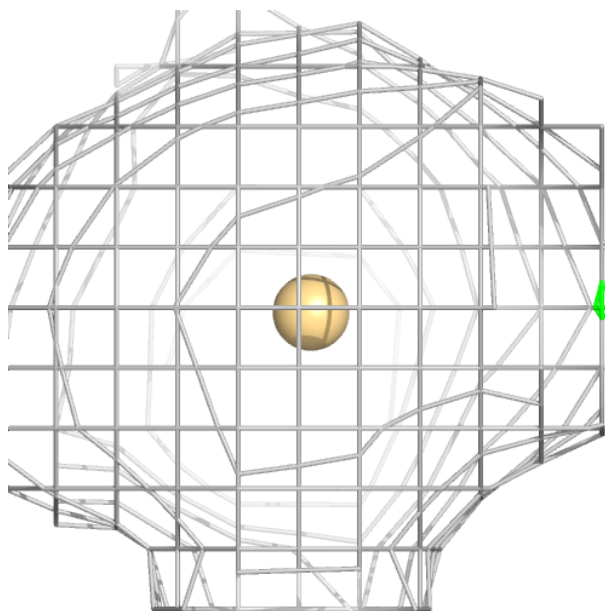
Electron density around CD FA 601:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



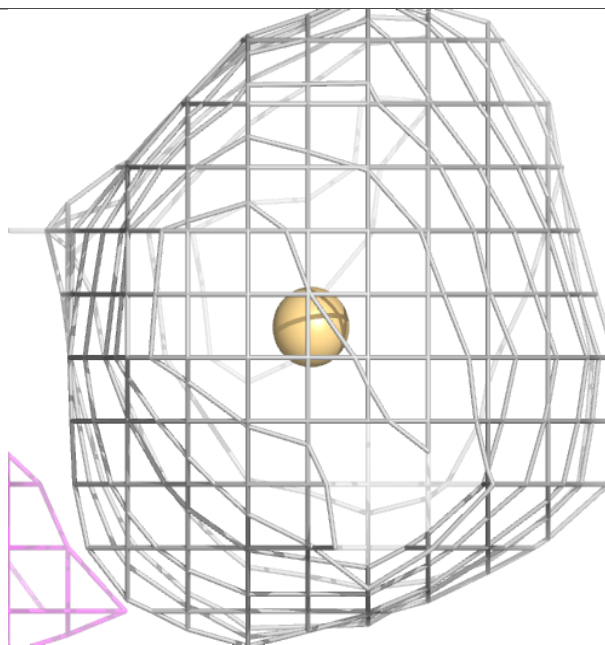
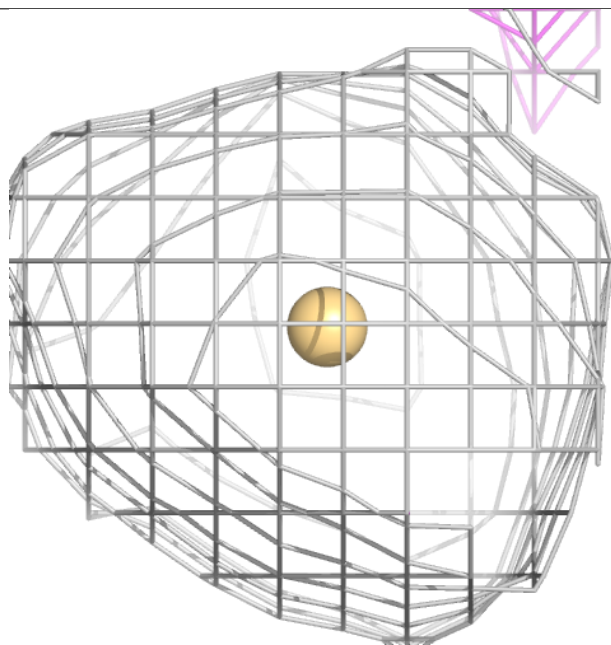
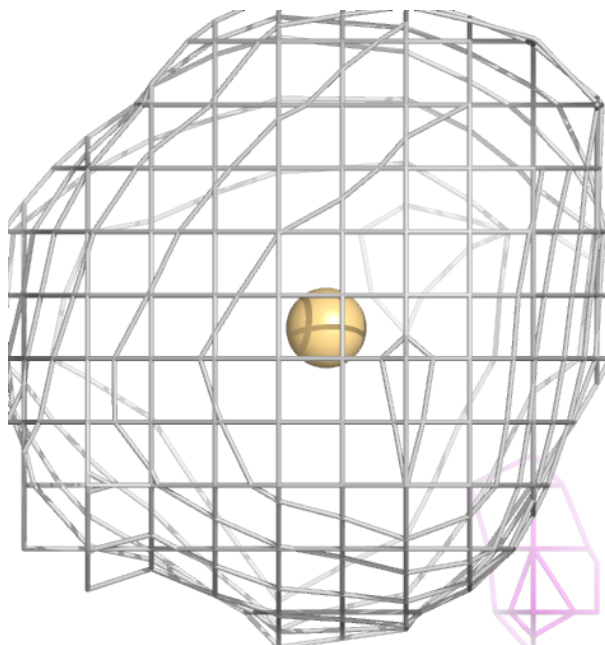
