



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:34 PM UTC

PDB ID : 1LVC / pdb_00001lvc
Title : Crystal structure of the adenylyl cyclase domain of anthrax edema factor (EF) in complex with calmodulin and 2' deoxy, 3' anthraniloyl ATP
Authors : Shen, Y.; Lee, Y.-S.; Soelaiman, S.; Bergson, P.; Lu, D.; Chen, A.; Beckingham, K.; Grabarek, Z.; Mrksich, M.; Tang, W.-J.
Deposited on : 2002-05-28
Resolution : 3.60 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:

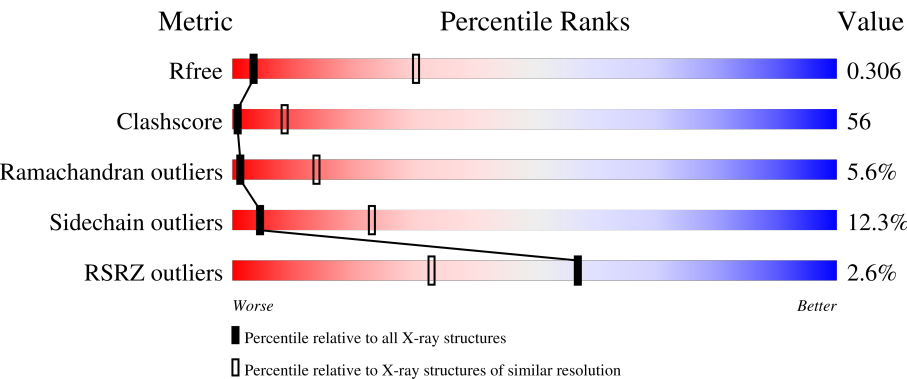
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	A	510	
1	B	510	
1	C	510	
2	D	149	

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Mol	Chain	Length	Quality of chain
2	E	149	6% 34% 54% 8%
2	F	149	5% 34% 50% 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15302 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 calmodulin-sensitive adenylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	65	0	0
			3952	2528	673	748	3			
1	B	465	Total	C	N	O	S	113	0	0
			3794	2431	642	718	3			
1	C	503	Total	C	N	O	S	166	0	0
			4094	2616	696	779	3			

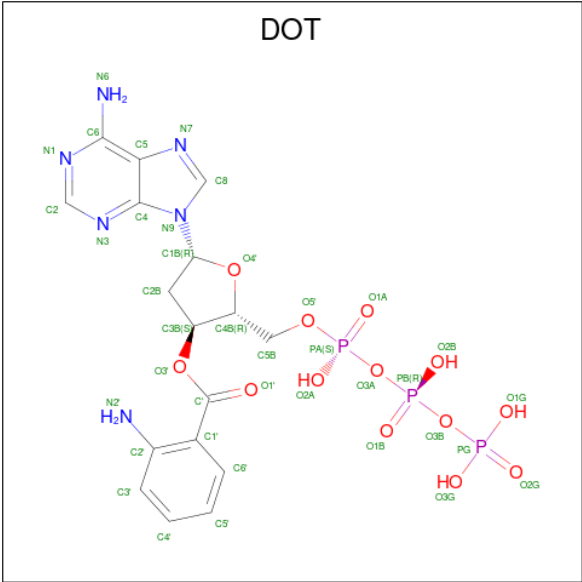
- Molecule 2 is a protein called calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			
2	E	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			
2	F	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			

- Molecule 3 is YTTERBIUM (III) ION (CCD ID: YB) (formula: Yb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Yb	0	0
			1	1		
3	B	1	Total	Yb	0	0
			1	1		
3	C	1	Total	Yb	0	0
			1	1		

- Molecule 4 is 3'-ANTHRANILOYL-2'-DEOXY-ADENOSINE-5'-TRIPHOSPHATE (CCD ID: DOT) (formula: C₁₇H₂₁N₆O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			39	17	6	13	3		
4	C	1	Total	C	N	O	P	0	0
			39	17	6	13	3		

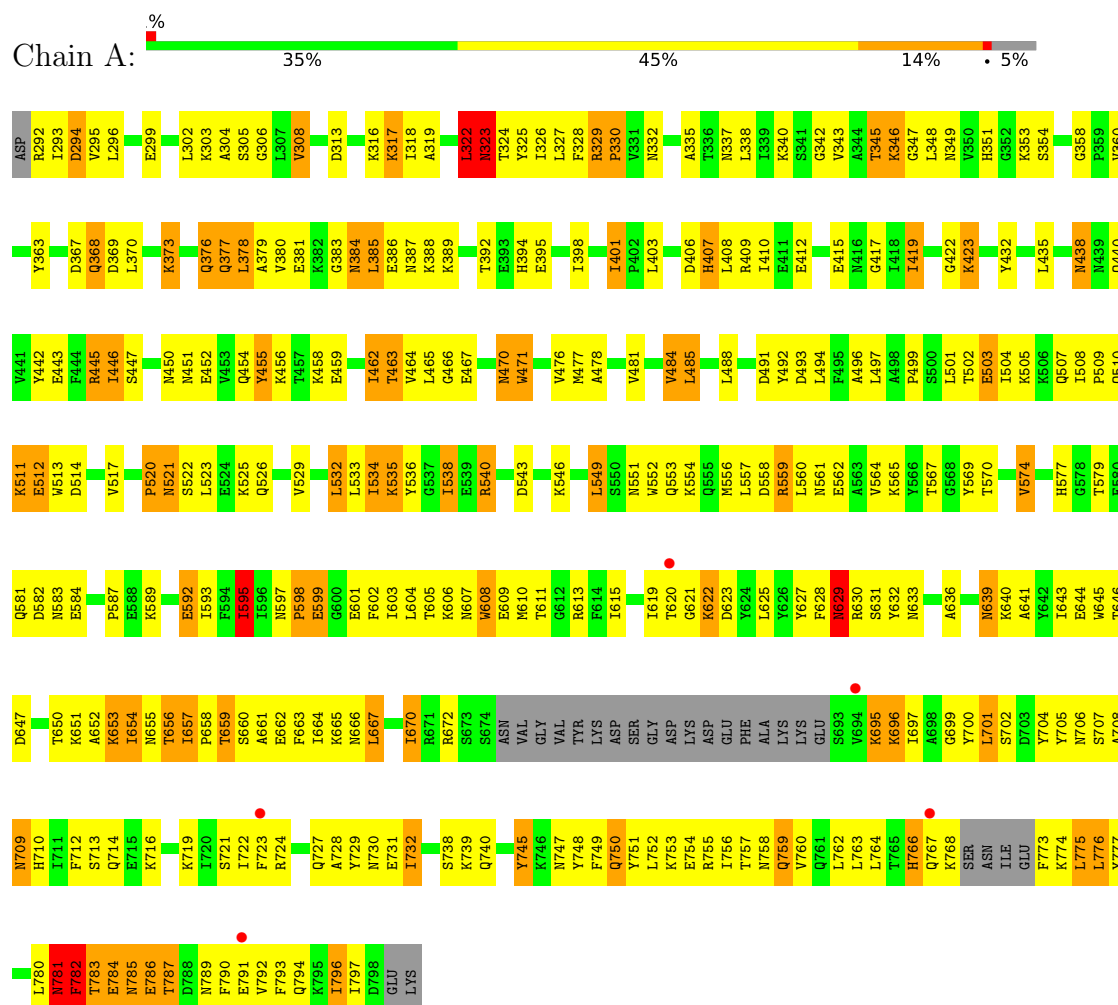
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	2	Total	Ca	0	0
			2	2		
5	E	2	Total	Ca	0	0
			2	2		
5	F	2	Total	Ca	0	0
			2	2		

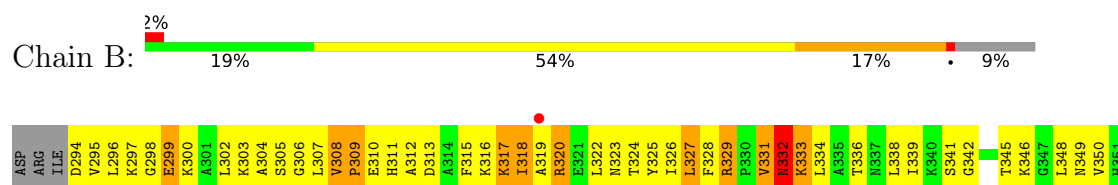
3 Residue-property plots

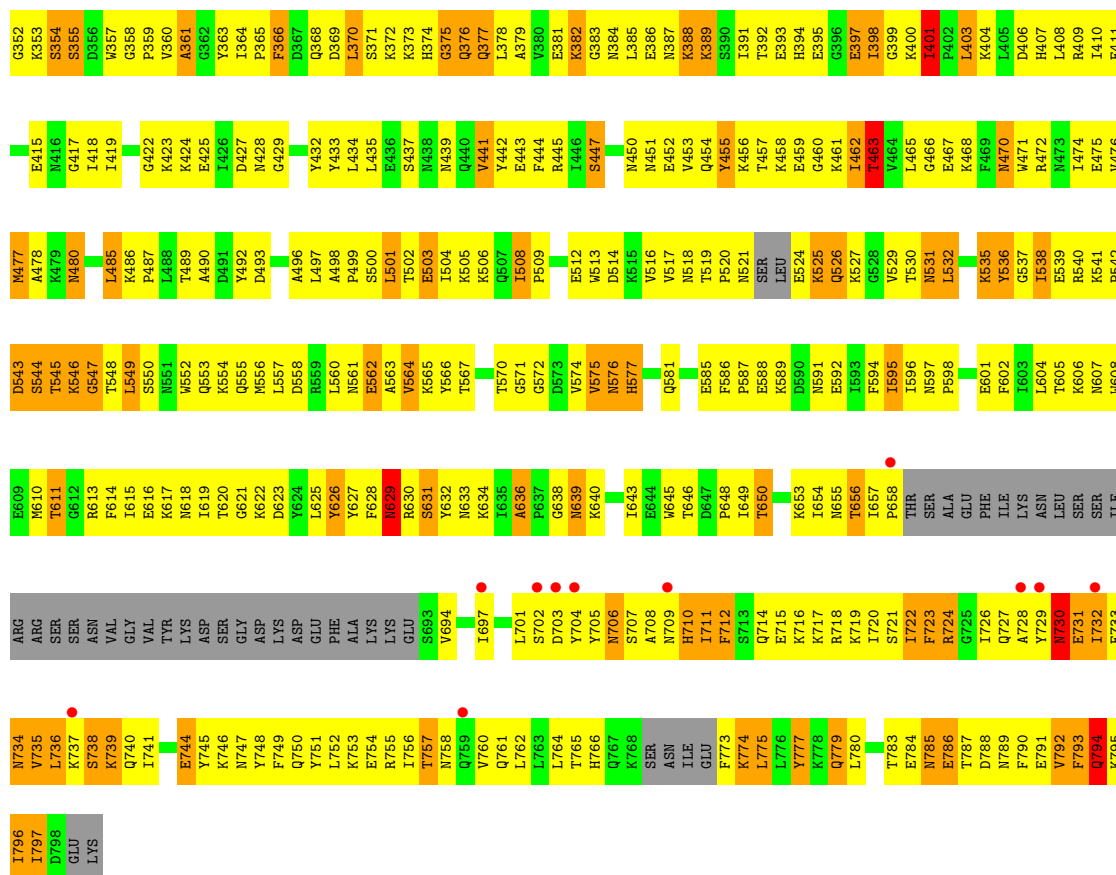
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: calmodulin-sensitive adenylate cyclase

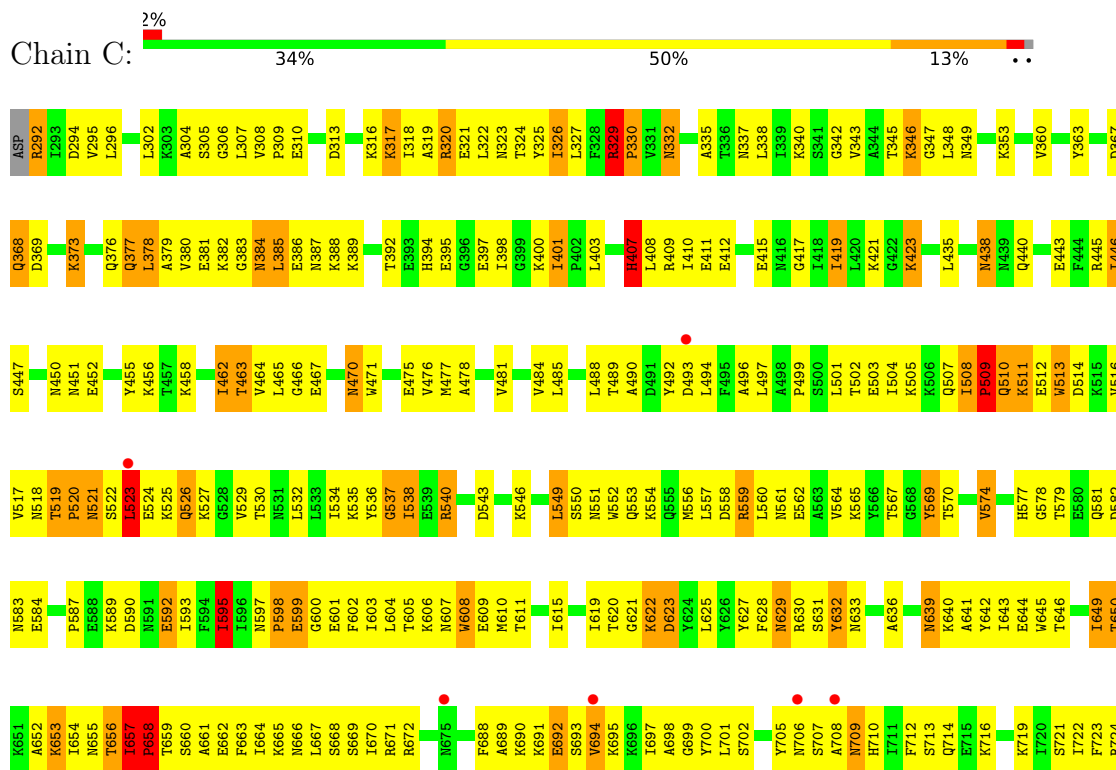


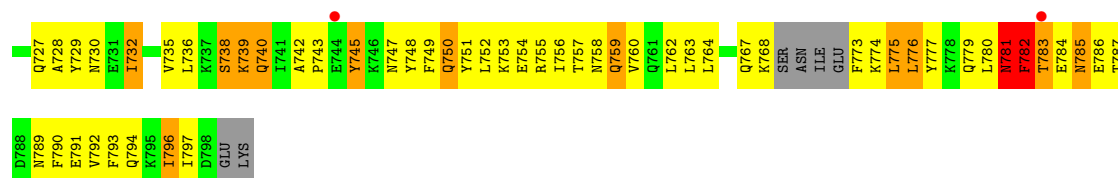
- Molecule 1: calmodulin-sensitive adenylate cyclase



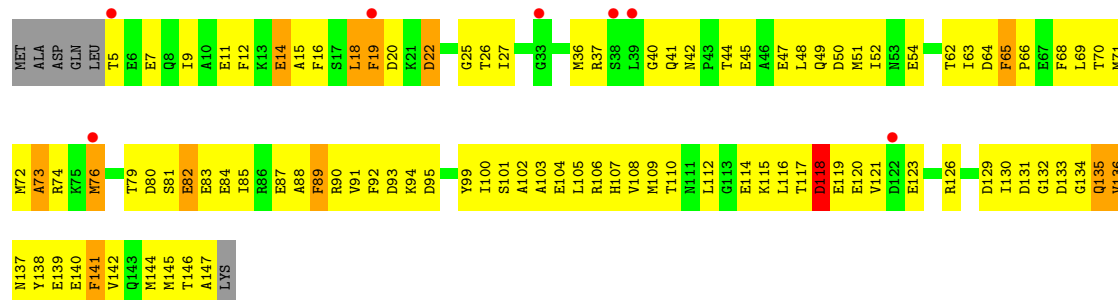


• Molecule 1: calmodulin-sensitive adenylate cyclase

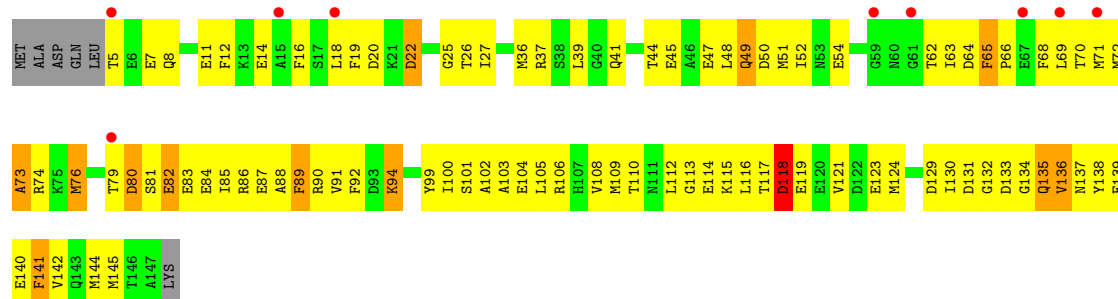




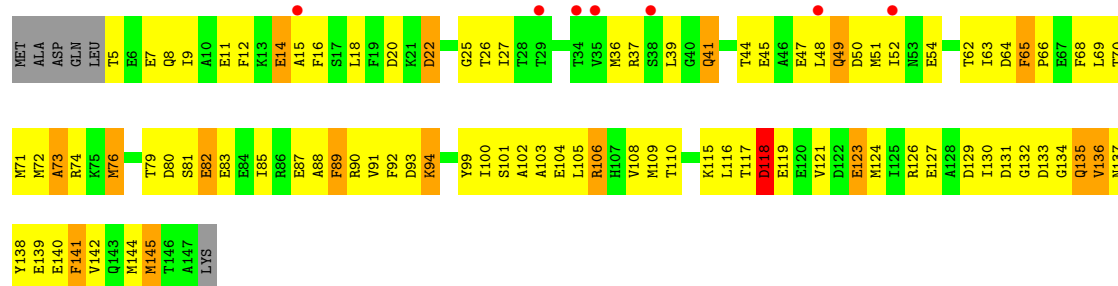
• Molecule 2: calmodulin



• Molecule 2: calmodulin



• Molecule 2: calmodulin



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	116.92Å 167.92Å 341.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.60 29.96 – 3.60	Depositor EDS
% Data completeness (in resolution range)	90.6 (29.96-3.60) 95.7 (29.96-3.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.00 (at 3.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.281 , 0.307 0.272 , 0.306	Depositor DCC
R_{free} test set	1945 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	98.5	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	15302	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: YB, DOT, CA

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	A	0.61	1/4027 (0.0%)	1.13	43/5419 (0.8%)
1	B	0.64	4/3867 (0.1%)	1.20	46/5204 (0.9%)
1	C	0.69	6/4172 (0.1%)	1.20	43/5613 (0.8%)
2	D	0.46	0/1137	0.82	1/1527 (0.1%)
2	E	0.44	0/1137	0.83	0/1527
2	F	0.41	0/1137	0.87	3/1527 (0.2%)
All	All	0.61	11/15477 (0.1%)	1.11	136/20817 (0.7%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	784	GLU	CA-C	-15.94	1.44	1.53
1	C	783	THR	C-N	-8.14	1.26	1.33
1	C	658	PRO	CA-C	-7.20	1.42	1.52
1	C	688	PHE	N-CA	6.86	1.54	1.46
1	C	693	SER	CA-C	6.80	1.61	1.53
1	B	738	SER	N-CA	-6.08	1.38	1.45
1	B	542	PRO	N-CA	5.44	1.53	1.47
1	B	537	GLY	C-N	5.43	1.39	1.33
1	A	322	LEU	N-CA	-5.16	1.39	1.46
1	C	738	SER	N-CA	5.07	1.52	1.46
1	B	730	ASN	CA-C	-5.04	1.46	1.52

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	783	THR	CA-C-N	-16.64	105.07	123.04
1	C	783	THR	C-N-CA	-16.64	105.07	123.04
1	B	538	ILE	CB-CA-C	-14.96	94.47	110.62
1	C	632	TYR	CA-C-N	-13.97	102.35	123.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	632	TYR	C-N-CA	-13.97	102.35	123.17
1	B	375	GLY	CA-C-N	-12.60	106.46	122.84
1	B	375	GLY	C-N-CA	-12.60	106.46	122.84
1	B	738	SER	N-CA-C	-12.09	91.12	109.86
1	B	538	ILE	N-CA-C	10.77	124.34	113.47
1	B	740	GLN	OE1-CD-NE2	-10.63	111.97	122.60
1	A	740	GLN	N-CA-C	-10.60	92.25	108.67
1	B	732	ILE	N-CA-C	-10.47	102.84	112.90
1	A	672	ARG	N-CA-C	-10.42	101.07	113.88
1	A	782	PHE	N-CA-C	-10.38	97.09	112.04
1	C	740	GLN	OE1-CD-NE2	-10.30	112.30	122.60
1	C	782	PHE	N-CA-C	-10.29	97.23	112.04
1	B	470	ASN	CA-C-N	-10.25	108.11	123.07
1	B	470	ASN	C-N-CA	-10.25	108.11	123.07
1	A	785	ASN	O-C-N	-10.23	110.28	122.05
1	C	767	GLN	OE1-CD-NE2	-10.14	112.45	122.60
1	C	510	GLN	OE1-CD-NE2	-10.13	112.47	122.60
1	A	787	THR	N-CA-C	-9.98	101.19	113.97
1	A	322	LEU	N-CA-C	-9.83	93.24	109.07
1	B	526	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	C	689	ALA	N-CA-C	9.52	125.84	114.04
1	A	785	ASN	CA-C-N	-9.51	103.38	121.54
1	A	785	ASN	C-N-CA	-9.51	103.38	121.54
1	B	376	GLN	OE1-CD-NE2	-9.41	113.19	122.60
1	C	470	ASN	N-CA-C	9.19	123.65	108.48
1	C	785	ASN	N-CA-C	9.18	130.35	110.80
1	C	538	ILE	N-CA-C	9.17	119.09	110.74
1	A	470	ASN	CA-CB-CG	-9.13	103.47	112.60
1	A	740	GLN	OE1-CD-NE2	-9.08	113.52	122.60
1	A	767	GLN	OE1-CD-NE2	-8.98	113.62	122.60
2	F	106	ARG	NE-CZ-NH2	8.73	127.06	119.20
1	C	509	PRO	CA-N-CD	-8.71	99.81	112.00
2	F	106	ARG	NE-CZ-NH1	-8.25	113.25	121.50
1	C	740	GLN	N-CA-C	-8.04	97.57	109.15
1	A	667	LEU	N-CA-C	-7.99	103.53	113.28
1	A	785	ASN	CA-C-O	-7.54	111.17	119.08
1	B	739	LYS	N-CA-C	7.51	126.80	110.80
1	B	730	ASN	CA-CB-CG	7.27	119.87	112.60
1	C	510	GLN	CG-CD-NE2	7.19	127.19	116.40
1	B	342	GLY	N-CA-C	7.07	123.49	115.08
1	C	784	GLU	CA-C-N	-7.03	108.11	121.54
1	C	784	GLU	C-N-CA	-7.03	108.11	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	613	ARG	NE-CZ-NH2	7.01	125.51	119.20
1	A	783	THR	CA-C-N	-6.94	108.29	121.54
1	A	783	THR	C-N-CA	-6.94	108.29	121.54
1	C	658	PRO	CA-N-CD	-6.94	102.29	112.00
1	A	346	LYS	N-CA-C	6.83	119.70	109.25
1	B	740	GLN	CG-CD-NE2	6.80	126.61	116.40
1	C	688	PHE	N-CA-C	6.79	119.79	108.73
1	A	783	THR	N-CA-C	6.78	125.25	110.80
1	C	346	LYS	N-CA-C	6.76	119.59	109.25
1	C	740	GLN	CG-CD-NE2	6.74	126.51	116.40
1	A	613	ARG	NE-CZ-NH1	-6.73	114.77	121.50
1	B	376	GLN	CG-CD-NE2	6.68	126.42	116.40
1	C	767	GLN	CG-CD-NE2	6.57	126.26	116.40
1	A	695	LYS	N-CA-C	-6.56	104.85	112.92
1	B	526	GLN	CG-CD-NE2	6.53	126.20	116.40
1	C	632	TYR	O-C-N	-6.50	113.94	122.59
1	B	470	ASN	O-C-N	-6.49	113.95	122.59
1	B	366	PHE	N-CA-C	-6.39	103.93	111.03
1	A	740	GLN	CG-CD-NE2	6.36	125.94	116.40
1	B	470	ASN	N-CA-C	6.35	124.33	110.80
1	C	470	ASN	CA-CB-CG	-6.23	106.37	112.60
1	B	546	LYS	N-CA-C	-6.22	99.10	109.24
1	B	329	ARG	N-CA-C	-6.22	100.99	110.07
1	B	779	GLN	N-CA-C	-6.21	104.76	112.90
1	C	320	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	B	308	VAL	CA-C-N	6.12	127.49	119.84
1	B	308	VAL	C-N-CA	6.12	127.49	119.84
1	C	592	GLU	N-CA-C	6.08	118.63	108.96
1	B	650	THR	N-CA-C	-6.05	107.72	114.62
2	F	106	ARG	CD-NE-CZ	6.01	132.81	124.40
1	C	512	GLU	N-CA-C	-5.99	105.06	112.90
1	A	767	GLN	CG-CD-NE2	5.89	125.24	116.40
1	B	777	TYR	N-CA-C	-5.89	103.65	112.54
1	A	592	GLU	N-CA-C	5.84	118.24	108.96
1	B	783	THR	N-CA-C	-5.83	106.08	113.43
1	C	781	ASN	N-CA-C	5.80	117.76	108.41
1	B	542	PRO	N-CA-C	5.79	119.95	111.03
1	A	783	THR	O-C-N	-5.79	114.89	122.59
1	C	660	SER	N-CA-C	-5.77	105.34	112.38
1	C	750	GLN	N-CA-C	-5.77	105.34	112.38
1	C	320	ARG	NE-CZ-NH1	-5.76	115.74	121.50
1	C	783	THR	N-CA-C	5.73	123.00	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	533	LEU	N-CA-C	-5.69	105.08	111.28
1	A	535	LYS	N-CA-C	5.68	119.03	111.75
1	B	358	GLY	CA-C-N	5.67	125.14	119.24
1	B	358	GLY	C-N-CA	5.67	125.14	119.24
1	B	377	GLN	N-CA-C	5.67	117.91	111.11
1	A	781	ASN	N-CA-C	5.63	117.47	108.41
1	A	738	SER	CA-C-N	-5.62	113.62	122.73
1	A	738	SER	C-N-CA	-5.62	113.62	122.73
1	B	470	ASN	CA-CB-CG	-5.62	106.98	112.60
1	C	745	TYR	N-CA-C	-5.61	105.17	111.28
1	C	513	TRP	N-CA-C	-5.58	105.73	112.54
1	A	745	TYR	N-CA-C	-5.58	105.20	111.28
1	B	542	PRO	CA-N-CD	-5.58	104.19	112.00
1	B	535	LYS	N-CA-C	5.57	118.28	111.82
1	A	595	ILE	N-CA-C	5.56	116.00	107.77
1	A	767	GLN	N-CA-C	5.53	119.80	112.72
1	A	308	VAL	N-CA-C	-5.52	102.95	108.96
1	A	750	GLN	N-CA-C	-5.50	105.67	112.38
1	A	786	GLU	N-CA-C	5.50	122.51	110.80
1	C	329	ARG	N-CA-C	-5.49	103.00	110.36
1	C	784	GLU	O-C-N	-5.48	117.36	121.47
1	C	508	ILE	CA-C-N	5.45	125.21	119.76
1	C	508	ILE	C-N-CA	5.45	125.21	119.76
1	B	441	VAL	N-CA-C	-5.45	107.32	111.62
1	B	532	LEU	N-CA-C	-5.29	104.42	112.04
1	B	401	ILE	CA-C-N	-5.28	114.35	119.78
1	B	401	ILE	C-N-CA	-5.28	114.35	119.78
1	A	470	ASN	N-CA-C	5.27	122.03	110.80
2	D	19	PHE	N-CA-C	5.27	118.27	107.37
1	B	543	ASP	CA-C-N	-5.26	111.49	121.54
1	B	543	ASP	C-N-CA	-5.26	111.49	121.54
1	C	382	LYS	N-CA-C	-5.25	106.58	112.87
1	C	693	SER	N-CA-C	5.20	118.42	111.24
1	A	785	ASN	N-CA-C	5.19	121.34	112.99
1	C	692	GLU	O-C-N	-5.18	117.17	123.13
1	C	784	GLU	N-CA-C	-5.16	104.55	108.78
1	A	512	GLU	N-CA-C	-5.16	105.73	112.23
1	C	595	ILE	N-CA-C	5.14	115.38	107.77
1	A	323	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	766	HIS	N-CA-C	-5.12	105.89	111.82
1	B	618	ASN	N-CA-C	5.10	119.58	112.90
1	B	545	THR	N-CA-C	-5.08	105.82	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	428	ASN	N-CA-C	-5.07	106.30	113.20
1	A	470	ASN	CA-C-N	-5.07	115.62	122.77
1	A	470	ASN	C-N-CA	-5.07	115.62	122.77
1	A	422	GLY	N-CA-C	5.04	118.88	112.13
1	B	636	ALA	CA-C-N	5.02	124.63	119.05
1	B	636	ALA	C-N-CA	5.02	124.63	119.05

