



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 06:04 AM EDT

PDB ID : 3PDI / pdb_00003pdi
Title : Precursor bound NifEN
Authors : Kaiser, J.T.; Hu, Y.; Wiig, J.A.; Rees, D.C.; Ribbe, M.W.
Deposited on : 2010-10-22
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

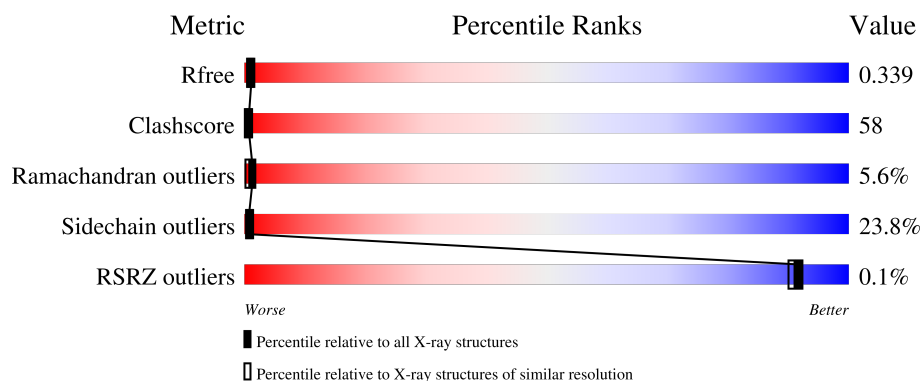
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	483	31% 40% 15% • 12%
1	C	483	28% 42% 16% • 12%
1	E	483	29% 43% 14% • 12%
1	G	483	27% 43% 16% • 12%
2	B	458	36% 40% 16% • 6%

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Mol	Chain	Length	Quality of chain
2	D	458	
2	F	458	
2	H	458	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SF4	A	501	-	-	X	-
3	SF4	C	501	-	-	X	-
3	SF4	E	501	-	-	X	-
3	SF4	G	501	-	-	X	-
4	CZL	G	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26112 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 Nitrogenase MoFe cofactor biosynthesis protein NifE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3280	2064	577	618	21			
1	C	427	Total	C	N	O	S	0	0	0
			3280	2064	577	618	21			
1	E	427	Total	C	N	O	S	0	0	0
			3280	2064	577	618	21			
1	G	427	Total	C	N	O	S	0	0	0
			3280	2064	577	618	21			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP C1DH03
A	-6	HIS	-	expression tag	UNP C1DH03
A	-5	HIS	-	expression tag	UNP C1DH03
A	-4	HIS	-	expression tag	UNP C1DH03
A	-3	HIS	-	expression tag	UNP C1DH03
A	-2	HIS	-	expression tag	UNP C1DH03
A	-1	HIS	-	expression tag	UNP C1DH03
A	0	HIS	-	expression tag	UNP C1DH03
C	-7	MET	-	expression tag	UNP C1DH03
C	-6	HIS	-	expression tag	UNP C1DH03
C	-5	HIS	-	expression tag	UNP C1DH03
C	-4	HIS	-	expression tag	UNP C1DH03
C	-3	HIS	-	expression tag	UNP C1DH03
C	-2	HIS	-	expression tag	UNP C1DH03
C	-1	HIS	-	expression tag	UNP C1DH03
C	0	HIS	-	expression tag	UNP C1DH03
E	-7	MET	-	expression tag	UNP C1DH03
E	-6	HIS	-	expression tag	UNP C1DH03
E	-5	HIS	-	expression tag	UNP C1DH03
E	-4	HIS	-	expression tag	UNP C1DH03
E	-3	HIS	-	expression tag	UNP C1DH03

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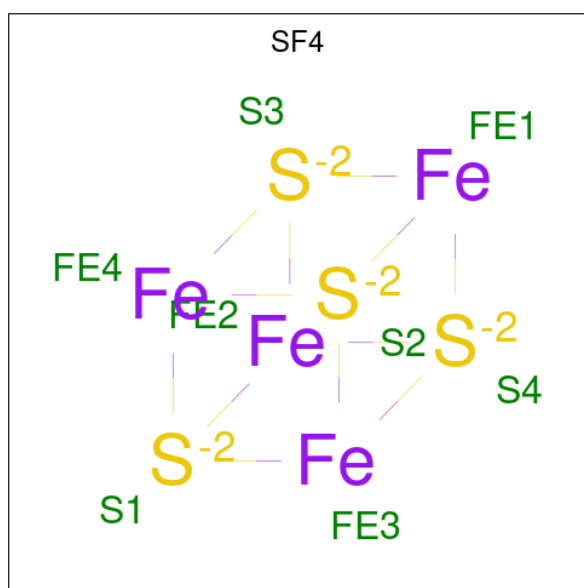
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	HIS	-	expression tag	UNP C1DH03
E	-1	HIS	-	expression tag	UNP C1DH03
E	0	HIS	-	expression tag	UNP C1DH03
G	-7	MET	-	expression tag	UNP C1DH03
G	-6	HIS	-	expression tag	UNP C1DH03
G	-5	HIS	-	expression tag	UNP C1DH03
G	-4	HIS	-	expression tag	UNP C1DH03
G	-3	HIS	-	expression tag	UNP C1DH03
G	-2	HIS	-	expression tag	UNP C1DH03
G	-1	HIS	-	expression tag	UNP C1DH03
G	0	HIS	-	expression tag	UNP C1DH03

- Molecule 2 is a protein called Nitrogenase MoFe cofactor biosynthesis protein NifN.

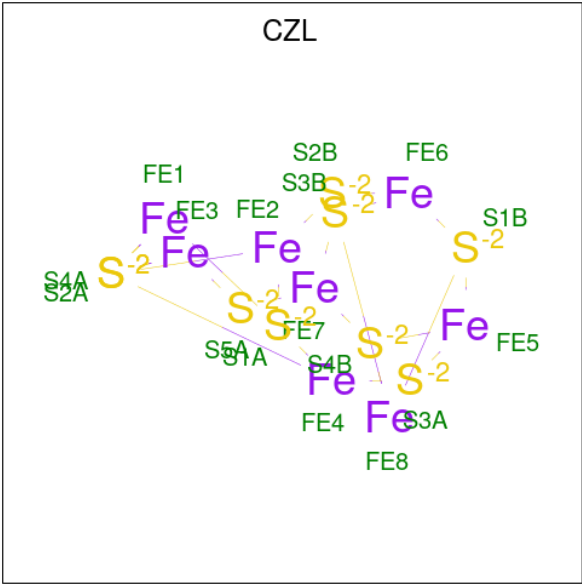
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	0	0
			3223	2025	573	610	15			
2	D	432	Total	C	N	O	S	0	0	0
			3223	2025	573	610	15			
2	F	432	Total	C	N	O	S	0	0	0
			3223	2025	573	610	15			
2	H	432	Total	C	N	O	S	0	0	0
			3223	2025	573	610	15			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

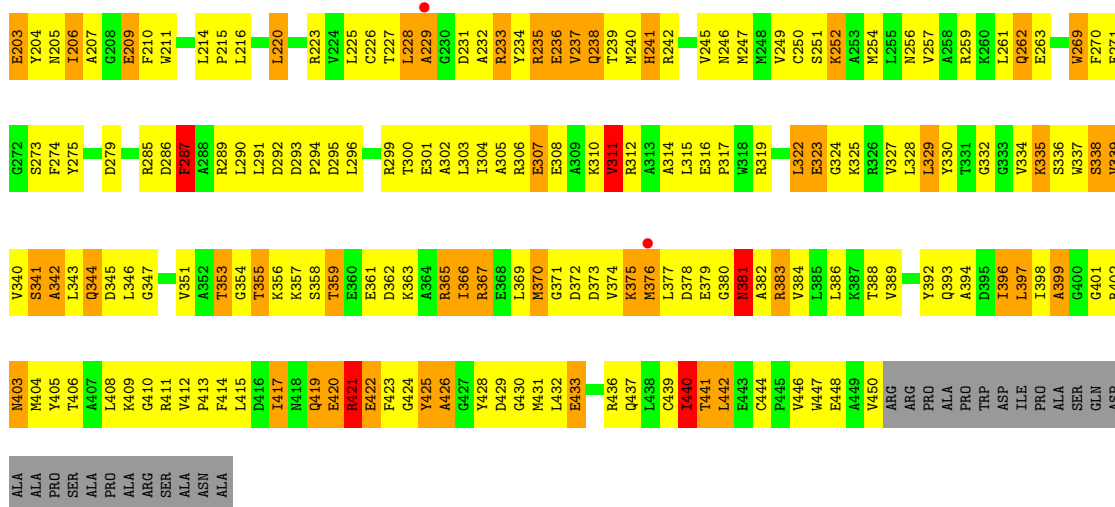


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	G	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is L-Cluster (Fe₈S₉) (CCD ID: CZL) (formula: Fe₈S₉).

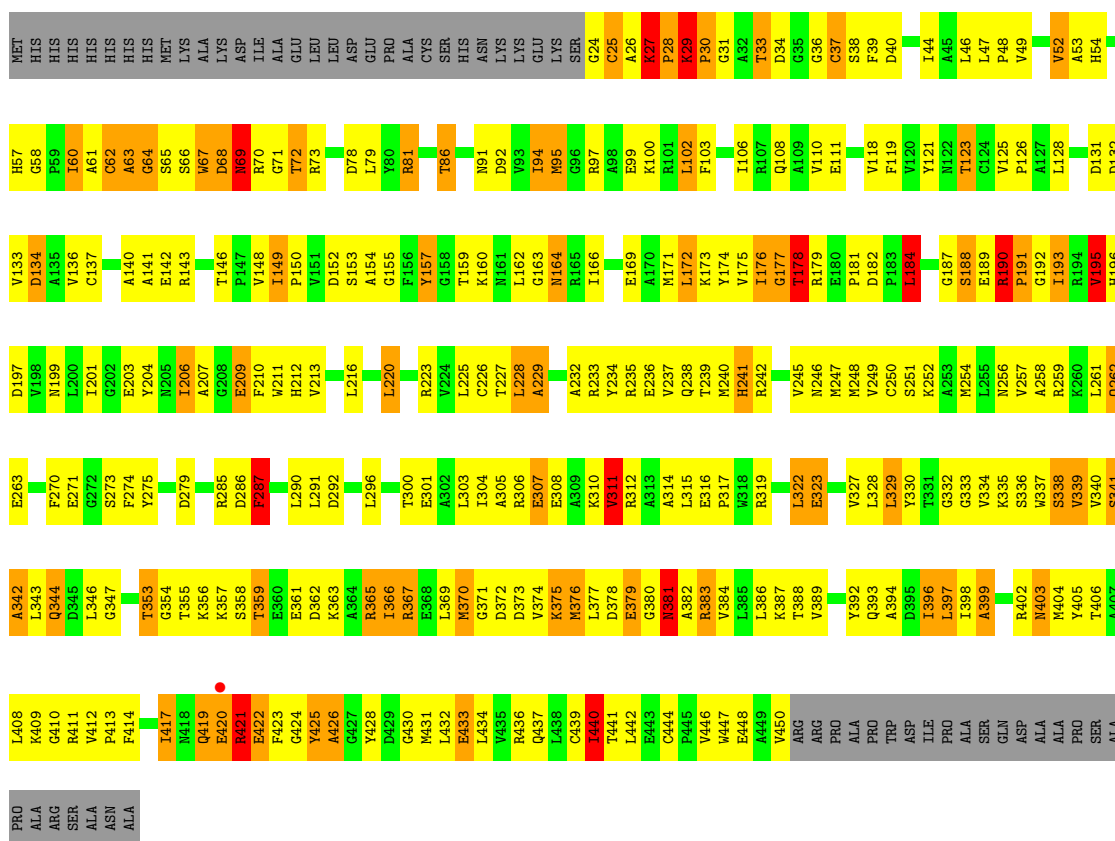


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			17	8	9		
4	C	1	Total	Fe	S	0	0
			17	8	9		
4	E	1	Total	Fe	S	0	0
			17	8	9		
4	G	1	Total	Fe	S	0	0
			17	8	9		



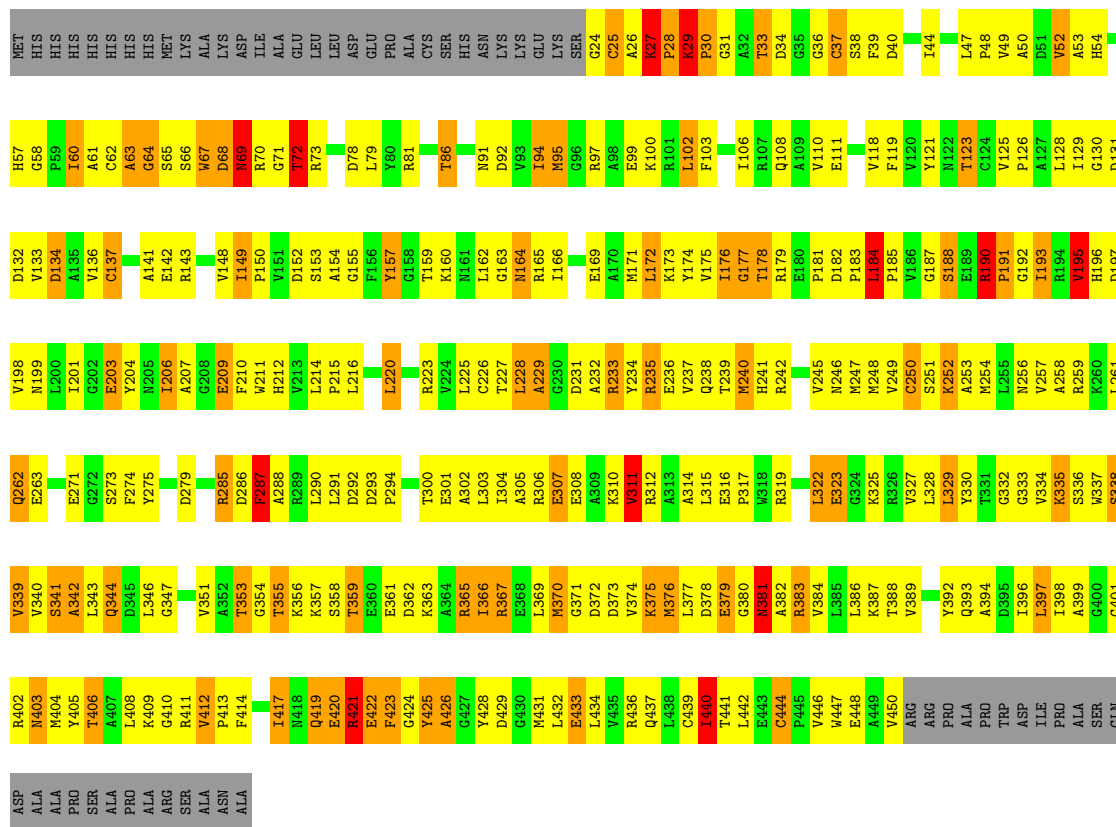
• Molecule 1: Nitrogenase MoFe cofactor biosynthesis protein NifE

Chain E: 29% 43% 14% 12%



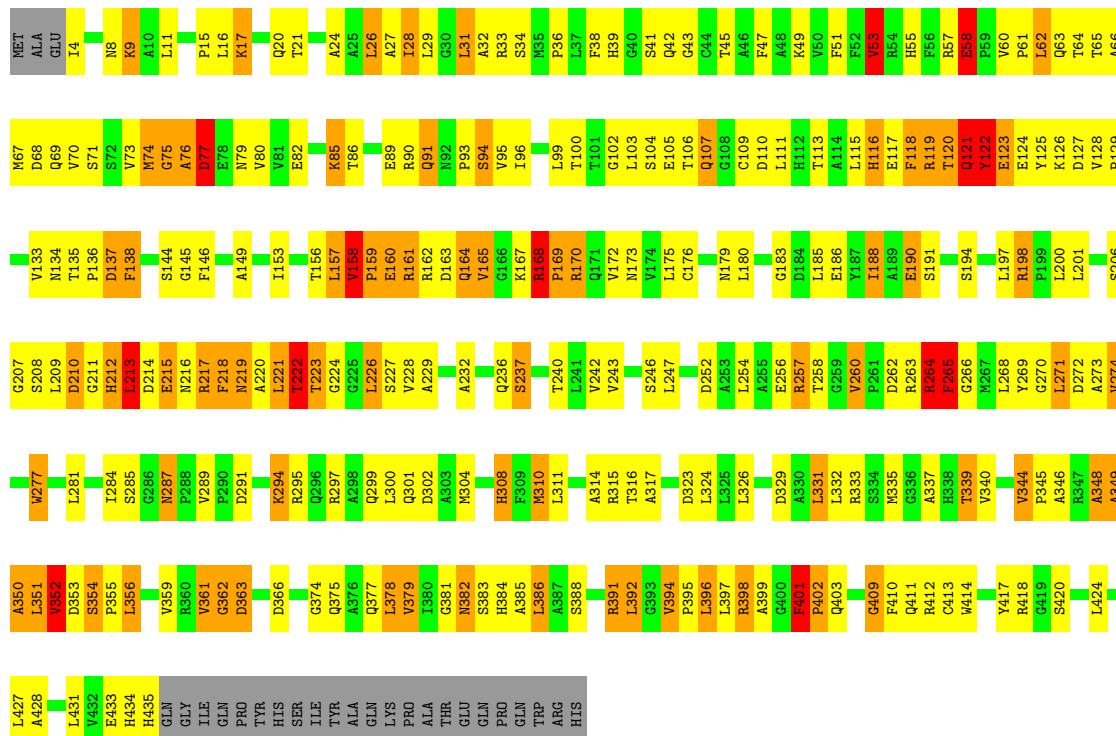
• Molecule 1: Nitrogenase MoFe cofactor biosynthesis protein NifE