Electron density around CD GA 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



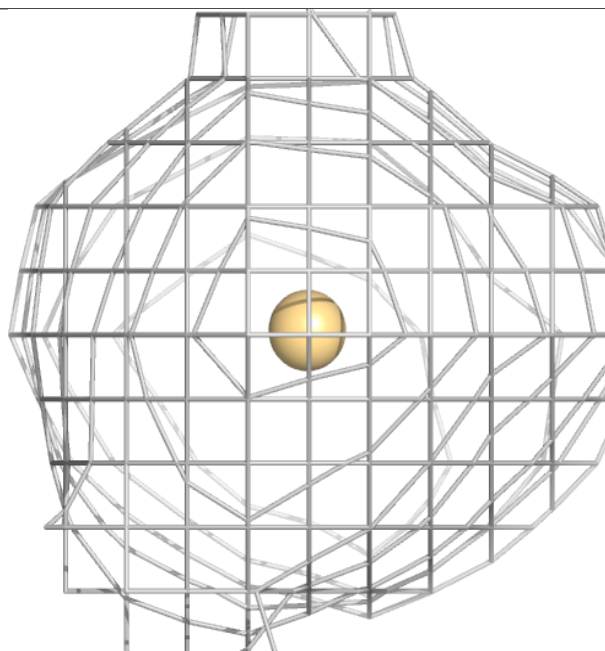
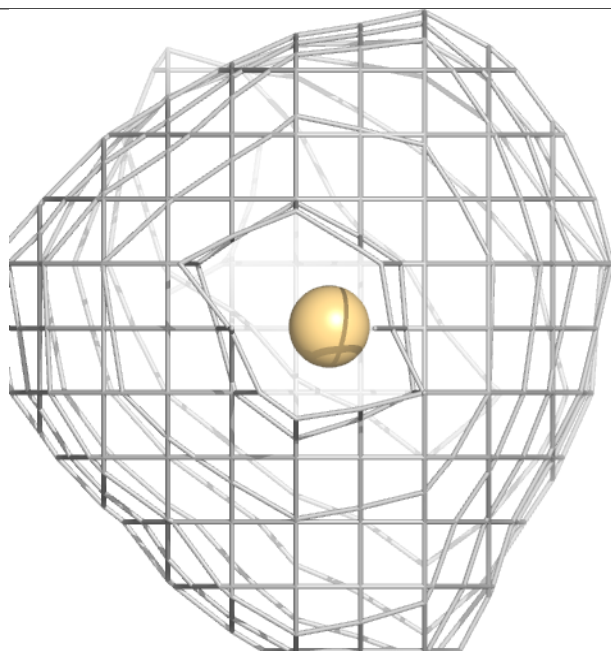
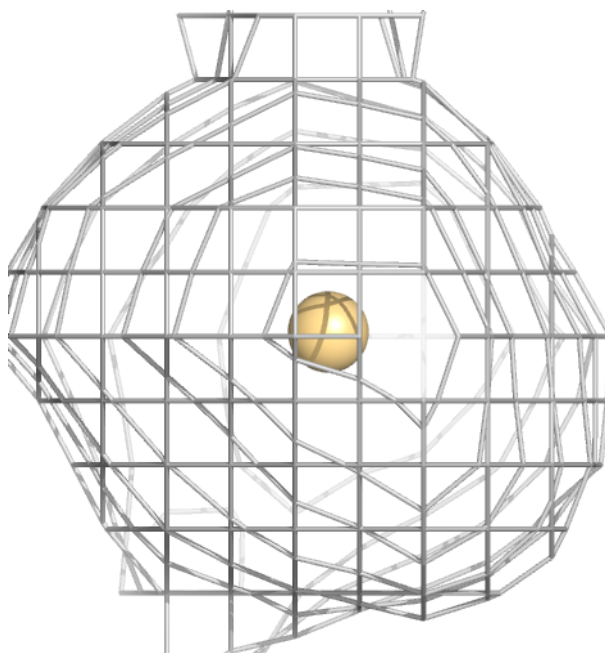