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	A	3952	0	3999	431	0
1	B	3794	0	3828	528	0
1	C	4094	0	4134	418	0
2	D	1125	0	1049	120	0
2	E	1125	0	1049	115	0
2	F	1125	0	1049	119	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	39	0	17	8	0
4	C	39	0	17	5	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
All	All	15302	0	15142	1658	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 56.

All (1658) 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:B:629:ASN:ND2	1:B:631:SER:H	1.14	1.44
1:C:456:LYS:HB2	1:C:470:ASN:O	1.22	1.34
1:C:456:LYS:CB	1:C:470:ASN:O	1.84	1.24
1:C:659:THR:HG22	1:C:661:ALA:H	1.08	1.14
1:A:456:LYS:HB2	1:A:470:ASN:O	1.46	1.11
1:B:629:ASN:ND2	1:B:631:SER:N	1.98	1.10
1:A:632:TYR:O	1:A:643:ILE:O	1.69	1.09
1:B:376:GLN:HB2	1:B:379:ALA:HB3	1.33	1.08
1:A:666:ASN:O	1:A:670:ILE:HB	1.52	1.07
1:B:538:ILE:HG22	1:B:538:ILE:O	1.52	1.06
1:A:456:LYS:CB	1:A:470:ASN:O	2.02	1.06
1:B:353:LYS:H	1:B:368:GLN:NE2	1.55	1.04
1:B:581:GLN:NE2	1:B:629:ASN:H	1.55	1.04
1:A:705:TYR:CE2	2:D:139:GLU:HB3	1.93	1.04
1:C:629:ASN:ND2	1:C:631:SER:H	1.56	1.03
1:A:759:GLN:HE21	1:A:759:GLN:HA	1.21	1.03
1:C:510:GLN:O	1:C:514:ASP:OD1	1.77	1.03
4:C:1999:DOT:N2'	4:C:1999:DOT:O1'	1.93	1.02
1:A:633:ASN:HD21	1:A:645:TRP:H	1.09	1.01
1:B:348:LEU:HD21	1:B:577:HIS:HB3	1.43	1.00
1:A:629:ASN:ND2	1:A:631:SER:H	1.57	1.00
1:C:510:GLN:C	1:C:514:ASP:OD1	2.05	1.00
1:A:605:THR:HG21	1:A:611:THR:HA	1.43	1.00
1:C:759:GLN:HA	1:C:759:GLN:HE21	1.21	0.99
1:C:605:THR:HG21	1:C:611:THR:HA	1.44	0.99
1:A:295:VAL:HG21	1:A:603:ILE:HG22	1.44	0.99
1:C:664:ILE:HG21	2:F:15:ALA:HB2	1.45	0.99
1:B:629:ASN:HD22	1:B:631:SER:N	1.60	0.98
1:B:456:LYS:HB2	1:B:470:ASN:O	1.63	0.98
1:B:353:LYS:N	1:B:368:GLN:HE22	1.62	0.97
1:B:657:ILE:HG12	1:B:658:PRO:HD2	1.47	0.96
1:C:295:VAL:HG21	1:C:603:ILE:HG22	1.45	0.96
4:A:999:DOT:N2'	4:A:999:DOT:O1'	1.92	0.96
1:B:777:TYR:HD1	1:B:780:LEU:HD12	1.30	0.95
1:B:581:GLN:HE21	1:B:629:ASN:H	1.10	0.95
1:B:456:LYS:CB	1:B:470:ASN:O	2.16	0.94
2:E:25:GLY:HA3	2:E:65:PHE:CE1	2.03	0.94
1:A:695:LYS:HB2	2:D:18:LEU:HD22	1.49	0.93
1:C:633:ASN:HD21	1:C:645:TRP:H	1.15	0.93
1:B:538:ILE:O	1:B:538:ILE:CG2	2.15	0.93
1:A:629:ASN:HD22	1:A:631:SER:H	1.10	0.93
1:A:324:THR:HG21	1:A:556:MET:CE	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:ASN:C	1:B:520:PRO:HD3	1.94	0.93
2:D:25:GLY:HA3	2:D:65:PHE:CE1	2.04	0.93
1:B:322:LEU:O	1:B:324:THR:HG23	1.70	0.91
1:B:376:GLN:HB2	1:B:379:ALA:CB	2.01	0.91
2:F:25:GLY:HA3	2:F:65:PHE:CE1	2.06	0.91
1:C:657:ILE:HD13	1:C:756:ILE:HD13	1.54	0.89
1:B:360:VAL:HG11	1:B:365:PRO:HG3	1.54	0.89
1:B:587:PRO:HD2	1:B:639:ASN:HD21	1.36	0.89
1:A:559:ARG:HB3	1:A:559:ARG:HH11	1.38	0.89
1:A:639:ASN:ND2	1:A:641:ALA:H	1.70	0.89
1:B:516:VAL:HA	1:B:520:PRO:HG2	1.55	0.89
1:A:521:ASN:ND2	1:A:522:SER:H	1.69	0.89
1:C:705:TYR:CE2	2:F:139:GLU:HB3	2.08	0.88
1:B:296:LEU:HD12	1:B:604:LEU:HD22	1.55	0.88
1:B:509:PRO:HG2	1:B:512:GLU:HB3	1.55	0.88
1:C:659:THR:HG22	1:C:661:ALA:N	1.88	0.88
1:B:734:ASN:C	1:B:736:LEU:H	1.77	0.88
1:C:622:LYS:HA	1:C:622:LYS:HE3	1.55	0.88
2:E:20:ASP:OD2	2:E:22:ASP:HB2	1.74	0.88
1:B:514:ASP:HA	1:B:517:VAL:HG12	1.56	0.87
1:B:709:ASN:HD21	1:B:720:ILE:HD11	1.38	0.87
1:B:654:ILE:HA	1:B:755:ARG:CD	2.04	0.87
1:B:561:ASN:O	1:B:564:VAL:HG22	1.74	0.87
2:D:20:ASP:OD2	2:D:22:ASP:HB2	1.75	0.87
1:A:324:THR:HG21	1:A:556:MET:HE1	1.57	0.86
1:A:712:PHE:HD2	1:A:716:LYS:HG2	1.38	0.86
2:E:100:ILE:HB	2:E:136:VAL:HG23	1.56	0.86
1:A:513:TRP:CD2	1:A:517:VAL:HG21	2.09	0.86
1:B:717:LYS:HD2	2:E:132:GLY:N	1.91	0.86
1:C:657:ILE:HG13	1:C:759:GLN:HG2	1.57	0.86
1:A:522:SER:O	1:A:525:LYS:HB3	1.76	0.86
1:C:639:ASN:ND2	1:C:641:ALA:H	1.73	0.86
2:F:100:ILE:HB	2:F:136:VAL:HG23	1.55	0.86
2:F:20:ASP:OD2	2:F:22:ASP:HB2	1.75	0.85
1:C:712:PHE:HD2	1:C:716:LYS:HG2	1.41	0.85
1:B:756:ILE:O	1:B:760:VAL:HG23	1.76	0.85
1:C:540:ARG:NH2	1:C:627:TYR:CD1	2.45	0.85
1:B:779:GLN:NE2	1:B:796:ILE:HG13	1.92	0.84
1:A:525:LYS:O	1:A:529:VAL:HG23	1.76	0.84
1:C:694:VAL:HG23	1:C:695:LYS:H	1.41	0.84
1:B:391:ILE:HD12	1:B:399:GLY:HA2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:LYS:HB3	1:C:470:ASN:O	1.74	0.84
1:A:712:PHE:CD2	1:A:716:LYS:HG2	2.13	0.84
1:B:625:LEU:HD23	1:B:626:TYR:N	1.93	0.83
1:B:308:VAL:HB	1:B:311:HIS:CD2	2.13	0.83
2:D:100:ILE:HB	2:D:136:VAL:HG23	1.58	0.83
1:B:332:ASN:C	1:B:332:ASN:HD22	1.86	0.83
2:D:76:MET:HE3	2:D:79:THR:HG23	1.59	0.83
1:B:728:ALA:HA	1:B:731:GLU:HG3	1.60	0.83
1:B:629:ASN:HD21	1:B:631:SER:H	1.22	0.83
1:A:747:ASN:O	1:A:750:GLN:HG2	1.79	0.82
1:A:695:LYS:HG3	2:D:18:LEU:HD13	1.61	0.82
1:C:747:ASN:O	1:C:750:GLN:HG2	1.79	0.82
2:F:36:MET:O	2:F:41:GLN:HB2	1.79	0.82
1:A:445:ARG:CZ	1:A:471:TRP:NE1	2.43	0.81
1:B:629:ASN:HD21	1:B:631:SER:HB2	1.43	0.81
1:B:324:THR:HG22	1:B:499:PRO:HA	1.61	0.81
1:B:728:ALA:HA	1:B:731:GLU:CG	2.10	0.81
1:C:510:GLN:O	1:C:510:GLN:HG3	1.80	0.81
1:C:712:PHE:CD2	1:C:716:LYS:HG2	2.15	0.81
1:A:657:ILE:HD11	1:A:704:TYR:CE1	2.14	0.81
2:F:76:MET:HE3	2:F:79:THR:HG23	1.61	0.81
1:B:629:ASN:HD22	1:B:631:SER:H	0.83	0.81
2:E:76:MET:HE3	2:E:79:THR:HG23	1.60	0.81
1:B:649:ILE:HG22	1:B:649:ILE:O	1.80	0.81
1:A:445:ARG:HG3	1:A:471:TRP:CZ2	2.15	0.80
1:A:540:ARG:NH2	1:A:627:TYR:CD1	2.49	0.80
1:B:527:LYS:O	1:B:531:ASN:HB2	1.81	0.80
1:A:445:ARG:HH22	1:A:456:LYS:HD3	1.45	0.80
1:C:377:GLN:HA	1:C:380:VAL:HG12	1.64	0.80
2:E:36:MET:O	2:E:41:GLN:HB2	1.81	0.80
1:A:714:GLN:NE2	2:D:126:ARG:HG3	1.97	0.79
1:C:633:ASN:HD21	1:C:645:TRP:N	1.79	0.79
1:B:543:ASP:OD1	1:B:544:SER:N	2.14	0.79
1:C:387:ASN:OD1	1:C:477:MET:HE2	1.82	0.79
1:A:639:ASN:C	1:A:639:ASN:HD22	1.91	0.79
1:B:577:HIS:CD2	1:B:577:HIS:H	1.99	0.79
1:B:706:ASN:ND2	1:B:708:ALA:HB3	1.97	0.79
1:A:445:ARG:NH2	1:A:456:LYS:HD3	1.96	0.79
1:A:622:LYS:HE3	1:A:622:LYS:HA	1.65	0.79
1:A:348:LEU:HD23	1:A:348:LEU:O	1.82	0.78
1:C:559:ARG:HH11	1:C:559:ARG:HB3	1.45	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:629:ASN:HD22	1:C:631:SER:H	1.26	0.78
1:B:654:ILE:HA	1:B:755:ARG:HD2	1.64	0.78
1:A:492:TYR:CD2	1:A:574:VAL:HG13	2.19	0.78
1:B:550:SER:H	1:B:553:GLN:HG3	1.47	0.78
1:B:391:ILE:CD1	1:B:399:GLY:HA2	2.14	0.78
1:C:318:ILE:HD12	1:C:318:ILE:H	1.48	0.78
1:B:706:ASN:HD21	1:B:708:ALA:HB3	1.48	0.78
1:A:629:ASN:HD22	1:A:631:SER:N	1.81	0.77
1:B:731:GLU:OE2	1:B:733:GLU:HB2	1.84	0.77
1:B:597:ASN:ND2	1:B:601:GLU:HB2	1.99	0.77
1:B:581:GLN:HE21	1:B:629:ASN:N	1.82	0.77
1:B:779:GLN:HE22	1:B:796:ILE:HG13	1.48	0.77
1:B:565:LYS:O	1:B:567:THR:N	2.18	0.77
1:B:626:TYR:CD2	1:B:627:TYR:N	2.53	0.77
1:A:445:ARG:HG3	1:A:471:TRP:CH2	2.20	0.77
1:B:394:HIS:O	1:B:397:GLU:HG2	1.85	0.77
1:C:639:ASN:C	1:C:639:ASN:HD22	1.91	0.76
2:D:36:MET:O	2:D:41:GLN:HB2	1.85	0.76
1:A:657:ILE:HD11	1:A:704:TYR:CZ	2.21	0.76
1:B:615:ILE:HD12	1:B:645:TRP:CH2	2.20	0.76
1:A:657:ILE:CG2	1:A:756:ILE:HD13	2.16	0.76
1:B:709:ASN:OD1	1:B:717:LYS:HG3	1.85	0.76
1:B:712:PHE:HD1	1:B:712:PHE:H	1.34	0.76
1:C:729:TYR:HB2	1:C:756:ILE:HG21	1.65	0.76
1:A:729:TYR:HB2	1:A:756:ILE:HG21	1.65	0.76
1:A:318:ILE:HD12	1:A:318:ILE:H	1.47	0.76
1:B:565:LYS:C	1:B:567:THR:H	1.90	0.76
1:B:657:ILE:HG12	1:B:658:PRO:CD	2.16	0.76
1:A:492:TYR:HD2	1:A:574:VAL:HG13	1.51	0.76
1:A:377:GLN:HA	1:A:380:VAL:HG12	1.67	0.75
1:A:581:GLN:HE21	1:A:629:ASN:H	1.32	0.75
1:C:633:ASN:ND2	1:C:644:GLU:HA	2.02	0.75
1:C:492:TYR:CD2	1:C:574:VAL:HG13	2.21	0.75
1:C:794:GLN:O	1:C:797:ILE:HG13	1.85	0.75
1:C:348:LEU:HD23	1:C:348:LEU:O	1.85	0.75
1:B:526:GLN:CD	1:B:526:GLN:H	1.94	0.75
1:A:794:GLN:O	1:A:797:ILE:HG13	1.87	0.75
1:B:353:LYS:H	1:B:368:GLN:HE22	0.81	0.75
1:B:463:THR:HG23	1:B:467:GLU:O	1.86	0.74
1:B:506:LYS:NZ	1:B:506:LYS:HB3	2.01	0.74
1:B:560:LEU:O	1:B:564:VAL:HG13	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:VAL:HG22	1:C:360:VAL:O	1.87	0.74
1:C:629:ASN:HD22	1:C:631:SER:N	1.84	0.74
1:C:493:ASP:OD2	1:C:577:HIS:HE1	1.70	0.74
1:C:629:ASN:ND2	1:C:631:SER:N	2.34	0.74
1:C:632:TYR:O	1:C:643:ILE:O	2.05	0.74
1:A:657:ILE:CG2	1:A:756:ILE:HA	2.17	0.74
1:B:308:VAL:HB	1:B:311:HIS:HD2	1.52	0.74
1:B:626:TYR:HD2	1:B:627:TYR:N	1.85	0.74
1:C:540:ARG:HB3	1:C:549:LEU:C	2.12	0.74
1:A:456:LYS:HB3	1:A:470:ASN:O	1.85	0.74
1:C:722:ILE:HD13	1:C:764:LEU:HD23	1.69	0.74
1:C:700:TYR:HB3	1:C:728:ALA:HB2	1.67	0.74
1:A:493:ASP:OD2	1:A:577:HIS:CE1	2.40	0.74
1:A:759:GLN:HE21	1:A:759:GLN:CA	1.97	0.74
1:B:710:HIS:CE1	1:B:711:ILE:HG23	2.23	0.74
1:B:727:GLN:HG3	1:B:786:GLU:CD	2.13	0.74
1:A:360:VAL:HG22	1:A:360:VAL:O	1.85	0.74
1:A:581:GLN:NE2	1:A:628:PHE:HA	2.03	0.73
1:B:747:ASN:O	1:B:751:TYR:HB2	1.87	0.73
1:B:777:TYR:CD1	1:B:780:LEU:HD12	2.20	0.73
1:B:779:GLN:OE1	1:B:796:ILE:HG21	1.87	0.73
1:C:324:THR:HG21	1:C:556:MET:CE	2.17	0.73
1:C:516:VAL:HG12	1:C:516:VAL:O	1.86	0.73
1:B:745:TYR:HB3	1:B:749:PHE:HE1	1.51	0.73
1:A:722:ILE:HD13	1:A:764:LEU:HD23	1.68	0.73
1:B:366:PHE:HA	1:B:477:MET:CE	2.18	0.73
1:C:759:GLN:HE21	1:C:759:GLN:CA	1.97	0.73
1:A:387:ASN:CG	1:A:477:MET:HE2	2.13	0.73
2:D:89:PHE:C	2:D:89:PHE:CD2	2.66	0.73
2:E:70:THR:O	2:E:73:ALA:HB3	1.88	0.73
1:B:312:ALA:O	1:B:315:PHE:HB2	1.87	0.73
1:B:650:THR:HA	1:B:653:LYS:HB2	1.70	0.73
2:F:89:PHE:C	2:F:89:PHE:CD2	2.66	0.73
1:A:322:LEU:HD12	1:A:322:LEU:N	2.04	0.72
1:A:493:ASP:OD2	1:A:577:HIS:HE1	1.72	0.72
1:B:606:LYS:H	1:B:610:MET:CE	2.02	0.72
1:C:629:ASN:HB3	1:C:632:TYR:CD2	2.24	0.72
1:B:366:PHE:HA	1:B:477:MET:HE1	1.71	0.72
2:E:89:PHE:C	2:E:89:PHE:CD2	2.65	0.72
2:E:25:GLY:HA3	2:E:65:PHE:HE1	1.51	0.72
2:F:106:ARG:O	2:F:110:THR:HG23	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:106:ARG:O	2:E:110:THR:HG23	1.89	0.72
1:C:581:GLN:NE2	1:C:629:ASN:H	1.86	0.72
1:C:581:GLN:HE21	1:C:629:ASN:H	1.35	0.72
2:D:44:THR:HG22	2:D:47:GLU:HG3	1.71	0.72
1:B:540:ARG:NH2	1:B:630:ARG:CZ	2.53	0.71
1:C:518:ASN:O	1:C:519:THR:HB	1.90	0.71
1:B:657:ILE:CG1	1:B:658:PRO:HD2	2.19	0.71
1:C:523:LEU:HD21	2:F:127:GLU:HB3	1.72	0.71
1:C:748:TYR:O	1:C:751:TYR:HB3	1.90	0.71
1:C:621:GLY:O	2:F:94:LYS:HE3	1.90	0.71
2:F:81:SER:O	2:F:83:GLU:N	2.23	0.71
1:A:657:ILE:HG22	1:A:756:ILE:HA	1.73	0.71
1:B:332:ASN:ND2	1:B:334:LEU:H	1.87	0.71
1:B:456:LYS:HB3	1:B:470:ASN:O	1.91	0.71
1:B:470:ASN:OD1	1:B:471:TRP:N	2.23	0.71
1:B:530:THR:HG22	2:E:92:PHE:CZ	2.25	0.71
1:B:697:ILE:HD13	1:B:732:ILE:CD1	2.21	0.71
1:A:351:HIS:CD2	4:A:999:DOT:H3B	2.26	0.71
1:C:401:ILE:HD13	1:C:478:ALA:HB2	1.73	0.71
2:E:44:THR:HG22	2:E:47:GLU:HG3	1.72	0.71
1:A:581:GLN:NE2	1:A:629:ASN:H	1.88	0.71
2:E:81:SER:O	2:E:83:GLU:N	2.24	0.71
1:B:777:TYR:HD1	1:B:780:LEU:CD1	2.02	0.71
1:C:318:ILE:HG23	1:C:322:LEU:HD13	1.73	0.71
1:A:387:ASN:OD1	1:A:477:MET:HE2	1.89	0.70
1:A:540:ARG:HB3	1:A:549:LEU:C	2.16	0.70
1:A:445:ARG:HH12	1:A:456:LYS:HB3	1.56	0.70
1:A:513:TRP:O	1:A:517:VAL:HG23	1.91	0.70
1:C:387:ASN:CG	1:C:477:MET:HE2	2.17	0.70
2:E:65:PHE:HB2	2:E:66:PRO:HD3	1.72	0.70
1:C:302:LEU:HD23	1:C:302:LEU:C	2.16	0.70
2:F:65:PHE:HB2	2:F:66:PRO:HD3	1.74	0.70
1:B:363:TYR:O	1:B:365:PRO:HD3	1.92	0.70
1:B:540:ARG:NH1	2:E:87:GLU:OE1	2.24	0.70
1:C:723:PHE:HB2	1:C:793:PHE:CE2	2.26	0.70
2:D:25:GLY:HA3	2:D:65:PHE:HE1	1.54	0.70
2:D:106:ARG:O	2:D:110:THR:HG23	1.92	0.70
1:C:633:ASN:HD22	1:C:644:GLU:HA	1.57	0.70
1:A:633:ASN:ND2	1:A:645:TRP:H	1.87	0.70
2:D:25:GLY:O	2:D:64:ASP:HA	1.92	0.70
2:D:70:THR:O	2:D:73:ALA:HB3	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:C	1:A:302:LEU:HD23	2.17	0.70
1:C:446:ILE:HG12	1:C:447:SER:N	2.07	0.69
2:D:65:PHE:HB2	2:D:66:PRO:HD3	1.73	0.69
2:F:81:SER:O	2:F:82:GLU:C	2.35	0.69
2:F:44:THR:HG22	2:F:47:GLU:HG3	1.74	0.69
1:B:540:ARG:NH2	1:B:630:ARG:NH2	2.40	0.69
1:A:445:ARG:HH22	1:A:456:LYS:CD	2.06	0.69
1:B:385:LEU:HA	1:B:388:LYS:HD3	1.74	0.69
2:E:81:SER:O	2:E:82:GLU:C	2.35	0.69
1:B:585:GLU:O	1:B:638:GLY:HA3	1.93	0.69
1:B:349:ASN:OD1	1:B:350:VAL:HG23	1.93	0.69
1:A:782:PHE:HD1	1:A:782:PHE:H	1.39	0.69
1:B:376:GLN:CB	1:B:379:ALA:HB3	2.17	0.69
1:C:782:PHE:HD1	1:C:782:PHE:H	1.39	0.69
2:F:25:GLY:HA3	2:F:65:PHE:HE1	1.55	0.69
1:A:723:PHE:HB2	1:A:793:PHE:CE2	2.27	0.69
1:B:332:ASN:C	1:B:332:ASN:ND2	2.49	0.69
1:B:478:ALA:HB1	1:B:486:LYS:O	1.92	0.69
1:C:367:ASP:O	1:C:369:ASP:N	2.26	0.69
1:C:492:TYR:HD2	1:C:574:VAL:HG13	1.54	0.69
2:D:133:ASP:OD1	2:D:135:GLN:HG3	1.93	0.69
1:C:501:LEU:O	1:C:504:ILE:HG22	1.93	0.68
1:A:477:MET:O	1:A:488:LEU:HD12	1.93	0.68
1:A:657:ILE:HG22	1:A:756:ILE:HD13	1.75	0.68
1:B:525:LYS:HB2	1:B:526:GLN:NE2	2.07	0.68
1:B:653:LYS:O	1:B:755:ARG:HD3	1.93	0.68
2:D:48:LEU:O	2:D:52:ILE:HG22	1.92	0.68
2:F:25:GLY:O	2:F:64:ASP:HA	1.93	0.68
1:C:324:THR:HG21	1:C:556:MET:HE1	1.76	0.68
1:C:657:ILE:HD13	1:C:756:ILE:CD1	2.23	0.68
1:A:748:TYR:O	1:A:751:TYR:HB3	1.94	0.68
1:A:759:GLN:HA	1:A:759:GLN:NE2	2.01	0.68
1:A:782:PHE:CD1	1:A:782:PHE:N	2.61	0.68
2:D:136:VAL:HA	2:D:140:GLU:OE1	1.92	0.68
1:B:454:GLN:HB3	1:B:472:ARG:O	1.93	0.68
1:C:782:PHE:CD1	1:C:782:PHE:N	2.62	0.68
1:C:793:PHE:O	1:C:796:ILE:HG12	1.94	0.68
2:F:70:THR:O	2:F:73:ALA:HB3	1.93	0.68
1:B:432:TYR:CD2	1:B:447:SER:HA	2.28	0.68
1:B:619:ILE:C	1:B:621:GLY:H	2.00	0.68
1:B:748:TYR:O	1:B:752:LEU:HG	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:ILE:HD13	1:C:532:LEU:HB3	1.75	0.68
1:B:720:ILE:HD12	1:B:721:SER:N	2.08	0.68
1:C:445:ARG:NH1	1:C:471:TRP:CD1	2.62	0.68
1:C:665:LYS:HE2	2:F:11:GLU:OE2	1.92	0.68
1:A:446:ILE:HG12	1:A:447:SER:N	2.09	0.68
1:A:501:LEU:O	1:A:504:ILE:HG22	1.94	0.68
1:C:514:ASP:HA	1:C:517:VAL:HG12	1.76	0.68
1:C:759:GLN:HA	1:C:759:GLN:NE2	2.01	0.68
1:C:463:THR:HG22	1:C:465:LEU:H	1.59	0.68
1:C:690:LYS:HG2	1:C:691:LYS:O	1.94	0.68
1:B:615:ILE:HD13	1:B:626:TYR:CE1	2.28	0.67
1:B:596:ILE:HG12	1:B:602:PHE:CE2	2.29	0.67
2:F:48:LEU:O	2:F:52:ILE:HG22	1.95	0.67
1:A:313:ASP:HA	1:A:316:LYS:HE2	1.77	0.67
1:B:462:ILE:HD11	1:B:466:GLY:HA2	1.76	0.67
1:C:313:ASP:HA	1:C:316:LYS:HE2	1.77	0.67
2:F:136:VAL:HA	2:F:140:GLU:OE1	1.95	0.67
1:A:367:ASP:O	1:A:369:ASP:N	2.28	0.67
1:A:388:LYS:O	1:A:392:THR:HG23	1.95	0.67
1:B:734:ASN:O	1:B:736:LEU:N	2.28	0.67
1:B:747:ASN:O	1:B:751:TYR:CB	2.43	0.67
1:B:760:VAL:O	1:B:764:LEU:HG	1.95	0.67
1:C:712:PHE:HB3	1:C:716:LYS:HG2	1.75	0.67
1:B:310:GLU:CD	1:B:310:GLU:H	2.03	0.67
1:B:388:LYS:O	1:B:392:THR:HG23	1.94	0.67
2:D:81:SER:O	2:D:82:GLU:C	2.37	0.67
1:B:432:TYR:HE2	1:B:447:SER:HB2	1.59	0.66
1:A:793:PHE:O	1:A:796:ILE:HG12	1.94	0.66
1:C:561:ASN:O	1:C:565:LYS:HG3	1.96	0.66
2:E:48:LEU:O	2:E:52:ILE:HG22	1.95	0.66
1:A:295:VAL:HG21	1:A:603:ILE:CG2	2.22	0.66
1:A:630:ARG:HE	2:D:87:GLU:CD	2.03	0.66
1:B:746:LYS:O	1:B:750:GLN:N	2.29	0.66
1:C:654:ILE:O	1:C:755:ARG:HG2	1.95	0.66
2:E:25:GLY:O	2:E:64:ASP:HA	1.94	0.66
1:A:463:THR:HG22	1:A:465:LEU:N	2.10	0.66
1:A:295:VAL:CG2	1:A:603:ILE:HG22	2.22	0.66
1:A:561:ASN:O	1:A:565:LYS:HG3	1.96	0.66
1:C:758:ASN:O	1:C:762:LEU:HB2	1.95	0.66
1:A:324:THR:HG21	1:A:556:MET:HE3	1.77	0.66
1:A:700:TYR:HD1	1:A:728:ALA:HA	1.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ASN:HB3	1:A:412:GLU:OE2	1.95	0.66
1:C:463:THR:HG22	1:C:465:LEU:N	2.10	0.66
2:D:101:SER:OG	2:D:104:GLU:HG3	1.96	0.66
1:A:670:ILE:HD12	1:A:745:TYR:CE1	2.31	0.66
1:B:324:THR:CG2	1:B:499:PRO:HA	2.26	0.66
1:B:616:GLU:HA	1:B:620:THR:HG22	1.78	0.66
2:D:81:SER:O	2:D:83:GLU:N	2.29	0.66
1:A:705:TYR:HE2	2:D:139:GLU:HB3	1.58	0.65
1:C:388:LYS:O	1:C:392:THR:HG23	1.96	0.65
1:C:705:TYR:HE2	2:F:139:GLU:HB3	1.55	0.65
1:B:366:PHE:HD1	1:B:477:MET:HE1	1.59	0.65
1:B:562:GLU:HA	1:B:565:LYS:HG3	1.77	0.65
1:C:540:ARG:NH2	1:C:627:TYR:CE1	2.65	0.65
2:E:115:LYS:O	2:E:116:LEU:HD23	1.95	0.65
1:A:758:ASN:O	1:A:762:LEU:HB2	1.96	0.65
2:E:101:SER:OG	2:E:104:GLU:HG3	1.97	0.65
1:B:535:LYS:C	1:B:536:TYR:HD2	2.03	0.65
1:B:792:VAL:HG12	1:B:792:VAL:O	1.96	0.65
1:A:377:GLN:O	1:A:379:ALA:N	2.29	0.65
1:A:521:ASN:ND2	1:A:522:SER:N	2.44	0.65
1:A:639:ASN:HD22	1:A:641:ALA:H	1.45	0.65
1:B:513:TRP:HH2	2:E:113:GLY:HA3	1.61	0.65
1:A:408:LEU:C	1:A:408:LEU:HD23	2.20	0.65
1:C:438:ASN:C	1:C:438:ASN:HD22	2.05	0.65
1:A:401:ILE:HD13	1:A:478:ALA:HB2	1.78	0.65
1:B:577:HIS:CD2	1:B:577:HIS:N	2.65	0.65
1:A:481:VAL:HG23	1:A:481:VAL:O	1.97	0.65
1:A:633:ASN:HD21	1:A:645:TRP:N	1.88	0.65
1:B:629:ASN:HD21	1:B:631:SER:N	1.84	0.65
1:B:722:ILE:HD13	1:B:764:LEU:HD21	1.78	0.65
2:E:92:PHE:CE2	2:E:108:VAL:HG11	2.32	0.65
1:C:295:VAL:HG21	1:C:603:ILE:CG2	2.24	0.64
1:C:337:ASN:HB3	1:C:412:GLU:OE2	1.98	0.64
1:C:740:GLN:H	1:C:740:GLN:CD	2.05	0.64
1:A:513:TRP:CE3	1:A:517:VAL:HG21	2.32	0.64
1:A:656:THR:O	1:A:755:ARG:HD2	1.97	0.64
1:B:306:GLY:O	1:B:336:THR:HB	1.96	0.64
1:C:530:THR:HG21	2:F:145:MET:CE	2.27	0.64
1:C:692:GLU:O	1:C:735:VAL:HG22	1.96	0.64
1:B:615:ILE:HD12	1:B:645:TRP:HH2	1.60	0.64
1:C:353:LYS:HG3	1:C:373:LYS:HD3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:92:PHE:CD2	2:E:108:VAL:HG21	2.32	0.64
2:F:140:GLU:O	2:F:142:VAL:N	2.30	0.64
1:C:349:ASN:HD21	1:C:398:ILE:HG13	1.62	0.64
1:C:463:THR:HB	1:C:467:GLU:H	1.63	0.64
1:A:445:ARG:NH2	1:A:471:TRP:NE1	2.45	0.64
1:B:377:GLN:HG2	1:B:378:LEU:HD22	1.80	0.64
1:B:654:ILE:HA	1:B:755:ARG:CG	2.26	0.64
1:C:522:SER:O	1:C:525:LYS:N	2.30	0.64
1:A:353:LYS:HG3	1:A:373:LYS:HD3	1.78	0.64
1:A:663:PHE:CE1	1:A:752:LEU:HD11	2.32	0.64
1:B:529:VAL:HG11	2:E:109:MET:HE1	1.80	0.64
1:B:606:LYS:H	1:B:610:MET:HE2	1.63	0.64
1:A:658:PRO:O	1:A:701:LEU:HD13	1.98	0.64
1:B:597:ASN:HD21	1:B:601:GLU:HB2	1.62	0.64
1:A:463:THR:HG22	1:A:465:LEU:H	1.61	0.63
1:A:696:LYS:HE2	1:A:696:LYS:HA	1.80	0.63
1:B:697:ILE:HD13	1:B:732:ILE:HD13	1.80	0.63
2:E:136:VAL:HA	2:E:140:GLU:OE1	1.98	0.63
1:A:633:ASN:HD22	1:A:644:GLU:HA	1.63	0.63
1:C:349:ASN:ND2	1:C:398:ILE:HG13	2.13	0.63
2:E:5:THR:OG1	2:E:8:GLN:HB2	1.98	0.63
1:A:445:ARG:NH2	1:A:471:TRP:HE1	1.95	0.63
1:B:712:PHE:CD1	1:B:712:PHE:N	2.66	0.63
1:A:438:ASN:HD22	1:A:438:ASN:C	2.05	0.63
1:B:712:PHE:HD1	1:B:712:PHE:N	1.97	0.63
1:B:722:ILE:HD13	1:B:764:LEU:CD2	2.29	0.63
1:B:728:ALA:CA	1:B:731:GLU:HG3	2.28	0.63
1:A:722:ILE:HD13	1:A:764:LEU:CD2	2.28	0.63
1:C:622:LYS:O	1:C:623:ASP:HB2	1.97	0.63
2:D:76:MET:HE3	2:D:79:THR:CG2	2.28	0.63
1:B:320:ARG:HH21	1:B:320:ARG:HG3	1.64	0.63
1:B:360:VAL:CG1	1:B:365:PRO:HG3	2.28	0.63
1:B:407:HIS:H	1:B:407:HIS:CD2	2.16	0.63
1:B:711:ILE:HG13	1:B:712:PHE:CD1	2.34	0.63