Chain G: 27% 43% 16% 12%



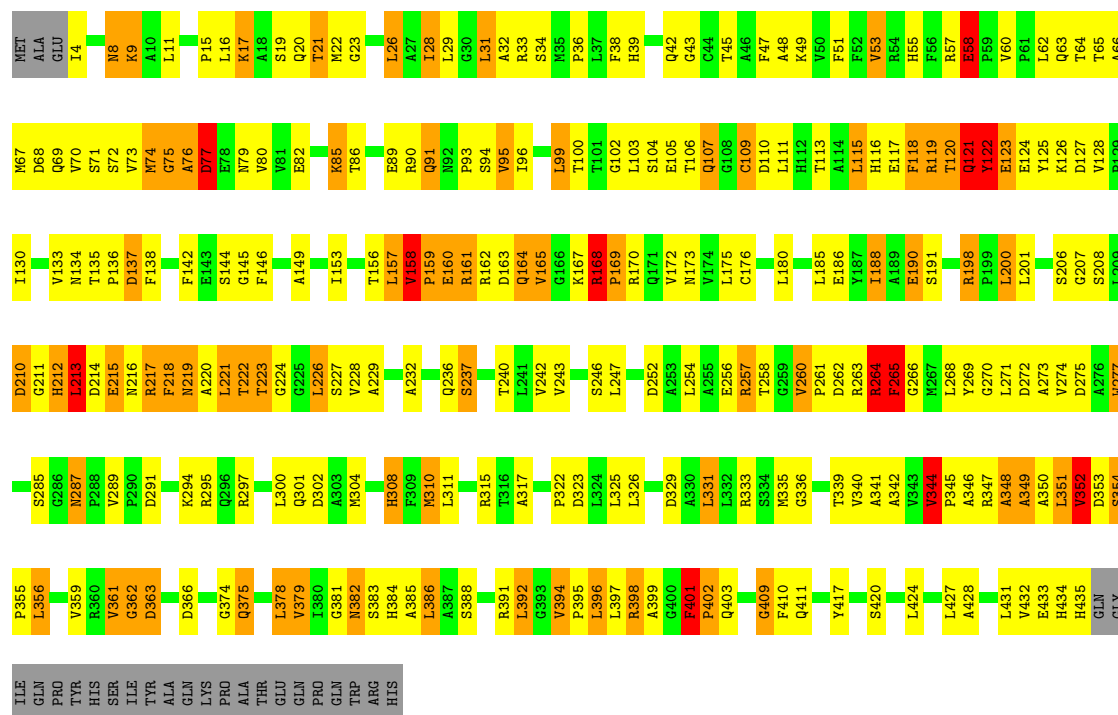
• Molecule 2: Nitrogenase MoFe cofactor biosynthesis protein NifN

Chain B: 36% 40% 16% 6%



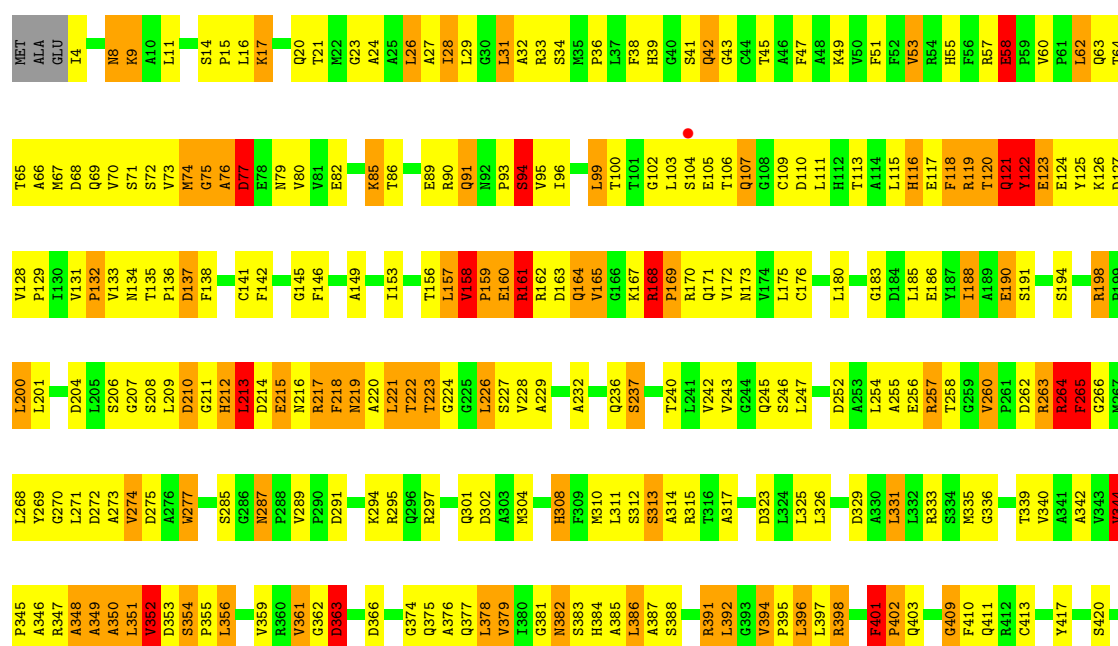
• Molecule 2: Nitrogenase MoFe cofactor biosynthesis protein NifN

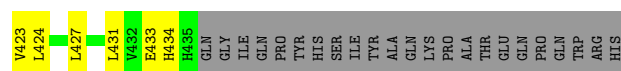
Chain D: 37% 39% 16% 6%



• Molecule 2: Nitrogenase MoFe cofactor biosynthesis protein NifN

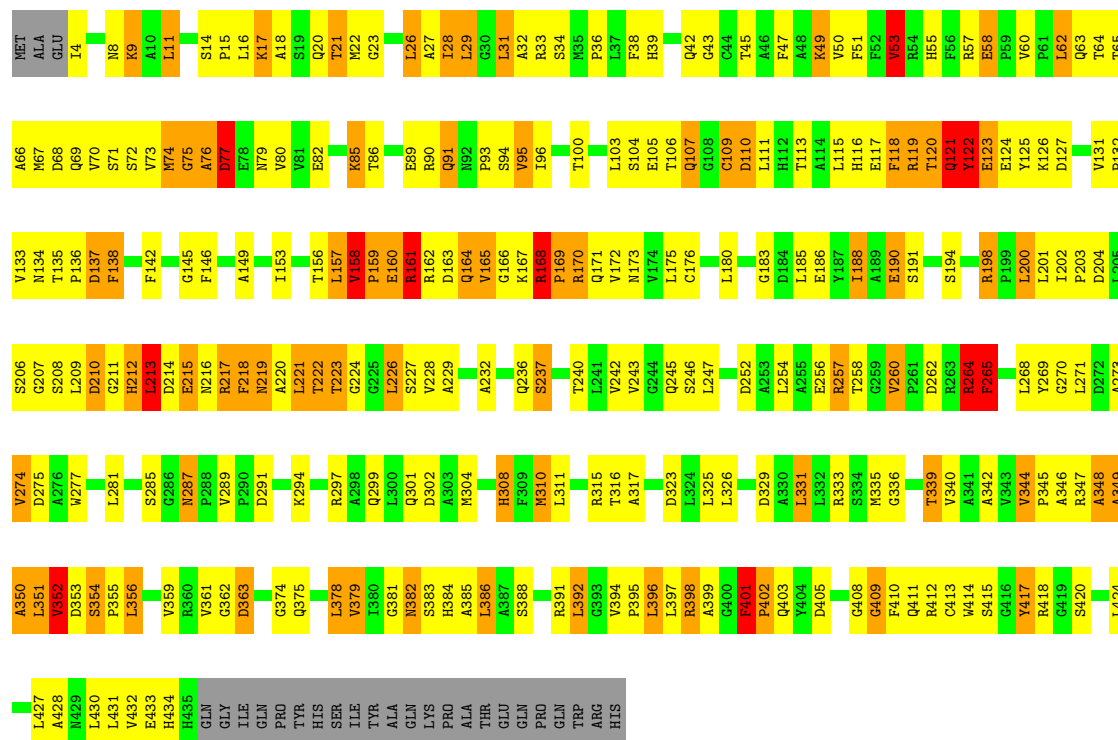
Chain F: 35% 40% 16% 6%





• Molecule 2: Nitrogenase MoFe cofactor biosynthesis protein NifN

Chain H: 35% 40% 16% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	146.07Å 95.22Å 149.98Å 90.00° 95.50° 90.00°	Depositor
Resolution (Å)	39.83 – 2.40 39.83 – 2.40	Depositor EDS
% Data completeness (in resolution range)	87.2 (39.83-2.40) 87.2 (39.83-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.294 , 0.341 0.291 , 0.339	Depositor DCC
R_{free} test set	13821 reflections (8.61%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.075 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	26112	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, CZL

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	0.78	2/3342 (0.1%)	1.12	24/4531 (0.5%)
1	C	0.74	0/3342	1.14	21/4531 (0.5%)
1	E	0.78	0/3342	1.13	19/4531 (0.4%)
1	G	0.73	1/3342 (0.0%)	1.15	24/4531 (0.5%)
2	B	0.88	4/3283 (0.1%)	1.23	19/4466 (0.4%)
2	D	0.91	4/3283 (0.1%)	1.24	22/4466 (0.5%)
2	F	0.88	3/3283 (0.1%)	1.23	20/4466 (0.4%)
2	H	0.88	4/3283 (0.1%)	1.23	24/4466 (0.5%)
All	All	0.82	18/26500 (0.1%)	1.18	173/35988 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	1
1	G	0	1
2	B	0	4
2	D	0	4
2	F	0	5
2	H	0	4
All	All	0	21

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	119	ARG	CA-C	7.86	1.62	1.53
2	D	119	ARG	CA-C	7.14	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	120	THR	CA-C	6.75	1.58	1.52
2	B	119	ARG	CA-C	6.70	1.61	1.53
2	F	344	VAL	CA-CB	-6.54	1.49	1.55
1	G	412	VAL	CA-C	6.46	1.57	1.52
2	H	119	ARG	CA-C	6.28	1.61	1.52
2	B	120	THR	CA-C	5.90	1.57	1.52
2	D	210	ASP	CA-CB	-5.78	1.49	1.54
2	D	120	THR	CA-C	5.63	1.57	1.52
2	D	344	VAL	CA-CB	-5.44	1.50	1.55
2	F	120	THR	CA-C	5.37	1.57	1.52
1	A	47	LEU	C-O	-5.17	1.19	1.24
2	H	210	ASP	CA-CB	-5.15	1.50	1.54
2	B	210	ASP	CA-CB	-5.13	1.50	1.54
2	H	53	VAL	CA-CB	5.11	1.60	1.54
1	A	109	ALA	CA-CB	-5.09	1.45	1.53
2	B	53	VAL	CA-CB	5.03	1.60	1.54

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	394	VAL	N-CA-C	12.75	119.64	109.19
2	B	394	VAL	N-CA-C	12.21	119.21	109.19
2	D	394	VAL	N-CA-C	10.87	118.10	109.19
1	C	178	THR	N-CA-C	-10.73	99.85	113.16
1	G	178	THR	N-CA-C	-10.49	100.16	113.16
1	E	178	THR	N-CA-C	-10.42	100.24	113.16
1	E	29	LYS	CA-C-N	9.69	131.95	119.84
1	E	29	LYS	C-N-CA	9.69	131.95	119.84
1	A	29	LYS	CA-C-N	9.68	131.94	119.84
1	A	29	LYS	C-N-CA	9.68	131.94	119.84
1	G	29	LYS	CA-C-N	9.56	131.79	119.84
1	G	29	LYS	C-N-CA	9.56	131.79	119.84
1	A	178	THR	N-CA-C	-9.24	101.71	113.16
1	C	29	LYS	CA-C-N	9.01	131.11	119.84
1	C	29	LYS	C-N-CA	9.01	131.11	119.84
2	F	122	TYR	N-CA-C	8.73	123.52	111.74
2	H	122	TYR	N-CA-C	8.56	123.29	111.74
2	B	122	TYR	N-CA-C	8.54	123.27	111.74
2	D	122	TYR	N-CA-C	8.33	122.98	111.74
1	A	190	ARG	CA-C-N	7.99	129.82	119.84
1	A	190	ARG	C-N-CA	7.99	129.82	119.84
2	D	409	GLY	N-CA-C	7.97	122.30	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	190	ARG	CA-C-N	7.96	129.79	119.84
1	E	190	ARG	C-N-CA	7.96	129.79	119.84
1	G	425	TYR	N-CA-C	7.91	122.56	113.15
2	B	409	GLY	N-CA-C	7.88	123.93	113.37
1	C	425	TYR	N-CA-C	7.83	122.46	113.15
1	G	50	ALA	N-CA-C	7.79	119.77	111.28
2	H	409	GLY	N-CA-C	7.67	123.44	114.16
1	E	425	TYR	N-CA-C	7.67	122.28	113.15
2	D	392	LEU	N-CA-C	-7.67	97.83	109.79
1	A	425	TYR	N-CA-C	7.62	122.42	113.20
1	C	190	ARG	CA-C-N	7.31	128.98	119.84
1	C	190	ARG	C-N-CA	7.31	128.98	119.84
2	D	344	VAL	N-CA-CB	-7.27	106.82	111.83
2	F	392	LEU	N-CA-C	-7.26	98.60	109.86
2	F	409	GLY	N-CA-C	7.24	123.07	113.37
1	C	184	LEU	CA-C-N	7.05	127.08	119.89
1	C	184	LEU	C-N-CA	7.05	127.08	119.89
1	C	50	ALA	N-CA-C	6.98	118.88	111.28
2	H	430	LEU	N-CA-C	-6.96	103.63	111.14
1	G	190	ARG	CA-C-N	6.95	128.53	119.84
1	G	190	ARG	C-N-CA	6.95	128.53	119.84
1	C	142	GLU	N-CA-C	6.93	119.43	111.11
2	H	392	LEU	N-CA-C	-6.86	99.08	109.79
1	E	184	LEU	CA-C-N	6.76	126.74	119.78
1	E	184	LEU	C-N-CA	6.76	126.74	119.78
2	F	58	GLU	CA-C-N	-6.76	113.34	120.03
2	F	58	GLU	C-N-CA	-6.76	113.34	120.03
2	D	58	GLU	CA-C-N	-6.66	113.44	120.03
2	D	58	GLU	C-N-CA	-6.66	113.44	120.03
2	B	58	GLU	CA-C-N	-6.55	113.55	120.03
2	B	58	GLU	C-N-CA	-6.55	113.55	120.03
2	H	60	VAL	CA-C-N	6.54	126.77	119.90
2	H	60	VAL	C-N-CA	6.54	126.77	119.90
1	G	184	LEU	CA-C-N	6.50	126.47	119.78
1	G	184	LEU	C-N-CA	6.50	126.47	119.78
2	H	213	LEU	N-CA-C	6.41	119.45	109.52
2	F	42	GLN	N-CA-C	6.36	118.30	111.36
1	A	184	LEU	CA-C-N	6.35	126.32	119.78
1	A	184	LEU	C-N-CA	6.35	126.32	119.78
1	A	50	ALA	N-CA-C	6.33	118.26	111.36
1	C	440	ILE	N-CA-CB	6.33	117.26	110.62
1	E	311	VAL	CB-CA-C	-6.32	103.75	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	ALA	N-CA-C	6.27	119.74	110.46
1	G	252	LYS	N-CA-C	-6.24	105.60	113.72
1	G	142	GLU	N-CA-C	6.24	118.59	111.11
2	F	213	LEU	N-CA-C	6.22	118.87	109.41
1	G	434	LEU	N-CA-C	-6.21	104.42	111.07
1	G	311	VAL	CB-CA-C	-6.18	103.93	112.02
1	C	252	LYS	N-CA-C	-6.15	105.73	113.72
2	B	158	VAL	N-CA-C	6.15	122.16	108.88
2	F	158	VAL	N-CA-C	6.11	122.09	108.88
1	A	225	LEU	N-CA-C	-6.11	104.70	111.36
2	H	209	LEU	N-CA-C	6.06	119.65	107.41
2	D	158	VAL	N-CA-C	5.94	121.72	108.88
2	B	392	LEU	N-CA-C	-5.94	100.53	109.79
2	F	94	SER	N-CA-C	-5.86	105.62	112.89
2	H	158	VAL	N-CA-C	5.86	121.54	108.88
1	E	213	VAL	CB-CA-C	-5.86	104.56	111.94
2	D	401	PHE	CA-C-N	-5.85	112.53	119.84
2	D	401	PHE	C-N-CA	-5.85	112.53	119.84
1	A	236	GLU	N-CA-C	-5.83	105.26	112.90
1	E	434	LEU	N-CA-C	-5.83	104.83	111.07
1	E	287	PHE	N-CA-C	-5.82	104.86	111.14
1	A	355	THR	N-CA-C	5.80	117.40	110.44
2	D	95	VAL	CB-CA-C	-5.79	103.75	111.80
2	B	144	SER	N-CA-C	-5.79	105.05	111.36
1	A	311	VAL	CB-CA-C	-5.78	104.45	112.02
2	B	213	LEU	N-CA-C	5.78	118.47	109.52
2	D	210	ASP	CB-CA-C	-5.77	106.16	114.87
2	H	243	VAL	N-CA-C	5.76	115.64	106.88
1	A	440	ILE	N-CA-CB	5.73	116.87	110.51
2	B	399	ALA	N-CA-C	-5.73	100.03	108.79
2	F	210	ASP	CB-CA-C	-5.72	106.23	114.87
1	E	333	GLY	N-CA-C	-5.64	107.98	114.69
2	D	399	ALA	N-CA-C	-5.63	100.38	108.60
2	B	210	ASP	CB-CA-C	-5.63	106.37	114.87
2	F	401	PHE	CA-C-N	-5.62	112.81	119.84
2	F	401	PHE	C-N-CA	-5.62	112.81	119.84
2	D	213	LEU	N-CA-C	5.62	117.95	109.41
1	A	182	ASP	CA-C-N	5.61	126.47	120.13
1	A	182	ASP	C-N-CA	5.61	126.47	120.13
1	C	311	VAL	CB-CA-C	-5.60	104.49	112.22
2	B	116	HIS	N-CA-C	-5.59	106.46	113.28
2	F	336	GLY	N-CA-C	-5.59	107.47	115.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	116	HIS	N-CA-C	-5.56	106.49	113.28
2	H	336	GLY	N-CA-C	-5.52	107.58	115.64
1	C	237	VAL	N-CA-C	-5.50	105.49	110.82
2	D	130	ILE	CA-C-N	-5.50	118.63	122.59
2	D	130	ILE	C-N-CA	-5.50	118.63	122.59
1	C	236	GLU	N-CA-C	-5.46	105.74	112.90
1	C	287	PHE	N-CA-C	-5.45	105.25	111.14
1	G	440	ILE	N-CA-CB	5.45	116.56	110.51
1	A	252	LYS	N-CA-C	-5.44	106.64	113.72
1	C	355	THR	N-CA-C	5.43	116.96	110.44
1	G	412	VAL	N-CA-C	5.42	114.06	107.61
1	E	440	ILE	N-CA-CB	5.41	116.51	110.51
2	H	138	PHE	N-CA-C	5.40	119.73	113.20
1	E	375	LYS	N-CA-C	-5.39	99.32	110.80
2	F	209	LEU	N-CA-C	5.33	119.01	107.49
1	A	333	GLY	N-CA-C	-5.32	108.36	114.69
2	H	95	VAL	CB-CA-C	-5.32	104.41	111.80
2	B	138	PHE	N-CA-C	5.30	119.61	113.20
2	H	379	VAL	N-CA-C	5.30	115.49	107.75
1	C	375	LYS	N-CA-C	-5.29	99.53	110.80
2	D	336	GLY	N-CA-C	-5.28	107.83	115.27
2	B	209	LEU	N-CA-C	5.26	118.86	107.49
1	A	287	PHE	N-CA-C	-5.24	105.48	111.14
1	G	333	GLY	N-CA-C	-5.24	108.84	115.08
2	B	401	PHE	N-CA-C	5.24	121.38	109.81
2	B	243	VAL	N-CA-C	5.23	114.82	106.88
2	D	60	VAL	CA-C-N	5.22	126.03	120.13
2	D	60	VAL	C-N-CA	5.22	126.03	120.13
1	A	444	CYS	CA-C-N	5.22	124.94	119.82
1	A	444	CYS	C-N-CA	5.22	124.94	119.82
1	C	401	GLY	N-CA-C	5.21	120.20	113.27
2	H	399	ALA	N-CA-C	-5.20	100.84	108.79
2	H	49	LYS	N-CA-C	-5.19	105.53	111.14
1	E	182	ASP	CA-C-N	5.18	125.98	120.13
1	E	182	ASP	C-N-CA	5.18	125.98	120.13
1	C	426	ALA	N-CA-C	5.18	117.99	110.17
2	D	379	VAL	N-CA-C	5.14	115.25	107.75
2	F	8	ASN	N-CA-C	5.14	121.74	110.80
2	B	294	LYS	N-CA-C	-5.13	105.76	112.23
1	E	426	ALA	N-CA-C	5.13	117.68	110.14
1	G	137	CYS	N-CA-C	-5.13	105.60	111.14
2	H	417	TYR	N-CA-C	5.13	116.56	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	415	SER	N-CA-C	5.13	117.48	110.55
1	G	375	LYS	N-CA-C	-5.13	99.88	110.80
1	A	142	GLU	N-CA-C	5.12	117.26	111.11
2	H	265	PHE	N-CA-C	5.11	121.69	110.80
2	D	8	ASN	N-CA-C	5.11	121.69	110.80
2	F	243	VAL	N-CA-C	5.11	114.65	106.88
1	A	375	LYS	N-CA-C	-5.11	99.91	110.80
2	D	243	VAL	N-CA-C	5.09	114.62	106.88
2	F	60	VAL	CA-C-N	5.09	125.25	119.90
2	F	60	VAL	C-N-CA	5.09	125.25	119.90
1	E	142	GLU	N-CA-C	5.09	117.22	111.11
2	H	210	ASP	CB-CA-C	-5.08	107.19	114.87
1	G	287	PHE	N-CA-C	-5.08	105.65	111.14
2	B	60	VAL	CA-C-N	5.08	125.87	120.13
2	B	60	VAL	C-N-CA	5.08	125.87	120.13
2	H	408	GLY	N-CA-C	5.07	120.30	114.16
1	G	426	ALA	N-CA-C	5.05	117.22	109.95
1	C	441	THR	N-CA-C	5.04	116.63	111.03
2	H	122	TYR	CB-CA-C	-5.04	104.57	111.73
1	G	444	CYS	CA-C-N	5.04	125.11	119.87
1	G	444	CYS	C-N-CA	5.04	125.11	119.87
1	G	355	THR	N-CA-C	5.04	116.49	110.44
2	H	264	ARG	N-CA-C	5.04	117.94	110.14
1	G	401	GLY	N-CA-C	5.03	119.96	113.27
2	H	401	PHE	N-CA-C	5.01	120.87	109.81