Electron density around CD AC 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



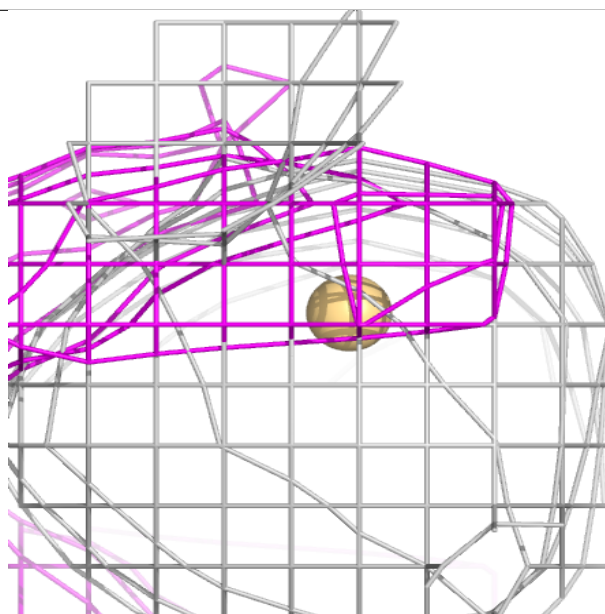
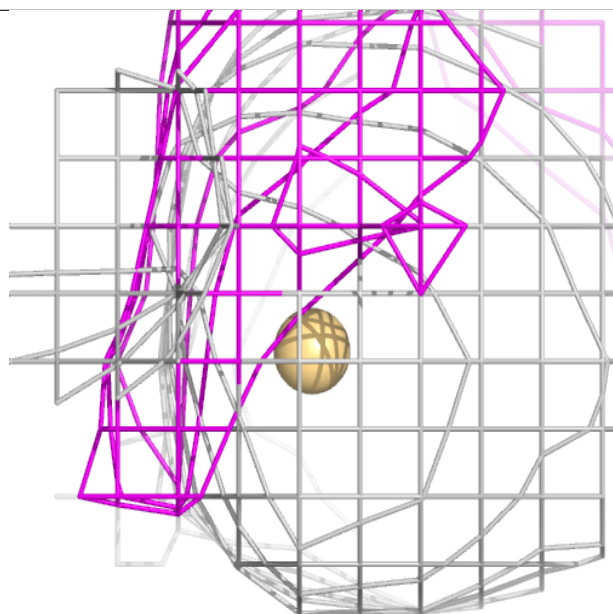
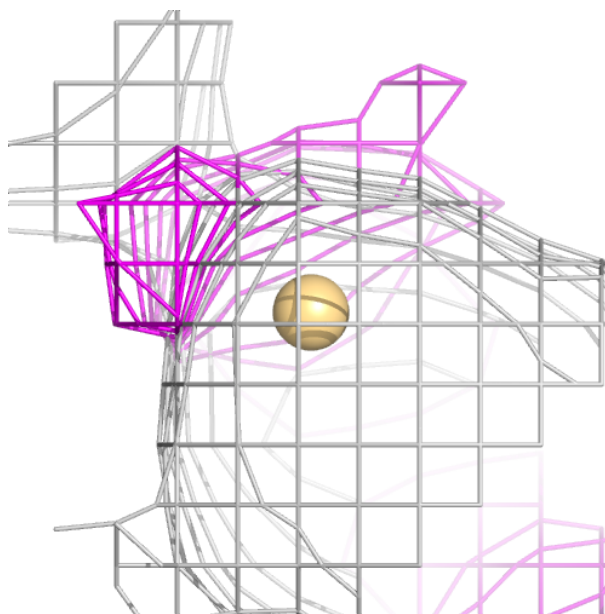
Electron density around CD HC 