1:A:349:ASN:HD21	1:A:398:ILE:HG13	1.62	0.63
1:A:653:LYS:O	1:A:755:ARG:HD3	1.99	0.63
1:B:432:TYR:HD2	1:B:447:SER:HA	1.61	0.63
1:B:656:THR:O	1:B:705:TYR:HE1	1.80	0.63
1:C:326:ILE:C	1:C:327:LEU:HD12	2.24	0.63
1:A:697:ILE:HD12	1:A:697:ILE:N	2.14	0.63
1:C:508:ILE:HG12	1:C:536:TYR:CD2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:653:LYS:O	1:C:656:THR:HG23	1.99	0.63
2:D:99:TYR:CD2	2:D:137:ASN:HB3	2.34	0.62
2:F:115:LYS:O	2:F:116:LEU:HD23	1.99	0.62
1:A:385:LEU:HD13	1:A:385:LEU:O	1.99	0.62
1:B:424:LYS:HE2	1:B:433:TYR:OH	1.98	0.62
1:C:722:ILE:HD13	1:C:764:LEU:CD2	2.29	0.62
1:C:722:ILE:HG23	1:C:760:VAL:HG13	1.81	0.62
1:C:327:LEU:HG	1:C:595:ILE:HG23	1.81	0.62
2:D:115:LYS:O	2:D:116:LEU:HD23	1.99	0.62
1:B:376:GLN:CB	1:B:379:ALA:CB	2.77	0.62
1:B:525:LYS:O	1:B:529:VAL:HG22	1.99	0.62
1:B:777:TYR:CD1	1:B:780:LEU:HB2	2.34	0.62
1:C:324:THR:HG23	1:C:324:THR:O	1.99	0.62
1:C:581:GLN:NE2	1:C:628:PHE:HA	2.14	0.62
2:E:133:ASP:OD1	2:E:135:GLN:HG3	2.00	0.62
2:F:133:ASP:OD1	2:F:135:GLN:HG3	1.99	0.62
1:A:318:ILE:HD12	1:A:318:ILE:N	2.14	0.62
1:B:649:ILE:O	1:B:649:ILE:CG2	2.48	0.62
2:E:140:GLU:O	2:E:142:VAL:N	2.31	0.62
1:B:333:LYS:O	1:B:336:THR:HG22	1.99	0.62
1:C:408:LEU:C	1:C:408:LEU:HD23	2.25	0.62
1:C:319:ALA:O	1:C:598:PRO:HA	1.99	0.62
1:C:602:PHE:O	1:C:603:ILE:HD13	1.99	0.62
1:C:700:TYR:CE1	1:C:727:GLN:HG2	2.35	0.62
1:B:633:ASN:O	1:B:634:LYS:HG3	2.00	0.62
1:B:361:ALA:O	1:B:409:ARG:NH2	2.30	0.62
1:B:419:ILE:HD12	1:B:435:LEU:HD22	1.81	0.62
1:B:445:ARG:HB3	1:B:471:TRP:CZ3	2.35	0.62
2:F:99:TYR:CD2	2:F:137:ASN:HB3	2.35	0.62
1:B:519:THR:N	1:B:520:PRO:HD3	2.15	0.61
1:B:723:PHE:O	1:B:727:GLN:N	2.30	0.61
1:C:525:LYS:HB2	2:F:124:MET:CE	2.30	0.61
1:A:622:LYS:O	1:A:623:ASP:HB2	2.00	0.61
1:B:514:ASP:HA	1:B:517:VAL:CG1	2.29	0.61
2:F:65:PHE:O	2:F:69:LEU:HG	2.00	0.61
1:B:649:ILE:CD1	2:E:86:ARG:HG3	2.29	0.61
1:B:653:LYS:O	1:B:653:LYS:HG3	1.99	0.61
1:C:481:VAL:HG23	1:C:481:VAL:O	2.00	0.61
1:A:299:GLU:HG3	1:A:303:LYS:HZ2	1.65	0.61
1:A:605:THR:CG2	1:A:611:THR:HA	2.25	0.61
1:A:712:PHE:HB3	1:A:716:LYS:HG2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:ASP:OD2	1:C:546:LYS:HG3	1.99	0.61
1:B:639:ASN:H	1:B:639:ASN:ND2	1.98	0.61
1:B:501:LEU:HB2	1:B:623:ASP:O	2.01	0.61
1:B:722:ILE:HG22	1:B:726:ILE:HD12	1.81	0.61
1:C:377:GLN:O	1:C:378:LEU:C	2.42	0.61
1:C:377:GLN:O	1:C:379:ALA:N	2.33	0.61
2:E:99:TYR:CD2	2:E:137:ASN:HB3	2.36	0.61
1:B:331:VAL:O	1:B:332:ASN:C	2.44	0.61
1:B:508:ILE:HG21	1:B:532:LEU:HD22	1.83	0.61
1:B:773:PHE:C	1:B:775:LEU:H	2.08	0.61
1:C:653:LYS:O	1:C:755:ARG:HD3	2.01	0.61
1:C:385:LEU:HD13	1:C:385:LEU:O	2.01	0.61
1:C:649:ILE:HD13	2:F:90:ARG:HE	1.66	0.61
1:B:554:LYS:O	1:B:555:GLN:C	2.43	0.61
1:C:639:ASN:ND2	1:C:639:ASN:C	2.59	0.61
1:C:663:PHE:HD2	1:C:664:ILE:HD12	1.66	0.61
1:A:349:ASN:ND2	1:A:398:ILE:HG13	2.16	0.61
1:A:792:VAL:HG12	1:A:796:ILE:HD11	1.83	0.61
1:C:657:ILE:HG22	1:C:658:PRO:N	2.16	0.61
1:C:776:LEU:N	1:C:776:LEU:HD12	2.15	0.61
2:F:63:ILE:N	2:F:63:ILE:HD12	2.16	0.61
1:B:339:ILE:HG12	1:B:489:THR:HG21	1.83	0.60
1:C:535:LYS:HE2	1:C:536:TYR:CZ	2.36	0.60
1:A:377:GLN:O	1:A:378:LEU:C	2.44	0.60
1:B:459:GLU:O	1:B:461:LYS:N	2.27	0.60
1:C:659:THR:HB	1:C:662:GLU:HG3	1.82	0.60
2:F:68:PHE:HA	2:F:71:MET:HE3	1.83	0.60
2:F:76:MET:HE3	2:F:79:THR:CG2	2.29	0.60
1:C:368:GLN:HB2	1:C:384:ASN:OD1	2.02	0.60
2:F:130:ILE:HG22	2:F:130:ILE:O	2.01	0.60
1:B:720:ILE:HD12	1:B:720:ILE:C	2.26	0.60
1:C:324:THR:O	1:C:324:THR:CG2	2.50	0.60
1:A:299:GLU:HG3	1:A:303:LYS:NZ	2.16	0.60
1:B:733:GLU:C	1:B:735:VAL:H	2.10	0.60
1:A:445:ARG:CZ	1:A:471:TRP:CD1	2.83	0.60
1:B:319:ALA:HB2	1:B:326:ILE:HD12	1.83	0.60
1:B:346:LYS:NZ	1:B:352:GLY:O	2.34	0.60
1:B:516:VAL:CA	1:B:520:PRO:HG2	2.28	0.60
1:A:538:ILE:HD11	2:D:91:VAL:HG21	1.83	0.60
1:A:632:TYR:C	1:A:643:ILE:O	2.42	0.60
2:F:7:GLU:O	2:F:11:GLU:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:117:THR:C	2:F:119:GLU:H	2.08	0.60
1:A:776:LEU:HD12	1:A:776:LEU:N	2.17	0.60
1:A:462:ILE:HD11	1:A:466:GLY:HA2	1.83	0.59
1:A:540:ARG:HD3	1:A:582:ASP:OD1	2.01	0.59
1:A:587:PRO:HB2	1:A:643:ILE:HD12	1.83	0.59
1:B:318:ILE:HD12	1:B:319:ALA:N	2.18	0.59
1:B:498:ALA:CB	1:B:619:ILE:HD13	2.32	0.59
1:B:615:ILE:HD12	1:B:645:TRP:CZ2	2.37	0.59
2:E:7:GLU:O	2:E:11:GLU:HG3	2.01	0.59
1:A:589:LYS:HE2	1:A:643:ILE:HG23	1.85	0.59
1:B:711:ILE:HG13	1:B:712:PHE:HD1	1.67	0.59
1:C:639:ASN:HD22	1:C:641:ALA:H	1.51	0.59
1:B:427:ASP:C	1:B:429:GLY:H	2.11	0.59
1:A:659:THR:OG1	1:A:660:SER:N	2.31	0.59
1:A:787:THR:O	1:A:791:GLU:HG2	2.02	0.59
1:B:432:TYR:CE2	1:B:447:SER:HB2	2.37	0.59
1:C:655:ASN:N	1:C:655:ASN:HD22	1.97	0.59
1:A:670:ILE:HG23	1:A:745:TYR:CE1	2.38	0.59
1:C:294:ASP:O	1:C:610:MET:HE1	2.03	0.59
1:C:605:THR:CG2	1:C:611:THR:HA	2.27	0.59
1:A:695:LYS:CB	2:D:18:LEU:HD22	2.30	0.59
1:B:554:LYS:O	1:B:557:LEU:N	2.35	0.59
1:C:583:ASN:ND2	4:C:1999:DOT:H1'	2.18	0.59
1:C:587:PRO:HB2	1:C:643:ILE:HD12	1.83	0.59
2:D:20:ASP:C	2:D:22:ASP:H	2.11	0.59
2:E:20:ASP:C	2:E:22:ASP:H	2.10	0.59
2:E:117:THR:C	2:E:119:GLU:H	2.09	0.59
1:A:432:TYR:CE1	1:A:471:TRP:HZ3	2.20	0.59
1:B:540:ARG:HH22	1:B:630:ARG:CZ	2.15	0.59
1:C:639:ASN:HD22	1:C:640:LYS:N	2.00	0.59
1:A:517:VAL:C	1:A:525:LYS:HZ1	2.10	0.59
1:A:592:GLU:HB3	1:A:604:LEU:HD21	1.85	0.59
1:A:639:ASN:ND2	1:A:639:ASN:C	2.60	0.59
1:B:629:ASN:HD21	1:B:631:SER:CB	2.14	0.59
1:B:752:LEU:O	1:B:756:ILE:HG13	2.02	0.59
1:C:631:SER:O	1:C:632:TYR:C	2.44	0.59
1:A:722:ILE:HG23	1:A:760:VAL:HG13	1.83	0.59
1:B:322:LEU:HA	1:B:503:GLU:OE1	2.02	0.59
1:B:540:ARG:HD2	1:B:627:TYR:CE1	2.38	0.59
1:B:546:LYS:HD2	1:B:546:LYS:N	2.18	0.59
1:B:733:GLU:O	1:B:735:VAL:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:ILE:HD12	1:A:697:ILE:H	1.67	0.58
4:C:1999:DOT:O1'	4:C:1999:DOT:H2'1	2.01	0.58
1:B:366:PHE:CD1	1:B:477:MET:HE1	2.37	0.58
1:B:606:LYS:N	1:B:610:MET:CE	2.65	0.58
2:E:76:MET:HE3	2:E:79:THR:CG2	2.30	0.58
1:C:661:ALA:C	1:C:663:PHE:H	2.11	0.58
1:C:698:ALA:O	1:C:701:LEU:HB2	2.02	0.58
1:C:792:VAL:HG12	1:C:796:ILE:HD11	1.84	0.58
1:A:652:ALA:O	1:A:653:LYS:C	2.46	0.58
1:B:605:THR:HG22	1:B:606:LYS:N	2.18	0.58
1:C:295:VAL:HG23	1:C:604:LEU:O	2.02	0.58
1:C:320:ARG:HG3	1:C:598:PRO:O	2.02	0.58
1:C:363:TYR:HD1	1:C:403:LEU:HD11	1.68	0.58
1:C:477:MET:O	1:C:488:LEU:HD12	2.03	0.58
1:A:521:ASN:CG	1:A:522:SER:N	2.60	0.58
1:A:621:GLY:O	2:D:94:LYS:HE3	2.03	0.58
1:B:761:GLN:OE1	1:B:765:THR:HG23	2.04	0.58
2:D:65:PHE:O	2:D:69:LEU:HG	2.04	0.58
2:D:117:THR:C	2:D:119:GLU:H	2.11	0.58
1:A:454:GLN:OE1	1:A:471:TRP:CE3	2.56	0.58
1:B:728:ALA:HA	1:B:731:GLU:HG2	1.86	0.58
1:C:318:ILE:HD12	1:C:318:ILE:N	2.17	0.58
1:C:659:THR:O	1:C:701:LEU:HD13	2.04	0.58
2:D:63:ILE:N	2:D:63:ILE:HD12	2.19	0.58
1:C:445:ARG:HH12	1:C:471:TRP:CD1	2.22	0.58
1:C:519:THR:O	1:C:525:LYS:HE2	2.04	0.58
1:C:664:ILE:CG2	2:F:15:ALA:HB2	2.24	0.58
2:E:68:PHE:HA	2:E:71:MET:HE3	1.86	0.58
1:B:606:LYS:HG3	1:B:610:MET:HE1	1.86	0.58
1:B:621:GLY:O	2:E:94:LYS:HE3	2.04	0.58
1:C:529:VAL:HG21	2:F:109:MET:HE1	1.86	0.58
1:C:707:SER:C	1:C:709:ASN:H	2.12	0.58
1:A:322:LEU:HD12	1:A:322:LEU:H	1.68	0.58
1:B:761:GLN:OE1	1:B:761:GLN:HA	2.03	0.58
1:C:450:ASN:O	1:C:451:ASN:HB2	2.04	0.58
2:D:68:PHE:HA	2:D:71:MET:HE3	1.86	0.58
2:D:140:GLU:O	2:D:142:VAL:N	2.37	0.58
1:C:558:ASP:O	1:C:562:GLU:HG3	2.03	0.58
2:F:5:THR:O	2:F:9:ILE:HG13	2.03	0.58
2:F:62:THR:C	2:F:63:ILE:HD12	2.29	0.58
1:B:354:SER:O	1:B:371:SER:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:ALA:HB3	1:C:604:LEU:HD13	1.86	0.57
1:C:584:GLU:OE1	1:C:630:ARG:HG3	2.04	0.57
2:D:133:ASP:OD1	2:D:135:GLN:O	2.22	0.57
1:A:440:GLN:H	1:A:440:GLN:CD	2.13	0.57
1:B:550:SER:N	1:B:553:GLN:HG3	2.19	0.57
1:C:324:THR:OG1	1:C:499:PRO:HA	2.04	0.57
1:C:697:ILE:HD11	1:C:735:VAL:HG21	1.85	0.57
1:A:295:VAL:HG23	1:A:604:LEU:O	2.04	0.57
1:A:540:ARG:NH1	1:A:630:ARG:HH21	2.03	0.57
1:B:307:LEU:HD21	1:B:328:PHE:CD1	2.40	0.57
1:B:629:ASN:HD22	1:B:629:ASN:C	2.11	0.57
1:C:302:LEU:HD12	1:C:602:PHE:HE1	1.69	0.57
2:F:131:ASP:OD1	2:F:133:ASP:OD2	2.22	0.57
1:A:790:PHE:O	1:A:793:PHE:HB3	2.05	0.57
1:C:462:ILE:HD11	1:C:466:GLY:HA2	1.85	0.57
1:A:385:LEU:HD13	1:A:385:LEU:C	2.29	0.57
1:B:586:PHE:N	1:B:587:PRO:HD3	2.20	0.57
1:B:657:ILE:CG1	1:B:658:PRO:CD	2.81	0.57
1:A:707:SER:C	1:A:709:ASN:H	2.12	0.57
1:B:605:THR:HG21	1:B:611:THR:OG1	2.03	0.57
2:E:65:PHE:O	2:E:69:LEU:HG	2.05	0.57
2:E:72:MET:C	2:E:74:ARG:H	2.12	0.57
1:A:583:ASN:ND2	4:A:999:DOT:H1'	2.19	0.57
1:C:669:SER:C	1:C:671:ARG:H	2.13	0.57
1:A:523:LEU:C	1:A:525:LYS:H	2.13	0.57
1:B:513:TRP:CH2	2:E:113:GLY:HA3	2.40	0.57
1:C:450:ASN:OD1	1:C:452:GLU:HG3	2.05	0.57
1:C:714:GLN:NE2	2:F:126:ARG:HG2	2.20	0.57
1:C:787:THR:O	1:C:791:GLU:HG2	2.05	0.57
2:F:89:PHE:C	2:F:89:PHE:HD2	2.13	0.57
1:A:574:VAL:HG13	1:A:574:VAL:O	2.05	0.56
1:C:324:THR:OG1	1:C:499:PRO:CA	2.53	0.56
1:C:363:TYR:CD1	1:C:403:LEU:HD11	2.40	0.56
2:F:137:ASN:OD1	2:F:139:GLU:HB2	2.05	0.56
1:A:505:LYS:HD3	2:D:112:LEU:O	2.05	0.56
1:A:781:ASN:ND2	1:A:783:THR:OG1	2.38	0.56
1:B:307:LEU:HD21	1:B:328:PHE:CE1	2.40	0.56
1:B:385:LEU:CD2	1:B:389:LYS:HE2	2.36	0.56
1:C:518:ASN:O	1:C:519:THR:CB	2.54	0.56
1:C:606:LYS:O	1:C:607:ASN:HB3	2.05	0.56
1:C:712:PHE:CD2	1:C:716:LYS:HE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:92:PHE:CD2	2:F:108:VAL:HG21	2.40	0.56
1:A:712:PHE:CD2	1:A:716:LYS:HE2	2.41	0.56
1:B:327:LEU:HG	1:B:595:ILE:HG23	1.88	0.56
1:B:509:PRO:HD2	1:B:536:TYR:HE1	1.69	0.56
1:B:562:GLU:O	1:B:564:VAL:N	2.38	0.56
1:B:597:ASN:HB2	1:B:598:PRO:HD2	1.87	0.56
1:B:728:ALA:C	1:B:730:ASN:H	2.13	0.56
2:E:133:ASP:OD1	2:E:135:GLN:O	2.23	0.56
2:F:20:ASP:C	2:F:22:ASP:H	2.11	0.56
2:F:72:MET:C	2:F:74:ARG:H	2.14	0.56
1:B:753:LYS:O	1:B:757:THR:OG1	2.23	0.56
1:C:295:VAL:HG22	1:C:296:LEU:N	2.19	0.56
1:A:318:ILE:H	1:A:318:ILE:CD1	2.17	0.56
1:A:378:LEU:HD22	1:B:378:LEU:HD11	1.87	0.56
1:A:384:ASN:O	1:A:385:LEU:C	2.48	0.56
1:B:415:GLU:C	1:B:417:GLY:H	2.11	0.56
1:B:606:LYS:H	1:B:610:MET:HE3	1.71	0.56
2:E:36:MET:C	2:E:41:GLN:HB2	2.31	0.56
1:A:318:ILE:HG23	1:A:322:LEU:HD13	1.86	0.56
1:A:509:PRO:HD3	1:A:536:TYR:HE1	1.70	0.56
1:A:581:GLN:HE21	1:A:629:ASN:N	2.03	0.56
1:C:639:ASN:ND2	1:C:641:ALA:N	2.50	0.56
1:B:785:ASN:O	1:B:786:GLU:C	2.48	0.56
1:A:385:LEU:CD1	1:A:389:LYS:HD2	2.36	0.56
1:B:415:GLU:C	1:B:417:GLY:N	2.61	0.56
1:B:506:LYS:HB3	1:B:506:LYS:HZ3	1.68	0.56
1:B:565:LYS:C	1:B:567:THR:N	2.55	0.56
1:B:751:TYR:O	1:B:754:GLU:N	2.39	0.56
1:C:607:ASN:HD21	1:C:609:GLU:HB2	1.71	0.56
2:E:63:ILE:HD12	2:E:63:ILE:N	2.20	0.56
1:A:394:HIS:O	1:A:395:GLU:C	2.49	0.56
1:B:308:VAL:O	1:B:311:HIS:HB2	2.06	0.56
2:E:89:PHE:C	2:E:89:PHE:HD2	2.11	0.56
1:A:308:VAL:HG23	1:A:492:TYR:OH	2.06	0.56
1:A:513:TRP:CE2	1:A:517:VAL:HG21	2.41	0.56
1:B:324:THR:HG22	1:B:499:PRO:CA	2.35	0.56
1:B:332:ASN:ND2	1:B:334:LEU:N	2.53	0.56
1:C:608:TRP:O	1:C:609:GLU:C	2.47	0.56
2:E:130:ILE:O	2:E:130:ILE:HG22	2.06	0.56
1:C:523:LEU:CD2	2:F:127:GLU:HB3	2.36	0.55
1:C:603:ILE:HG22	1:C:604:LEU:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:697:ILE:HD13	1:C:732:ILE:HG12	1.88	0.55
2:D:7:GLU:O	2:D:11:GLU:HG3	2.05	0.55
2:F:140:GLU:C	2:F:142:VAL:N	2.64	0.55
1:B:400:LYS:HD2	1:B:475:GLU:OE2	2.05	0.55
1:B:454:GLN:CB	1:B:472:ARG:O	2.54	0.55
1:C:628:PHE:CD1	1:C:628:PHE:C	2.84	0.55
2:D:92:PHE:CE2	2:D:108:VAL:HG11	2.41	0.55
1:A:368:GLN:HB2	1:A:384:ASN:OD1	2.07	0.55
1:A:450:ASN:O	1:A:451:ASN:HB2	2.06	0.55
1:B:616:GLU:HG3	1:B:617:LYS:N	2.20	0.55
1:B:654:ILE:HA	1:B:755:ARG:HG2	1.87	0.55
1:A:293:ILE:O	1:A:293:ILE:HG13	2.06	0.55
1:A:322:LEU:HB3	1:A:503:GLU:OE2	2.05	0.55
1:A:540:ARG:NH1	1:A:630:ARG:NH2	2.54	0.55
1:B:298:GLY:O	1:B:299:GLU:C	2.48	0.55
1:B:536:TYR:N	1:B:536:TYR:CD2	2.73	0.55
1:C:527:LYS:NZ	2:F:145:MET:O	2.39	0.55
1:C:652:ALA:O	1:C:656:THR:HG22	2.07	0.55
1:C:775:LEU:HB2	1:C:776:LEU:HD12	1.87	0.55
2:E:117:THR:C	2:E:119:GLU:N	2.64	0.55
1:A:463:THR:HB	1:A:467:GLU:H	1.70	0.55
1:A:581:GLN:HE21	1:A:628:PHE:HA	1.70	0.55
1:A:639:ASN:HD22	1:A:640:LYS:N	2.05	0.55
1:B:309:PRO:O	1:B:310:GLU:C	2.50	0.55
1:B:529:VAL:HG23	1:B:530:THR:H	1.71	0.55
1:C:534:ILE:HA	1:C:538:ILE:HB	1.88	0.55
1:C:589:LYS:HE2	1:C:643:ILE:HG23	1.87	0.55
1:C:667:LEU:HA	1:C:670:ILE:HG22	1.88	0.55
2:E:105:LEU:O	2:E:105:LEU:HD23	2.06	0.55
1:A:602:PHE:O	1:A:603:ILE:HD13	2.07	0.55
1:A:670:ILE:HG23	1:A:745:TYR:CZ	2.41	0.55
1:B:549:LEU:N	1:B:549:LEU:HD23	2.22	0.55
1:C:540:ARG:HD3	1:C:582:ASP:OD1	2.07	0.55
1:C:694:VAL:HG23	1:C:695:LYS:N	2.15	0.55
1:C:706:ASN:O	1:C:709:ASN:HB2	2.05	0.55
1:A:327:LEU:HG	1:A:595:ILE:HG23	1.89	0.55
1:A:494:LEU:HD23	1:A:497:LEU:HG	1.89	0.55
1:B:400:LYS:NZ	1:B:475:GLU:OE2	2.35	0.55
1:B:616:GLU:CG	1:B:617:LYS:N	2.68	0.55
1:C:409:ARG:O	1:C:410:ILE:C	2.49	0.55
2:F:36:MET:C	2:F:41:GLN:HB2	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:GLN:C	1:A:379:ALA:N	2.64	0.55
1:A:540:ARG:HH12	1:A:630:ARG:NH2	2.05	0.55
1:B:332:ASN:HD22	1:B:333:LYS:N	2.04	0.55
1:B:557:LEU:HD11	1:B:575:VAL:HG12	1.89	0.55
1:B:625:LEU:HD23	1:B:625:LEU:C	2.32	0.55
1:C:295:VAL:CG2	1:C:603:ILE:HG22	2.27	0.55
1:C:667:LEU:HB2	2:F:14:GLU:OE2	2.07	0.55
2:D:72:MET:C	2:D:74:ARG:H	2.13	0.55
1:B:445:ARG:HB2	1:B:471:TRP:CH2	2.42	0.54
1:B:527:LYS:O	1:B:527:LYS:HG2	2.07	0.54
1:B:616:GLU:O	1:B:621:GLY:HA3	2.07	0.54
1:B:726:ILE:HA	1:B:729:TYR:HB2	1.88	0.54
1:C:385:LEU:HD13	1:C:385:LEU:C	2.31	0.54
1:C:440:GLN:CD	1:C:440:GLN:H	2.14	0.54
2:D:130:ILE:HG22	2:D:130:ILE:O	2.06	0.54
2:D:140:GLU:C	2:D:142:VAL:N	2.65	0.54
1:A:664:ILE:HD13	2:D:15:ALA:HB2	1.88	0.54
1:B:775:LEU:H	1:B:775:LEU:HD22	1.72	0.54
1:C:340:LYS:C	1:C:342:GLY:H	2.15	0.54
1:C:629:ASN:HB3	1:C:632:TYR:CE2	2.42	0.54
2:F:100:ILE:HB	2:F:136:VAL:CG2	2.33	0.54
1:C:669:SER:HA	1:C:672:ARG:HG2	1.90	0.54
1:C:790:PHE:O	1:C:793:PHE:HB3	2.07	0.54
2:D:44:THR:CG2	2:D:47:GLU:HG3	2.37	0.54
1:A:445:ARG:NE	1:A:471:TRP:CE2	2.75	0.54
1:A:604:LEU:C	1:A:604:LEU:HD23	2.33	0.54
1:A:663:PHE:HE1	1:A:752:LEU:HD11	1.73	0.54
1:A:768:LYS:O	1:A:768:LYS:HG2	2.08	0.54
2:E:87:GLU:O	2:E:91:VAL:HG23	2.08	0.54
2:F:117:THR:C	2:F:119:GLU:N	2.64	0.54
1:A:456:LYS:HD3	1:A:471:TRP:CD1	2.43	0.54
1:A:603:ILE:HG22	1:A:604:LEU:H	1.72	0.54
1:A:700:TYR:CE1	1:A:731:GLU:HG2	2.42	0.54
1:B:530:THR:HG22	2:E:92:PHE:HZ	1.70	0.54
1:C:318:ILE:H	1:C:318:ILE:CD1	2.18	0.54
1:A:408:LEU:HD23	1:A:408:LEU:O	2.08	0.54
1:A:523:LEU:C	1:A:525:LYS:N	2.62	0.54
1:A:583:ASN:O	1:A:629:ASN:OD1	2.25	0.54
1:B:524:GLU:O	1:B:525:LYS:C	2.51	0.54
1:C:602:PHE:C	1:C:603:ILE:HD13	2.33	0.54
1:A:706:ASN:O	1:A:709:ASN:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:GLU:HG2	1:B:605:THR:O	2.08	0.54
1:C:381:GLU:C	1:C:383:GLY:N	2.66	0.54
1:C:462:ILE:CD1	1:C:466:GLY:HA2	2.38	0.54
1:C:650:THR:C	1:C:652:ALA:N	2.63	0.54
2:E:137:ASN:OD1	2:E:139:GLU:HB2	2.08	0.54
1:B:737:LYS:C	1:B:738:SER:O	2.47	0.54
1:C:322:LEU:O	1:C:323:ASN:C	2.50	0.54
1:C:494:LEU:HD23	1:C:497:LEU:HG	1.90	0.54
1:A:608:TRP:O	1:A:609:GLU:C	2.50	0.54
1:B:774:LYS:O	1:B:774:LYS:HG3	2.08	0.54
1:B:785:ASN:HD22	1:B:787:THR:HG22	1.73	0.54
1:C:505:LYS:HE3	1:C:513:TRP:CG	2.43	0.54
1:C:521:ASN:O	1:C:524:GLU:HB2	2.08	0.54
1:B:732:ILE:HG22	1:B:732:ILE:O	2.07	0.54
1:C:385:LEU:CD1	1:C:389:LYS:HD2	2.37	0.54
1:A:775:LEU:HB2	1:A:776:LEU:HD12	1.89	0.53
1:B:761:GLN:O	1:B:765:THR:N	2.38	0.53
2:F:140:GLU:C	2:F:142:VAL:H	2.16	0.53
1:A:450:ASN:OD1	1:A:452:GLU:HG3	2.08	0.53
1:A:462:ILE:CD1	1:A:466:GLY:HA2	2.38	0.53
1:B:654:ILE:HG13	1:B:654:ILE:O	2.08	0.53
1:B:727:GLN:HG3	1:B:786:GLU:OE2	2.08	0.53
2:D:36:MET:C	2:D:41:GLN:HB2	2.33	0.53
2:D:117:THR:C	2:D:119:GLU:N	2.65	0.53
1:A:324:THR:OG1	1:A:499:PRO:HB3	2.08	0.53
1:A:326:ILE:C	1:A:327:LEU:HD12	2.33	0.53
1:A:602:PHE:C	1:A:603:ILE:HD13	2.34	0.53
1:A:639:ASN:ND2	1:A:641:ALA:N	2.50	0.53
1:A:665:LYS:HG3	2:D:11:GLU:OE1	2.08	0.53
1:A:764:LEU:O	1:A:768:LYS:N	2.40	0.53
1:B:502:THR:O	1:B:505:LYS:HG2	2.08	0.53
1:B:654:ILE:HG22	1:B:755:ARG:HG2	1.90	0.53
1:B:721:SER:O	1:B:723:PHE:N	2.41	0.53
1:C:327:LEU:HD12	1:C:327:LEU:N	2.22	0.53
2:D:62:THR:C	2:D:63:ILE:HD12	2.33	0.53
1:A:295:VAL:HG22	1:A:296:LEU:N	2.23	0.53
1:A:438:ASN:C	1:A:438:ASN:ND2	2.66	0.53
1:B:315:PHE:O	1:B:316:LYS:C	2.51	0.53
1:B:581:GLN:NE2	1:B:629:ASN:N	2.39	0.53
1:C:581:GLN:HE21	1:C:629:ASN:N	2.05	0.53
2:E:140:GLU:C	2:E:142:VAL:N	2.64	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:44:THR:CG2	2:F:47:GLU:HG3	2.38	0.53
1:A:540:ARG:HH12	1:A:630:ARG:HH21	1.57	0.53
1:B:381:GLU:HG2	1:B:465:LEU:HD11	1.90	0.53
2:D:137:ASN:OD1	2:D:139:GLU:HB2	2.08	0.53
1:A:383:GLY:O	1:A:386:GLU:HB2	2.08	0.53
1:B:294:ASP:O	1:B:610:MET:HE1	2.09	0.53
1:B:443:GLU:OE1	1:B:456:LYS:HE2	2.09	0.53
1:B:654:ILE:O	1:B:655:ASN:ND2	2.40	0.53
1:B:732:ILE:O	1:B:735:VAL:HG12	2.09	0.53
1:C:317:LYS:HB3	1:C:318:ILE:HD12	1.91	0.53
2:F:92:PHE:CE2	2:F:108:VAL:HG11	2.43	0.53
2:F:27:ILE:CG1	2:F:63:ILE:HB	2.39	0.53
2:F:101:SER:OG	2:F:104:GLU:HG3	2.09	0.53
2:F:105:LEU:HD23	2:F:105:LEU:O	2.08	0.53
1:A:445:ARG:HH22	1:A:456:LYS:CG	2.21	0.53
1:A:509:PRO:O	1:A:511:LYS:N	2.40	0.53
1:A:697:ILE:HD11	1:A:731:GLU:O	2.09	0.53
2:D:105:LEU:HD23	2:D:105:LEU:O	2.08	0.53
1:A:319:ALA:O	1:A:598:PRO:HA	2.09	0.53
1:B:574:VAL:O	1:B:575:VAL:HG23	2.09	0.53
1:B:793:PHE:HA	1:B:796:ILE:HG12	1.91	0.53
1:B:596:ILE:HG12	1:B:602:PHE:CD2	2.44	0.53
1:B:626:TYR:CD2	1:B:626:TYR:C	2.87	0.53
1:C:384:ASN:OD1	1:C:384:ASN:N	2.42	0.53
1:C:377:GLN:C	1:C:379:ALA:N	2.66	0.52
1:C:394:HIS:O	1:C:395:GLU:C	2.53	0.52
1:A:477:MET:C	1:A:488:LEU:HD12	2.34	0.52
1:A:534:ILE:HG22	1:A:535:LYS:N	2.24	0.52
1:B:619:ILE:C	1:B:621:GLY:N	2.67	0.52
1:C:338:LEU:O	1:C:343:VAL:HG23	2.09	0.52
2:E:140:GLU:C	2:E:142:VAL:H	2.17	0.52
1:A:324:THR:HG23	1:A:324:THR:O	2.07	0.52
1:A:338:LEU:O	1:A:343:VAL:HG23	2.10	0.52
1:A:360:VAL:O	1:A:360:VAL:CG2	2.57	0.52
1:B:296:LEU:HB2	1:B:604:LEU:HB3	1.92	0.52
1:C:574:VAL:HG13	1:C:574:VAL:O	2.09	0.52
2:E:44:THR:CG2	2:E:47:GLU:HG3	2.37	0.52
1:B:338:LEU:O	1:B:339:ILE:C	2.50	0.52
1:B:391:ILE:HD13	1:B:398:ILE:HG22	1.90	0.52
1:B:557:LEU:CD1	1:B:575:VAL:HG12	2.40	0.52
1:B:714:GLN:OE1	1:B:718:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASP:O	1:A:610:MET:HE1	2.10	0.52