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	ILE	Peptide
2	B	118	PHE	Peptide
2	B	121	GLN	Peptide
2	B	159	PRO	Peptide
2	B	264	ARG	Peptide
1	C	94	ILE	Peptide
2	D	118	PHE	Peptide
2	D	121	GLN	Peptide
2	D	159	PRO	Peptide
2	D	264	ARG	Peptide
1	E	94	ILE	Peptide
2	F	118	PHE	Peptide

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Mol	Chain	Res	Type	Group
2	F	121	GLN	Peptide
2	F	159	PRO	Peptide
2	F	264	ARG	Peptide
2	F	363	ASP	Peptide
1	G	94	ILE	Peptide
2	H	118	PHE	Peptide
2	H	121	GLN	Peptide
2	H	159	PRO	Peptide
2	H	264	ARG	Peptide

5.2 Too-close contacts [i](#)

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	3280	0	3271	404	0
1	C	3280	0	3271	422	0
1	E	3280	0	3270	412	0
1	G	3280	0	3271	404	0
2	B	3223	0	3197	413	5
2	D	3223	0	3197	416	2
2	F	3223	0	3197	406	0
2	H	3223	0	3197	399	7
3	A	8	0	0	2	0
3	C	8	0	0	2	0
3	E	8	0	0	3	0
3	G	8	0	0	4	0
4	A	17	0	0	3	0
4	C	17	0	0	3	0
4	E	17	0	0	2	0
4	G	17	0	0	4	0
All	All	26112	0	25871	3036	7

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 58.