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



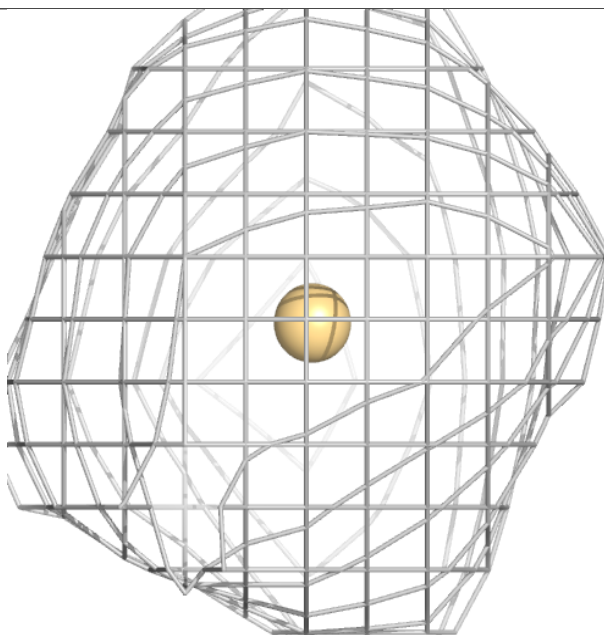
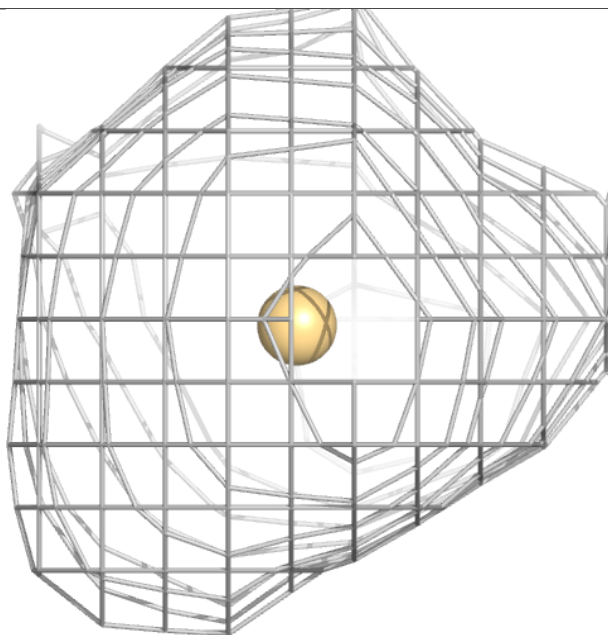
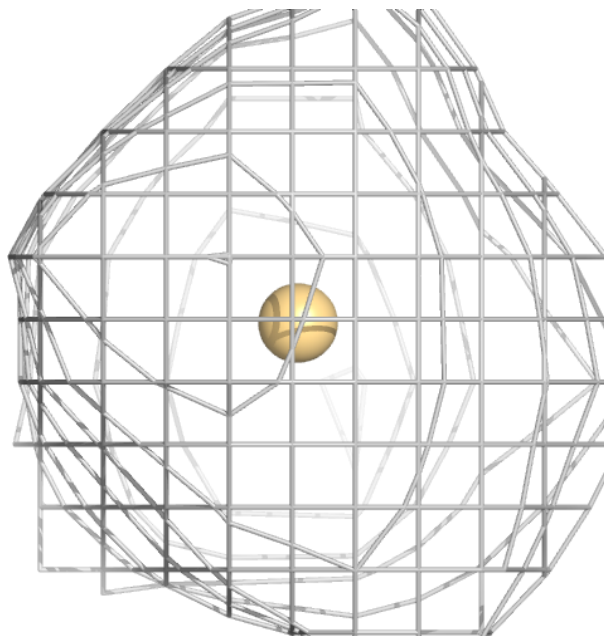
Electron density around CD EC 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