1:A:540:ARG:NH2	1:A:627:TYR:CE1	2.77	0.52
1:B:744:GLU:OE1	1:B:744:GLU:HA	2.08	0.52
1:C:308:VAL:HG23	1:C:492:TYR:OH	2.10	0.52
1:C:509:PRO:HD2	1:C:536:TYR:CZ	2.45	0.52
1:C:781:ASN:ND2	1:C:783:THR:OG1	2.42	0.52
2:E:37:ARG:HG2	2:E:41:GLN:O	2.10	0.52
1:A:633:ASN:ND2	1:A:644:GLU:HA	2.25	0.52
1:B:309:PRO:O	1:B:312:ALA:N	2.42	0.52
1:A:636:ALA:O	1:A:640:LYS:HA	2.10	0.52
1:B:298:GLY:O	1:B:300:LYS:N	2.43	0.52
1:B:306:GLY:O	1:B:336:THR:CB	2.57	0.52
1:B:311:HIS:ND1	1:B:564:VAL:HB	2.24	0.52
1:B:423:LYS:HB3	1:B:434:LEU:CD2	2.39	0.52
1:B:516:VAL:O	1:B:520:PRO:HD2	2.10	0.52
1:B:540:ARG:HD2	1:B:627:TYR:CZ	2.44	0.52
1:B:785:ASN:ND2	1:B:787:THR:CG2	2.73	0.52
1:C:636:ALA:O	1:C:640:LYS:HA	2.10	0.52
2:D:92:PHE:CD2	2:D:108:VAL:HG21	2.44	0.52
2:D:140:GLU:C	2:D:142:VAL:H	2.18	0.52
2:E:85:ILE:O	2:E:88:ALA:HB3	2.10	0.52
2:F:65:PHE:CD1	2:F:65:PHE:N	2.77	0.52
1:B:509:PRO:CD	1:B:536:TYR:HE1	2.21	0.52
1:B:748:TYR:O	1:B:752:LEU:CG	2.58	0.52
2:D:89:PHE:C	2:D:89:PHE:HD2	2.14	0.52
1:B:536:TYR:HD2	1:B:536:TYR:N	2.09	0.51
1:B:733:GLU:C	1:B:735:VAL:N	2.68	0.51
1:B:749:PHE:O	1:B:752:LEU:HB2	2.11	0.51
1:C:292:ARG:HA	1:C:292:ARG:NE	2.25	0.51
2:E:62:THR:C	2:E:63:ILE:HD12	2.35	0.51
1:C:657:ILE:CG1	1:C:759:GLN:HG2	2.37	0.51
2:D:37:ARG:HG2	2:D:41:GLN:O	2.11	0.51
2:E:131:ASP:OD1	2:E:133:ASP:OD2	2.27	0.51
1:A:509:PRO:HD3	1:A:536:TYR:CE1	2.44	0.51
1:A:517:VAL:HA	1:A:525:LYS:NZ	2.25	0.51
1:B:525:LYS:NZ	2:E:114:GLU:OE2	2.43	0.51
1:B:540:ARG:NH1	1:B:627:TYR:CD1	2.79	0.51
1:B:574:VAL:C	1:B:575:VAL:HG23	2.35	0.51
1:C:346:LYS:O	1:C:346:LYS:HG3	2.10	0.51
1:A:318:ILE:HG23	1:A:322:LEU:CD1	2.41	0.51
1:A:607:ASN:O	1:A:610:MET:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:LYS:HG2	1:B:393:GLU:OE2	2.11	0.51
1:C:666:ASN:O	1:C:670:ILE:HG22	2.10	0.51
1:A:324:THR:O	1:A:324:THR:CG2	2.58	0.51
1:A:384:ASN:O	1:A:387:ASN:N	2.44	0.51
1:A:607:ASN:HD21	1:A:609:GLU:HB2	1.75	0.51
1:A:628:PHE:CD1	1:A:628:PHE:C	2.88	0.51
1:B:513:TRP:O	1:B:517:VAL:HG12	2.10	0.51
1:B:730:ASN:HA	1:B:733:GLU:HB3	1.93	0.51
1:B:787:THR:HG23	1:B:788:ASP:N	2.25	0.51
1:C:384:ASN:O	1:C:385:LEU:C	2.51	0.51
1:C:657:ILE:HG23	1:C:658:PRO:HD2	1.91	0.51
2:E:27:ILE:CG1	2:E:63:ILE:HB	2.40	0.51
1:A:558:ASP:O	1:A:562:GLU:HG3	2.11	0.51
1:A:606:LYS:O	1:A:607:ASN:HB3	2.11	0.51
1:B:327:LEU:CG	1:B:595:ILE:HG23	2.40	0.51
1:B:355:SER:HB2	1:B:371:SER:HA	1.91	0.51
1:C:510:GLN:O	1:C:510:GLN:CG	2.57	0.51
1:C:774:LYS:O	1:C:777:TYR:N	2.38	0.51
1:A:419:ILE:O	1:A:419:ILE:HG13	2.11	0.51
1:A:445:ARG:NE	1:A:471:TRP:NE1	2.59	0.51
1:A:697:ILE:O	1:A:701:LEU:HG	2.10	0.51
1:A:705:TYR:CE2	2:D:139:GLU:CB	2.81	0.51
1:B:717:LYS:CD	2:E:132:GLY:N	2.70	0.51
1:C:383:GLY:O	1:C:386:GLU:HB2	2.10	0.51
2:F:37:ARG:HG2	2:F:41:GLN:O	2.10	0.51
1:A:652:ALA:O	1:A:654:ILE:N	2.44	0.51
1:C:381:GLU:C	1:C:383:GLY:H	2.19	0.51
2:E:44:THR:HG23	2:E:47:GLU:H	1.76	0.51
1:B:791:GLU:C	1:B:793:PHE:H	2.19	0.51
2:D:44:THR:HG23	2:D:47:GLU:H	1.75	0.51
1:A:340:LYS:C	1:A:342:GLY:H	2.18	0.50
1:B:508:ILE:HA	1:B:536:TYR:HD1	1.75	0.50
1:A:502:THR:O	1:A:505:LYS:N	2.44	0.50
1:B:622:LYS:O	1:B:623:ASP:HB2	2.12	0.50
1:C:650:THR:C	1:C:652:ALA:H	2.19	0.50
1:B:300:LYS:HA	1:B:303:LYS:NZ	2.25	0.50
1:B:576:ASN:OD1	1:B:576:ASN:N	2.44	0.50
1:B:722:ILE:O	1:B:726:ILE:HG13	2.11	0.50
2:F:44:THR:HG23	2:F:47:GLU:H	1.76	0.50
1:A:494:LEU:HB3	1:A:579:THR:HG22	1.93	0.50
1:A:667:LEU:HA	1:A:670:ILE:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:LYS:O	1:A:777:TYR:N	2.39	0.50
1:B:616:GLU:HA	1:B:620:THR:CG2	2.40	0.50
2:D:27:ILE:CG1	2:D:63:ILE:HB	2.42	0.50
2:E:65:PHE:CD1	2:E:65:PHE:N	2.75	0.50
1:A:697:ILE:H	1:A:697:ILE:CD1	2.25	0.50
1:B:369:ASP:OD2	1:B:442:TYR:OH	2.19	0.50
1:B:606:LYS:N	1:B:610:MET:HE3	2.27	0.50
1:B:649:ILE:HD12	2:E:86:ARG:HG3	1.92	0.50
1:B:746:LYS:CG	1:B:750:GLN:HB2	2.41	0.50
1:C:540:ARG:HB3	1:C:549:LEU:O	2.11	0.50
1:C:668:SER:HA	2:F:14:GLU:HG3	1.94	0.50
1:B:404:LYS:HG3	1:B:452:GLU:HA	1.93	0.50
1:A:324:THR:HA	1:A:499:PRO:HA	1.94	0.50
1:C:525:LYS:HB2	2:F:124:MET:HE3	1.92	0.50
1:A:346:LYS:O	1:A:346:LYS:HG3	2.12	0.50
1:A:607:ASN:O	1:A:608:TRP:C	2.54	0.50
1:B:387:ASN:C	1:B:389:LYS:N	2.69	0.50
2:F:5:THR:N	2:F:8:GLN:HB2	2.27	0.50
2:F:144:MET:SD	2:F:144:MET:C	2.95	0.50
1:B:453:VAL:CG1	1:B:474:ILE:HD12	2.42	0.50
1:A:367:ASP:C	1:A:369:ASP:H	2.20	0.49
1:C:360:VAL:O	1:C:360:VAL:CG2	2.57	0.49
1:C:400:LYS:HD2	1:C:475:GLU:OE1	2.12	0.49
1:C:438:ASN:C	1:C:438:ASN:ND2	2.66	0.49
2:E:100:ILE:HB	2:E:136:VAL:CG2	2.37	0.49
1:A:348:LEU:HD12	1:A:577:HIS:CB	2.42	0.49
1:B:489:THR:HG23	1:B:490:ALA:O	2.12	0.49
1:C:363:TYR:CD1	1:C:403:LEU:CD1	2.95	0.49
1:C:592:GLU:HB3	1:C:604:LEU:HD21	1.93	0.49
1:C:739:LYS:HE2	1:C:739:LYS:HA	1.94	0.49
1:A:722:ILE:HG21	1:A:764:LEU:HD21	1.94	0.49
1:C:318:ILE:CG2	1:C:322:LEU:HD13	2.42	0.49
2:F:121:VAL:C	2:F:123:GLU:N	2.70	0.49
1:A:780:LEU:HD12	1:A:780:LEU:O	2.12	0.49
1:B:530:THR:OG1	2:E:145:MET:SD	2.70	0.49
1:B:629:ASN:ND2	1:B:629:ASN:C	2.70	0.49
1:C:320:ARG:HH21	1:C:600:GLY:HA3	1.77	0.49
1:C:655:ASN:N	1:C:655:ASN:ND2	2.60	0.49
2:D:42:ASN:ND2	2:D:147:ALA:HB2	2.27	0.49
2:D:138:TYR:O	2:D:139:GLU:C	2.55	0.49
2:E:37:ARG:HA	2:E:41:GLN:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:ASN:OD1	1:A:601:GLU:HB2	2.13	0.49
1:B:315:PHE:CE2	1:B:560:LEU:HD23	2.47	0.49
1:B:605:THR:CG2	1:B:606:LYS:N	2.76	0.49
1:B:709:ASN:OD1	1:B:709:ASN:O	2.30	0.49
1:B:709:ASN:ND2	1:B:720:ILE:HD11	2.19	0.49
1:B:773:PHE:O	1:B:775:LEU:N	2.46	0.49
1:B:793:PHE:C	1:B:795:LYS:H	2.20	0.49
1:A:340:LYS:C	1:A:342:GLY:N	2.67	0.49
1:B:313:ASP:C	1:B:315:PHE:N	2.68	0.49
1:B:629:ASN:ND2	1:B:631:SER:HB2	2.21	0.49
1:C:522:SER:C	1:C:524:GLU:N	2.71	0.49
1:C:540:ARG:HH12	1:C:630:ARG:NH2	2.10	0.49
1:A:325:TYR:CE1	1:A:619:ILE:HG12	2.47	0.49
1:C:502:THR:O	1:C:505:LYS:N	2.45	0.49
1:A:557:LEU:O	1:A:560:LEU:HB2	2.11	0.49
1:A:629:ASN:ND2	1:A:631:SER:N	2.41	0.49
1:B:587:PRO:CD	1:B:639:ASN:HD21	2.18	0.49
1:B:639:ASN:ND2	1:B:639:ASN:N	2.58	0.49
1:B:655:ASN:H	1:B:755:ARG:HD2	1.78	0.49
1:C:305:SER:OG	1:C:306:GLY:N	2.45	0.49
1:C:325:TYR:CE2	1:C:598:PRO:HD2	2.48	0.49
1:C:561:ASN:O	1:C:564:VAL:HG22	2.12	0.49
1:C:581:GLN:HE21	1:C:628:PHE:HA	1.77	0.49
2:F:117:THR:O	2:F:119:GLU:N	2.46	0.49
1:A:721:SER:O	1:A:722:ILE:C	2.55	0.49
1:B:721:SER:C	1:B:723:PHE:N	2.68	0.49
1:C:335:ALA:O	1:C:338:LEU:HB2	2.12	0.49
1:C:340:LYS:C	1:C:342:GLY:N	2.68	0.49
1:C:557:LEU:O	1:C:560:LEU:HB2	2.12	0.49
1:C:607:ASN:O	1:C:610:MET:N	2.44	0.49
2:E:117:THR:O	2:E:119:GLU:N	2.46	0.49
1:A:526:GLN:CD	2:D:144:MET:HE2	2.38	0.49
1:B:294:ASP:O	1:B:606:LYS:HE3	2.12	0.49
1:B:728:ALA:C	1:B:731:GLU:HG3	2.37	0.49
1:B:795:LYS:O	1:B:797:ILE:HG12	2.12	0.49
1:C:670:ILE:O	1:C:745:TYR:HE1	1.95	0.49
1:A:403:LEU:HD13	1:A:476:VAL:HG21	1.93	0.48
1:A:409:ARG:O	1:A:410:ILE:C	2.54	0.48
1:A:700:TYR:HE1	1:A:731:GLU:HG2	1.77	0.48
1:B:562:GLU:C	1:B:564:VAL:N	2.70	0.48
1:B:773:PHE:C	1:B:775:LEU:N	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:ILE:HG23	1:C:322:LEU:CD1	2.41	0.48
1:C:780:LEU:HD12	1:C:780:LEU:O	2.12	0.48
2:D:65:PHE:CD1	2:D:65:PHE:N	2.78	0.48
2:D:121:VAL:C	2:D:123:GLU:N	2.71	0.48
1:B:437:SER:C	1:B:439:ASN:H	2.21	0.48
1:C:401:ILE:HD13	1:C:478:ALA:CB	2.42	0.48
1:C:669:SER:C	1:C:671:ARG:N	2.70	0.48
2:D:19:PHE:CD2	2:D:19:PHE:C	2.89	0.48
1:A:325:TYR:CE2	1:A:598:PRO:HD2	2.49	0.48
1:B:315:PHE:HA	1:B:318:ILE:HD11	1.95	0.48
1:B:562:GLU:C	1:B:564:VAL:H	2.22	0.48
1:B:722:ILE:HG23	1:B:760:VAL:HG13	1.95	0.48
2:D:79:THR:C	2:D:81:SER:H	2.22	0.48
2:F:121:VAL:C	2:F:123:GLU:H	2.22	0.48
1:A:432:TYR:CD1	1:A:471:TRP:CZ3	3.01	0.48
1:B:359:PRO:HG2	1:B:444:PHE:CD2	2.49	0.48
2:E:50:ASP:OD1	2:E:51:MET:N	2.47	0.48
1:A:304:ALA:HB3	1:A:604:LEU:HD13	1.95	0.48
1:A:587:PRO:HB2	1:A:643:ILE:CD1	2.44	0.48
1:B:717:LYS:HD2	2:E:132:GLY:CA	2.43	0.48
1:B:721:SER:O	1:B:722:ILE:C	2.56	0.48
1:A:793:PHE:O	1:A:794:GLN:C	2.56	0.48
1:B:331:VAL:O	1:B:331:VAL:HG12	2.13	0.48
1:B:423:LYS:O	1:B:434:LEU:CD2	2.62	0.48
1:C:527:LYS:HZ1	2:F:145:MET:C	2.22	0.48
1:C:630:ARG:HE	2:F:87:GLU:CD	2.21	0.48
1:C:667:LEU:O	1:C:671:ARG:HB2	2.14	0.48
1:A:381:GLU:C	1:A:383:GLY:N	2.71	0.48
1:A:508:ILE:HG21	1:A:532:LEU:HD13	1.96	0.48
1:B:338:LEU:HD11	1:B:409:ARG:NE	2.28	0.48
1:C:367:ASP:C	1:C:369:ASP:H	2.22	0.48
1:C:583:ASN:ND2	4:C:1999:DOT:C1B	2.77	0.48
2:D:137:ASN:O	2:D:138:TYR:C	2.56	0.48
1:A:401:ILE:HD13	1:A:478:ALA:CB	2.44	0.48
1:A:543:ASP:OD2	1:A:546:LYS:HG3	2.13	0.48
1:B:535:LYS:HB3	1:B:536:TYR:CD2	2.48	0.48
1:B:746:LYS:HG3	1:B:750:GLN:HB2	1.95	0.48
1:C:419:ILE:O	1:C:419:ILE:HG13	2.12	0.48
1:C:721:SER:O	1:C:722:ILE:C	2.55	0.48
1:C:740:GLN:CD	1:C:740:GLN:N	2.72	0.48
2:D:100:ILE:HB	2:D:136:VAL:CG2	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:MET:C	2:D:144:MET:SD	2.97	0.48
1:A:323:ASN:C	1:A:323:ASN:HD22	2.22	0.48
1:A:423:LYS:HB3	1:A:423:LYS:NZ	2.28	0.48
1:A:504:ILE:O	1:A:505:LYS:C	2.55	0.48
1:B:333:LYS:O	1:B:336:THR:CG2	2.61	0.48
1:B:543:ASP:HB3	1:B:546:LYS:O	2.14	0.48
2:D:117:THR:O	2:D:119:GLU:N	2.46	0.48
2:F:102:ALA:O	2:F:103:ALA:C	2.56	0.48
1:A:408:LEU:C	1:A:408:LEU:CD2	2.86	0.48
1:A:540:ARG:NH2	2:D:87:GLU:OE1	2.45	0.48
1:A:652:ALA:O	1:A:655:ASN:N	2.38	0.48
1:A:730:ASN:C	1:A:732:ILE:H	2.22	0.48
1:B:400:LYS:HA	1:B:476:VAL:O	2.14	0.48
1:B:526:GLN:HE21	2:E:124:MET:CE	2.27	0.48
1:B:529:VAL:HG23	1:B:530:THR:N	2.28	0.48
1:C:304:ALA:HB3	1:C:604:LEU:CD1	2.43	0.48
2:E:65:PHE:H	2:E:65:PHE:HD1	1.56	0.48
1:B:726:ILE:O	1:B:729:TYR:CB	2.62	0.47
1:A:559:ARG:HB3	1:A:559:ARG:NH1	2.19	0.47
1:B:497:LEU:HD13	1:B:556:MET:HG2	1.96	0.47
1:B:720:ILE:O	1:B:724:ARG:HG2	2.14	0.47
1:C:403:LEU:CD1	1:C:476:VAL:HG21	2.44	0.47
1:C:527:LYS:HZ3	2:F:145:MET:HA	1.79	0.47
1:C:793:PHE:O	1:C:794:GLN:C	2.57	0.47
1:A:462:ILE:HD11	1:A:466:GLY:CA	2.43	0.47
1:A:493:ASP:OD2	4:A:999:DOT:O1A	2.33	0.47
1:A:583:ASN:HD21	4:A:999:DOT:H1'	1.79	0.47
2:D:121:VAL:C	2:D:123:GLU:H	2.22	0.47
2:F:45:GLU:O	2:F:49:GLN:HG2	2.15	0.47
1:A:561:ASN:O	1:A:564:VAL:HG22	2.14	0.47
1:A:657:ILE:HG21	1:A:756:ILE:HD13	1.92	0.47
1:A:789:ASN:N	1:A:789:ASN:HD22	2.11	0.47
1:B:381:GLU:O	1:B:382:LYS:C	2.55	0.47
1:A:317:LYS:HB3	1:A:318:ILE:HD12	1.97	0.47
1:A:419:ILE:HD12	1:A:435:LEU:HD22	1.97	0.47
1:B:587:PRO:HD2	1:B:639:ASN:ND2	2.18	0.47
1:B:735:VAL:O	1:B:735:VAL:HG22	2.15	0.47
1:B:773:PHE:HE1	1:B:777:TYR:HB2	1.78	0.47
1:C:445:ARG:NH1	1:C:471:TRP:NE1	2.61	0.47
1:A:504:ILE:CG2	1:A:505:LYS:N	2.77	0.47
1:A:534:ILE:HA	1:A:538:ILE:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ILE:CD1	2:D:88:ALA:HA	2.45	0.47
1:A:628:PHE:HD1	1:A:629:ASN:O	1.98	0.47
1:B:456:LYS:HG3	1:B:457:THR:O	2.14	0.47
1:B:615:ILE:HD13	1:B:626:TYR:CZ	2.50	0.47
1:B:785:ASN:ND2	1:B:787:THR:HG22	2.29	0.47
1:C:699:GLY:O	1:C:702:SER:N	2.46	0.47
1:A:370:LEU:HD11	1:A:455:TYR:CE1	2.49	0.47
1:B:357:TRP:CZ2	1:B:370:LEU:HA	2.49	0.47
1:B:514:ASP:CA	1:B:517:VAL:HG12	2.38	0.47
1:B:750:GLN:O	1:B:753:LYS:HB3	2.15	0.47
1:B:785:ASN:HD22	1:B:787:THR:CG2	2.27	0.47
1:C:408:LEU:HD23	1:C:408:LEU:O	2.14	0.47
1:C:540:ARG:NH1	1:C:630:ARG:NH2	2.63	0.47
1:C:607:ASN:O	1:C:608:TRP:C	2.58	0.47
1:C:789:ASN:N	1:C:789:ASN:HD22	2.12	0.47
2:D:22:ASP:HB3	2:D:26:THR:OG1	2.15	0.47
2:D:45:GLU:O	2:D:49:GLN:HG2	2.15	0.47
2:E:19:PHE:C	2:E:19:PHE:CD2	2.91	0.47
1:B:338:LEU:O	1:B:341:SER:N	2.47	0.47
1:B:377:GLN:HG3	1:B:465:LEU:HD23	1.97	0.47
1:B:574:VAL:O	1:B:575:VAL:CG2	2.63	0.47
1:B:614:PHE:C	1:B:614:PHE:CD2	2.93	0.47
1:C:349:ASN:HD21	1:C:398:ILE:CG1	2.27	0.47
1:C:415:GLU:C	1:C:417:GLY:H	2.23	0.47
2:D:5:THR:O	2:D:9:ILE:HG13	2.15	0.47
2:F:37:ARG:HA	2:F:41:GLN:O	2.15	0.47
1:A:329:ARG:O	1:A:330:PRO:O	2.33	0.47
1:A:443:GLU:HB2	1:A:458:LYS:HG2	1.97	0.47
1:B:498:ALA:HB3	1:B:619:ILE:HD13	1.95	0.47
1:B:648:PRO:C	1:B:650:THR:H	2.22	0.47
1:C:363:TYR:HD1	1:C:403:LEU:CD1	2.27	0.47
1:C:583:ASN:O	1:C:629:ASN:OD1	2.32	0.47
1:C:657:ILE:CG2	1:C:658:PRO:N	2.78	0.47
1:B:327:LEU:HA	1:B:594:PHE:O	2.14	0.47
1:B:328:PHE:HB2	1:B:594:PHE:HB3	1.97	0.47
1:C:527:LYS:NZ	2:F:145:MET:C	2.74	0.46
1:C:597:ASN:OD1	1:C:601:GLU:HB2	2.14	0.46
1:C:629:ASN:HD21	1:C:631:SER:H	1.52	0.46
1:A:327:LEU:HB2	1:A:496:ALA:O	2.14	0.46
1:B:327:LEU:HD13	1:B:496:ALA:HB3	1.96	0.46
1:B:360:VAL:O	1:B:361:ALA:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:ASN:HA	1:B:761:GLN:HB2	1.97	0.46
1:C:517:VAL:O	1:C:517:VAL:HG22	2.13	0.46
1:C:722:ILE:HG21	1:C:764:LEU:HD21	1.97	0.46
1:A:299:GLU:CG	1:A:303:LYS:NZ	2.79	0.46
1:C:302:LEU:HD12	1:C:602:PHE:CE1	2.48	0.46
1:C:419:ILE:HD12	1:C:435:LEU:HD22	1.97	0.46
1:C:658:PRO:HB2	1:C:701:LEU:CD1	2.44	0.46
2:D:37:ARG:HA	2:D:41:GLN:O	2.15	0.46
2:F:137:ASN:O	2:F:138:TYR:C	2.57	0.46
1:A:700:TYR:HD1	1:A:728:ALA:CA	2.28	0.46
1:A:722:ILE:HG12	1:A:763:LEU:HB2	1.98	0.46
1:B:418:ILE:HG22	1:B:419:ILE:HG23	1.96	0.46
1:B:450:ASN:O	1:B:451:ASN:HB2	2.15	0.46
1:B:476:VAL:HG12	1:B:477:MET:N	2.30	0.46
1:B:480:ASN:HA	1:B:485:LEU:HD12	1.97	0.46
1:C:659:THR:C	1:C:701:LEU:HD13	2.40	0.46
2:E:22:ASP:HB3	2:E:26:THR:OG1	2.15	0.46
1:A:747:ASN:O	1:A:748:TYR:C	2.56	0.46
1:B:327:LEU:HD23	1:B:595:ILE:HG23	1.98	0.46
1:B:368:GLN:H	1:B:384:ASN:ND2	2.13	0.46
1:C:462:ILE:HD11	1:C:466:GLY:CA	2.45	0.46
1:C:663:PHE:O	1:C:667:LEU:HG	2.16	0.46
2:D:42:ASN:HD21	2:D:147:ALA:HB2	1.80	0.46
2:E:137:ASN:O	2:E:138:TYR:C	2.58	0.46
1:A:345:THR:HB	1:A:491:ASP:HA	1.97	0.46
1:A:657:ILE:HD11	1:A:704:TYR:CD1	2.50	0.46
1:B:324:THR:CB	1:B:499:PRO:HA	2.46	0.46
1:B:346:LYS:HD3	1:B:364:ILE:CD1	2.46	0.46
1:B:501:LEU:HA	1:B:504:ILE:HG12	1.98	0.46
1:B:509:PRO:HD2	1:B:536:TYR:CE1	2.51	0.46
1:B:707:SER:C	1:B:709:ASN:H	2.24	0.46
1:B:728:ALA:C	1:B:730:ASN:N	2.73	0.46
1:C:325:TYR:CD2	1:C:597:ASN:HA	2.51	0.46
2:D:87:GLU:O	2:D:91:VAL:HG23	2.15	0.46
1:A:324:THR:OG1	1:A:499:PRO:CA	2.64	0.46
1:A:663:PHE:CE1	1:A:752:LEU:CD1	2.98	0.46
1:B:332:ASN:HD21	1:B:334:LEU:H	1.62	0.46
1:B:368:GLN:H	1:B:384:ASN:HD21	1.64	0.46
1:B:622:LYS:O	1:B:623:ASP:CB	2.64	0.46
1:C:522:SER:C	1:C:524:GLU:H	2.24	0.46
2:E:121:VAL:C	2:E:123:GLU:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ALA:O	1:A:662:GLU:C	2.58	0.46
1:B:350:VAL:HG22	1:B:398:ILE:HG13	1.98	0.46
1:B:423:LYS:HB3	1:B:434:LEU:HD22	1.97	0.46
1:B:597:ASN:CG	1:B:601:GLU:HB2	2.41	0.46
1:B:613:ARG:O	1:B:616:GLU:HG2	2.15	0.46
1:C:385:LEU:HD11	1:C:389:LYS:HD2	1.97	0.46
1:C:540:ARG:HD3	1:C:582:ASP:CG	2.41	0.46
1:C:593:ILE:O	1:C:604:LEU:HA	2.15	0.46
2:F:65:PHE:H	2:F:65:PHE:HD1	1.58	0.46
1:A:292:ARG:HG3	1:A:292:ARG:HH11	1.79	0.46
1:A:349:ASN:HD21	1:A:398:ILE:CG1	2.28	0.46
1:A:463:THR:CG2	1:A:465:LEU:H	2.28	0.46
1:B:745:TYR:HB3	1:B:749:PHE:CE1	2.41	0.46
1:C:504:ILE:CG2	1:C:505:LYS:N	2.78	0.46
1:C:747:ASN:O	1:C:748:TYR:C	2.56	0.46
2:D:50:ASP:OD1	2:D:51:MET:N	2.48	0.46
2:F:50:ASP:OD1	2:F:51:MET:N	2.48	0.46
1:B:315:PHE:O	1:B:318:ILE:CD1	2.64	0.46
2:D:118:ASP:N	2:D:118:ASP:OD2	2.48	0.46
2:F:22:ASP:HB3	2:F:26:THR:OG1	2.16	0.46
1:A:714:GLN:HE22	2:D:126:ARG:HG3	1.75	0.45
1:A:789:ASN:N	1:A:789:ASN:ND2	2.63	0.45
1:B:630:ARG:HE	2:E:87:GLU:CD	2.24	0.45
1:B:777:TYR:HA	1:B:780:LEU:HD12	1.97	0.45
1:C:463:THR:CG2	1:C:465:LEU:H	2.28	0.45
1:C:583:ASN:HD21	4:C:1999:DOT:H1'	1.79	0.45
1:C:749:PHE:C	1:C:751:TYR:N	2.71	0.45
2:F:87:GLU:O	2:F:91:VAL:HG23	2.15	0.45
1:A:302:LEU:C	1:A:302:LEU:CD2	2.88	0.45
1:A:432:TYR:CD1	1:A:471:TRP:HZ3	2.33	0.45
1:A:654:ILE:O	1:A:654:ILE:HG13	2.14	0.45
1:A:655:ASN:OD1	1:A:758:ASN:HB3	2.16	0.45
1:A:697:ILE:N	1:A:697:ILE:CD1	2.80	0.45
1:B:408:LEU:O	1:B:411:GLU:HB3	2.16	0.45
1:B:549:LEU:N	1:B:549:LEU:CD2	2.79	0.45
1:C:403:LEU:HD13	1:C:476:VAL:HG21	1.97	0.45
2:E:12:PHE:O	2:E:16:PHE:HB2	2.16	0.45
2:E:89:PHE:HE1	2:E:138:TYR:N	2.14	0.45
2:E:121:VAL:C	2:E:123:GLU:N	2.72	0.45
1:A:323:ASN:C	1:A:323:ASN:ND2	2.74	0.45
1:B:744:GLU:HG2	1:C:397:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:597:ASN:C	1:C:599:GLU:H	2.24	0.45
1:C:604:LEU:C	1:C:604:LEU:HD23	2.42	0.45
1:C:639:ASN:HD21	1:C:641:ALA:CB	2.29	0.45
2:E:129:ASP:OD1	2:E:132:GLY:N	2.44	0.45
2:F:99:TYR:HD2	2:F:137:ASN:HB3	1.79	0.45
1:A:327:LEU:HD12	1:A:327:LEU:N	2.32	0.45
1:A:456:LYS:HD3	1:A:471:TRP:HD1	1.81	0.45
1:A:625:LEU:HD12	1:A:625:LEU:HA	1.64	0.45
1:B:302:LEU:HD13	1:B:594:PHE:CZ	2.52	0.45
1:B:626:TYR:HD2	1:B:626:TYR:C	2.21	0.45
1:B:716:LYS:O	1:B:720:ILE:HG23	2.17	0.45
1:B:717:LYS:HB3	1:B:717:LYS:HE3	1.67	0.45
1:B:787:THR:HG23	1:B:788:ASP:H	1.81	0.45
1:B:790:PHE:O	1:B:794:GLN:HB2	2.17	0.45
1:C:322:LEU:HD12	1:C:322:LEU:N	2.31	0.45
1:C:324:THR:HG21	1:C:556:MET:HE3	1.94	0.45
1:C:415:GLU:C	1:C:417:GLY:N	2.74	0.45
1:C:423:LYS:NZ	1:C:423:LYS:HB3	2.32	0.45
1:C:773:PHE:O	1:C:774:LYS:C	2.60	0.45
2:D:12:PHE:O	2:D:16:PHE:HB2	2.16	0.45
2:E:45:GLU:O	2:E:49:GLN:HG2	2.16	0.45
2:E:105:LEU:O	2:E:109:MET:HG2	2.16	0.45
2:F:92:PHE:O	2:F:94:LYS:N	2.38	0.45
1:B:308:VAL:HG23	1:B:492:TYR:OH	2.16	0.45
1:B:322:LEU:O	1:B:323:ASN:C	2.59	0.45
1:B:394:HIS:O	1:B:395:GLU:C	2.59	0.45
1:B:581:GLN:O	1:B:629:ASN:HA	2.15	0.45
1:B:703:ASP:O	1:B:705:TYR:O	2.35	0.45
1:B:723:PHE:O	1:B:726:ILE:N	2.49	0.45
1:C:509:PRO:C	1:C:511:LYS:H	2.25	0.45
1:C:522:SER:O	1:C:524:GLU:N	2.49	0.45
1:C:789:ASN:N	1:C:789:ASN:ND2	2.63	0.45
2:F:89:PHE:CE1	2:F:138:TYR:N	2.85	0.45
1:A:535:LYS:NZ	1:A:536:TYR:HE2	2.14	0.45
1:B:455:TYR:H	1:B:455:TYR:HD2	1.64	0.45
1:B:462:ILE:HG12	1:B:463:THR:O	2.17	0.45
1:B:470:ASN:CG	1:B:471:TRP:N	2.69	0.45
1:B:589:LYS:HA	1:B:608:TRP:CZ3	2.51	0.45
2:D:102:ALA:O	2:D:103:ALA:C	2.59	0.45
2:E:89:PHE:HD2	2:E:90:ARG:N	2.14	0.45
1:A:325:TYR:CD2	1:A:597:ASN:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:C	1:A:385:LEU:CD1	2.90	0.45
1:A:513:TRP:CD2	1:A:517:VAL:CG2	2.92	0.45
1:B:636:ALA:O	1:B:640:LYS:HA	2.17	0.45
1:C:671:ARG:C	1:C:672:ARG:HE	2.25	0.45
1:C:721:SER:O	1:C:724:ARG:N	2.50	0.45
1:C:730:ASN:C	1:C:732:ILE:H	2.24	0.45
2:E:83:GLU:O	2:E:84:GLU:C	2.60	0.45
2:E:89:PHE:CE1	2:E:138:TYR:N	2.85	0.45
1:A:663:PHE:HE1	1:A:752:LEU:CD1	2.30	0.45
1:A:667:LEU:HA	1:A:670:ILE:HG21	1.99	0.45
1:C:658:PRO:HB2	1:C:701:LEU:HD13	1.98	0.45
1:C:776:LEU:N	1:C:776:LEU:CD1	2.79	0.45
1:A:335:ALA:O	1:A:338:LEU:HB2	2.16	0.45