All (3036) 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:A:190:ARG:CB	1:A:191:PRO:HD2	1.56	1.33
1:A:190:ARG:HB3	1:A:191:PRO:CD	1.54	1.31
2:H:119:ARG:HA	2:H:122:TYR:CE2	1.66	1.30
2:B:119:ARG:CA	2:B:122:TYR:HE2	1.42	1.29
2:B:119:ARG:HA	2:B:122:TYR:CE2	1.64	1.29
2:H:119:ARG:CA	2:H:122:TYR:HE2	1.44	1.28
1:E:190:ARG:CB	1:E:191:PRO:HD2	1.62	1.27
2:F:119:ARG:CA	2:F:122:TYR:HE2	1.47	1.27
1:E:190:ARG:HB3	1:E:191:PRO:CD	1.63	1.26
1:G:190:ARG:HB3	1:G:191:PRO:CD	1.64	1.26
1:C:190:ARG:HB3	1:C:191:PRO:CD	1.63	1.26
2:D:119:ARG:HA	2:D:122:TYR:CE2	1.69	1.26
2:D:119:ARG:CA	2:D:122:TYR:HE2	1.46	1.25
1:G:190:ARG:CB	1:G:191:PRO:HD2	1.64	1.23
2:F:119:ARG:HA	2:F:122:TYR:CE2	1.72	1.22
1:C:190:ARG:CB	1:C:191:PRO:HD2	1.64	1.21
2:D:122:TYR:N	2:D:122:TYR:HD1	1.37	1.19
2:B:122:TYR:N	2:B:122:TYR:HD1	1.36	1.16
2:B:308:HIS:CE1	1:C:441:THR:HG22	1.82	1.14
1:A:29:LYS:NZ	1:A:29:LYS:H	1.44	1.13
1:A:441:THR:HG22	2:D:308:HIS:CE1	1.84	1.13
1:E:441:THR:HG22	2:H:308:HIS:CE1	1.84	1.13
2:B:173:ASN:HB2	2:B:240:THR:HG22	1.30	1.12
2:F:122:TYR:N	2:F:122:TYR:HD1	1.34	1.11
1:E:29:LYS:NZ	1:E:29:LYS:H	1.46	1.11
2:F:308:HIS:HE1	1:G:441:THR:HG22	1.08	1.11
2:H:173:ASN:HB2	2:H:240:THR:HG22	1.32	1.11
1:A:419:GLN:HA	1:A:419:GLN:HE21	0.96	1.10
1:C:29:LYS:NZ	1:C:29:LYS:H	1.47	1.10
2:H:242:VAL:HB	2:H:264:ARG:HB3	1.33	1.10
2:F:173:ASN:HB2	2:F:240:THR:HG22	1.33	1.09
1:E:441:THR:HG22	2:H:308:HIS:HE1	0.92	1.08
2:D:119:ARG:CA	2:D:122:TYR:CE2	2.32	1.08
2:B:118:PHE:O	2:B:119:ARG:HD2	1.52	1.08
2:D:173:ASN:HB2	2:D:240:THR:HG22	1.34	1.08
2:F:122:TYR:N	2:F:122:TYR:CD1	2.10	1.08
1:G:419:GLN:HE21	1:G:419:GLN:HA	0.97	1.07
2:H:122:TYR:N	2:H:122:TYR:HD1	1.38	1.07
2:B:122:TYR:N	2:B:122:TYR:CD1	2.13	1.07
2:H:68:ASP:HB3	2:H:70:VAL:HG22	1.35	1.06
1:E:419:GLN:HA	1:E:419:GLN:HE21	0.97	1.06
2:H:122:TYR:N	2:H:122:TYR:CD1	2.15	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:242:VAL:HB	2:D:264:ARG:HB3	1.34	1.05
2:H:119:ARG:CA	2:H:122:TYR:CE2	2.29	1.05
2:D:122:TYR:N	2:D:122:TYR:CD1	2.15	1.05
1:A:441:THR:HG22	2:D:308:HIS:HE1	0.92	1.04
2:F:107:GLN:N	2:F:107:GLN:HE21	1.54	1.04
2:F:118:PHE:O	2:F:119:ARG:HD2	1.56	1.04
1:G:29:LYS:H	1:G:29:LYS:NZ	1.53	1.04
2:F:68:ASP:HB3	2:F:70:VAL:HG22	1.35	1.04
1:C:419:GLN:HA	1:C:419:GLN:HE21	0.90	1.04
2:D:118:PHE:O	2:D:119:ARG:HD2	1.56	1.04
1:A:57:HIS:HD2	1:A:86:THR:HG21	1.19	1.03
1:C:419:GLN:HA	1:C:419:GLN:NE2	1.65	1.03
2:F:119:ARG:CA	2:F:122:TYR:CE2	2.33	1.03
1:A:322:LEU:HD21	1:A:439:CYS:SG	1.99	1.03
2:F:242:VAL:HB	2:F:264:ARG:HB3	1.40	1.03
2:H:208:SER:HA	2:H:223:THR:O	1.59	1.03
2:B:119:ARG:CA	2:B:122:TYR:CE2	2.28	1.02
1:E:206:ILE:HG13	1:E:419:GLN:HB3	1.39	1.02
1:E:57:HIS:CD2	1:E:86:THR:HG21	1.95	1.02
2:B:242:VAL:HB	2:B:264:ARG:HB3	1.38	1.02
2:B:308:HIS:HE1	1:C:441:THR:HG22	0.92	1.02
2:H:118:PHE:O	2:H:119:ARG:HD2	1.60	1.02
2:B:107:GLN:N	2:B:107:GLN:HE21	1.57	1.01
2:D:208:SER:HA	2:D:223:THR:O	1.61	1.00
2:B:68:ASP:HB3	2:B:70:VAL:HG22	1.40	1.00
1:A:57:HIS:CD2	1:A:86:THR:HG21	1.96	1.00
1:G:419:GLN:HA	1:G:419:GLN:NE2	1.69	1.00
2:H:34:SER:H	2:H:221:LEU:HD22	1.24	0.99
1:G:57:HIS:CD2	1:G:86:THR:HG21	1.98	0.99
1:G:57:HIS:HD2	1:G:86:THR:HG21	1.21	0.99
2:B:301:GLN:HE21	1:C:450:VAL:HG12	1.20	0.99
2:F:208:SER:HA	2:F:223:THR:O	1.61	0.99
2:B:34:SER:H	2:B:221:LEU:HD22	1.28	0.99
1:A:172:LEU:HD12	1:A:173:LYS:N	1.76	0.99
2:D:107:GLN:HE21	2:D:107:GLN:N	1.59	0.99
2:D:16:LEU:H	2:D:363:ASP:HB3	1.27	0.98
1:G:172:LEU:HD12	1:G:173:LYS:N	1.76	0.98
1:E:172:LEU:HD12	1:E:173:LYS:N	1.78	0.98
2:D:68:ASP:HB3	2:D:70:VAL:HG22	1.42	0.98
2:F:119:ARG:HA	2:F:122:TYR:HE2	0.83	0.97
1:G:319:ARG:O	1:G:323:GLU:HB2	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:107:GLN:N	2:H:107:GLN:HE21	1.62	0.97
2:D:34:SER:H	2:D:221:LEU:HD22	1.27	0.97
1:E:450:VAL:HG12	2:H:301:GLN:HE21	1.27	0.97
1:E:176:ILE:O	1:E:178:THR:N	1.98	0.97
1:A:174:TYR:CE2	1:A:238:GLN:HG2	2.00	0.96
2:D:119:ARG:HA	2:D:122:TYR:HE2	0.79	0.96
2:D:351:LEU:C	2:D:353:ASP:H	1.74	0.96
1:G:206:ILE:HG13	1:G:419:GLN:HB3	1.45	0.96
2:F:308:HIS:CE1	1:G:441:THR:HG22	2.00	0.96
1:A:206:ILE:HB	1:A:419:GLN:C	1.90	0.96
2:F:34:SER:H	2:F:221:LEU:HD22	1.31	0.96
1:C:57:HIS:CD2	1:C:86:THR:HG21	2.00	0.96
1:E:57:HIS:HD2	1:E:86:THR:HG21	1.23	0.96
1:E:419:GLN:HA	1:E:419:GLN:NE2	1.69	0.96
2:H:118:PHE:C	2:H:122:TYR:CE2	2.44	0.96
2:B:16:LEU:H	2:B:363:ASP:HB3	1.31	0.96
1:C:57:HIS:HD2	1:C:86:THR:HG21	1.31	0.96
1:G:206:ILE:HB	1:G:419:GLN:C	1.90	0.96
1:C:174:TYR:CE2	1:C:238:GLN:HG2	2.01	0.95
1:A:450:VAL:HG12	2:D:301:GLN:HE21	1.27	0.95
1:C:206:ILE:HG13	1:C:419:GLN:HB3	1.47	0.95
1:A:206:ILE:HG13	1:A:419:GLN:HB3	1.47	0.95
2:B:20:GLN:HG3	2:B:145:GLY:HA2	1.46	0.95
1:E:201:ILE:HG23	1:E:228:LEU:HD23	1.48	0.95
1:E:206:ILE:HB	1:E:419:GLN:C	1.91	0.95
1:A:367:ARG:HG2	1:A:367:ARG:HH11	1.31	0.95
1:E:108:GLN:HE22	2:F:11:LEU:H	1.07	0.95
2:F:100:THR:HG22	2:F:135:THR:H	1.32	0.95
2:D:39:HIS:CD2	2:D:65:THR:HG21	2.01	0.94
1:E:154:ALA:HB3	1:E:157:TYR:HE1	1.32	0.94
1:E:319:ARG:O	1:E:323:GLU:HB2	1.66	0.94
2:F:351:LEU:C	2:F:353:ASP:H	1.75	0.94
1:C:367:ARG:HH11	1:C:367:ARG:HG2	1.31	0.94
2:H:118:PHE:CA	2:H:122:TYR:OH	2.16	0.94
1:A:319:ARG:O	1:A:323:GLU:HB2	1.66	0.94
2:F:20:GLN:HG3	2:F:145:GLY:HA2	1.47	0.94
1:A:176:ILE:O	1:A:178:THR:N	2.00	0.94
2:H:32:ALA:HA	2:H:224:GLY:HA3	1.49	0.94
1:E:193:ILE:H	1:E:193:ILE:HD12	1.29	0.94
2:F:32:ALA:HA	2:F:224:GLY:HA3	1.50	0.94
1:C:29:LYS:H	1:C:29:LYS:HZ1	1.13	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:GLN:HA	1:A:419:GLN:NE2	1.66	0.93
1:G:174:TYR:CE2	1:G:238:GLN:HG2	2.03	0.93
2:H:119:ARG:HA	2:H:122:TYR:HE2	0.77	0.93
1:C:206:ILE:HB	1:C:419:GLN:C	1.93	0.93
1:C:319:ARG:O	1:C:323:GLU:HB2	1.68	0.93
2:D:158:VAL:HG11	2:D:232:ALA:O	1.69	0.93
1:A:29:LYS:H	1:A:29:LYS:HZ1	1.12	0.93
2:B:351:LEU:C	2:B:353:ASP:H	1.74	0.93
1:C:419:GLN:HE21	1:C:419:GLN:CA	1.80	0.93
1:G:176:ILE:O	1:G:178:THR:N	2.02	0.93
2:B:208:SER:HA	2:B:223:THR:O	1.69	0.93
1:C:172:LEU:HD12	1:C:173:LYS:N	1.84	0.93
1:C:322:LEU:HD21	1:C:439:CYS:SG	2.08	0.92
1:G:201:ILE:HG23	1:G:228:LEU:HD23	1.51	0.92
1:E:322:LEU:HD21	1:E:439:CYS:SG	2.09	0.92
1:C:37:CYS:SG	2:D:43:GLY:HA3	2.09	0.92
1:G:37:CYS:CB	1:G:155:GLY:HA2	1.99	0.92
1:G:367:ARG:HG2	1:G:367:ARG:HH11	1.31	0.92
2:B:118:PHE:C	2:B:122:TYR:CE2	2.47	0.92
1:C:37:CYS:HB3	1:C:155:GLY:CA	2.00	0.92
1:G:322:LEU:HD21	1:G:439:CYS:SG	2.09	0.92
1:E:29:LYS:H	1:E:29:LYS:HZ1	1.13	0.92
1:E:174:TYR:CE2	1:E:238:GLN:HG2	2.05	0.92
1:G:209:GLU:OE1	1:G:426:ALA:HB2	1.70	0.92
1:A:419:GLN:HE21	1:A:419:GLN:CA	1.83	0.92
2:F:39:HIS:CD2	2:F:65:THR:HG21	2.05	0.92
2:F:158:VAL:HG11	2:F:232:ALA:O	1.70	0.92
2:H:118:PHE:HA	2:H:122:TYR:CZ	2.05	0.92
2:H:100:THR:HG22	2:H:135:THR:H	1.35	0.91
2:H:351:LEU:C	2:H:353:ASP:H	1.75	0.91
2:D:100:THR:HG22	2:D:135:THR:H	1.34	0.91
2:F:16:LEU:H	2:F:363:ASP:HB3	1.34	0.91
2:D:118:PHE:C	2:D:122:TYR:CE2	2.48	0.91
1:G:37:CYS:HB3	1:G:155:GLY:CA	2.01	0.91
2:H:16:LEU:H	2:H:363:ASP:HB3	1.33	0.91
2:D:39:HIS:HD2	2:D:65:THR:HG21	1.35	0.91
1:A:209:GLU:OE1	1:A:426:ALA:HB2	1.70	0.90
2:B:32:ALA:HA	2:B:224:GLY:HA3	1.53	0.90
1:E:37:CYS:HB3	1:E:155:GLY:CA	2.00	0.90
2:H:118:PHE:C	2:H:122:TYR:CZ	2.48	0.90
2:H:158:VAL:HG11	2:H:232:ALA:O	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:217:ARG:HD3	2:H:219:ASN:H	1.36	0.90
1:C:199:ASN:HD21	1:C:225:LEU:HB2	1.36	0.90
1:E:367:ARG:HG2	1:E:367:ARG:HH11	1.35	0.90
1:C:176:ILE:O	1:C:178:THR:N	2.04	0.90
2:F:118:PHE:C	2:F:122:TYR:CE2	2.50	0.90
2:B:119:ARG:HA	2:B:122:TYR:HE2	0.74	0.90
2:B:118:PHE:C	2:B:122:TYR:CZ	2.50	0.90
1:C:193:ILE:H	1:C:193:ILE:HD12	1.35	0.90
2:D:120:THR:N	2:D:122:TYR:CZ	2.40	0.90
2:H:20:GLN:HG3	2:H:145:GLY:HA2	1.52	0.90
2:B:118:PHE:CA	2:B:122:TYR:OH	2.19	0.90
1:C:154:ALA:HB3	1:C:157:TYR:HE1	1.35	0.90
2:F:118:PHE:O	2:F:119:ARG:CD	2.20	0.90
1:A:29:LYS:HB3	1:A:30:PRO:HD2	1.53	0.89
2:B:158:VAL:HG11	2:B:232:ALA:O	1.73	0.89
2:B:120:THR:N	2:B:122:TYR:CZ	2.41	0.89
2:H:39:HIS:CD2	2:H:65:THR:HG21	2.08	0.89
2:F:118:PHE:CA	2:F:122:TYR:OH	2.22	0.88
1:A:37:CYS:HB3	1:A:155:GLY:CA	2.03	0.88
1:E:37:CYS:CB	1:E:155:GLY:HA2	2.03	0.88
2:B:39:HIS:CD2	2:B:65:THR:HG21	2.08	0.88
1:E:199:ASN:HD21	1:E:225:LEU:HB2	1.38	0.88
2:D:217:ARG:HD3	2:D:219:ASN:H	1.37	0.88
1:A:191:PRO:HB3	1:E:314:ALA:HB2	1.53	0.88
1:A:174:TYR:OH	1:A:234:TYR:O	1.91	0.88
1:E:419:GLN:HE21	1:E:419:GLN:CA	1.86	0.87
2:F:212:HIS:HB3	2:F:223:THR:CG2	2.05	0.87
2:H:17:LYS:HG3	2:H:345:PRO:HB2	1.54	0.87
2:B:85:LYS:HD2	2:B:118:PHE:CE1	2.10	0.87
1:G:29:LYS:H	1:G:29:LYS:HZ1	1.13	0.87
1:G:108:GLN:HE22	2:H:11:LEU:H	1.19	0.87
1:A:199:ASN:HD21	1:A:225:LEU:HB2	1.37	0.87
2:B:118:PHE:O	2:B:119:ARG:CD	2.22	0.87
2:F:118:PHE:HA	2:F:122:TYR:CZ	2.09	0.87
2:D:20:GLN:HG3	2:D:145:GLY:HA2	1.56	0.87
1:E:37:CYS:HB3	1:E:155:GLY:HA2	1.54	0.87
2:F:122:TYR:HD1	2:F:122:TYR:H	1.21	0.87
2:B:118:PHE:HA	2:B:122:TYR:CZ	2.10	0.87
2:B:382:ASN:HD21	2:B:384:HIS:HB2	1.37	0.87
2:F:120:THR:N	2:F:122:TYR:CZ	2.43	0.86
1:E:206:ILE:HG13	1:E:419:GLN:CB	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:GLU:O	1:A:311:VAL:HG23	1.75	0.86
2:D:118:PHE:C	2:D:122:TYR:CZ	2.53	0.86
2:D:118:PHE:HA	2:D:122:TYR:CZ	2.10	0.86
1:A:201:ILE:HG23	1:A:228:LEU:HD23	1.57	0.86
2:D:32:ALA:HA	2:D:224:GLY:HA3	1.56	0.86
2:D:118:PHE:CA	2:D:122:TYR:OH	2.22	0.86
1:G:193:ILE:H	1:G:193:ILE:HD12	1.39	0.86
2:B:308:HIS:HE1	1:C:441:THR:CG2	1.86	0.86
1:E:307:GLU:O	1:E:311:VAL:HG23	1.76	0.86
2:F:17:LYS:HG3	2:F:345:PRO:HB2	1.57	0.86
2:F:118:PHE:C	2:F:122:TYR:CZ	2.54	0.86
2:H:118:PHE:O	2:H:119:ARG:CD	2.22	0.86
2:F:217:ARG:HD3	2:F:219:ASN:H	1.39	0.86
1:C:177:GLY:HA3	1:C:241:HIS:NE2	1.90	0.85
2:H:213:LEU:HD23	2:H:214:ASP:H	1.41	0.85
2:D:118:PHE:O	2:D:119:ARG:CD	2.22	0.85
1:E:29:LYS:HB3	1:E:30:PRO:HD2	1.58	0.85
1:G:209:GLU:OE1	1:G:419:GLN:OE1	1.94	0.85
2:B:242:VAL:HB	2:B:264:ARG:CB	2.07	0.85
1:E:209:GLU:OE1	1:E:419:GLN:OE1	1.93	0.85
1:A:29:LYS:HZ1	1:A:29:LYS:N	1.75	0.85
2:D:382:ASN:HD21	2:D:384:HIS:HB2	1.40	0.85
2:F:39:HIS:HD2	2:F:65:THR:HG21	1.39	0.85
1:G:29:LYS:HB3	1:G:30:PRO:HD2	1.59	0.85
2:D:17:LYS:HG3	2:D:345:PRO:HB2	1.57	0.85
2:H:264:ARG:O	2:H:265:PHE:HB2	1.74	0.85
1:C:209:GLU:OE1	1:C:426:ALA:HB2	1.76	0.85
1:C:30:PRO:HA	2:D:63:GLN:OE1	1.77	0.85
1:A:154:ALA:HB3	1:A:157:TYR:HE1	1.39	0.85
2:H:351:LEU:O	2:H:352:VAL:HG12	1.77	0.85
1:C:307:GLU:HG2	1:C:428:TYR:CD2	2.12	0.84
2:H:382:ASN:HD21	2:H:384:HIS:HB2	1.41	0.84
2:D:242:VAL:HB	2:D:264:ARG:CB	2.07	0.84