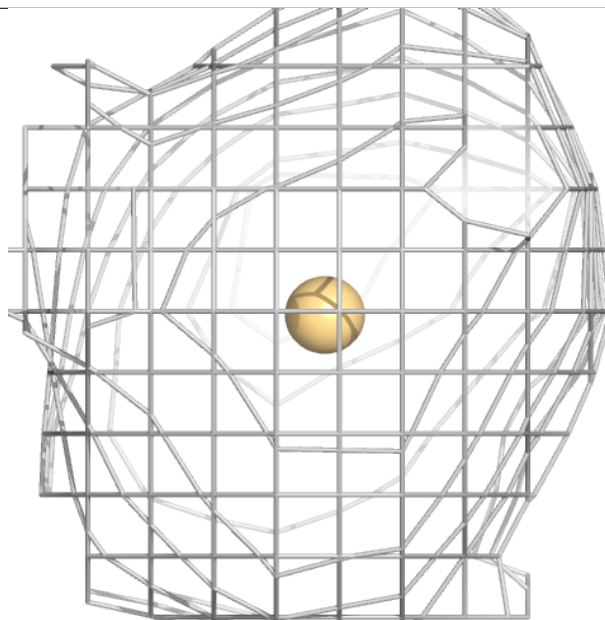
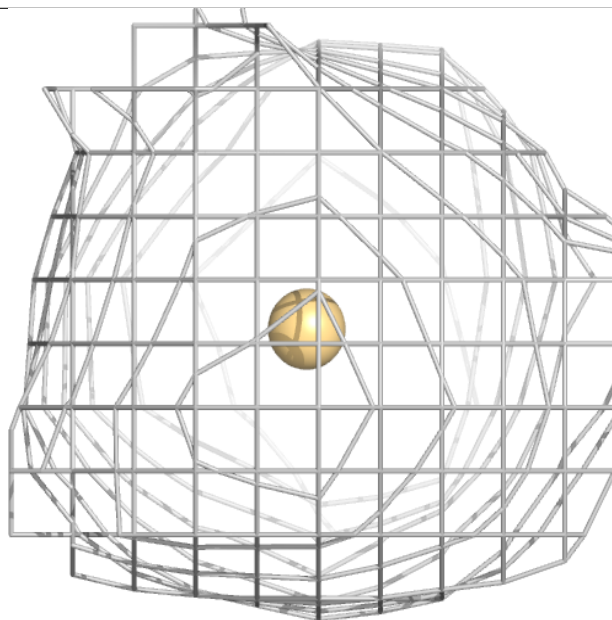
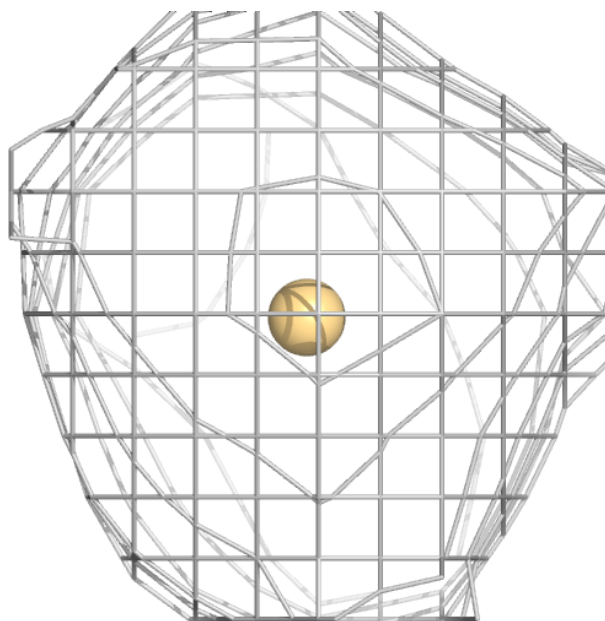
Electron density around CD NC 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