1:A:597:ASN:C	1:A:599:GLU:H	2.24	0.45
1:B:408:LEU:O	1:B:411:GLU:N	2.48	0.45
1:C:537:GLY:HA2	1:C:552:TRP:NE1	2.31	0.45
2:F:130:ILE:O	2:F:130:ILE:CG2	2.65	0.45
1:A:520:PRO:O	1:A:521:ASN:O	2.36	0.45
1:A:581:GLN:O	1:A:629:ASN:HA	2.17	0.45
1:A:695:LYS:CG	2:D:18:LEU:HD13	2.39	0.45
1:B:312:ALA:HB1	1:B:602:PHE:CZ	2.52	0.45
1:B:422:GLY:O	1:B:433:TYR:CD2	2.70	0.45
1:B:723:PHE:O	1:B:724:ARG:C	2.60	0.45
1:B:786:GLU:O	1:B:789:ASN:N	2.44	0.45
1:C:329:ARG:O	1:C:330:PRO:O	2.35	0.45
1:C:659:THR:HB	1:C:662:GLU:H	1.82	0.45
1:A:323:ASN:ND2	1:A:323:ASN:O	2.50	0.44
1:A:667:LEU:O	1:A:670:ILE:HG22	2.16	0.44
1:A:722:ILE:CG1	1:A:763:LEU:HB2	2.47	0.44
1:B:313:ASP:C	1:B:315:PHE:H	2.25	0.44
1:B:345:THR:HG21	1:B:574:VAL:HG23	1.99	0.44
1:B:508:ILE:HA	1:B:536:TYR:CD1	2.52	0.44
1:B:540:ARG:CZ	1:B:627:TYR:CE1	3.00	0.44
1:B:773:PHE:C	1:B:775:LEU:HD22	2.42	0.44
1:C:309:PRO:O	1:C:310:GLU:C	2.60	0.44
1:C:478:ALA:HA	1:C:488:LEU:HD12	1.99	0.44
1:C:768:LYS:HD2	1:C:797:ILE:O	2.17	0.44
1:C:776:LEU:HD12	1:C:776:LEU:H	1.80	0.44
1:A:749:PHE:C	1:A:751:TYR:N	2.72	0.44
1:B:517:VAL:HG22	1:B:517:VAL:O	2.17	0.44
1:C:722:ILE:CG1	1:C:763:LEU:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:776:LEU:CD1	1:C:776:LEU:H	2.31	0.44
2:F:100:ILE:HD12	2:F:141:PHE:CD1	2.52	0.44
1:A:445:ARG:HD2	1:A:445:ARG:N	2.32	0.44
1:A:509:PRO:HG2	1:A:512:GLU:HB2	2.00	0.44
1:A:584:GLU:OE1	1:A:630:ARG:HG3	2.17	0.44
1:A:752:LEU:O	1:A:753:LYS:C	2.60	0.44
1:B:550:SER:H	1:B:553:GLN:CG	2.24	0.44
1:B:628:PHE:CD1	1:B:628:PHE:C	2.96	0.44
1:B:732:ILE:O	1:B:735:VAL:HB	2.17	0.44
1:C:663:PHE:CD2	1:C:664:ILE:HD12	2.49	0.44
1:A:299:GLU:CG	1:A:303:LYS:HZ2	2.28	0.44
1:A:381:GLU:C	1:A:383:GLY:H	2.24	0.44
1:A:760:VAL:HG11	1:A:773:PHE:HE1	1.83	0.44
1:B:348:LEU:N	1:B:348:LEU:HD22	2.32	0.44
1:B:391:ILE:CD1	1:B:399:GLY:CA	2.90	0.44
1:B:478:ALA:HB2	1:B:487:PRO:HA	1.99	0.44
1:C:527:LYS:NZ	2:F:145:MET:HA	2.31	0.44
1:C:699:GLY:C	1:C:701:LEU:N	2.74	0.44
2:D:26:THR:HA	2:D:63:ILE:O	2.17	0.44
2:E:99:TYR:CE2	2:E:137:ASN:HB3	2.52	0.44
2:E:99:TYR:HD2	2:E:137:ASN:HB3	1.82	0.44
1:A:415:GLU:C	1:A:417:GLY:N	2.76	0.44
1:A:639:ASN:HD21	1:A:641:ALA:CB	2.30	0.44
1:A:667:LEU:HB3	2:D:14:GLU:OE2	2.17	0.44
1:B:353:LYS:N	1:B:368:GLN:NE2	2.40	0.44
1:C:625:LEU:HA	1:C:625:LEU:HD12	1.66	0.44
2:D:42:ASN:ND2	2:D:147:ALA:CB	2.81	0.44
2:E:100:ILE:HD12	2:E:141:PHE:CD1	2.52	0.44
2:E:105:LEU:HD23	2:E:109:MET:HG2	2.00	0.44
1:A:700:TYR:CE1	1:A:727:GLN:O	2.71	0.44
1:C:327:LEU:HB2	1:C:496:ALA:O	2.18	0.44
1:C:400:LYS:CE	1:C:475:GLU:OE1	2.66	0.44
1:C:504:ILE:O	1:C:505:LYS:C	2.58	0.44
1:C:712:PHE:HB3	1:C:716:LYS:CG	2.44	0.44
2:D:146:THR:HG22	2:D:147:ALA:N	2.31	0.44
2:F:89:PHE:HE1	2:F:138:TYR:N	2.16	0.44
1:A:367:ASP:C	1:A:369:ASP:N	2.76	0.44
1:C:661:ALA:C	1:C:663:PHE:N	2.76	0.44
2:D:141:PHE:O	2:D:141:PHE:CD2	2.70	0.44
2:D:145:MET:HG3	2:D:145:MET:O	2.18	0.44
1:A:774:LYS:O	1:A:775:LEU:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:LEU:HD23	1:B:453:VAL:HB	1.99	0.44
1:B:489:THR:HG23	1:B:490:ALA:N	2.31	0.44
1:C:384:ASN:O	1:C:387:ASN:N	2.51	0.44
2:D:65:PHE:HB2	2:D:66:PRO:CD	2.46	0.44
1:A:329:ARG:C	1:A:330:PRO:O	2.61	0.44
1:A:415:GLU:C	1:A:417:GLY:H	2.24	0.44
1:A:499:PRO:HD2	1:A:625:LEU:HB3	1.99	0.44
1:A:597:ASN:HB2	1:A:598:PRO:HD2	1.99	0.44
1:A:776:LEU:HD12	1:A:776:LEU:H	1.81	0.44
1:B:649:ILE:HD12	2:E:86:ARG:CG	2.48	0.44
1:C:477:MET:C	1:C:488:LEU:HD12	2.43	0.44
1:C:550:SER:OG	1:C:553:GLN:HB2	2.17	0.44
1:C:659:THR:HB	1:C:662:GLU:CG	2.47	0.44
1:C:700:TYR:HD1	1:C:728:ALA:HA	1.82	0.44
2:D:65:PHE:H	2:D:65:PHE:HD1	1.59	0.44
2:D:83:GLU:O	2:D:84:GLU:C	2.59	0.44
2:D:131:ASP:OD1	2:D:133:ASP:OD2	2.35	0.44
2:F:79:THR:C	2:F:81:SER:H	2.25	0.44
2:F:141:PHE:O	2:F:141:PHE:CD2	2.70	0.44
1:A:385:LEU:HD11	1:A:389:LYS:HD2	1.99	0.43
1:A:730:ASN:C	1:A:732:ILE:N	2.76	0.43
1:A:757:THR:O	1:A:758:ASN:C	2.61	0.43
1:A:768:LYS:O	1:A:768:LYS:CG	2.65	0.43
1:B:516:VAL:C	1:B:520:PRO:HG2	2.43	0.43
1:B:703:ASP:O	1:B:704:TYR:C	2.60	0.43
1:B:727:GLN:O	1:B:730:ASN:O	2.35	0.43
1:B:773:PHE:O	1:B:773:PHE:CD1	2.71	0.43
1:C:325:TYR:CE1	1:C:619:ILE:HG12	2.53	0.43
1:C:712:PHE:HD2	1:C:716:LYS:HE2	1.81	0.43
2:D:26:THR:HG22	2:D:64:ASP:OD1	2.18	0.43
2:D:99:TYR:CE2	2:D:137:ASN:HB3	2.53	0.43
2:E:26:THR:HA	2:E:63:ILE:O	2.18	0.43
1:A:322:LEU:HA	1:A:503:GLU:OE2	2.18	0.43
1:C:332:ASN:O	1:C:335:ALA:N	2.39	0.43
1:C:597:ASN:HB2	1:C:598:PRO:HD2	2.00	0.43
2:E:26:THR:HG22	2:E:64:ASP:OD1	2.19	0.43
1:A:305:SER:OG	1:A:306:GLY:N	2.50	0.43
1:A:384:ASN:OD1	1:A:384:ASN:N	2.49	0.43
1:A:773:PHE:O	1:A:774:LYS:C	2.60	0.43
1:B:553:GLN:O	1:B:556:MET:HB3	2.18	0.43
1:B:607:ASN:OD1	1:B:610:MET:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:639:ASN:N	1:B:639:ASN:HD22	2.16	0.43
1:C:302:LEU:C	1:C:302:LEU:CD2	2.88	0.43
2:D:129:ASP:OD1	2:D:132:GLY:N	2.47	0.43
2:F:12:PHE:O	2:F:16:PHE:HB2	2.18	0.43
1:A:529:VAL:HG21	2:D:109:MET:HE1	2.00	0.43
1:C:519:THR:OG1	1:C:520:PRO:HD2	2.18	0.43
2:F:26:THR:HG22	2:F:64:ASP:OD1	2.19	0.43
2:F:99:TYR:CE2	2:F:137:ASN:HB3	2.54	0.43
1:A:345:THR:HG21	1:A:574:VAL:CG2	2.49	0.43
1:A:514:ASP:HA	1:A:517:VAL:HB	2.01	0.43
1:A:707:SER:C	1:A:709:ASN:N	2.76	0.43
1:B:371:SER:O	1:B:372:LYS:C	2.60	0.43
1:B:383:GLY:O	1:B:386:GLU:HB2	2.19	0.43
1:B:508:ILE:HG22	1:B:509:PRO:HD2	2.01	0.43
1:B:549:LEU:HD11	1:B:554:LYS:HG2	1.99	0.43
1:A:370:LEU:HD11	1:A:455:TYR:CD1	2.53	0.43
1:B:326:ILE:HG23	1:B:497:LEU:HD21	2.00	0.43
1:B:441:VAL:HA	1:B:461:LYS:HG2	2.01	0.43
1:B:607:ASN:O	1:B:610:MET:N	2.52	0.43
1:B:747:ASN:O	1:B:751:TYR:HB3	2.17	0.43
1:C:722:ILE:HG12	1:C:763:LEU:HB2	1.99	0.43
2:E:39:LEU:O	2:E:39:LEU:HG	2.18	0.43
1:A:302:LEU:HD12	1:A:602:PHE:HE1	1.84	0.43
1:A:478:ALA:C	1:A:488:LEU:HD11	2.44	0.43
1:A:650:THR:O	1:A:651:LYS:C	2.62	0.43
1:A:700:TYR:HB3	1:A:728:ALA:HB2	2.00	0.43
1:A:712:PHE:CE2	1:A:716:LYS:HE2	2.54	0.43
1:A:762:LEU:O	1:A:766:HIS:HB2	2.19	0.43
1:B:400:LYS:C	1:B:401:ILE:CG2	2.90	0.43
1:B:744:GLU:HG2	1:C:397:GLU:CG	2.48	0.43
1:C:408:LEU:C	1:C:408:LEU:CD2	2.90	0.43
1:C:516:VAL:O	1:C:516:VAL:CG1	2.58	0.43
2:E:44:THR:HG22	2:E:47:GLU:CG	2.45	0.43
2:F:26:THR:HA	2:F:63:ILE:O	2.17	0.43
1:A:345:THR:HG21	1:A:574:VAL:HG22	2.00	0.43
1:A:445:ARG:HH22	1:A:456:LYS:HG2	1.83	0.43
1:B:320:ARG:HH21	1:B:320:ARG:CG	2.31	0.43
1:B:323:ASN:ND2	1:B:500:SER:CB	2.82	0.43
1:B:368:GLN:C	1:B:370:LEU:H	2.26	0.43
1:B:570:THR:O	1:B:572:GLY:N	2.51	0.43
1:B:727:GLN:HG3	1:B:786:GLU:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:745:TYR:O	1:B:749:PHE:CD1	2.72	0.43
1:C:320:ARG:HA	1:C:598:PRO:O	2.19	0.43
1:C:329:ARG:HD2	1:C:590:ASP:OD2	2.18	0.43
1:C:463:THR:CG2	1:C:464:VAL:N	2.82	0.43
2:D:95:ASP:OD1	2:D:104:GLU:OE2	2.36	0.43
1:A:304:ALA:HB3	1:A:604:LEU:CD1	2.49	0.43
1:A:337:ASN:CB	1:A:412:GLU:OE2	2.64	0.43
1:A:354:SER:N	4:A:999:DOT:O2G	2.42	0.43
1:A:385:LEU:HD23	1:C:640:LYS:HB3	2.00	0.43
1:B:318:ILE:HD12	1:B:319:ALA:H	1.83	0.43
1:B:629:ASN:ND2	1:B:631:SER:CA	2.79	0.43
1:C:324:THR:OG1	1:C:499:PRO:HB3	2.18	0.43
1:C:551:ASN:O	1:C:552:TRP:C	2.61	0.43
1:C:757:THR:O	1:C:758:ASN:C	2.61	0.43
1:C:773:PHE:CD2	1:C:774:LYS:N	2.87	0.43
2:E:92:PHE:CZ	2:E:108:VAL:HG11	2.53	0.43
1:A:647:ASP:OD2	2:D:90:ARG:NE	2.52	0.43
1:A:663:PHE:CD1	1:A:752:LEU:HD11	2.54	0.43
1:B:313:ASP:O	1:B:315:PHE:N	2.52	0.43
1:B:327:LEU:CD2	1:B:595:ILE:HG23	2.48	0.43
1:B:555:GLN:O	1:B:558:ASP:HB2	2.19	0.43
1:C:321:GLU:HB3	1:C:322:LEU:HD12	2.00	0.43
1:C:332:ASN:O	1:C:335:ALA:HB3	2.19	0.43
1:C:456:LYS:HB2	1:C:470:ASN:C	2.24	0.43
1:C:522:SER:HA	1:C:525:LYS:HG3	2.00	0.43
1:C:712:PHE:CE2	1:C:716:LYS:HE2	2.54	0.43
1:C:754:GLU:O	1:C:758:ASN:ND2	2.52	0.43
2:F:118:ASP:OD2	2:F:118:ASP:N	2.52	0.43
1:A:700:TYR:CD1	1:A:728:ALA:HA	2.47	0.42
1:A:773:PHE:CD2	1:A:774:LYS:N	2.86	0.42
1:A:776:LEU:N	1:A:776:LEU:CD1	2.81	0.42
1:B:606:LYS:HB2	1:B:610:MET:HE2	2.01	0.42
1:B:755:ARG:O	1:B:756:ILE:C	2.61	0.42
1:C:502:THR:O	1:C:503:GLU:C	2.62	0.42
1:C:774:LYS:O	1:C:775:LEU:C	2.62	0.42
2:E:102:ALA:O	2:E:103:ALA:C	2.61	0.42
2:E:118:ASP:N	2:E:118:ASP:OD2	2.52	0.42
2:E:145:MET:HE2	2:E:145:MET:HB2	1.72	0.42
2:F:145:MET:O	2:F:145:MET:HG3	2.19	0.42
1:A:797:ILE:HD12	1:A:797:ILE:C	2.44	0.42
1:B:317:LYS:O	1:B:320:ARG:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:GLU:O	1:B:417:GLY:N	2.52	0.42
1:B:434:LEU:HA	1:B:445:ARG:HA	2.01	0.42
1:B:597:ASN:OD1	1:B:597:ASN:C	2.61	0.42
1:B:726:ILE:O	1:B:729:TYR:HB2	2.19	0.42
1:B:774:LYS:O	1:B:774:LYS:CG	2.66	0.42
1:C:385:LEU:C	1:C:385:LEU:CD1	2.92	0.42
2:E:27:ILE:HG13	2:E:63:ILE:HB	2.01	0.42
1:A:340:LYS:O	1:A:342:GLY:N	2.52	0.42
1:A:440:GLN:O	1:A:458:LYS:HE2	2.20	0.42
1:A:721:SER:O	1:A:724:ARG:N	2.53	0.42
1:B:315:PHE:O	1:B:318:ILE:HD12	2.19	0.42
1:B:526:GLN:HG3	2:E:124:MET:HE2	2.00	0.42
1:C:666:ASN:N	1:C:666:ASN:HD22	2.15	0.42
1:C:712:PHE:N	1:C:712:PHE:CD1	2.87	0.42
2:D:89:PHE:HD2	2:D:90:ARG:N	2.17	0.42
2:F:27:ILE:HG13	2:F:63:ILE:HB	2.00	0.42
1:A:665:LYS:HE2	2:D:11:GLU:OE1	2.19	0.42
1:A:667:LEU:C	1:A:670:ILE:HG22	2.44	0.42
1:A:713:SER:O	1:A:714:GLN:C	2.61	0.42
1:B:728:ALA:CA	1:B:731:GLU:CG	2.90	0.42
1:C:549:LEU:CD1	1:C:554:LYS:HE2	2.49	0.42
1:C:691:LYS:HB2	1:C:694:VAL:HG13	2.02	0.42
2:D:89:PHE:CE1	2:D:138:TYR:N	2.87	0.42
2:F:5:THR:O	2:F:9:ILE:CG1	2.66	0.42
1:A:318:ILE:CG2	1:A:322:LEU:HD13	2.49	0.42
1:A:376:GLN:H	1:A:376:GLN:HG3	1.68	0.42
1:A:403:LEU:CD1	1:A:476:VAL:HG21	2.49	0.42
1:B:628:PHE:O	1:B:629:ASN:C	2.62	0.42
1:B:757:THR:O	1:B:760:VAL:N	2.52	0.42
1:C:295:VAL:CG2	1:C:296:LEU:N	2.81	0.42
1:C:307:LEU:HA	1:C:492:TYR:HE1	1.85	0.42
2:E:65:PHE:HB2	2:E:66:PRO:CD	2.45	0.42
2:F:65:PHE:HB2	2:F:66:PRO:CD	2.46	0.42
1:A:540:ARG:HD3	1:A:582:ASP:CG	2.45	0.42
1:A:699:GLY:O	1:A:702:SER:N	2.53	0.42
1:B:387:ASN:O	1:B:388:LYS:C	2.62	0.42
1:B:654:ILE:C	1:B:655:ASN:ND2	2.78	0.42
1:B:773:PHE:HA	1:B:775:LEU:HD22	2.00	0.42
1:C:489:THR:OG1	1:C:490:ALA:N	2.53	0.42
2:E:140:GLU:O	2:E:141:PHE:C	2.63	0.42
1:A:508:ILE:CG2	1:A:532:LEU:HD13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ASN:O	1:A:552:TRP:C	2.62	0.42
1:B:530:THR:HG22	2:E:92:PHE:CE1	2.54	0.42
1:C:628:PHE:CD1	1:C:628:PHE:O	2.73	0.42
1:C:664:ILE:HD12	1:C:664:ILE:N	2.35	0.42
1:C:797:ILE:C	1:C:797:ILE:HD12	2.44	0.42
2:E:72:MET:C	2:E:74:ARG:N	2.78	0.42
2:F:92:PHE:CB	2:F:100:ILE:HD13	2.50	0.42
1:A:463:THR:CG2	1:A:464:VAL:N	2.82	0.42
1:A:551:ASN:C	1:A:553:GLN:N	2.77	0.42
1:B:715:GLU:O	1:B:719:LYS:HB2	2.19	0.42
1:B:751:TYR:O	1:B:752:LEU:C	2.63	0.42
1:C:502:THR:OG1	1:C:503:GLU:N	2.52	0.42
1:C:667:LEU:HA	1:C:670:ILE:CG2	2.49	0.42
1:C:700:TYR:CD1	1:C:728:ALA:HA	2.55	0.42
2:F:145:MET:HE2	2:F:145:MET:HB2	1.69	0.42
1:A:351:HIS:NE2	4:A:999:DOT:H3B	2.34	0.42
1:A:505:LYS:C	1:A:507:GLN:N	2.78	0.42
1:A:776:LEU:H	1:A:776:LEU:CD1	2.32	0.42
1:B:525:LYS:NZ	2:E:114:GLU:HG2	2.35	0.42
1:B:556:MET:O	1:B:560:LEU:HD12	2.19	0.42
1:B:732:ILE:O	1:B:735:VAL:CG1	2.67	0.42
1:C:713:SER:O	1:C:714:GLN:C	2.62	0.42
2:E:79:THR:C	2:E:81:SER:H	2.27	0.42
2:F:129:ASP:OD1	2:F:132:GLY:N	2.44	0.42
2:F:144:MET:SD	2:F:144:MET:O	2.77	0.42
1:A:295:VAL:HG23	1:A:604:LEU:C	2.45	0.42
1:A:484:VAL:CG1	1:A:485:LEU:N	2.82	0.42
1:A:593:ILE:HB	1:A:605:THR:OG1	2.20	0.42
1:A:712:PHE:CD1	1:A:712:PHE:N	2.88	0.42
1:B:520:PRO:O	1:B:521:ASN:C	2.62	0.42
1:B:751:TYR:CE2	1:B:755:ARG:HG3	2.55	0.42
1:C:363:TYR:HB3	1:C:476:VAL:HG11	2.02	0.42
1:C:478:ALA:CA	1:C:488:LEU:HD12	2.50	0.42
1:C:530:THR:HG21	2:F:145:MET:HE3	2.01	0.42
1:C:652:ALA:O	1:C:653:LYS:C	2.63	0.42
2:D:44:THR:HG22	2:D:47:GLU:CG	2.44	0.42
2:F:20:ASP:C	2:F:22:ASP:N	2.78	0.42
1:A:363:TYR:HB3	1:A:476:VAL:HG11	2.01	0.41
1:A:502:THR:OG1	1:A:503:GLU:N	2.52	0.41
1:B:453:VAL:HG12	1:B:474:ILE:HD12	2.02	0.41
1:B:546:LYS:O	1:B:547:GLY:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:MET:C	1:B:558:ASP:N	2.77	0.41
1:B:629:ASN:ND2	1:B:630:ARG:N	2.67	0.41
1:B:722:ILE:O	1:B:726:ILE:CG1	2.68	0.41
1:C:593:ILE:HB	1:C:605:THR:OG1	2.20	0.41
1:A:523:LEU:O	1:A:525:LYS:N	2.52	0.41
1:A:540:ARG:CZ	1:A:627:TYR:CE1	3.03	0.41
1:A:658:PRO:HG3	1:A:752:LEU:HD22	2.02	0.41
1:A:754:GLU:O	1:A:758:ASN:ND2	2.53	0.41
1:B:374:HIS:ND1	1:B:375:GLY:N	2.68	0.41
1:B:383:GLY:O	1:B:384:ASN:C	2.62	0.41
1:B:629:ASN:HB3	1:B:632:TYR:CZ	2.55	0.41
1:B:762:LEU:O	1:B:766:HIS:HB2	2.20	0.41
1:B:786:GLU:O	1:B:787:THR:C	2.63	0.41
1:C:511:LYS:N	1:C:514:ASP:OD1	2.51	0.41
2:D:130:ILE:O	2:D:130:ILE:CG2	2.68	0.41
2:F:68:PHE:CE1	2:F:72:MET:HG2	2.55	0.41
1:A:540:ARG:HB3	1:A:549:LEU:O	2.20	0.41
1:B:410:ILE:HD13	1:B:419:ILE:HD11	2.01	0.41
1:B:445:ARG:CB	1:B:471:TRP:CZ3	3.02	0.41
1:B:461:LYS:HG3	1:B:462:ILE:H	1.85	0.41
2:D:99:TYR:HD2	2:D:137:ASN:HB3	1.79	0.41
2:E:144:MET:SD	2:E:144:MET:C	3.04	0.41
2:F:39:LEU:HG	2:F:39:LEU:O	2.20	0.41
2:F:132:GLY:C	2:F:134:GLY:H	2.28	0.41
1:A:502:THR:O	1:A:503:GLU:C	2.63	0.41
1:A:505:LYS:O	1:A:507:GLN:N	2.54	0.41
1:A:517:VAL:HG13	2:D:114:GLU:OE2	2.20	0.41
1:A:662:GLU:O	1:A:666:ASN:HB2	2.20	0.41
1:B:350:VAL:CG2	1:B:398:ILE:HG13	2.51	0.41
1:C:340:LYS:O	1:C:342:GLY:N	2.54	0.41
1:C:713:SER:O	1:C:716:LYS:HB3	2.19	0.41
2:E:132:GLY:C	2:E:134:GLY:H	2.28	0.41
1:A:294:ASP:O	1:A:294:ASP:CG	2.63	0.41
1:A:664:ILE:C	1:A:666:ASN:H	2.28	0.41
1:A:670:ILE:HD12	1:A:745:TYR:CD1	2.54	0.41
1:B:403:LEU:HB2	1:B:476:VAL:HG23	2.01	0.41
1:B:558:ASP:C	1:B:560:LEU:N	2.77	0.41
1:B:656:THR:O	1:B:705:TYR:CE1	2.69	0.41
2:D:145:MET:HB2	2:D:145:MET:HE2	1.64	0.41
2:F:85:ILE:O	2:F:88:ALA:HB3	2.20	0.41
2:F:140:GLU:O	2:F:141:PHE:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ASP:OD2	1:A:442:TYR:OH	2.29	0.41
1:A:583:ASN:ND2	4:A:999:DOT:C1B	2.82	0.41
1:B:410:ILE:HD12	1:B:435:LEU:HD21	2.02	0.41
1:B:784:GLU:HB2	1:B:788:ASP:HB2	2.03	0.41
1:C:478:ALA:C	1:C:488:LEU:HD11	2.46	0.41
1:C:558:ASP:O	1:C:559:ARG:C	2.62	0.41
1:C:581:GLN:O	1:C:629:ASN:HA	2.20	0.41
2:D:92:PHE:O	2:D:94:LYS:N	2.44	0.41
2:F:9:ILE:O	2:F:9:ILE:HG22	2.19	0.41
1:A:388:LYS:HD3	1:C:642:TYR:HB2	2.02	0.41
1:B:526:GLN:CD	1:B:526:GLN:N	2.72	0.41
1:B:775:LEU:N	1:B:775:LEU:HD13	2.35	0.41
1:C:505:LYS:C	1:C:507:GLN:N	2.78	0.41
1:C:540:ARG:CZ	1:C:627:TYR:CE1	3.03	0.41
1:C:691:LYS:HB2	1:C:694:VAL:CG1	2.51	0.41
1:A:458:LYS:O	1:A:459:GLU:C	2.64	0.41
1:A:529:VAL:HG11	2:D:109:MET:HE1	2.03	0.41
1:B:629:ASN:HD22	1:B:630:ARG:N	2.19	0.41
1:C:463:THR:HB	1:C:467:GLU:N	2.33	0.41
1:C:742:ALA:O	1:C:743:PRO:C	2.63	0.41
2:D:40:GLY:O	2:D:41:GLN:HG2	2.21	0.41
2:D:79:THR:O	2:D:81:SER:N	2.53	0.41
2:D:121:VAL:O	2:D:123:GLU:N	2.54	0.41
2:F:44:THR:HG22	2:F:47:GLU:CG	2.45	0.41
1:A:406:ASP:O	1:A:407:HIS:C	2.64	0.41
1:A:712:PHE:HD2	1:A:716:LYS:HE2	1.83	0.41
1:A:768:LYS:HD2	1:A:797:ILE:O	2.21	0.41
1:B:457:THR:HG21	1:B:468:LYS:HA	2.01	0.41
1:B:616:GLU:CG	1:B:617:LYS:H	2.33	0.41
1:B:745:TYR:HD2	1:B:749:PHE:CZ	2.39	0.41
1:B:785:ASN:O	1:B:787:THR:N	2.54	0.41
1:C:407:HIS:CD2	1:C:407:HIS:H	2.35	0.41
1:C:421:LYS:HA	1:C:435:LEU:HD23	2.02	0.41
1:C:456:LYS:HD3	1:C:471:TRP:CE2	2.56	0.41
1:C:540:ARG:NH1	1:C:630:ARG:HH21	2.18	0.41
1:C:569:TYR:CE2	1:C:574:VAL:HG23	2.56	0.41
1:C:628:PHE:HD1	1:C:629:ASN:O	2.03	0.41
1:C:752:LEU:O	1:C:753:LYS:C	2.62	0.41
2:D:72:MET:C	2:D:74:ARG:N	2.79	0.41
2:D:92:PHE:CB	2:D:100:ILE:HD13	2.51	0.41
2:D:120:GLU:O	2:D:123:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:81:SER:C	2:F:83:GLU:N	2.79	0.41
1:A:295:VAL:CG2	1:A:296:LEU:N	2.84	0.41
1:B:302:LEU:C	1:B:304:ALA:H	2.29	0.41
1:B:427:ASP:C	1:B:429:GLY:N	2.75	0.41
1:B:703:ASP:O	1:B:703:ASP:OD1	2.38	0.41
1:B:746:LYS:HG2	1:B:750:GLN:HB2	2.03	0.41
1:C:540:ARG:HH12	1:C:630:ARG:HH21	1.69	0.41
1:C:621:GLY:HA2	2:F:94:LYS:O	2.21	0.41
1:C:657:ILE:CG2	1:C:658:PRO:HD2	2.51	0.41
1:C:777:TYR:CD1	1:C:780:LEU:HD21	2.56	0.41
2:D:107:HIS:O	2:D:108:VAL:C	2.64	0.41
2:D:108:VAL:O	2:D:112:LEU:HG	2.21	0.41
2:F:121:VAL:O	2:F:123:GLU:N	2.54	0.41
1:A:326:ILE:HG22	1:A:328:PHE:CE1	2.57	0.40
1:A:593:ILE:HG13	1:A:611:THR:HG21	2.03	0.40
1:B:338:LEU:HD11	1:B:409:ARG:CZ	2.51	0.40
1:B:381:GLU:C	1:B:383:GLY:N	2.76	0.40
1:B:501:LEU:O	1:B:501:LEU:HD23	2.20	0.40
1:B:508:ILE:CG2	1:B:532:LEU:HD22	2.50	0.40
1:C:629:ASN:CB	1:C:632:TYR:CE2	3.03	0.40
1:C:654:ILE:H	1:C:654:ILE:HG13	1.59	0.40
2:D:85:ILE:O	2:D:88:ALA:HB3	2.20	0.40
2:E:80:ASP:C	2:E:82:GLU:N	2.79	0.40
2:E:108:VAL:O	2:E:112:LEU:HG	2.21	0.40
2:E:115:LYS:HD2	2:E:115:LYS:HA	1.96	0.40
1:A:777:TYR:CD1	1:A:780:LEU:HD21	2.55	0.40
1:B:509:PRO:HG2	1:B:512:GLU:CB	2.40	0.40
1:C:494:LEU:HB3	1:C:579:THR:HG22	2.04	0.40
1:C:785:ASN:OD1	1:C:786:GLU:HG2	2.22	0.40
2:D:132:GLY:C	2:D:134:GLY:H	2.28	0.40
2:F:89:PHE:HD2	2:F:90:ARG:N	2.18	0.40
2:F:129:ASP:OD1	2:F:129:ASP:C	2.64	0.40
1:A:549:LEU:CD1	1:A:554:LYS:HE2	2.51	0.40
1:B:297:LYS:HA	1:B:602:PHE:O	2.21	0.40
1:B:717:LYS:HD2	2:E:132:GLY:H	1.78	0.40
1:C:411:GLU:O	1:C:412:GLU:C	2.64	0.40
1:C:510:GLN:HE21	1:C:510:GLN:HA	1.86	0.40
1:C:526:GLN:HB3	2:F:144:MET:CE	2.52	0.40
1:C:587:PRO:HB2	1:C:643:ILE:CD1	2.49	0.40
1:C:736:LEU:C	1:C:738:SER:H	2.28	0.40
1:C:779:GLN:HG3	1:C:779:GLN:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:41:GLN:HE21	2:E:41:GLN:HA	1.86	0.40
2:E:81:SER:C	2:E:83:GLU:N	2.79	0.40
1:A:377:GLN:C	1:A:379:ALA:H	2.29	0.40
1:A:520:PRO:C	1:A:521:ASN:O	2.65	0.40
1:A:785:ASN:OD1	1:A:786:GLU:HG2	2.22	0.40
1:B:310:GLU:CB	1:B:567:THR:HG21	2.51	0.40
1:B:317:LYS:O	1:B:318:ILE:C	2.64	0.40
1:B:329:ARG:HE	1:B:329:ARG:HB3	1.61	0.40
1:C:317:LYS:HE2	1:C:317:LYS:HB2	1.96	0.40
2:E:89:PHE:CD1	2:E:138:TYR:HA	2.57	0.40
1:A:432:TYR:CE1	1:A:471:TRP:CZ3	3.07	0.40
1:A:517:VAL:CA	1:A:525:LYS:NZ	2.85	0.40
1:B:325:TYR:HB2	1:B:498:ALA:HB3	2.03	0.40
1:B:717:LYS:CD	2:E:132:GLY:H	2.32	0.40
1:B:777:TYR:CD1	1:B:780:LEU:CD1	2.92	0.40
1:C:440:GLN:O	1:C:458:LYS:HE2	2.21	0.40
1:C:443:GLU:HB2	1:C:458:LYS:HG2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A	479/510 (94%)	386 (81%)	71 (15%)	22 (5%)	2	17
1	B	457/510 (90%)	335 (73%)	89 (20%)	33 (7%)	1	10
1	C	499/510 (98%)	384 (77%)	93 (19%)	22 (4%)	2	18
2	D	141/149 (95%)	105 (74%)	28 (20%)	8 (6%)	1	13
2	E	141/149 (95%)	108 (77%)	24 (17%)	9 (6%)	1	12
2	F	141/149 (95%)	108 (77%)	23 (16%)	10 (7%)	1	10
All	All	1858/1977 (94%)	1426 (77%)	328 (18%)	104 (6%)	1	14