2:B:163:ASP:O	2:B:165:VAL:N	2.11	0.84
1:A:307:GLU:HG2	1:A:428:TYR:CD2	2.12	0.84
1:C:201:ILE:HG23	1:C:228:LEU:HD23	1.57	0.84
1:A:193:ILE:HD12	1:A:193:ILE:H	1.43	0.84
1:E:307:GLU:HG2	1:E:428:TYR:CD2	2.12	0.84
1:A:30:PRO:HA	2:B:63:GLN:OE1	1.76	0.84
1:C:411:ARG:HH22	2:D:214:ASP:HA	1.43	0.84
1:G:154:ALA:HB3	1:G:157:TYR:HE1	1.43	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLU:OE1	1:A:426:ALA:CB	2.26	0.83
1:E:29:LYS:H	1:E:29:LYS:HZ2	1.26	0.83
1:E:37:CYS:SG	2:F:43:GLY:HA3	2.18	0.83
1:G:419:GLN:HE21	1:G:419:GLN:CA	1.88	0.83
1:A:37:CYS:CB	1:A:155:GLY:HA2	2.08	0.83
1:C:386:LEU:HD21	2:D:216:ASN:HB3	1.59	0.83
2:H:242:VAL:HB	2:H:264:ARG:CB	2.08	0.83
2:D:85:LYS:HD2	2:D:118:PHE:CE1	2.13	0.83
2:B:39:HIS:HD2	2:B:65:THR:HG21	1.41	0.83
2:B:100:THR:HG22	2:B:135:THR:H	1.42	0.83
2:F:301:GLN:HE21	1:G:450:VAL:HG12	1.44	0.83
2:B:201:LEU:O	2:B:226:LEU:HD21	1.79	0.83
2:D:264:ARG:O	2:D:265:PHE:HB2	1.76	0.83
1:E:30:PRO:HA	2:F:63:GLN:OE1	1.78	0.83
2:F:351:LEU:O	2:F:352:VAL:HG12	1.78	0.83
2:D:85:LYS:HD2	2:D:118:PHE:HE1	1.44	0.83
1:E:154:ALA:HB3	1:E:157:TYR:CE1	2.14	0.83
2:B:122:TYR:HD1	2:B:122:TYR:H	1.25	0.83
1:C:361:GLU:HG3	4:C:502:CZL:S3B	2.19	0.82
1:G:307:GLU:HG2	1:G:428:TYR:CD2	2.13	0.82
2:B:217:ARG:HD3	2:B:219:ASN:H	1.43	0.82
1:G:199:ASN:HD21	1:G:225:LEU:HB2	1.41	0.82
1:C:307:GLU:O	1:C:311:VAL:HG23	1.78	0.82
1:E:209:GLU:OE1	1:E:426:ALA:HB2	1.78	0.82
2:B:264:ARG:O	2:B:265:PHE:HB2	1.75	0.82
1:C:37:CYS:HB3	1:C:155:GLY:HA2	1.62	0.82
1:G:177:GLY:HA3	1:G:241:HIS:NE2	1.95	0.82
2:H:85:LYS:HD2	2:H:118:PHE:CE1	2.13	0.82
2:D:126:LYS:NZ	2:D:127:ASP:H	1.78	0.82
1:A:206:ILE:HB	1:A:419:GLN:O	1.80	0.82
1:E:123:THR:HG22	3:E:501:SF4:S4	2.19	0.82
2:H:122:TYR:HD1	2:H:122:TYR:H	1.28	0.82
1:G:362:ASP:O	1:G:366:ILE:HG13	1.80	0.82
2:B:85:LYS:HD2	2:B:118:PHE:HE1	1.44	0.82
2:H:39:HIS:HD2	2:H:65:THR:HG21	1.43	0.82
1:A:29:LYS:H	1:A:29:LYS:HZ2	1.24	0.81
1:A:206:ILE:HG13	1:A:419:GLN:CB	2.09	0.81
2:F:85:LYS:HD2	2:F:118:PHE:CE1	2.15	0.81
1:A:209:GLU:OE1	1:A:419:GLN:OE1	1.99	0.81
1:A:206:ILE:C	1:A:419:GLN:O	2.24	0.81
1:C:206:ILE:HG13	1:C:419:GLN:CB	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:159:PRO:HG3	2:F:257:ARG:HH11	1.46	0.81
2:F:212:HIS:HB3	2:F:223:THR:HG22	1.59	0.81
2:H:120:THR:N	2:H:122:TYR:CZ	2.47	0.81
2:D:381:GLY:O	2:D:398:ARG:HA	1.78	0.81
1:C:29:LYS:H	1:C:29:LYS:HZ2	1.28	0.81
1:A:66:SER:O	1:A:69:ASN:ND2	2.14	0.81
1:G:206:ILE:HG13	1:G:419:GLN:CB	2.10	0.81
2:D:159:PRO:HG3	2:D:257:ARG:HH11	1.46	0.81
1:G:72:THR:HG23	1:G:204:TYR:O	1.79	0.81
2:H:163:ASP:O	2:H:165:VAL:N	2.14	0.81
2:F:264:ARG:O	2:F:265:PHE:HB2	1.79	0.81
2:H:119:ARG:N	2:H:122:TYR:CE2	2.47	0.81
2:H:397:LEU:HD23	2:H:427:LEU:HD21	1.62	0.81
1:E:174:TYR:CE2	1:E:234:TYR:CZ	2.69	0.80
2:B:126:LYS:NZ	2:B:127:ASP:H	1.79	0.80
1:C:209:GLU:OE1	1:C:419:GLN:OE1	1.98	0.80
1:E:29:LYS:HZ1	1:E:29:LYS:N	1.79	0.80
1:E:91:ASN:O	1:E:94:ILE:HG13	1.81	0.80
2:F:242:VAL:HB	2:F:264:ARG:CB	2.10	0.80
2:H:212:HIS:HB3	2:H:223:THR:CG2	2.11	0.80
1:C:37:CYS:CB	1:C:155:GLY:HA2	2.10	0.80
1:G:367:ARG:HG2	1:G:367:ARG:NH1	1.93	0.80
2:B:213:LEU:HD23	2:B:214:ASP:H	1.44	0.80
1:G:209:GLU:OE1	1:G:426:ALA:CB	2.29	0.80
2:D:133:VAL:HG12	2:D:135:THR:HG23	1.63	0.80
2:H:315:ARG:CG	2:H:340:VAL:HG21	2.11	0.80
1:G:57:HIS:HA	1:G:86:THR:CG2	2.12	0.80
2:D:163:ASP:O	2:D:165:VAL:N	2.14	0.80
1:G:26:ALA:O	1:G:27:LYS:HB3	1.80	0.80
2:H:67:MET:HE2	2:H:71:SER:HB2	1.64	0.80
1:C:29:LYS:HB3	1:C:30:PRO:HD2	1.61	0.80
1:E:29:LYS:NZ	1:E:29:LYS:N	2.30	0.79
2:H:117:GLU:C	2:H:122:TYR:OH	2.25	0.79
1:C:154:ALA:HB3	1:C:157:TYR:CE1	2.16	0.79
2:D:213:LEU:HD23	2:D:214:ASP:H	1.46	0.79
1:E:206:ILE:HB	1:E:419:GLN:O	1.80	0.79
2:D:201:LEU:O	2:D:226:LEU:HD21	1.81	0.79
1:E:177:GLY:HA3	1:E:241:HIS:NE2	1.97	0.79
1:C:91:ASN:O	1:C:94:ILE:HG13	1.82	0.79
2:D:120:THR:N	2:D:122:TYR:CE2	2.50	0.79
2:H:168:ARG:HE	2:H:169:PRO:HD3	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:HIS:HB3	2:B:223:THR:CG2	2.13	0.79
1:C:383:ARG:CA	2:D:217:ARG:HH12	1.96	0.79
2:H:159:PRO:CG	2:H:257:ARG:HH11	1.94	0.79
2:B:258:THR:OG1	2:B:260:VAL:HG23	1.82	0.79
2:B:351:LEU:C	2:B:353:ASP:N	2.40	0.79
2:F:85:LYS:HD2	2:F:118:PHE:HE1	1.46	0.79
2:F:159:PRO:CG	2:F:257:ARG:HH11	1.94	0.79
1:G:37:CYS:HB3	1:G:155:GLY:HA2	1.61	0.79
1:G:206:ILE:HB	1:G:419:GLN:O	1.83	0.79
2:B:120:THR:N	2:B:122:TYR:CE2	2.51	0.79
2:F:163:ASP:O	2:F:165:VAL:N	2.15	0.79
1:C:27:LYS:HD3	2:D:66:ALA:HB1	1.65	0.79
1:C:409:LYS:HB3	2:D:218:PHE:CZ	2.18	0.79
2:D:42:GLN:HA	2:D:64:THR:HG21	1.62	0.79
2:H:85:LYS:HD2	2:H:118:PHE:HE1	1.48	0.79
2:B:221:LEU:O	2:B:223:THR:N	2.16	0.79
1:C:29:LYS:HZ1	1:C:29:LYS:N	1.81	0.79
2:F:42:GLN:HA	2:F:64:THR:HG21	1.65	0.79
2:H:118:PHE:CA	2:H:122:TYR:CZ	2.65	0.79
2:F:213:LEU:HD23	2:F:214:ASP:H	1.48	0.79
1:E:193:ILE:HD12	1:E:193:ILE:N	1.97	0.78
2:F:118:PHE:HA	2:F:122:TYR:OH	1.83	0.78
2:H:126:LYS:NZ	2:H:127:ASP:H	1.80	0.78
2:B:17:LYS:HG3	2:B:345:PRO:HB2	1.64	0.78
2:B:159:PRO:HG3	2:B:257:ARG:HH11	1.47	0.78
2:B:351:LEU:O	2:B:352:VAL:HG12	1.82	0.78
1:G:29:LYS:HZ1	1:G:29:LYS:N	1.81	0.78
1:A:174:TYR:CE2	1:A:234:TYR:CZ	2.71	0.78
1:A:252:LYS:HB2	1:A:361:GLU:OE2	1.82	0.78
2:F:119:ARG:N	2:F:122:TYR:CE2	2.51	0.78
1:G:175:VAL:O	1:G:176:ILE:C	2.26	0.78
2:B:119:ARG:N	2:B:122:TYR:CE2	2.50	0.78
2:F:315:ARG:CG	2:F:340:VAL:HG21	2.13	0.78
1:G:177:GLY:CA	1:G:241:HIS:CE1	2.66	0.78
2:B:119:ARG:C	2:B:122:TYR:CE2	2.61	0.78
1:G:37:CYS:HB2	1:G:155:GLY:HA2	1.63	0.78
2:H:118:PHE:HA	2:H:122:TYR:OH	1.80	0.78
1:E:66:SER:O	1:E:69:ASN:ND2	2.16	0.78
2:F:133:VAL:HG12	2:F:135:THR:HG23	1.66	0.78
2:F:201:LEU:O	2:F:226:LEU:HD21	1.84	0.78
2:F:382:ASN:HD21	2:F:384:HIS:HB2	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LYS:HD3	2:B:66:ALA:HB1	1.64	0.78
1:A:386:LEU:HD21	2:B:216:ASN:HB3	1.63	0.78
1:C:175:VAL:O	1:C:176:ILE:C	2.26	0.78
1:E:175:VAL:O	1:E:176:ILE:C	2.23	0.78
1:E:206:ILE:C	1:E:419:GLN:O	2.27	0.78
1:C:57:HIS:HA	1:C:86:THR:HG22	1.66	0.78
2:F:126:LYS:NZ	2:F:127:ASP:H	1.82	0.78
1:G:413:PRO:HA	1:G:447:TRP:CZ2	2.19	0.78
1:E:386:LEU:HD21	2:F:216:ASN:HB3	1.65	0.78
2:F:240:THR:HG21	2:F:254:LEU:HD11	1.66	0.78
1:A:362:ASP:O	1:A:366:ILE:HG13	1.83	0.77
2:D:168:ARG:HE	2:D:169:PRO:HD3	1.48	0.77
1:E:72:THR:HG23	1:E:204:TYR:O	1.85	0.77
2:F:351:LEU:C	2:F:353:ASP:N	2.42	0.77
2:H:159:PRO:HG3	2:H:257:ARG:HH11	1.49	0.77
2:H:270:GLY:O	2:H:274:VAL:HG23	1.84	0.77
1:A:91:ASN:O	1:A:94:ILE:HG13	1.84	0.77
2:F:67:MET:HE2	2:F:71:SER:HB2	1.65	0.77
2:B:64:THR:HG22	2:B:66:ALA:H	1.50	0.77
2:B:326:LEU:HD11	2:B:350:ALA:HB1	1.66	0.77
1:C:177:GLY:CA	1:C:241:HIS:CE1	2.67	0.77
2:D:351:LEU:O	2:D:352:VAL:HG12	1.84	0.77
2:H:133:VAL:HG12	2:H:135:THR:HG23	1.66	0.77
1:A:26:ALA:O	1:A:27:LYS:HB3	1.85	0.77
2:D:122:TYR:HD1	2:D:122:TYR:H	1.28	0.77
1:E:361:GLU:HG3	4:E:502:CZL:S3B	2.25	0.77
2:D:351:LEU:C	2:D:353:ASP:N	2.40	0.77
2:B:168:ARG:HE	2:B:169:PRO:HD3	1.49	0.77
1:C:174:TYR:OH	1:C:234:TYR:O	2.02	0.77
1:C:206:ILE:HB	1:C:419:GLN:O	1.83	0.77
1:A:29:LYS:NZ	1:A:29:LYS:N	2.27	0.77
2:B:119:ARG:N	2:B:122:TYR:OH	2.16	0.77
2:B:126:LYS:HZ3	2:B:127:ASP:H	1.32	0.77
2:D:119:ARG:N	2:D:122:TYR:CE2	2.52	0.77
1:E:362:ASP:O	1:E:366:ILE:HG13	1.85	0.77
2:F:39:HIS:HA	2:F:65:THR:OG1	1.84	0.77
2:H:64:THR:HG22	2:H:66:ALA:H	1.48	0.77
1:E:94:ILE:HD12	1:E:94:ILE:O	1.85	0.77
1:A:27:LYS:HD3	2:B:66:ALA:CB	2.15	0.77
1:C:26:ALA:O	1:C:27:LYS:HB3	1.85	0.77
1:E:26:ALA:O	1:E:27:LYS:HB3	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:120:THR:N	2:F:122:TYR:CE2	2.52	0.76
2:D:212:HIS:HB3	2:D:223:THR:CG2	2.14	0.76
2:D:240:THR:HG21	2:D:254:LEU:HD11	1.67	0.76
1:A:57:HIS:HA	1:A:86:THR:CG2	2.16	0.76
2:D:118:PHE:HA	2:D:122:TYR:OH	1.85	0.76
2:F:26:LEU:HA	2:F:29:LEU:HB2	1.67	0.76
1:A:72:THR:HG23	1:A:204:TYR:O	1.85	0.76
2:F:64:THR:HG22	2:F:66:ALA:H	1.49	0.76
2:H:173:ASN:CB	2:H:240:THR:HG22	2.14	0.76
2:H:212:HIS:HB3	2:H:223:THR:HG22	1.66	0.76
2:H:381:GLY:O	2:H:398:ARG:HA	1.84	0.76
1:E:206:ILE:CG1	1:E:419:GLN:HB3	2.13	0.76
2:H:119:ARG:N	2:H:122:TYR:OH	2.19	0.76
2:B:118:PHE:CA	2:B:122:TYR:CZ	2.69	0.76
1:A:175:VAL:O	1:A:176:ILE:C	2.29	0.76
2:B:315:ARG:CG	2:B:340:VAL:HG21	2.15	0.76
1:C:57:HIS:HA	1:C:86:THR:CG2	2.16	0.76
1:A:177:GLY:HA2	1:A:241:HIS:CE1	2.21	0.75
2:B:42:GLN:HA	2:B:64:THR:HG21	1.67	0.75
2:B:159:PRO:CG	2:B:257:ARG:HH11	1.99	0.75
1:G:177:GLY:HA2	1:G:241:HIS:CE1	2.20	0.75
1:A:37:CYS:HB3	1:A:155:GLY:HA2	1.65	0.75
1:A:154:ALA:HB3	1:A:157:TYR:CE1	2.21	0.75
1:A:191:PRO:HG2	1:E:310:LYS:NZ	2.01	0.75
2:B:117:GLU:C	2:B:122:TYR:OH	2.29	0.75
1:C:174:TYR:CE2	1:C:234:TYR:CZ	2.75	0.75
2:F:125:TYR:O	2:F:126:LYS:HB3	1.86	0.75
1:G:91:ASN:O	1:G:94:ILE:HG13	1.86	0.75
1:G:252:LYS:HB2	1:G:361:GLU:OE2	1.85	0.75
2:D:217:ARG:C	2:D:218:PHE:HD2	1.94	0.75
2:F:173:ASN:CB	2:F:240:THR:HG22	2.15	0.75
2:B:118:PHE:HA	2:B:122:TYR:OH	1.86	0.75
2:D:159:PRO:CG	2:D:257:ARG:HH11	1.98	0.75
2:D:168:ARG:HG3	2:D:236:GLN:HB2	1.67	0.75
2:H:201:LEU:O	2:H:226:LEU:HD21	1.85	0.75
2:B:212:HIS:HB3	2:B:223:THR:HG22	1.68	0.75
1:C:209:GLU:OE1	1:C:426:ALA:CB	2.34	0.75
1:E:66:SER:HB3	2:F:47:PHE:CE1	2.22	0.75
1:E:108:GLN:CD	2:F:11:LEU:HB3	2.11	0.75
1:E:381:ASN:HD22	1:E:381:ASN:H	1.34	0.75
2:B:168:ARG:HG3	2:B:236:GLN:HB2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:117:GLU:C	2:D:122:TYR:OH	2.29	0.75
2:H:168:ARG:HG3	2:H:236:GLN:HB2	1.67	0.75
2:D:39:HIS:HA	2:D:65:THR:OG1	1.87	0.75
2:D:159:PRO:CB	2:D:257:ARG:HD3	2.17	0.75
1:G:190:ARG:O	1:G:192:GLY:N	2.20	0.75
1:A:191:PRO:CB	1:E:314:ALA:HB2	2.17	0.74
2:D:212:HIS:HB3	2:D:223:THR:HG22	1.69	0.74
1:E:108:GLN:NE2	2:F:11:LEU:H	1.81	0.74
2:F:168:ARG:HG3	2:F:236:GLN:HB2	1.68	0.74
1:E:57:HIS:HA	1:E:86:THR:CG2	2.17	0.74
1:C:220:LEU:HG	1:C:300:THR:HG22	1.69	0.74
2:F:20:GLN:HG3	2:F:145:GLY:CA	2.17	0.74
2:B:107:GLN:N	2:B:107:GLN:NE2	2.34	0.74
2:B:20:GLN:HG3	2:B:145:GLY:CA	2.17	0.74
2:B:173:ASN:CB	2:B:240:THR:HG22	2.12	0.74
2:D:16:LEU:H	2:D:363:ASP:CB	1.98	0.74
2:D:118:PHE:CA	2:D:122:TYR:CZ	2.70	0.74
2:D:119:ARG:C	2:D:122:TYR:CE2	2.65	0.74
2:F:168:ARG:HE	2:F:169:PRO:HD3	1.51	0.74
1:A:190:ARG:O	1:A:192:GLY:N	2.19	0.74
1:A:361:GLU:HG3	4:A:502:CZL:S3B	2.27	0.74
1:E:67:TRP:CZ3	2:F:15:PRO:O	2.40	0.74
2:F:121:GLN:N	2:F:122:TYR:CE1	2.56	0.74
2:F:159:PRO:HB2	2:F:257:ARG:HB2	1.67	0.74
2:H:125:TYR:O	2:H:126:LYS:HB3	1.86	0.74
2:D:16:LEU:N	2:D:363:ASP:HB3	2.00	0.74
2:D:382:ASN:ND2	2:D:384:HIS:HB2	2.03	0.74
1:A:383:ARG:CA	2:B:217:ARG:HH12	2.00	0.74
1:C:206:ILE:CG1	1:C:419:GLN:HB3	2.17	0.74