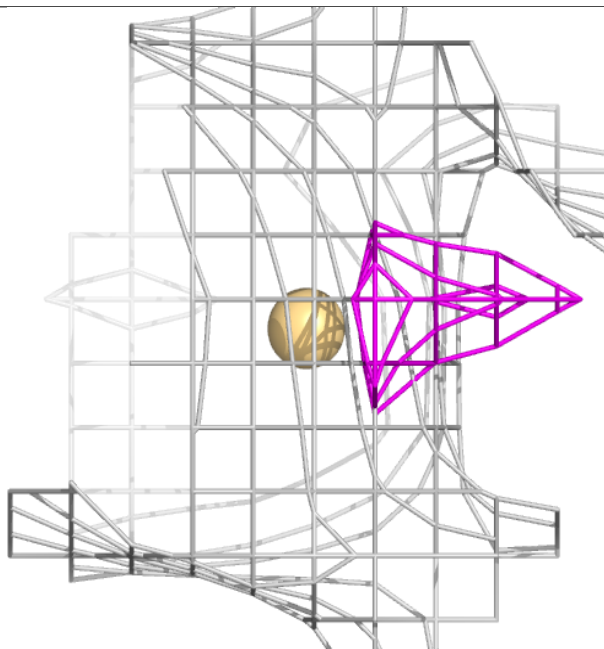
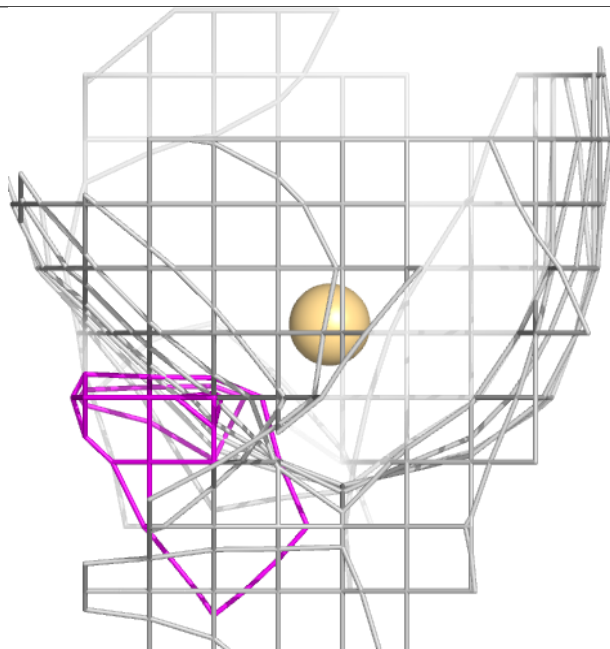
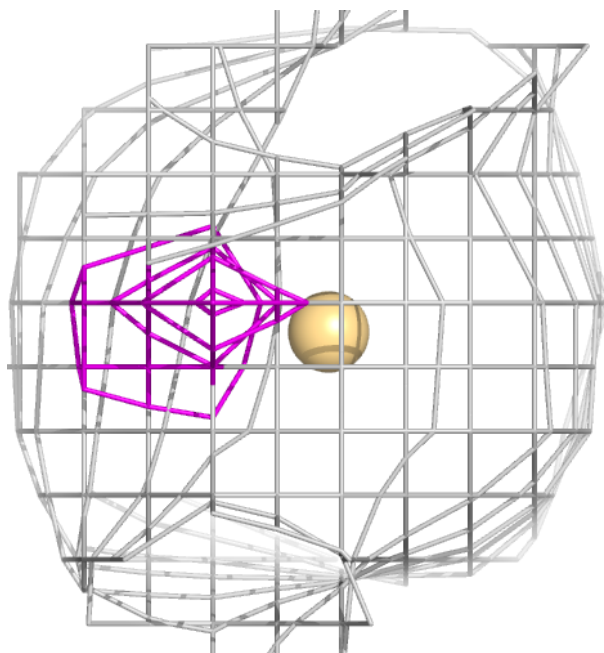
Electron density around CD BC 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



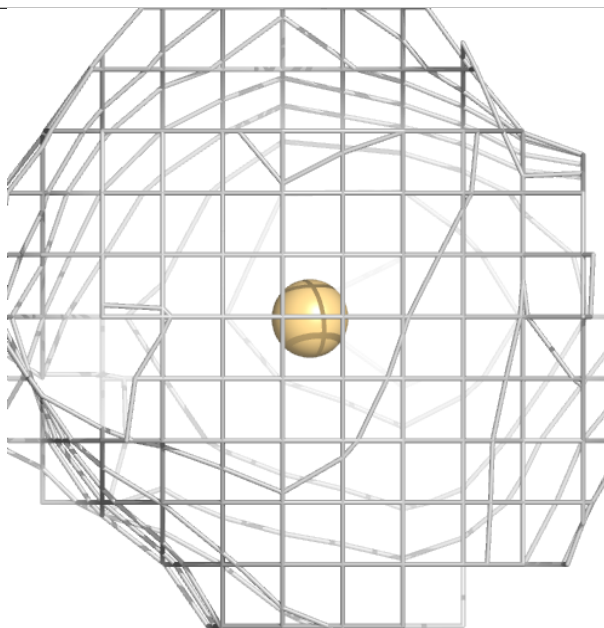