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	GLN
1	A	521	ASN
1	B	566	TYR
1	B	571	GLY
1	B	757	THR
1	C	368	GLN
1	C	519	THR
1	C	521	ASN
2	D	82	GLU
2	E	82	GLU
2	F	82	GLU
1	A	378	LEU
1	A	629	ASN
1	A	653	LYS
1	B	299	GLU
1	B	460	GLY
1	B	525	LYS
1	B	547	GLY
1	B	575	VAL
1	B	722	ILE
1	B	734	ASN
1	B	735	VAL
1	B	736	LEU
1	B	739	LYS
1	B	774	LYS
1	B	786	GLU
1	B	796	ILE
1	C	378	LEU
1	C	569	TYR
2	D	93	ASP
2	D	141	PHE
2	E	141	PHE
2	F	93	ASP
2	F	141	PHE
1	A	294	ASP
1	A	317	LYS
1	A	347	GLY
1	A	377	GLN
1	A	510	GLN
1	B	309	PRO
1	B	317	LYS
1	B	354	SER

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Mol	Chain	Res	Type
1	B	463	THR
1	B	563	ALA
1	B	591	ASN
1	B	702	SER
1	B	706	ASN
1	B	793	PHE
1	C	317	LYS
1	C	332	ASN
1	C	623	ASP
2	D	73	ALA
2	D	76	MET
2	D	80	ASP
2	E	73	ALA
2	E	76	MET
2	F	73	ALA
2	F	76	MET
2	F	80	ASP
1	A	330	PRO
1	A	332	ASN
1	A	511	LYS
1	A	520	PRO
1	A	708	ALA
1	B	332	ASN
1	B	361	ALA
1	B	629	ASN
1	B	794	GLN
1	C	347	GLY
1	C	407	HIS
1	C	523	LEU
1	C	708	ALA
2	D	118	ASP
2	E	80	ASP
2	E	118	ASP
2	F	94	LYS
2	F	118	ASP
1	A	503	GLU
1	A	569	TYR
1	A	608	TRP
1	B	694	VAL
1	B	792	VAL
1	C	330	PRO
1	C	377	GLN