1:E:174:TYR:OH	1:E:234:TYR:O	2.04	0.74
1:G:38:SER:OG	1:G:162:LEU:HD12	1.87	0.74
2:B:159:PRO:HB2	2:B:257:ARG:HB2	1.69	0.74
2:B:363:ASP:OD2	2:B:363:ASP:N	2.20	0.74
1:C:367:ARG:HG2	1:C:367:ARG:NH1	1.94	0.74
2:F:119:ARG:C	2:F:122:TYR:CE2	2.65	0.74
1:G:30:PRO:HA	2:H:63:GLN:OE1	1.87	0.74
2:B:302:ASP:CB	2:D:211:GLY:HA3	2.17	0.74
1:E:106:ILE:O	1:E:110:VAL:HG22	1.87	0.73
1:E:417:ILE:HG22	1:E:417:ILE:O	1.87	0.73
2:F:107:GLN:N	2:F:107:GLN:NE2	2.36	0.73
2:B:198:ARG:HG3	2:B:198:ARG:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:168:ARG:HB2	2:D:169:PRO:HD3	1.69	0.73
1:G:67:TRP:CZ3	2:H:15:PRO:O	2.41	0.73
1:A:57:HIS:HA	1:A:86:THR:HG22	1.70	0.73
1:A:66:SER:HB3	2:B:47:PHE:CE1	2.23	0.73
2:B:125:TYR:O	2:B:126:LYS:HB3	1.87	0.73
1:C:206:ILE:C	1:C:419:GLN:O	2.32	0.73
2:H:297:ARG:HD2	2:H:417:TYR:OH	1.88	0.73
2:B:382:ASN:ND2	2:B:384:HIS:HB2	2.03	0.73
2:D:121:GLN:N	2:D:122:TYR:CE1	2.57	0.73
2:D:125:TYR:O	2:D:126:LYS:HB3	1.87	0.73
1:E:209:GLU:OE1	1:E:426:ALA:CB	2.36	0.73
1:G:62:CYS:SG	1:G:123:THR:HG21	2.28	0.73
1:G:154:ALA:HB3	1:G:157:TYR:CE1	2.24	0.73
2:D:67:MET:HE2	2:D:71:SER:HB2	1.71	0.73
1:A:367:ARG:HG2	1:A:367:ARG:NH1	1.93	0.73
1:C:67:TRP:CZ3	2:D:15:PRO:O	2.42	0.73
1:E:38:SER:OG	1:E:162:LEU:HD12	1.87	0.73
1:G:174:TYR:CE2	1:G:234:TYR:CZ	2.76	0.73
2:H:242:VAL:CB	2:H:264:ARG:HB3	2.16	0.73
1:C:193:ILE:HD12	1:C:193:ILE:N	2.03	0.73
1:C:413:PRO:HA	1:C:447:TRP:CZ2	2.23	0.73
1:A:206:ILE:HG13	1:A:419:GLN:CG	2.19	0.73
1:E:177:GLY:CA	1:E:241:HIS:CE1	2.72	0.73
1:A:314:ALA:HB2	1:E:191:PRO:HB3	1.70	0.73
1:C:29:LYS:NZ	1:C:29:LYS:N	2.31	0.73
2:F:119:ARG:N	2:F:122:TYR:OH	2.21	0.73
1:G:206:ILE:C	1:G:419:GLN:O	2.32	0.73
2:H:149:ALA:O	2:H:153:ILE:HG13	1.88	0.73
2:B:240:THR:HG21	2:B:254:LEU:HD11	1.71	0.72
2:D:107:GLN:N	2:D:107:GLN:NE2	2.36	0.72
1:G:174:TYR:OH	1:G:234:TYR:O	2.06	0.72
1:G:307:GLU:O	1:G:311:VAL:HG23	1.87	0.72
1:G:367:ARG:HH11	1:G:367:ARG:CG	2.02	0.72
2:B:121:GLN:N	2:B:122:TYR:CE1	2.57	0.72
1:C:191:PRO:HB3	1:G:314:ALA:HB2	1.69	0.72
2:D:315:ARG:CG	2:D:340:VAL:HG21	2.18	0.72
1:E:57:HIS:HA	1:E:86:THR:HG22	1.70	0.72
2:F:117:GLU:C	2:F:122:TYR:OH	2.32	0.72
2:F:118:PHE:CA	2:F:122:TYR:CZ	2.71	0.72
2:F:270:GLY:O	2:F:274:VAL:HG23	1.90	0.72
1:G:206:ILE:CG1	1:G:419:GLN:HB3	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLY:CA	1:A:241:HIS:CE1	2.72	0.72
1:A:367:ARG:HH11	1:A:367:ARG:CG	2.01	0.72
1:C:108:GLN:HE22	2:D:11:LEU:H	1.37	0.72
1:C:177:GLY:HA2	1:C:241:HIS:CE1	2.24	0.72
1:E:252:LYS:HB2	1:E:361:GLU:OE2	1.88	0.72
2:H:120:THR:N	2:H:122:TYR:CE2	2.57	0.72
1:A:436:ARG:O	1:A:440:ILE:HG23	1.88	0.72
2:B:106:THR:C	2:B:107:GLN:HE21	1.97	0.72
1:C:66:SER:O	1:C:69:ASN:ND2	2.21	0.72
1:C:383:ARG:HG2	1:C:384:VAL:H	1.55	0.72
2:B:67:MET:HE2	2:B:71:SER:HB2	1.72	0.72
2:B:302:ASP:HB2	2:D:211:GLY:HA3	1.70	0.72
1:C:190:ARG:O	1:C:192:GLY:N	2.22	0.72
1:G:301:GLU:O	1:G:304:ILE:HG13	1.90	0.72
2:H:240:THR:HG21	2:H:254:LEU:HD11	1.72	0.72
1:E:382:ALA:HB3	2:F:217:ARG:HG3	1.71	0.72
1:E:441:THR:CG2	2:H:308:HIS:HE1	1.87	0.72
1:G:193:ILE:HD12	1:G:193:ILE:N	2.04	0.72
1:C:382:ALA:HB3	2:D:217:ARG:HG3	1.70	0.72
1:A:174:TYR:HE2	1:A:238:GLN:HG2	1.53	0.72
1:C:66:SER:HB3	2:D:47:PHE:CE1	2.25	0.72
2:F:159:PRO:CB	2:F:257:ARG:HD3	2.19	0.72
1:G:29:LYS:H	1:G:29:LYS:HZ2	1.37	0.72
2:H:119:ARG:C	2:H:122:TYR:CE2	2.67	0.72
1:A:383:ARG:HA	2:B:217:ARG:HH12	1.55	0.72
2:B:218:PHE:CD2	2:B:218:PHE:N	2.58	0.72
1:C:362:ASP:O	1:C:366:ILE:HG13	1.90	0.72
2:D:119:ARG:N	2:D:122:TYR:OH	2.23	0.72
2:H:168:ARG:HB2	2:H:169:PRO:HD3	1.71	0.72
2:D:126:LYS:HZ3	2:D:127:ASP:H	1.36	0.71
1:G:27:LYS:HD3	2:H:66:ALA:HB1	1.71	0.71
1:A:177:GLY:HA3	1:A:241:HIS:NE2	2.05	0.71
1:C:94:ILE:HD12	1:C:94:ILE:O	1.90	0.71
1:E:367:ARG:HG2	1:E:367:ARG:NH1	1.97	0.71
2:H:119:ARG:N	2:H:122:TYR:CZ	2.59	0.71
2:B:26:LEU:HA	2:B:29:LEU:HB2	1.72	0.71
2:B:344:VAL:HG22	2:B:345:PRO:HD2	1.71	0.71
2:D:39:HIS:HD2	2:D:65:THR:CG2	2.01	0.71
1:A:108:GLN:HE22	2:B:11:LEU:H	1.37	0.71
1:C:27:LYS:HD3	2:D:66:ALA:CB	2.19	0.71
2:D:397:LEU:HD23	2:D:427:LEU:HD21	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:397:LEU:HD22	1:E:398:ILE:N	2.06	0.71
1:G:381:ASN:HD22	1:G:381:ASN:H	1.38	0.71
2:H:159:PRO:CB	2:H:257:ARG:HD3	2.20	0.71
1:A:409:LYS:HB3	2:B:218:PHE:CZ	2.25	0.71
2:B:67:MET:CE	2:B:71:SER:HB2	2.20	0.71
2:D:64:THR:HG22	2:D:66:ALA:H	1.55	0.71
2:F:397:LEU:HD23	2:F:427:LEU:HD21	1.70	0.71
2:B:133:VAL:HG12	2:B:135:THR:HG23	1.72	0.71
2:B:159:PRO:CB	2:B:257:ARG:HD3	2.21	0.71
2:B:381:GLY:O	2:B:398:ARG:HA	1.90	0.71
2:D:218:PHE:CD2	2:D:218:PHE:N	2.58	0.71
2:F:159:PRO:HB3	2:F:257:ARG:HD3	1.72	0.71
2:H:221:LEU:O	2:H:223:THR:N	2.23	0.71
2:H:344:VAL:HG22	2:H:345:PRO:HD2	1.70	0.71
1:A:383:ARG:HG2	1:A:384:VAL:H	1.56	0.71
2:D:363:ASP:N	2:D:363:ASP:OD2	2.22	0.71
1:A:62:CYS:SG	1:A:123:THR:HG21	2.30	0.70
2:H:16:LEU:H	2:H:363:ASP:CB	2.03	0.70
2:D:159:PRO:HB2	2:D:257:ARG:HB2	1.73	0.70
1:E:193:ILE:H	1:E:193:ILE:CD1	2.02	0.70
1:E:262:GLN:HG3	1:E:263:GLU:N	2.05	0.70
2:H:121:GLN:N	2:H:122:TYR:CE1	2.59	0.70
1:A:301:GLU:O	1:A:304:ILE:HG13	1.91	0.70
2:D:20:GLN:HG2	2:D:135:THR:HB	1.73	0.70
2:D:221:LEU:O	2:D:223:THR:N	2.24	0.70
1:E:220:LEU:HG	1:E:300:THR:HG22	1.72	0.70
2:F:221:LEU:O	2:F:223:THR:N	2.24	0.70
2:H:124:GLU:CD	2:H:126:LYS:H	2.00	0.70
2:H:382:ASN:ND2	2:H:384:HIS:HB2	2.05	0.70
1:C:174:TYR:HE2	1:C:238:GLN:HG2	1.51	0.70
1:E:108:GLN:NE2	2:F:11:LEU:HB3	2.06	0.70
1:A:383:ARG:H	2:B:217:ARG:HH22	1.39	0.70
2:D:220:ALA:O	2:D:221:LEU:HB3	1.89	0.70
1:E:67:TRP:CH2	2:F:15:PRO:O	2.44	0.70
2:F:16:LEU:H	2:F:363:ASP:CB	2.04	0.70
1:G:332:GLY:H	1:G:334:VAL:HG22	1.56	0.70
2:H:118:PHE:C	2:H:122:TYR:OH	2.35	0.70
2:H:198:ARG:O	2:H:198:ARG:HG3	1.91	0.70
1:C:397:LEU:HD22	1:C:398:ILE:N	2.06	0.70
1:E:367:ARG:HH11	1:E:367:ARG:CG	2.04	0.70
2:F:363:ASP:OD2	2:F:363:ASP:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:381:GLY:O	2:F:398:ARG:HA	1.91	0.70
2:B:118:PHE:C	2:B:122:TYR:OH	2.35	0.70
2:D:173:ASN:CB	2:D:240:THR:HG22	2.16	0.70
2:H:20:GLN:HG3	2:H:145:GLY:CA	2.21	0.70
2:H:217:ARG:C	2:H:218:PHE:HD2	2.00	0.70
1:C:191:PRO:CB	1:G:314:ALA:HB2	2.20	0.69
1:C:314:ALA:HB2	1:G:191:PRO:HB3	1.73	0.69
1:G:410:GLY:O	1:G:412:VAL:HG23	1.91	0.69
2:B:119:ARG:N	2:B:122:TYR:CZ	2.61	0.69
1:C:206:ILE:HG13	1:C:419:GLN:CG	2.21	0.69
1:E:329:LEU:HD13	1:E:340:VAL:HG22	1.74	0.69
2:H:218:PHE:N	2:H:218:PHE:CD2	2.56	0.69
2:H:379:VAL:O	2:H:396:LEU:HD23	1.92	0.69
1:C:383:ARG:HA	2:D:217:ARG:HH12	1.58	0.69
2:D:242:VAL:CB	2:D:264:ARG:HB3	2.17	0.69
2:F:121:GLN:C	2:F:122:TYR:CD1	2.69	0.69
2:F:168:ARG:HH21	2:F:169:PRO:HG3	1.56	0.69
1:G:197:ASP:OD2	1:G:223:ARG:HD3	1.92	0.69
1:G:383:ARG:HG2	1:G:384:VAL:H	1.56	0.69
1:E:413:PRO:HA	1:E:447:TRP:CZ2	2.27	0.69
1:A:106:ILE:O	1:A:110:VAL:HG22	1.92	0.69
2:F:39:HIS:HD2	2:F:65:THR:CG2	2.04	0.69
2:B:16:LEU:H	2:B:363:ASP:CB	2.03	0.69
1:C:367:ARG:HH11	1:C:367:ARG:CG	2.03	0.69
1:G:57:HIS:HA	1:G:86:THR:HG22	1.73	0.69
2:H:159:PRO:HB2	2:H:257:ARG:HB2	1.72	0.69
2:H:363:ASP:OD2	2:H:363:ASP:N	2.25	0.69
1:A:314:ALA:HB2	1:E:191:PRO:CB	2.22	0.69
2:H:42:GLN:HA	2:H:64:THR:HG21	1.73	0.69
1:A:37:CYS:HB2	1:A:155:GLY:HA2	1.74	0.69
1:A:206:ILE:CG1	1:A:419:GLN:HB3	2.21	0.69
2:B:159:PRO:HB3	2:B:257:ARG:HD3	1.75	0.69
1:C:359:THR:HG22	4:C:502:CZL:S2A	2.33	0.69
1:E:177:GLY:HA2	1:E:241:HIS:CE1	2.28	0.69
1:E:403:ASN:OD1	1:E:403:ASN:N	2.26	0.69
1:E:421:ARG:CZ	1:E:422:GLU:H	2.06	0.69
2:F:326:LEU:HD11	2:F:350:ALA:HB1	1.74	0.69
1:G:48:PRO:HG2	1:G:229:ALA:HB1	1.75	0.69
1:G:66:SER:HB3	2:H:47:PHE:CE1	2.28	0.69
2:H:67:MET:CE	2:H:71:SER:HB2	2.22	0.69
2:H:289:VAL:HG23	2:H:294:LYS:HD3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:168:ARG:CB	2:D:169:PRO:HD3	2.22	0.69
2:F:344:VAL:HG22	2:F:345:PRO:HD2	1.74	0.69
1:A:220:LEU:HG	1:A:300:THR:HG22	1.75	0.69
2:B:217:ARG:C	2:B:218:PHE:HD2	2.01	0.69
1:C:197:ASP:OD2	1:C:223:ARG:HD3	1.93	0.69
1:G:417:ILE:O	1:G:417:ILE:HG22	1.93	0.69
2:H:107:GLN:N	2:H:107:GLN:NE2	2.39	0.69
2:B:220:ALA:O	2:B:221:LEU:HB3	1.91	0.68
2:D:93:PRO:HG3	2:D:96:ILE:HD11	1.75	0.68
1:G:71:GLY:HA2	1:G:420:GLU:O	1.92	0.68
2:H:168:ARG:CB	2:H:169:PRO:HD3	2.24	0.68
1:A:209:GLU:HG2	1:A:210:PHE:N	2.07	0.68
1:E:332:GLY:H	1:E:334:VAL:HG22	1.57	0.68
2:B:159:PRO:HB2	2:B:257:ARG:CB	2.24	0.68
2:D:20:GLN:HG3	2:D:145:GLY:CA	2.22	0.68
2:D:106:THR:C	2:D:107:GLN:HE21	2.01	0.68
1:E:190:ARG:O	1:E:192:GLY:N	2.21	0.68
1:E:206:ILE:HG13	1:E:419:GLN:CG	2.24	0.68
1:E:381:ASN:HD22	1:E:381:ASN:N	1.91	0.68
2:H:34:SER:H	2:H:221:LEU:CD2	2.03	0.68
2:D:121:GLN:C	2:D:122:TYR:CD1	2.72	0.68
2:D:344:VAL:HG22	2:D:345:PRO:HD2	1.74	0.68
2:F:100:THR:CG2	2:F:135:THR:H	2.05	0.68
2:F:333:ARG:HB2	2:F:333:ARG:HH11	1.58	0.68
1:C:339:VAL:O	1:C:343:LEU:HD23	1.94	0.68
2:F:191:SER:HB3	2:F:277:TRP:HZ3	1.58	0.68
2:F:218:PHE:N	2:F:218:PHE:CD2	2.61	0.68
2:D:159:PRO:HB2	2:D:257:ARG:CB	2.24	0.68
2:D:159:PRO:HB3	2:D:257:ARG:HD3	1.75	0.68
1:E:404:MET:HB2	1:E:414:PHE:CE1	2.29	0.68
1:G:220:LEU:HG	1:G:300:THR:HG22	1.74	0.68
1:A:207:ALA:HB2	1:A:421:ARG:O	1.94	0.68
2:B:57:ARG:O	2:B:58:GLU:CD	2.37	0.68
1:C:27:LYS:HD2	1:C:27:LYS:O	1.93	0.68
1:C:252:LYS:HB2	1:C:361:GLU:OE2	1.94	0.68
1:C:381:ASN:H	1:C:381:ASN:HD22	1.40	0.68
1:G:359:THR:HG22	4:G:502:CZL:S2A	2.34	0.68
2:H:351:LEU:C	2:H:353:ASP:N	2.42	0.68
1:A:381:ASN:H	1:A:381:ASN:HD22	1.40	0.68
2:D:67:MET:CE	2:D:71:SER:HB2	2.24	0.68
1:E:383:ARG:HG2	1:E:384:VAL:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:409:LYS:HB3	2:F:218:PHE:CZ	2.28	0.68
1:G:381:ASN:HD22	1:G:381:ASN:N	1.92	0.68
1:C:383:ARG:H	2:D:217:ARG:HH22	1.42	0.68
2:F:383:SER:OG	2:F:403:GLN:HA	1.94	0.68
1:G:37:CYS:CB	1:G:155:GLY:CA	2.67	0.68
2:H:188:ILE:HD11	2:H:268:LEU:HD12	1.74	0.68
1:C:36:GLY:HA2	2:D:43:GLY:HA2	1.76	0.67
2:D:258:THR:OG1	2:D:260:VAL:HG23	1.94	0.67
2:D:382:ASN:HB2	2:D:402:PRO:O	1.93	0.67
2:H:106:THR:C	2:H:107:GLN:HE21	2.02	0.67
1:A:36:GLY:HA2	2:B:43:GLY:HA2	1.76	0.67
1:A:332:GLY:H	1:A:334:VAL:HG22	1.58	0.67
1:E:410:GLY:O	1:E:412:VAL:HG23	1.94	0.67
1:G:206:ILE:HG13	1:G:419:GLN:CG	2.23	0.67
2:B:124:GLU:CD	2:B:126:LYS:H	2.02	0.67
1:E:450:VAL:HG12	2:H:301:GLN:NE2	2.05	0.67
2:F:333:ARG:HB2	2:F:333:ARG:NH1	2.10	0.67
2:H:126:LYS:O	2:H:127:ASP:HB2	1.94	0.67
1:A:382:ALA:HB3	2:B:217:ARG:HG3	1.75	0.67
2:B:207:GLY:O	2:B:223:THR:O	2.12	0.67
1:C:123:THR:O	1:C:126:PRO:HD2	1.93	0.67
2:F:289:VAL:HG23	2:F:294:LYS:HD3	1.76	0.67
2:F:315:ARG:HG2	2:F:340:VAL:HG21	1.75	0.67