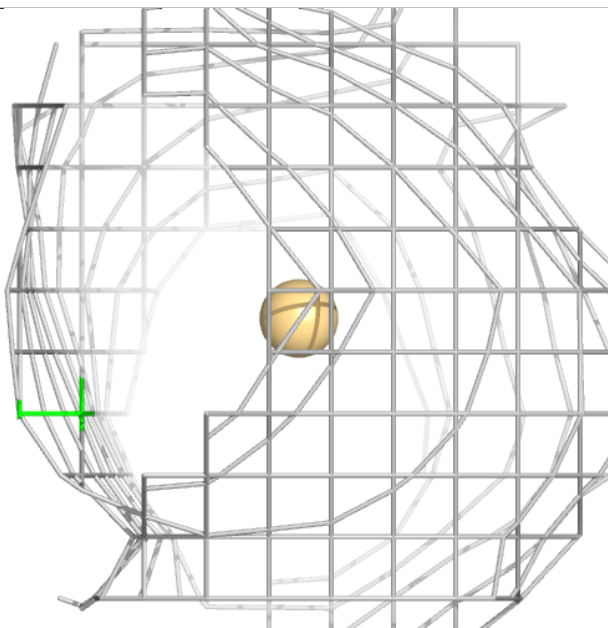
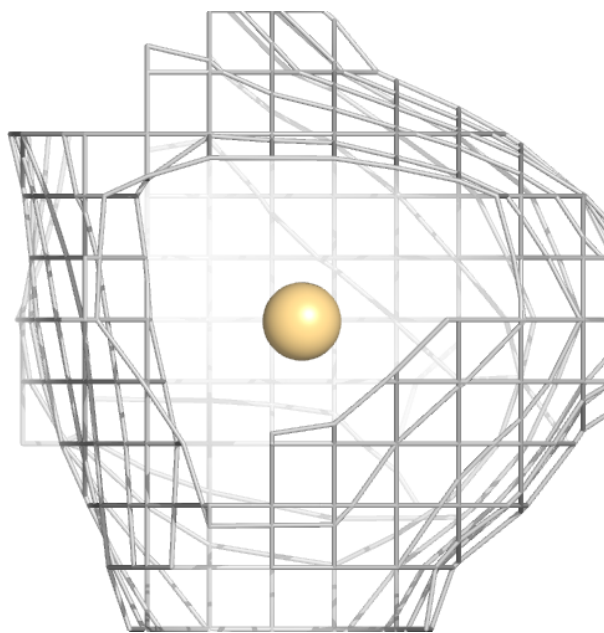
Electron density around CD JC 601:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



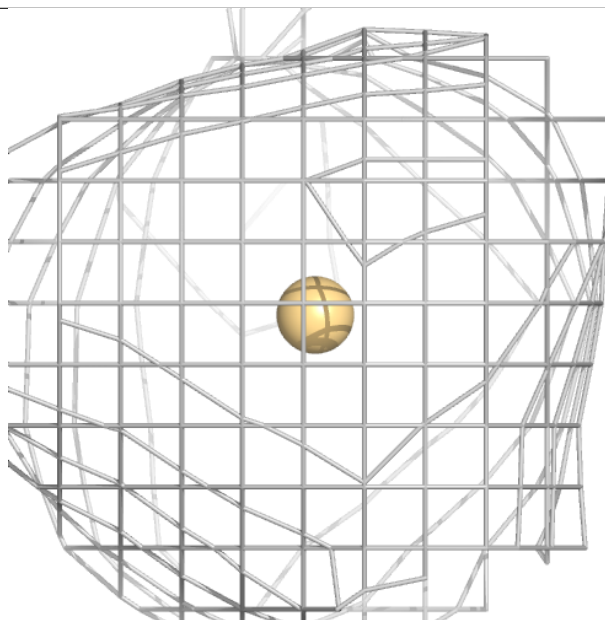
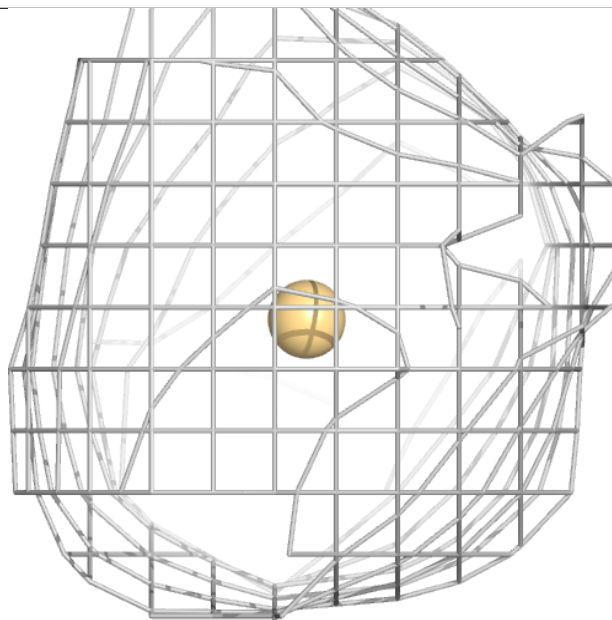