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Mol	Chain	Res	Type
1	C	658	PRO
2	D	54	GLU
2	E	49	GLN
2	E	54	GLU
2	E	94	LYS
2	F	54	GLU
1	A	598	PRO
1	A	784	GLU
1	B	295	VAL
1	B	373	LYS
1	C	578	GLY
1	C	608	TRP
2	F	49	GLN
1	A	358	GLY
1	C	537	GLY
1	C	598	PRO
1	C	694	VAL
1	A	534	ILE
1	C	520	PRO
1	C	657	ILE

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	A	433/455 (95%)	377 (87%)	56 (13%)	4	22
1	B	414/455 (91%)	347 (84%)	67 (16%)	2	15
1	C	448/455 (98%)	394 (88%)	54 (12%)	5	23
2	D	121/127 (95%)	113 (93%)	8 (7%)	15	43
2	E	121/127 (95%)	113 (93%)	8 (7%)	15	43
2	F	121/127 (95%)	110 (91%)	11 (9%)	9	33
All	All	1658/1746 (95%)	1454 (88%)	204 (12%)	4	23

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	LEU
1	A	323	ASN
1	A	329	ARG
1	A	345	THR
1	A	373	LYS
1	A	376	GLN
1	A	384	ASN
1	A	385	LEU
1	A	401	ILE
1	A	407	HIS
1	A	419	ILE
1	A	423	LYS
1	A	438	ASN
1	A	445	ARG
1	A	446	ILE
1	A	455	TYR
1	A	462	ILE
1	A	463	THR
1	A	471	TRP
1	A	484	VAL
1	A	485	LEU
1	A	532	LEU
1	A	538	ILE
1	A	540	ARG
1	A	549	LEU
1	A	559	ARG
1	A	567	THR
1	A	570	THR
1	A	574	VAL
1	A	595	ILE
1	A	599	GLU
1	A	615	ILE
1	A	620	THR
1	A	622	LYS
1	A	629	ASN
1	A	639	ASN
1	A	646	THR
1	A	654	ILE
1	A	656	THR
1	A	657	ILE
1	A	659	THR
1	A	670	ILE
1	A	696	LYS

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Mol	Chain	Res	Type
1	A	701	LEU
1	A	709	ASN
1	A	710	HIS
1	A	719	LYS
1	A	732	ILE
1	A	739	LYS
1	A	759	GLN
1	A	775	LEU
1	A	776	LEU
1	A	781	ASN
1	A	782	PHE
1	A	784	GLU
1	A	796	ILE
1	B	305	SER
1	B	318	ILE
1	B	320	ARG
1	B	327	LEU
1	B	331	VAL
1	B	332	ASN
1	B	333	LYS
1	B	355	SER
1	B	370	LEU
1	B	382	LYS
1	B	388	LYS
1	B	389	LYS
1	B	397	GLU
1	B	398	ILE
1	B	401	ILE
1	B	403	LEU
1	B	406	ASP
1	B	425	GLU
1	B	447	SER
1	B	455	TYR
1	B	458	LYS
1	B	462	ILE
1	B	463	THR
1	B	477	MET
1	B	480	ASN
1	B	485	LEU
1	B	493	ASP
1	B	501	LEU
1	B	503	GLU

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Mol	Chain	Res	Type
1	B	508	ILE
1	B	531	ASN
1	B	536	TYR
1	B	539	GLU
1	B	541	LYS
1	B	544	SER
1	B	545	THR
1	B	548	THR
1	B	549	LEU
1	B	552	TRP
1	B	562	GLU
1	B	564	VAL
1	B	576	ASN
1	B	577	HIS
1	B	588	GLU
1	B	595	ILE
1	B	611	THR
1	B	626	TYR
1	B	629	ASN
1	B	631	SER
1	B	639	ASN
1	B	643	ILE
1	B	646	THR
1	B	656	THR
1	B	701	LEU
1	B	710	HIS
1	B	711	ILE
1	B	712	PHE
1	B	723	PHE
1	B	724	ARG
1	B	730	ASN
1	B	731	GLU
1	B	741	ILE
1	B	744	GLU
1	B	775	LEU
1	B	785	ASN
1	B	794	GLN
1	B	797	ILE
1	C	292	ARG
1	C	326	ILE
1	C	329	ARG
1	C	345	THR

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Mol	Chain	Res	Type
1	C	373	LYS
1	C	376	GLN
1	C	384	ASN
1	C	385	LEU
1	C	401	ILE
1	C	407	HIS
1	C	419	ILE
1	C	423	LYS
1	C	438	ASN
1	C	446	ILE
1	C	455	TYR
1	C	462	ILE
1	C	463	THR
1	C	484	VAL
1	C	485	LEU
1	C	509	PRO
1	C	511	LYS
1	C	523	LEU
1	C	526	GLN
1	C	540	ARG
1	C	549	LEU
1	C	559	ARG
1	C	567	THR
1	C	570	THR
1	C	574	VAL
1	C	595	ILE
1	C	599	GLU
1	C	615	ILE
1	C	620	THR
1	C	622	LYS
1	C	629	ASN
1	C	639	ASN
1	C	646	THR
1	C	649	ILE
1	C	650	THR
1	C	653	LYS
1	C	656	THR
1	C	657	ILE
1	C	658	PRO
1	C	709	ASN
1	C	710	HIS
1	C	719	LYS

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Mol	Chain	Res	Type
1	C	732	ILE
1	C	739	LYS
1	C	759	GLN
1	C	775	LEU
1	C	776	LEU
1	C	781	ASN
1	C	782	PHE
1	C	796	ILE
2	D	14	GLU
2	D	18	LEU
2	D	22	ASP
2	D	65	PHE
2	D	89	PHE
2	D	118	ASP
2	D	135	GLN
2	D	136	VAL
2	E	14	GLU
2	E	18	LEU
2	E	22	ASP
2	E	65	PHE
2	E	89	PHE
2	E	118	ASP
2	E	135	GLN
2	E	136	VAL
2	F	14	GLU
2	F	18	LEU
2	F	22	ASP
2	F	41	GLN
2	F	65	PHE
2	F	89	PHE
2	F	118	ASP
2	F	123	GLU
2	F	135	GLN
2	F	136	VAL
2	F	145	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	ASN
1	A	349	ASN
1	A	376	GLN