2:H:121:GLN:C	2:H:122:TYR:CD1	2.72	0.67
2:H:159:PRO:HB3	2:H:257:ARG:HD3	1.75	0.67
2:H:315:ARG:HG2	2:H:340:VAL:HG21	1.76	0.67
2:B:16:LEU:N	2:B:363:ASP:HB3	2.05	0.67
2:B:191:SER:HB3	2:B:277:TRP:HZ3	1.59	0.67
2:F:159:PRO:HB2	2:F:257:ARG:CB	2.24	0.67
1:G:174:TYR:CE1	1:G:237:VAL:HB	2.30	0.67
2:H:213:LEU:HD13	2:H:218:PHE:HB3	1.77	0.67
1:E:37:CYS:HB2	1:E:155:GLY:HA2	1.76	0.67
1:G:339:VAL:O	1:G:343:LEU:HD23	1.95	0.67
1:A:174:TYR:CE1	1:A:237:VAL:HB	2.30	0.67
1:A:411:ARG:HH22	2:B:214:ASP:HA	1.59	0.67
2:D:158:VAL:HG13	2:D:158:VAL:O	1.92	0.67
2:H:382:ASN:HB2	2:H:402:PRO:O	1.94	0.67
2:B:121:GLN:C	2:B:122:TYR:CD1	2.72	0.67
2:B:270:GLY:O	2:B:274:VAL:HG23	1.95	0.67
1:C:62:CYS:SG	1:C:123:THR:HG21	2.34	0.67
2:F:93:PRO:HG3	2:F:96:ILE:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:258:THR:OG1	2:F:260:VAL:HG23	1.94	0.67
2:H:16:LEU:N	2:H:363:ASP:HB3	2.06	0.67
2:H:220:ALA:O	2:H:221:LEU:HB3	1.95	0.67
2:D:104:SER:O	2:D:109:CYS:HB3	1.94	0.67
2:B:93:PRO:HG3	2:B:96:ILE:CG1	2.25	0.67
2:B:149:ALA:O	2:B:153:ILE:HG13	1.95	0.67
1:C:48:PRO:HB3	1:C:72:THR:HG21	1.77	0.67
2:F:119:ARG:N	2:F:122:TYR:CZ	2.63	0.67
2:F:302:ASP:CB	2:H:211:GLY:HA3	2.25	0.67
2:H:326:LEU:HD11	2:H:350:ALA:HB1	1.75	0.67
1:C:71:GLY:HA2	1:C:420:GLU:O	1.95	0.66
2:D:124:GLU:CD	2:D:126:LYS:H	2.03	0.66
1:A:450:VAL:HG12	2:D:301:GLN:NE2	2.06	0.66
2:B:176:CYS:O	2:B:247:LEU:HD11	1.95	0.66
1:C:403:ASN:OD1	1:C:403:ASN:N	2.28	0.66
2:H:93:PRO:HG3	2:H:96:ILE:HD11	1.77	0.66
2:D:252:ASP:O	2:D:256:GLU:HG2	1.95	0.66
2:F:67:MET:CE	2:F:71:SER:HB2	2.25	0.66
2:F:93:PRO:HG3	2:F:96:ILE:CG1	2.26	0.66
1:C:177:GLY:HA3	1:C:241:HIS:CE1	2.30	0.66
2:H:39:HIS:HD2	2:H:65:THR:CG2	2.08	0.66
2:H:382:ASN:C	2:H:382:ASN:HD22	2.02	0.66
1:E:197:ASP:OD2	1:E:223:ARG:HD3	1.95	0.66
1:G:68:ASP:HA	1:G:81:ARG:HH22	1.59	0.66
1:G:398:ILE:HG23	1:G:417:ILE:HG12	1.78	0.66
1:A:30:PRO:HD3	2:B:64:THR:O	1.95	0.66
1:A:94:ILE:HD12	1:A:94:ILE:O	1.96	0.66
1:C:37:CYS:HB3	1:C:155:GLY:HA3	1.77	0.66
2:F:297:ARG:HD2	2:F:417:TYR:OH	1.95	0.66
2:H:349:ALA:O	2:H:350:ALA:C	2.39	0.66
1:A:397:LEU:HD22	1:A:398:ILE:N	2.11	0.66
1:E:172:LEU:HD12	1:E:172:LEU:C	2.20	0.66
1:A:67:TRP:CZ3	2:B:15:PRO:O	2.48	0.66
2:B:301:GLN:NE2	1:C:450:VAL:HG12	2.03	0.66
1:C:68:ASP:HA	1:C:81:ARG:HH22	1.60	0.66
1:C:106:ILE:O	1:C:110:VAL:HG22	1.94	0.66
1:A:176:ILE:O	1:A:177:GLY:C	2.39	0.66
1:C:310:LYS:NZ	1:G:191:PRO:HG2	2.11	0.66
1:E:27:LYS:O	1:E:27:LYS:HD2	1.96	0.66
1:E:346:LEU:O	1:E:346:LEU:HD23	1.96	0.66
1:G:174:TYR:HE2	1:G:238:GLN:HG2	1.57	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:258:THR:OG1	2:H:260:VAL:HG23	1.96	0.66
1:A:380:GLY:HA3	1:A:384:VAL:HG23	1.78	0.66
2:B:168:ARG:HB2	2:B:169:PRO:HD3	1.78	0.66
1:C:301:GLU:O	1:C:304:ILE:HG13	1.96	0.66
2:F:212:HIS:HB3	2:F:223:THR:HG21	1.78	0.66
1:A:38:SER:OG	1:A:162:LEU:HD12	1.95	0.65
1:A:71:GLY:HA2	1:A:420:GLU:O	1.96	0.65
1:A:322:LEU:CD2	1:A:439:CYS:SG	2.82	0.65
1:C:332:GLY:H	1:C:334:VAL:HG22	1.60	0.65
1:E:199:ASN:HB2	1:E:246:ASN:ND2	2.12	0.65
2:F:104:SER:O	2:F:109:CYS:HB3	1.96	0.65
2:F:382:ASN:HD22	2:F:382:ASN:C	2.04	0.65
1:A:381:ASN:HD22	1:A:381:ASN:N	1.92	0.65
2:B:39:HIS:HD2	2:B:65:THR:CG2	2.09	0.65
2:D:119:ARG:N	2:D:122:TYR:CZ	2.64	0.65
2:F:16:LEU:N	2:F:363:ASP:HB3	2.08	0.65
2:F:198:ARG:HG3	2:F:198:ARG:O	1.95	0.65
1:C:417:ILE:HG22	1:C:417:ILE:O	1.97	0.65
2:D:289:VAL:HG23	2:D:294:LYS:HD3	1.77	0.65
2:D:379:VAL:O	2:D:396:LEU:HD23	1.96	0.65
2:F:217:ARG:C	2:F:218:PHE:HD2	2.04	0.65
2:B:93:PRO:HG3	2:B:96:ILE:HD11	1.77	0.65
2:B:315:ARG:HG2	2:B:340:VAL:HG21	1.76	0.65
2:F:149:ALA:O	2:F:153:ILE:HG13	1.97	0.65
1:G:245:VAL:CG1	1:G:290:LEU:HD23	2.26	0.65
1:G:380:GLY:HA3	1:G:384:VAL:HG23	1.76	0.65
2:H:126:LYS:HZ3	2:H:127:ASP:H	1.45	0.65
1:E:108:GLN:HE22	2:F:11:LEU:N	1.89	0.65
2:F:118:PHE:C	2:F:122:TYR:OH	2.40	0.65
2:H:118:PHE:N	2:H:122:TYR:OH	2.28	0.65
1:A:108:GLN:NE2	2:B:11:LEU:HB3	2.11	0.65
2:B:289:VAL:HG23	2:B:294:LYS:HD3	1.77	0.65
1:C:262:GLN:HG3	1:C:263:GLU:N	2.12	0.65
1:C:380:GLY:HA3	1:C:384:VAL:HG23	1.78	0.65
1:E:436:ARG:O	1:E:440:ILE:HG23	1.96	0.65
1:G:346:LEU:HD23	1:G:346:LEU:O	1.97	0.65
1:G:421:ARG:CZ	1:G:422:GLU:H	2.09	0.65
2:H:39:HIS:HA	2:H:65:THR:OG1	1.96	0.65
2:H:117:GLU:C	2:H:122:TYR:HH	2.04	0.65
1:A:206:ILE:HB	1:A:420:GLU:N	2.11	0.65
2:B:126:LYS:O	2:B:127:ASP:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:20:GLN:HG2	2:H:135:THR:HB	1.78	0.65
1:A:330:TYR:HB3	1:A:399:ALA:HB2	1.78	0.65
1:C:206:ILE:CG2	1:C:420:GLU:HA	2.27	0.65
2:D:126:LYS:O	2:D:127:ASP:HB2	1.96	0.65
2:F:126:LYS:O	2:F:127:ASP:HB2	1.96	0.65
2:F:382:ASN:HB2	2:F:402:PRO:O	1.96	0.65
1:A:413:PRO:HA	1:A:447:TRP:CZ2	2.32	0.65
1:E:176:ILE:O	1:E:177:GLY:C	2.40	0.65
2:F:106:THR:C	2:F:107:GLN:HE21	2.05	0.65
2:H:160:GLU:CG	2:H:161:ARG:H	2.10	0.65
2:D:159:PRO:HB2	2:D:257:ARG:CG	2.27	0.65
2:D:168:ARG:NE	2:D:169:PRO:HD3	2.11	0.65
1:E:27:LYS:HD3	2:F:66:ALA:HB1	1.79	0.65
1:E:206:ILE:HB	1:E:420:GLU:N	2.11	0.65
1:G:37:CYS:HB3	1:G:155:GLY:HA3	1.79	0.65
1:G:397:LEU:HD22	1:G:398:ILE:N	2.12	0.65
2:H:82:GLU:O	2:H:86:THR:OG1	2.10	0.65
1:C:209:GLU:HG2	1:C:210:PHE:N	2.07	0.64
2:D:326:LEU:HD11	2:D:350:ALA:HB1	1.79	0.64
1:G:436:ARG:O	1:G:440:ILE:HG23	1.97	0.64
2:H:159:PRO:HB2	2:H:257:ARG:CB	2.28	0.64
1:A:174:TYR:CZ	1:A:234:TYR:CE2	2.86	0.64
2:D:26:LEU:HA	2:D:29:LEU:HB2	1.80	0.64
2:F:28:ILE:HD12	2:F:34:SER:OG	1.97	0.64
1:G:245:VAL:HG13	1:G:290:LEU:HD23	1.76	0.64
2:B:382:ASN:HB2	2:B:402:PRO:O	1.96	0.64
1:C:329:LEU:HD13	1:C:340:VAL:HG22	1.79	0.64
1:G:403:ASN:N	1:G:403:ASN:OD1	2.30	0.64
2:H:168:ARG:NE	2:H:169:PRO:HD3	2.12	0.64
2:F:160:GLU:CG	2:F:161:ARG:H	2.09	0.64
2:F:302:ASP:HB2	2:H:211:GLY:HA3	1.79	0.64
2:F:340:VAL:O	2:F:340:VAL:HG12	1.97	0.64
2:D:198:ARG:HG3	2:D:198:ARG:O	1.98	0.64
1:E:71:GLY:HA2	1:E:420:GLU:O	1.98	0.64
1:E:206:ILE:HB	1:E:420:GLU:HA	1.80	0.64
1:G:174:TYR:CZ	1:G:238:GLN:HG2	2.32	0.64
1:A:37:CYS:HB3	1:A:155:GLY:HA3	1.76	0.64
2:D:315:ARG:HG2	2:D:340:VAL:HG21	1.79	0.64
1:E:123:THR:O	1:E:126:PRO:HD2	1.96	0.64
1:E:369:LEU:HD23	1:E:370:MET:HB3	1.79	0.64
2:F:420:SER:O	2:F:424:LEU:HD12	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:329:LEU:HD13	1:G:340:VAL:HG22	1.80	0.64
1:C:191:PRO:CG	1:G:314:ALA:HB2	2.27	0.64
1:C:381:ASN:HD22	1:C:381:ASN:N	1.95	0.64
2:D:100:THR:CG2	2:D:135:THR:H	2.10	0.64
2:D:149:ALA:O	2:D:153:ILE:HG13	1.97	0.64
2:D:160:GLU:CG	2:D:161:ARG:H	2.11	0.64
2:D:270:GLY:O	2:D:274:VAL:HG23	1.97	0.64
1:E:125:VAL:HB	1:E:126:PRO:HD3	1.80	0.64
2:F:378:LEU:HD13	2:F:379:VAL:N	2.11	0.64
1:G:176:ILE:O	1:G:177:GLY:C	2.41	0.64
1:G:177:GLY:HA3	1:G:241:HIS:CE1	2.32	0.64
1:A:128:LEU:HD23	2:B:106:THR:HG21	1.80	0.64
1:A:193:ILE:C	1:A:195:VAL:H	2.06	0.64
1:A:369:LEU:HD23	1:A:370:MET:HB3	1.78	0.64
1:A:417:ILE:O	1:A:417:ILE:HG22	1.96	0.64
2:B:160:GLU:CG	2:B:161:ARG:H	2.10	0.64
1:C:287:PHE:O	1:C:291:LEU:HD23	1.97	0.64
1:C:369:LEU:HD23	1:C:370:MET:HB3	1.79	0.64
1:G:172:LEU:HD12	1:G:172:LEU:C	2.22	0.64
1:G:421:ARG:NH2	1:G:422:GLU:HB3	2.12	0.64
2:B:349:ALA:O	2:B:350:ALA:C	2.41	0.64
2:B:378:LEU:HD13	2:B:379:VAL:N	2.13	0.64
1:C:346:LEU:O	1:C:346:LEU:HD23	1.98	0.64
1:E:68:ASP:HA	1:E:81:ARG:HH22	1.62	0.64
1:A:432:LEU:O	1:A:436:ARG:HD2	1.98	0.63
2:D:217:ARG:C	2:D:218:PHE:CD2	2.76	0.63
1:E:123:THR:CG2	3:E:501:SF4:S4	2.85	0.63
1:E:174:TYR:CZ	1:E:234:TYR:CE2	2.86	0.63
1:A:172:LEU:HD12	1:A:172:LEU:C	2.23	0.63
1:A:193:ILE:HD12	1:A:193:ILE:N	2.14	0.63
1:A:398:ILE:HG23	1:A:417:ILE:HG12	1.80	0.63
1:C:38:SER:OG	1:C:162:LEU:HD12	1.98	0.63
1:C:398:ILE:HG23	1:C:417:ILE:HG12	1.80	0.63
1:C:420:GLU:HG2	1:C:421:ARG:N	2.13	0.63
1:A:68:ASP:HA	1:A:81:ARG:HH22	1.62	0.63
1:A:403:ASN:N	1:A:403:ASN:OD1	2.31	0.63
1:C:37:CYS:HB2	1:C:155:GLY:HA2	1.80	0.63
2:D:382:ASN:C	2:D:382:ASN:HD22	2.06	0.63
2:F:207:GLY:O	2:F:223:THR:O	2.16	0.63
2:F:220:ALA:O	2:F:221:LEU:HB3	1.97	0.63
1:A:206:ILE:CG2	1:A:420:GLU:HA	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:ARG:CB	2:B:169:PRO:HD3	2.29	0.63
1:C:206:ILE:HB	1:C:420:GLU:N	2.13	0.63
2:D:176:CYS:O	2:D:247:LEU:HD11	1.98	0.63
1:E:411:ARG:HH22	2:F:214:ASP:HA	1.63	0.63
1:G:206:ILE:CG2	1:G:420:GLU:HA	2.27	0.63
1:A:206:ILE:HG13	1:A:419:GLN:HG3	1.80	0.63
2:B:76:ALA:O	2:B:77:ASP:C	2.42	0.63
2:B:246:SER:HB3	2:B:323:ASP:OD2	1.98	0.63
1:C:30:PRO:HD3	2:D:64:THR:O	1.97	0.63
1:E:174:TYR:CZ	1:E:238:GLN:HG2	2.32	0.63
1:A:191:PRO:HG2	1:E:310:LYS:HZ3	1.60	0.63
1:A:420:GLU:HG2	1:A:421:ARG:N	2.14	0.63
1:C:108:GLN:CD	2:D:11:LEU:HB3	2.23	0.63
1:C:123:THR:HG22	3:C:501:SF4:S4	2.38	0.63
2:F:168:ARG:HB2	2:F:169:PRO:HD3	1.81	0.63
2:H:168:ARG:HH21	2:H:169:PRO:HG3	1.63	0.63
2:D:31:LEU:O	2:D:221:LEU:HD21	1.99	0.63
2:F:124:GLU:CD	2:F:126:LYS:H	2.06	0.63
2:F:379:VAL:O	2:F:396:LEU:HD23	1.97	0.63
2:H:26:LEU:HA	2:H:29:LEU:HB2	1.80	0.63
2:H:93:PRO:HG3	2:H:96:ILE:CG1	2.29	0.63
2:B:242:VAL:CB	2:B:264:ARG:HB3	2.21	0.63
1:E:206:ILE:CG2	1:E:420:GLU:HA	2.28	0.63
2:F:38:PHE:HB2	2:F:45:THR:CG2	2.29	0.63
2:H:31:LEU:O	2:H:221:LEU:HD21	1.99	0.63
1:A:389:VAL:HG13	1:A:394:ALA:HB3	1.80	0.63
1:A:37:CYS:SG	2:B:43:GLY:HA3	2.39	0.62
2:B:117:GLU:C	2:B:122:TYR:HH	2.07	0.62
1:C:102:LEU:CD2	1:C:106:ILE:HD11	2.29	0.62
2:F:126:LYS:HZ3	2:F:127:ASP:H	1.45	0.62
1:A:262:GLN:HG3	1:A:263:GLU:N	2.13	0.62
1:C:72:THR:HG23	1:C:204:TYR:O	1.99	0.62
1:C:193:ILE:C	1:C:195:VAL:H	2.08	0.62
2:D:168:ARG:HH21	2:D:169:PRO:HG3	1.64	0.62
1:E:355:THR:HB	1:E:377:LEU:HD11	1.80	0.62
1:G:66:SER:O	1:G:69:ASN:ND2	2.32	0.62
1:G:355:THR:HB	1:G:377:LEU:HD11	1.79	0.62
1:G:404:MET:HB2	1:G:414:PHE:CE1	2.33	0.62
1:A:346:LEU:HD23	1:A:346:LEU:O	2.00	0.62
1:C:125:VAL:HB	1:C:126:PRO:HD3	1.80	0.62
1:E:48:PRO:HG2	1:E:229:ALA:HB1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:GLY:HA3	1:E:384:VAL:HG23	1.80	0.62
1:G:193:ILE:H	1:G:193:ILE:CD1	2.11	0.62
1:G:206:ILE:HB	1:G:420:GLU:N	2.13	0.62
1:A:421:ARG:CZ	1:A:422:GLU:H	2.12	0.62
2:B:379:VAL:O	2:B:396:LEU:HD23	1.98	0.62
1:C:27:LYS:HD2	1:C:27:LYS:C	2.25	0.62
1:C:176:ILE:O	1:C:177:GLY:C	2.43	0.62
1:C:404:MET:HB2	1:C:414:PHE:CE1	2.34	0.62
1:E:48:PRO:HB3	1:E:72:THR:HG21	1.81	0.62
2:H:191:SER:HB3	2:H:277:TRP:HZ3	1.64	0.62
1:E:382:ALA:HB2	1:E:406:THR:HB	1.82	0.62
2:F:100:THR:HG22	2:F:135:THR:N	2.11	0.62
1:G:373:ASP:CG	1:G:374:VAL:H	2.08	0.62
2:H:164:GLN:O	2:H:167:LYS:HG2	2.00	0.62
1:A:421:ARG:NH2	1:A:422:GLU:HB3	2.14	0.62
2:B:104:SER:O	2:B:109:CYS:HB3	1.98	0.62
1:C:174:TYR:CZ	1:C:238:GLN:HG2	2.34	0.62