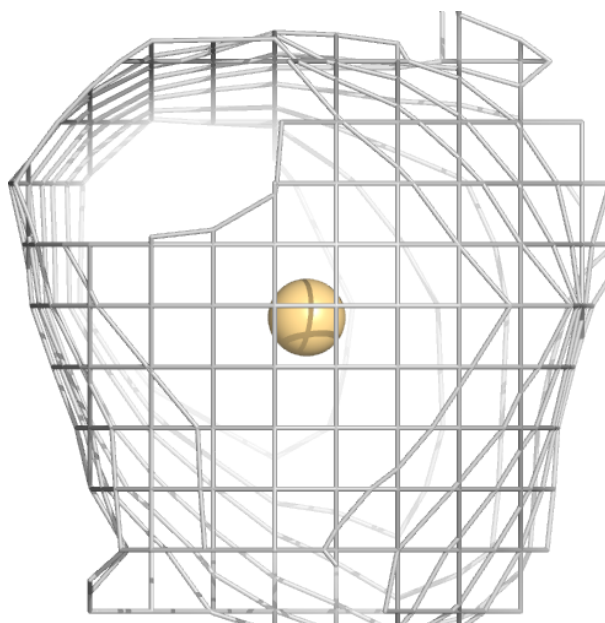
Electron density around CD KB 601:

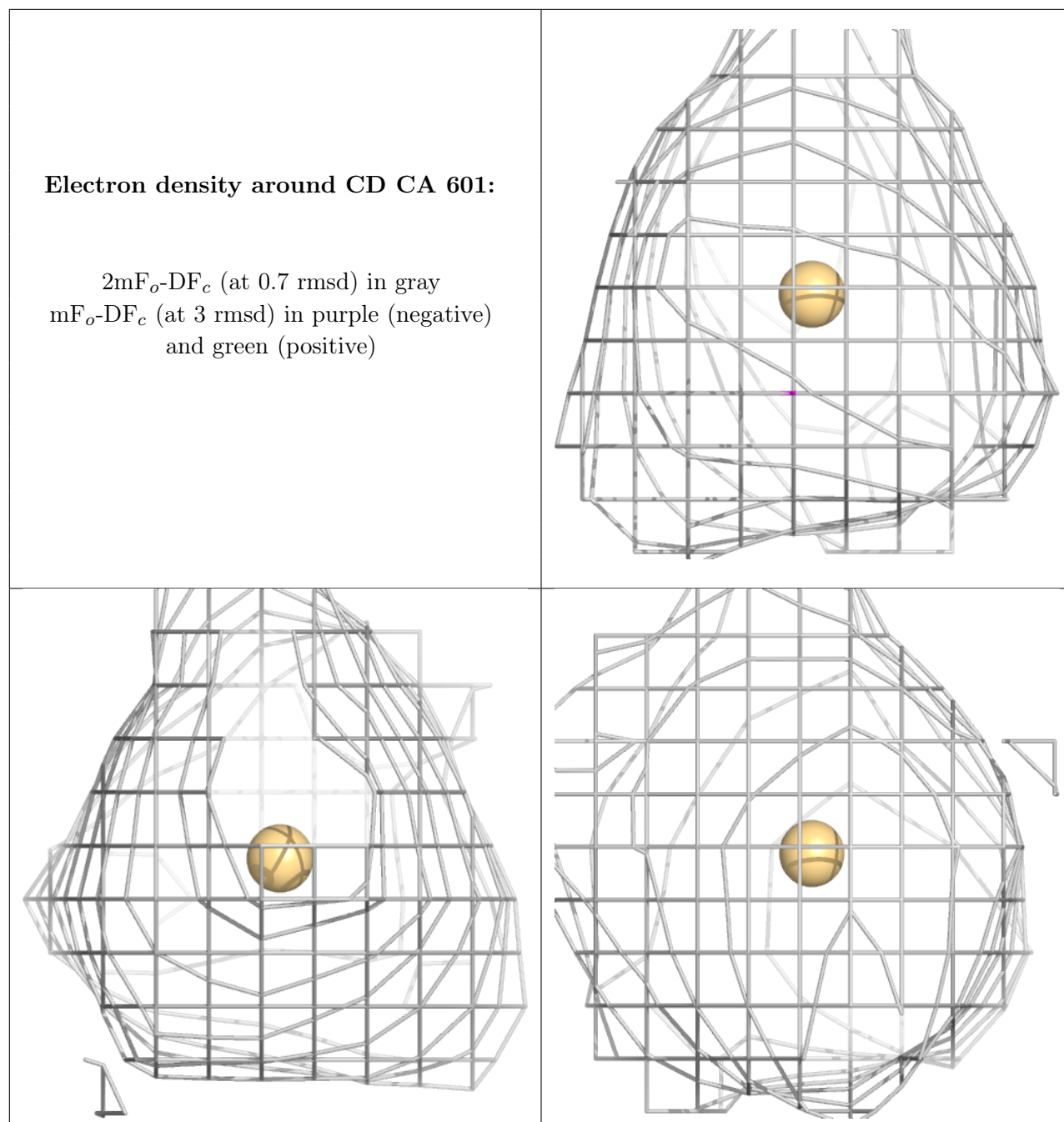
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CD FC 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.