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Mol	Chain	Res	Type
1	A	407	HIS
1	A	416	ASN
1	A	438	ASN
1	A	451	ASN
1	A	507	GLN
1	A	510	GLN
1	A	521	ASN
1	A	526	GLN
1	A	555	GLN
1	A	581	GLN
1	A	583	ASN
1	A	607	ASN
1	A	618	ASN
1	A	629	ASN
1	A	633	ASN
1	A	639	ASN
1	A	666	ASN
1	A	714	GLN
1	A	727	GLN
1	A	740	GLN
1	A	758	ASN
1	A	759	GLN
1	A	766	HIS
1	A	781	ASN
1	B	323	ASN
1	B	332	ASN
1	B	368	GLN
1	B	384	ASN
1	B	394	HIS
1	B	407	HIS
1	B	439	ASN
1	B	507	GLN
1	B	510	GLN
1	B	518	ASN
1	B	526	GLN
1	B	531	ASN
1	B	551	ASN
1	B	555	GLN
1	B	581	GLN
1	B	629	ASN
1	B	639	ASN
1	B	706	ASN

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Mol	Chain	Res	Type
1	B	709	ASN
1	B	727	GLN
1	B	730	ASN
1	B	750	GLN
1	B	785	ASN
1	C	323	ASN
1	C	349	ASN
1	C	376	GLN
1	C	377	GLN
1	C	407	HIS
1	C	438	ASN
1	C	451	ASN
1	C	507	GLN
1	C	510	GLN
1	C	518	ASN
1	C	555	GLN
1	C	581	GLN
1	C	583	ASN
1	C	607	ASN
1	C	618	ASN
1	C	629	ASN
1	C	633	ASN
1	C	639	ASN
1	C	655	ASN
1	C	666	ASN
1	C	714	GLN
1	C	727	GLN
1	C	730	ASN
1	C	747	ASN
1	C	759	GLN
1	C	781	ASN
2	D	41	GLN
2	D	60	ASN
2	E	41	GLN
2	E	60	ASN
2	E	107	HIS
2	F	41	GLN
2	F	60	ASN
2	F	107	HIS

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 ⓘ

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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	DOT	C	1999	3	41,42,42	5.54	25 (60%)	60,64,64	6.55	29 (48%)
4	DOT	A	999	3	41,42,42	5.55	25 (60%)	60,64,64	6.55	26 (43%)

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	DOT	C	1999	3	-	3/30/42/42	0/4/4/4
4	DOT	A	999	3	-	7/30/42/42	0/4/4/4

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	DOT	C1'-C2'	19.06	1.70	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1999	DOT	C1'-C2'	18.95	1.70	1.41
4	A	999	DOT	C3'-C2'	16.01	1.74	1.40
4	C	1999	DOT	C3'-C2'	16.00	1.74	1.40
4	C	1999	DOT	PB-O3A	13.41	1.74	1.59
4	A	999	DOT	PB-O3A	13.34	1.73	1.59
4	C	1999	DOT	C8-N7	7.71	1.46	1.31
4	A	999	DOT	C8-N7	7.67	1.46	1.31
4	A	999	DOT	C6'-C1'	6.79	1.50	1.39
4	C	1999	DOT	C6'-C1'	6.78	1.50	1.39
4	A	999	DOT	PB-O3B	6.25	1.66	1.59
4	C	1999	DOT	PB-O3B	6.19	1.66	1.59
4	A	999	DOT	C5-C4	6.06	1.49	1.39
4	C	1999	DOT	C5-C4	5.98	1.49	1.39
4	C	1999	DOT	C1B-N9	5.49	1.57	1.46
4	A	999	DOT	C1B-N9	5.46	1.56	1.46
4	A	999	DOT	C2-N1	5.24	1.43	1.33
4	C	1999	DOT	C2-N1	5.22	1.43	1.33
4	C	1999	DOT	C5'-C4'	5.15	1.49	1.38
4	A	999	DOT	C5'-C4'	5.15	1.49	1.38
4	A	999	DOT	C5'-C6'	5.11	1.47	1.38
4	C	1999	DOT	C5'-C6'	5.09	1.47	1.38
4	A	999	DOT	C2B-C3B	-4.94	1.42	1.52
4	C	1999	DOT	C2B-C3B	-4.89	1.42	1.52
4	C	1999	DOT	C8-N9	4.88	1.45	1.37
4	A	999	DOT	C8-N9	4.85	1.45	1.37
4	C	1999	DOT	O3'-C3B	4.08	1.53	1.46
4	A	999	DOT	O3'-C3B	4.02	1.53	1.46
4	A	999	DOT	C4'-C3'	3.87	1.45	1.38
4	C	1999	DOT	C4'-C3'	3.79	1.45	1.38
4	A	999	DOT	PA-O1A	3.34	1.62	1.50
4	C	1999	DOT	PA-O1A	3.33	1.62	1.50
4	A	999	DOT	O3'-C'	3.15	1.41	1.34
4	C	1999	DOT	O3'-C'	3.15	1.41	1.34
4	C	1999	DOT	C3B-C4B	2.94	1.63	1.52
4	A	999	DOT	C3B-C4B	2.93	1.63	1.52
4	C	1999	DOT	C1'-C'	2.84	1.56	1.50
4	A	999	DOT	C1'-C'	2.84	1.56	1.50
4	A	999	DOT	C6-N1	2.66	1.43	1.35
4	C	1999	DOT	C5B-C4B	2.64	1.59	1.51
4	C	1999	DOT	C6-N1	2.64	1.43	1.35
4	A	999	DOT	C5B-C4B	2.63	1.59	1.51
4	A	999	DOT	C2-N3	2.58	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1999	DOT	C2-N3	2.57	1.38	1.33
4	C	1999	DOT	PB-O1B	-2.43	1.42	1.50
4	A	999	DOT	PB-O1B	-2.42	1.42	1.50
4	A	999	DOT	C5-C6	2.12	1.46	1.41
4	C	1999	DOT	C5-C6	2.12	1.46	1.41
4	A	999	DOT	O1'-C'	2.10	1.28	1.22
4	C	1999	DOT	O1'-C'	2.08	1.28	1.22

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	DOT	C3'-C2'-N2'	26.45	171.91	120.11
4	C	1999	DOT	C3'-C2'-N2'	26.44	171.90	120.11
4	A	999	DOT	C1'-C2'-N2'	-23.22	90.26	122.68
4	C	1999	DOT	C1'-C2'-N2'	-23.19	90.30	122.68
4	A	999	DOT	C3'-C2'-C1'	-22.49	94.08	118.16
4	C	1999	DOT	C3'-C2'-C1'	-22.45	94.13	118.16
4	C	1999	DOT	C6'-C1'-C2'	12.50	131.62	118.96
4	A	999	DOT	C6'-C1'-C2'	12.50	131.61	118.96
4	C	1999	DOT	C2'-C1'-C'	-12.29	104.95	121.10
4	A	999	DOT	C2'-C1'-C'	-12.28	104.95	121.10
4	C	1999	DOT	O3'-C'-O1'	-10.41	106.63	123.55
4	A	999	DOT	O3'-C'-O1'	-10.38	106.67	123.55
4	A	999	DOT	C4'-C3'-C2'	9.97	134.54	121.03
4	C	1999	DOT	C4'-C3'-C2'	9.94	134.50	121.03
4	C	1999	DOT	O3'-C'-C1'	7.80	124.12	111.71
4	A	999	DOT	O3'-C'-C1'	7.79	124.10	111.71
4	C	1999	DOT	N6-C6-N1	-6.41	104.11	118.38
4	A	999	DOT	N6-C6-N1	-6.35	104.23	118.38
4	C	1999	DOT	C6'-C1'-C'	-4.43	109.69	118.66
4	A	999	DOT	C6'-C1'-C'	-4.41	109.72	118.66
4	A	999	DOT	C2B-C1B-N9	4.13	124.32	114.63
4	A	999	DOT	O3'-C3B-C4B	4.10	118.83	109.37
4	C	1999	DOT	O3'-C3B-C4B	4.08	118.80	109.37
4	C	1999	DOT	C3B-C2B-C1B	4.00	110.52	102.89
4	C	1999	DOT	C4-N9-C8	-4.00	101.54	105.74
4	A	999	DOT	C3B-C2B-C1B	3.99	110.49	102.89
4	A	999	DOT	C4-N9-C8	-3.97	101.57	105.74
4	A	999	DOT	O3'-C3B-C2B	3.83	118.44	109.21
4	C	1999	DOT	O3'-C3B-C2B	3.82	118.43	109.21
4	C	1999	DOT	O3G-PG-O3B	-3.62	92.50	104.64
4	A	999	DOT	C3B-O3'-C'	3.49	124.89	117.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1999	DOT	C3B-O3'-C'	3.48	124.88	117.33
4	C	1999	DOT	O2A-PA-O1A	3.22	127.44	112.44
4	A	999	DOT	O2A-PA-O1A	3.22	127.44	112.44
4	A	999	DOT	O5'-PA-O1A	-3.21	96.21	108.94
4	C	1999	DOT	O5'-PA-O1A	-3.20	96.23	108.94
4	A	999	DOT	C5-C4-N9	2.67	108.72	105.81
4	A	999	DOT	C4'-C5'-C6'	-2.67	116.94	120.24
4	C	1999	DOT	C5-C4-N9	2.67	108.72	105.81
4	C	1999	DOT	C4'-C5'-C6'	-2.67	116.95	120.24
4	A	999	DOT	C5B-C4B-C3B	2.35	120.14	114.57
4	C	1999	DOT	C5B-C4B-C3B	2.33	120.10	114.57
4	C	1999	DOT	C2B-C1B-N9	2.29	120.01	114.63
4	C	1999	DOT	N3-C4-N9	-2.28	123.29	127.17
4	C	1999	DOT	C1B-N9-C8	2.24	134.78	126.95
4	A	999	DOT	C1B-N9-C8	2.24	134.78	126.95
4	A	999	DOT	N3-C4-N9	-2.22	123.39	127.17
4	C	1999	DOT	O1G-PG-O3B	2.15	111.83	104.64
4	C	1999	DOT	C5-N7-C8	-2.13	100.10	103.45
4	A	999	DOT	C5-N7-C8	-2.11	100.13	103.45
4	C	1999	DOT	C6-C5-N7	-2.05	128.15	132.09
4	A	999	DOT	N9-C8-N7	2.04	116.83	113.94
4	A	999	DOT	C6-C5-N7	-2.03	128.18	132.09
4	C	1999	DOT	N9-C8-N7	2.03	116.81	113.94
4	C	1999	DOT	O2A-PA-O3A	-2.00	101.86	107.27

There are no chirality outliers.

All (10) torsion outliers are listed below:

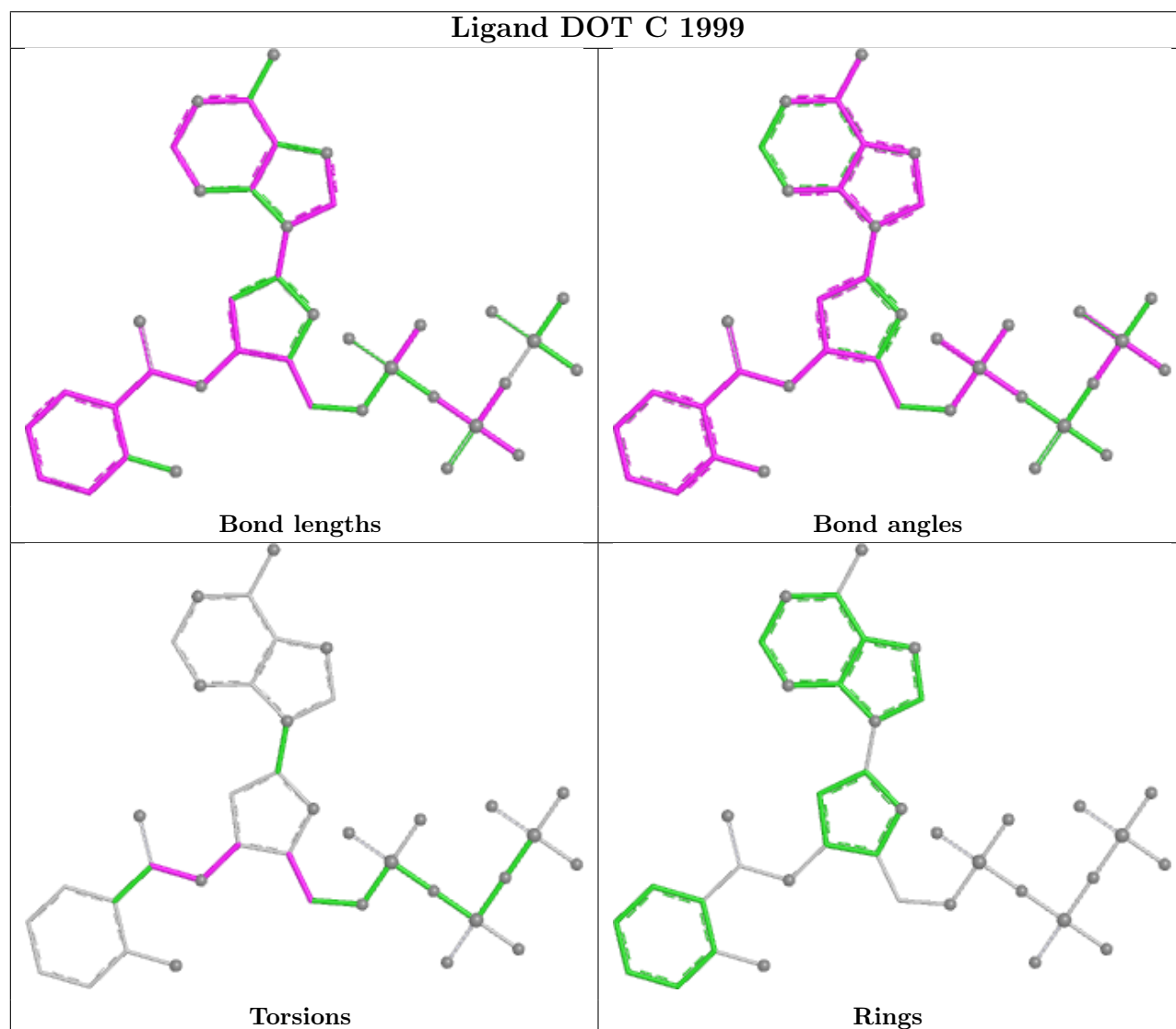
Mol	Chain	Res	Type	Atoms
4	A	999	DOT	O4'-C4B-C5B-O5'
4	A	999	DOT	O1'-C'-O3'-C3B
4	A	999	DOT	C1'-C'-O3'-C3B
4	C	1999	DOT	C2B-C3B-O3'-C'
4	C	1999	DOT	O1'-C'-O3'-C3B
4	A	999	DOT	C3B-C4B-C5B-O5'
4	C	1999	DOT	O4'-C4B-C5B-O5'
4	A	999	DOT	PG-O3B-PB-O2B
4	A	999	DOT	O4'-C1B-N9-C4
4	A	999	DOT	C2B-C3B-O3'-C'

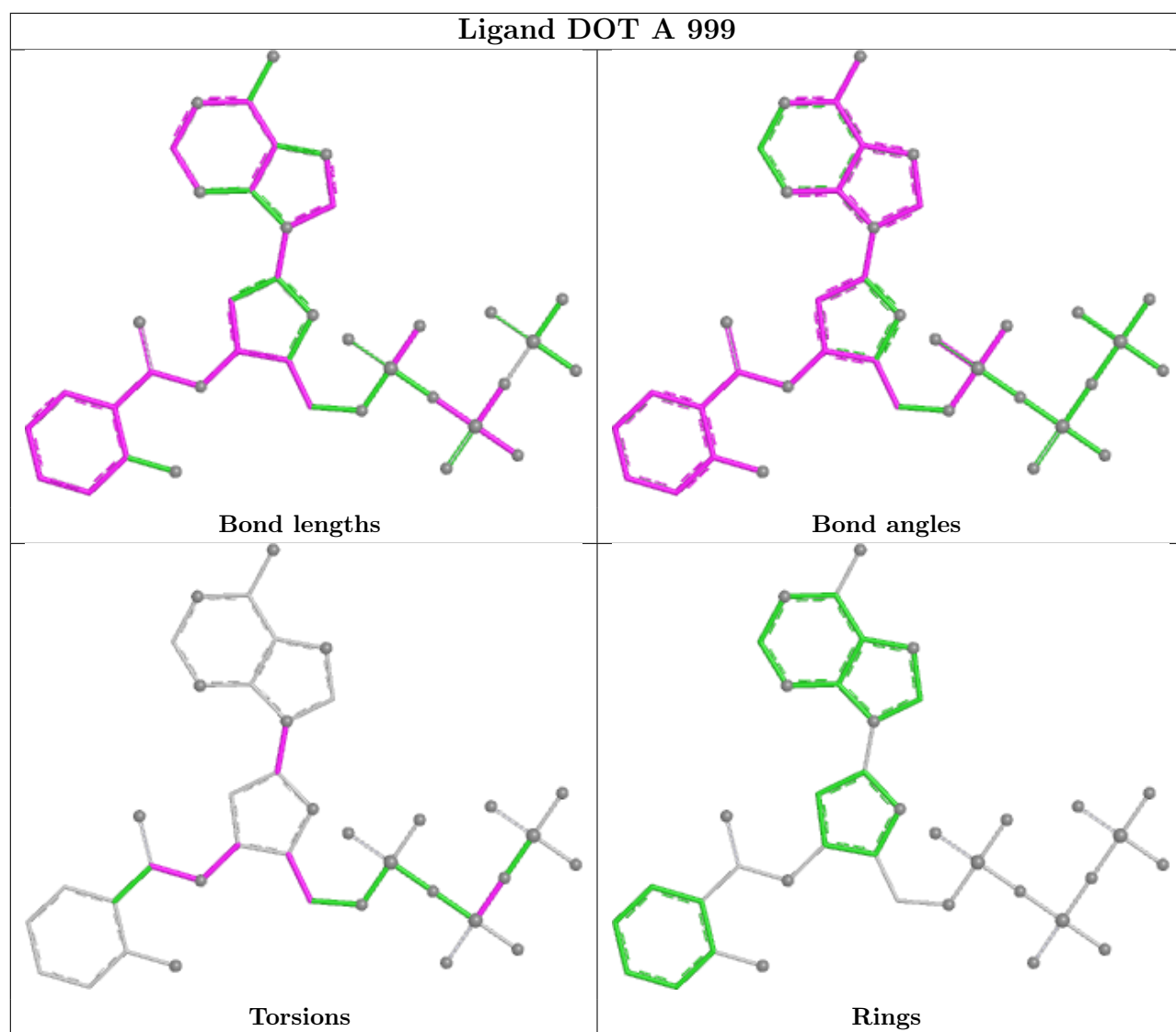
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1999	DOT	5	0
4	A	999	DOT	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	A	485/510 (95%)	0.03	5 (1%) 79 54	14, 57, 137, 162	16 (3%)
1	B	457/510 (89%)	0.14	12 (2%) 57 33	10, 57, 158, 165	12 (2%)
1	C	491/510 (96%)	0.05	8 (1%) 70 43	13, 59, 137, 162	19 (3%)
2	D	143/149 (95%)	0.62	7 (4%) 35 20	49, 143, 180, 183	0
2	E	143/149 (95%)	0.59	9 (6%) 26 16	48, 144, 180, 182	0
2	F	143/149 (95%)	0.46	7 (4%) 35 20	49, 143, 180, 183	0
All	All	1862/1977 (94%)	0.18	48 (2%) 57 33	10, 66, 166, 183	47 (2%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	697	ILE	16.1
2	E	18	LEU	3.8
2	E	61	GLY	3.8
2	E	15	ALA	3.8
1	C	744	GLU	3.7
2	F	38	SER	3.7
1	B	704	TYR	3.3
2	F	48	LEU	3.3
1	C	523	LEU	3.2
1	B	759	GLN	3.2
1	A	791	GLU	3.2
1	C	708	ALA	3.1
2	D	33	GLY	3.1
1	A	620	THR	3.0
2	F	29	THR	3.0
1	A	694	VAL	3.0
1	C	675	ASN	2.9
2	E	59	GLY	2.9
2	F	52	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	658	PRO	2.9
1	A	723	PHE	2.7
2	D	38	SER	2.7
1	A	767	GLN	2.6
2	F	35	VAL	2.6
2	E	71	MET	2.6
2	F	15	ALA	2.6
2	E	79	THR	2.5
2	F	34	THR	2.5
2	E	67	GLU	2.5
1	B	732	ILE	2.5
1	B	319	ALA	2.4
2	D	76	MET	2.4
1	B	728	ALA	2.3
1	B	702	SER	2.3
2	D	19	PHE	2.3
1	C	493	ASP	2.2
2	E	5	THR	2.2
1	C	783	THR	2.2
1	B	703	ASP	2.2
1	B	737	LYS	2.2
1	C	694	VAL	2.2
2	D	122	ASP	2.1
2	D	39	LEU	2.1
2	E	69	LEU	2.1
1	B	709	ASN	2.1
1	C	706	ASN	2.0
1	B	729	TYR	2.0
2	D	5	THR	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

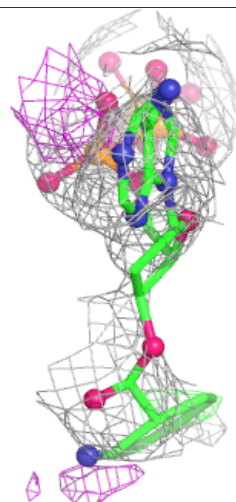
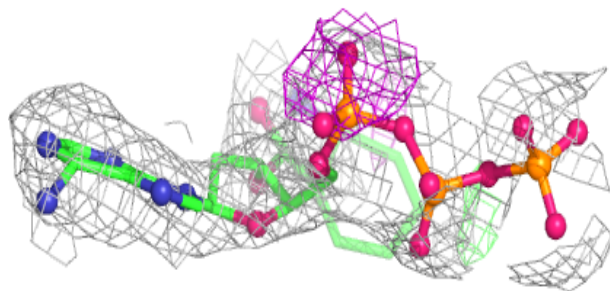
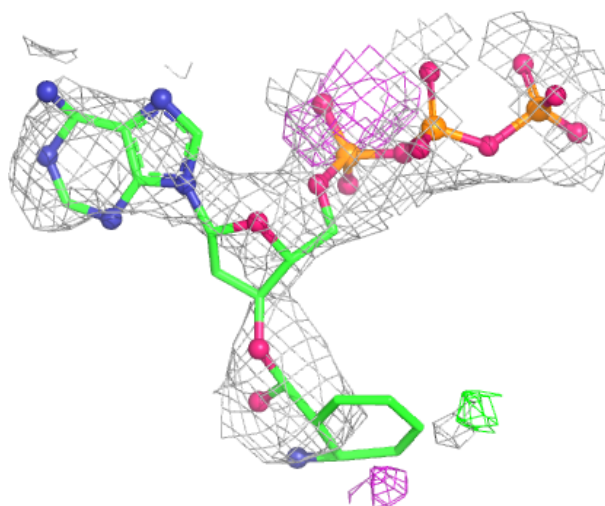
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	CA	F	804	1/1	0.77	0.14	70,70,70,70	0
5	CA	F	805	1/1	0.80	0.13	82,82,82,82	0
4	DOT	A	999	39/39	0.89	0.16	52,80,92,92	0
4	DOT	C	1999	39/39	0.92	0.12	45,80,83,84	0
3	YB	A	901	1/1	0.93	0.11	135,135,135,135	0
3	YB	B	902	1/1	0.93	0.10	142,142,142,142	0
5	CA	E	802	1/1	0.97	0.13	75,75,75,75	0
3	YB	C	903	1/1	0.97	0.12	124,124,124,124	0
5	CA	D	800	1/1	0.97	0.04	65,65,65,65	0
5	CA	D	801	1/1	0.98	0.04	51,51,51,51	0
5	CA	E	803	1/1	0.98	0.06	70,70,70,70	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.

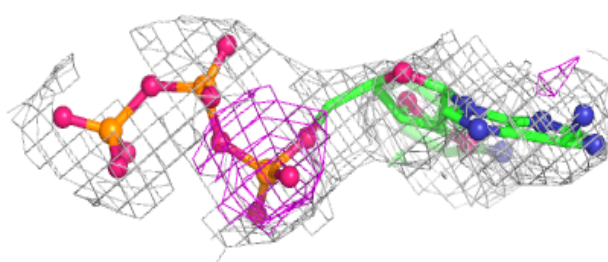
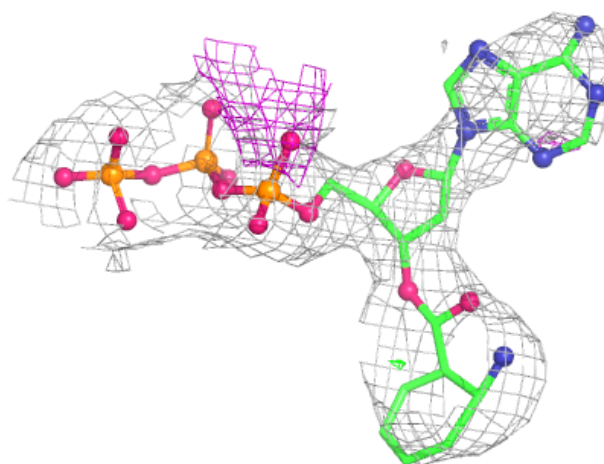
Electron density around DOT A 999:

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



Electron density around DOT C 1999:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.