2:F:126:LYS:HG3	2:F:127:ASP:N	2.15	0.62
2:F:242:VAL:CB	2:F:264:ARG:HB3	2.26	0.62
1:G:94:ILE:O	1:G:95:MET:O	2.18	0.62
1:C:421:ARG:CZ	1:C:422:GLU:H	2.12	0.62
2:D:164:GLN:O	2:D:167:LYS:HG2	2.00	0.62
2:D:213:LEU:HG	2:D:223:THR:HG23	1.81	0.62
2:D:246:SER:HB3	2:D:323:ASP:OD2	1.99	0.62
2:F:388:SER:O	2:F:392:LEU:HD22	1.99	0.62
1:G:36:GLY:HA2	2:H:43:GLY:HA2	1.82	0.62
1:G:92:ASP:HA	1:G:97:ARG:HB3	1.81	0.62
2:B:8:ASN:O	2:B:9:LYS:CB	2.46	0.62
1:C:330:TYR:HB3	1:C:399:ALA:HB2	1.81	0.62
2:F:158:VAL:HG13	2:F:158:VAL:O	2.00	0.62
2:F:168:ARG:CB	2:F:169:PRO:HD3	2.29	0.62
2:H:4:ILE:N	2:H:353:ASP:OD2	2.33	0.62
1:A:383:ARG:H	2:B:217:ARG:NH2	1.97	0.62
2:B:348:ALA:O	2:B:349:ALA:O	2.18	0.62
2:D:118:PHE:C	2:D:122:TYR:OH	2.40	0.62
2:H:213:LEU:CD2	2:H:214:ASP:H	2.13	0.62
1:A:410:GLY:O	1:A:412:VAL:HG23	2.00	0.62
2:B:31:LEU:O	2:B:221:LEU:HD21	2.00	0.62
2:B:38:PHE:HB2	2:B:45:THR:CG2	2.30	0.62
1:C:206:ILE:HG13	1:C:419:GLN:HG3	1.81	0.62
1:G:108:GLN:CD	2:H:11:LEU:HB3	2.24	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:PHE:N	2:B:122:TYR:OH	2.33	0.61
1:E:118:VAL:C	1:E:119:PHE:HD1	2.08	0.61
1:E:383:ARG:CA	2:F:217:ARG:HH12	2.13	0.61
2:F:164:GLN:O	2:F:167:LYS:HG2	2.00	0.61
2:F:349:ALA:O	2:F:350:ALA:C	2.43	0.61
1:G:92:ASP:OD2	1:G:97:ARG:HG2	1.98	0.61
2:H:388:SER:O	2:H:392:LEU:HD22	2.00	0.61
1:C:172:LEU:HD12	1:C:172:LEU:C	2.24	0.61
1:C:193:ILE:H	1:C:193:ILE:CD1	2.10	0.61
1:C:245:VAL:CG1	1:C:290:LEU:HD23	2.31	0.61
1:E:94:ILE:O	1:E:95:MET:O	2.19	0.61
1:G:125:VAL:HB	1:G:126:PRO:HD3	1.80	0.61
2:H:158:VAL:O	2:H:158:VAL:HG13	2.00	0.61
1:A:27:LYS:CD	2:B:66:ALA:HB1	2.30	0.61
1:C:421:ARG:NH2	1:C:422:GLU:HB3	2.16	0.61
1:G:94:ILE:O	1:G:94:ILE:HD12	2.00	0.61
2:H:126:LYS:HG3	2:H:127:ASP:N	2.15	0.61
1:A:172:LEU:HD12	1:A:173:LYS:CA	2.30	0.61
2:D:34:SER:H	2:D:221:LEU:CD2	2.09	0.61
2:F:382:ASN:ND2	2:F:384:HIS:HB2	2.14	0.61
1:G:389:VAL:HG13	1:G:394:ALA:HB3	1.83	0.61
2:B:388:SER:O	2:B:392:LEU:HD22	2.01	0.61
2:D:191:SER:HB3	2:D:277:TRP:HZ3	1.65	0.61
1:E:193:ILE:C	1:E:195:VAL:H	2.06	0.61
2:F:168:ARG:NE	2:F:169:PRO:HD3	2.15	0.61
1:G:67:TRP:CH2	2:H:15:PRO:O	2.53	0.61
1:G:155:GLY:N	3:G:501:SF4:S4	2.72	0.61
1:C:174:TYR:CZ	1:C:234:TYR:CE2	2.88	0.61
2:D:42:GLN:CA	2:D:64:THR:HG21	2.30	0.61
2:D:93:PRO:HG3	2:D:96:ILE:CG1	2.30	0.61
1:E:172:LEU:HD12	1:E:173:LYS:CA	2.30	0.61
1:E:174:TYR:CE1	1:E:237:VAL:HB	2.35	0.61
1:E:432:LEU:O	1:E:436:ARG:HD2	2.01	0.61
1:G:37:CYS:SG	2:H:43:GLY:HA3	2.41	0.61
1:G:262:GLN:HG3	1:G:263:GLU:N	2.14	0.61
1:A:329:LEU:HD13	1:A:340:VAL:HG22	1.82	0.61
2:D:117:GLU:C	2:D:122:TYR:HH	2.09	0.61
1:E:154:ALA:O	1:E:157:TYR:CD1	2.53	0.61
2:H:75:GLY:O	2:H:76:ALA:HB2	2.01	0.61
2:H:160:GLU:CD	2:H:161:ARG:H	2.08	0.61
1:A:174:TYR:CZ	1:A:238:GLN:HG2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LYS:NZ	1:E:191:PRO:HG2	2.16	0.61
1:E:339:VAL:O	1:E:343:LEU:HD23	2.00	0.61
1:G:48:PRO:HB3	1:G:72:THR:HG21	1.81	0.61
2:H:17:LYS:HG3	2:H:345:PRO:CB	2.28	0.61
2:H:333:ARG:NH1	2:H:333:ARG:HB2	2.15	0.61
1:A:108:GLN:CD	2:B:11:LEU:HB3	2.26	0.61
1:A:404:MET:HB2	1:A:414:PHE:CE1	2.36	0.61
1:G:404:MET:HE3	1:G:405:TYR:CE2	2.36	0.61
2:B:126:LYS:HZ3	2:B:127:ASP:N	1.99	0.61
2:D:317:ALA:HB3	2:D:379:VAL:HG22	1.81	0.61
1:C:67:TRP:CH2	2:D:15:PRO:O	2.54	0.60
1:C:314:ALA:HB2	1:G:191:PRO:CB	2.31	0.60
1:E:421:ARG:NH2	1:E:422:GLU:HB3	2.16	0.60
1:G:193:ILE:C	1:G:195:VAL:H	2.07	0.60
2:H:33:ARG:N	2:H:221:LEU:HD23	2.15	0.60
1:A:355:THR:HB	1:A:377:LEU:HD11	1.82	0.60
1:A:373:ASP:CG	1:A:374:VAL:H	2.09	0.60
2:B:340:VAL:O	2:B:340:VAL:HG12	2.01	0.60
1:C:410:GLY:O	1:C:412:VAL:HG23	2.01	0.60
2:D:8:ASN:O	2:D:9:LYS:CB	2.48	0.60
1:E:398:ILE:HG23	1:E:417:ILE:HG12	1.83	0.60
1:G:306:ARG:NH2	1:G:307:GLU:OE1	2.35	0.60
1:G:369:LEU:HD23	1:G:370:MET:HB3	1.83	0.60
2:H:100:THR:CG2	2:H:135:THR:H	2.12	0.60
1:C:432:LEU:O	1:C:436:ARG:HD2	2.01	0.60
2:F:93:PRO:HG3	2:F:96:ILE:CD1	2.32	0.60
1:A:125:VAL:HB	1:A:126:PRO:HD3	1.82	0.60
2:F:331:LEU:O	2:F:331:LEU:HD22	2.01	0.60
1:G:382:ALA:HB2	1:G:406:THR:HB	1.84	0.60
2:H:28:ILE:HG13	2:H:29:LEU:N	2.15	0.60
1:A:48:PRO:HB3	1:A:72:THR:HG21	1.84	0.60
1:A:67:TRP:CD1	1:A:67:TRP:C	2.79	0.60
1:A:339:VAL:O	1:A:343:LEU:HD23	2.02	0.60
2:B:27:ALA:HB2	2:B:146:PHE:CD1	2.36	0.60
1:C:172:LEU:HD12	1:C:173:LYS:CA	2.32	0.60
1:E:68:ASP:HB3	2:F:384:HIS:HE1	1.67	0.60
2:B:158:VAL:O	2:B:158:VAL:HG13	2.00	0.60
2:B:160:GLU:CD	2:B:161:ARG:H	2.10	0.60
1:C:108:GLN:NE2	2:D:11:LEU:HB3	2.16	0.60
2:D:118:PHE:N	2:D:122:TYR:OH	2.35	0.60
2:F:159:PRO:HG3	2:F:257:ARG:NH1	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:67:TRP:C	1:G:67:TRP:CD1	2.79	0.60
1:G:432:LEU:O	1:G:436:ARG:HD2	2.02	0.60
1:A:356:LYS:HG2	1:A:376:MET:SD	2.42	0.60
2:B:168:ARG:HH21	2:B:169:PRO:HG3	1.66	0.60
2:B:186:GLU:O	2:B:190:GLU:HG2	2.02	0.60
2:D:388:SER:O	2:D:392:LEU:HD22	2.01	0.60
1:E:177:GLY:HA3	1:E:241:HIS:CE1	2.35	0.60
1:G:108:GLN:NE2	2:H:11:LEU:H	1.95	0.60
2:H:160:GLU:O	2:H:161:ARG:C	2.45	0.60
2:B:213:LEU:CD2	2:B:214:ASP:H	2.15	0.60
1:G:54:HIS:HD2	1:G:121:TYR:OH	1.85	0.60
2:H:38:PHE:HB2	2:H:45:THR:CG2	2.32	0.60
2:F:176:CYS:O	2:F:247:LEU:HD11	2.01	0.60
1:G:362:ASP:C	1:G:366:ILE:HG13	2.27	0.60
1:G:420:GLU:HG2	1:G:421:ARG:N	2.15	0.60
2:H:104:SER:O	2:H:109:CYS:HB3	2.02	0.60
1:C:128:LEU:HD23	2:D:106:THR:HG21	1.84	0.60
1:C:207:ALA:HB2	1:C:421:ARG:O	2.02	0.60
1:C:310:LYS:HZ3	1:G:191:PRO:HG2	1.67	0.60
2:D:349:ALA:O	2:D:350:ALA:C	2.45	0.60
1:E:209:GLU:HG2	1:E:210:PHE:N	2.13	0.60
1:E:397:LEU:HD22	1:E:398:ILE:H	1.67	0.60
1:G:106:ILE:O	1:G:110:VAL:HG22	2.02	0.60
1:C:436:ARG:O	1:C:440:ILE:HG23	2.01	0.59
1:E:420:GLU:HG2	1:E:421:ARG:N	2.16	0.59
1:A:92:ASP:HA	1:A:97:ARG:HB3	1.84	0.59
1:C:245:VAL:HG13	1:C:290:LEU:HD23	1.83	0.59
2:F:186:GLU:O	2:F:190:GLU:HG2	2.02	0.59
1:G:359:THR:CG2	4:G:502:CZL:S2A	2.90	0.59
1:A:94:ILE:O	1:A:95:MET:O	2.21	0.59
2:B:168:ARG:NE	2:B:169:PRO:HD3	2.16	0.59
2:B:213:LEU:HD13	2:B:218:PHE:HB3	1.83	0.59
1:A:419:GLN:HE22	1:A:424:GLY:H	1.50	0.59
2:B:38:PHE:HB2	2:B:45:THR:HG22	1.85	0.59
1:C:355:THR:HB	1:C:377:LEU:HD11	1.84	0.59
2:D:331:LEU:O	2:D:331:LEU:HD22	2.02	0.59
1:A:67:TRP:O	1:A:81:ARG:NH2	2.36	0.59
2:B:212:HIS:HB3	2:B:223:THR:HG21	1.84	0.59
2:B:382:ASN:ND2	2:B:384:HIS:H	2.01	0.59
1:C:383:ARG:H	2:D:217:ARG:NH2	2.00	0.59
1:E:27:LYS:HD2	1:E:27:LYS:C	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:245:VAL:HG13	1:E:290:LEU:HD23	1.83	0.59
1:G:232:ALA:HA	1:G:236:GLU:OE1	2.03	0.59
1:C:149:ILE:HD12	1:C:149:ILE:N	2.17	0.59
2:D:156:THR:HG22	2:D:157:LEU:HD13	1.83	0.59
1:E:164:ASN:O	1:E:254:MET:HE2	2.01	0.59
1:E:174:TYR:HE2	1:E:238:GLN:HG2	1.60	0.59
1:E:389:VAL:HG13	1:E:394:ALA:HB3	1.84	0.59
1:A:92:ASP:OD2	1:A:97:ARG:HG2	2.02	0.59
2:B:20:GLN:HG2	2:B:135:THR:HB	1.85	0.59
1:G:172:LEU:HD12	1:G:173:LYS:CA	2.32	0.59
1:C:389:VAL:HG13	1:C:394:ALA:HB3	1.85	0.59
2:D:300:LEU:O	2:D:300:LEU:HD12	2.02	0.59
2:F:433:GLU:HG3	2:F:434:HIS:CD2	2.37	0.59
2:H:212:HIS:HB3	2:H:223:THR:HG21	1.83	0.59
1:C:199:ASN:ND2	1:C:225:LEU:HB2	2.14	0.59
1:C:382:ALA:HB2	1:C:406:THR:HB	1.85	0.59
2:D:213:LEU:HD13	2:D:218:PHE:HB3	1.84	0.59
2:D:297:ARG:HD2	2:D:417:TYR:OH	2.03	0.59
1:E:245:VAL:CG1	1:E:290:LEU:HD23	2.33	0.59
2:H:76:ALA:O	2:H:77:ASP:C	2.44	0.59
2:D:410:PHE:CE2	2:D:411:GLN:HB2	2.38	0.59
1:E:421:ARG:NH2	1:E:422:GLU:H	2.00	0.59
1:G:108:GLN:NE2	2:H:11:LEU:HB3	2.17	0.59
2:H:100:THR:HG22	2:H:135:THR:N	2.13	0.59
1:A:196:HIS:HB3	1:A:291:LEU:HD11	1.85	0.58
1:C:337:TRP:O	1:C:337:TRP:CE3	2.56	0.58
1:E:36:GLY:HA2	2:F:43:GLY:HA2	1.84	0.58
2:H:93:PRO:HG3	2:H:96:ILE:CD1	2.33	0.58
1:A:27:LYS:HD2	1:A:27:LYS:O	2.02	0.58
2:B:382:ASN:C	2:B:382:ASN:HD22	2.10	0.58
1:E:373:ASP:CG	1:E:374:VAL:H	2.11	0.58
2:F:160:GLU:CD	2:F:161:ARG:H	2.11	0.58
1:A:382:ALA:HB2	1:A:406:THR:HB	1.85	0.58
2:B:173:ASN:HB2	2:B:240:THR:CG2	2.20	0.58
1:C:92:ASP:OD2	1:C:97:ARG:HG2	2.04	0.58
1:C:154:ALA:O	1:C:157:TYR:CD1	2.56	0.58
1:E:27:LYS:HD3	2:F:66:ALA:CB	2.33	0.58
1:E:206:ILE:HB	1:E:420:GLU:CA	2.33	0.58
1:E:330:TYR:HB3	1:E:399:ALA:HB2	1.86	0.58
2:F:75:GLY:O	2:F:76:ALA:HB2	2.02	0.58
2:F:159:PRO:CG	2:F:257:ARG:NH1	2.65	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:252:ASP:O	2:H:256:GLU:HG2	2.04	0.58
1:A:359:THR:HG22	4:A:502:CZL:S2A	2.43	0.58
2:B:100:THR:CG2	2:B:135:THR:H	2.16	0.58
1:C:94:ILE:O	1:C:95:MET:O	2.22	0.58
2:D:348:ALA:O	2:D:349:ALA:O	2.21	0.58
1:E:29:LYS:CB	1:E:30:PRO:HD2	2.30	0.58
1:E:327:VAL:HG21	1:E:343:LEU:CD1	2.34	0.58
2:F:246:SER:HB3	2:F:323:ASP:OD2	2.03	0.58
2:H:213:LEU:HG	2:H:223:THR:HG23	1.86	0.58
2:D:76:ALA:O	2:D:77:ASP:C	2.47	0.58
2:D:160:GLU:CD	2:D:161:ARG:H	2.12	0.58
2:D:331:LEU:HD22	2:D:331:LEU:C	2.28	0.58
2:F:76:ALA:O	2:F:77:ASP:C	2.45	0.58
2:F:118:PHE:N	2:F:122:TYR:OH	2.36	0.58
2:B:297:ARG:HD2	2:B:417:TYR:OH	2.03	0.58
1:C:232:ALA:HA	1:C:236:GLU:OE1	2.04	0.58
1:E:362:ASP:C	1:E:366:ILE:HG13	2.28	0.58
2:F:38:PHE:CD2	2:F:45:THR:HG22	2.38	0.58
2:F:213:LEU:HD13	2:F:218:PHE:HB3	1.85	0.58
1:G:29:LYS:HG3	2:H:66:ALA:HB3	1.85	0.58
1:E:92:ASP:OD2	1:E:97:ARG:HG2	2.03	0.58
2:B:211:GLY:HA3	2:D:302:ASP:CB	2.34	0.58
1:C:174:TYR:CE1	1:C:237:VAL:HB	2.39	0.58
2:F:38:PHE:HB2	2:F:45:THR:HG22	1.86	0.58
1:C:27:LYS:CD	2:D:66:ALA:HB1	2.32	0.58
1:C:190:ARG:HB3	1:C:191:PRO:HD2	0.73	0.58
1:C:409:LYS:HB3	2:D:218:PHE:HZ	1.65	0.58
1:E:92:ASP:HA	1:E:97:ARG:HB3	1.85	0.58
2:F:188:ILE:HD11	2:F:268:LEU:HD12	1.86	0.58
2:D:385:ALA:O	2:D:386:LEU:C	2.46	0.58
1:G:30:PRO:HD3	2:H:64:THR:O	2.03	0.58
1:A:204:TYR:CE1	1:A:229:ALA:HB3	2.39	0.57
2:D:17:LYS:HG3	2:D:345:PRO:CB	2.32	0.57
1:G:193:ILE:C	1:G:195:VAL:N	2.62	0.57
1:G:199:ASN:ND2	1:G:225:LEU:HB2	2.17	0.57
2:H:8:ASN:O	2:H:9:LYS:CB	2.51	0.57
2:H:156:THR:HG22	2:H:157:LEU:HD13	1.86	0.57
2:H:217:ARG:C	2:H:218:PHE:CD2	2.82	0.57
2:H:397:LEU:CD2	2:H:427:LEU:HD21	2.33	0.57
2:H:410:PHE:CE2	2:H:411:GLN:HB2	2.39	0.57
2:D:38:PHE:HB2	2:D:45:THR:CG2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:HIS:HD2	1:E:121:TYR:OH	1.87	0.57
2:H:126:LYS:HG3	2:H:127:ASP:H	1.68	0.57
1:A:37:CYS:CB	1:A:155:GLY:CA	2.72	0.57
1:A:247:MET:HE1	1:A:274:PHE:CE2	2.40	0.57
1:A:370:MET:HG2	1:A:370:MET:O	2.02	0.57
1:A:404:MET:HE3	1:A:405:TYR:CE2	2.39	0.57
2:D:20:GLN:HG2	2:D:135:THR:CB	2.35	0.57
1:A:362:ASP:C	1:A:366:ILE:HG13	2.28	0.57
2:B:42:GLN:CA	2:B:64:THR:HG21	2.35	0.57
2:B:191:SER:CB	2:B:277:TRP:HZ3	2.16	0.57
2:D:168:ARG:HB2	2:D:169:PRO:CD	2.34	0.57
2:D:382:ASN:ND2	2:D:384:HIS:H	2.02	0.57
1:G:287:PHE:O	1:G:291:LEU:HD23	2.04	0.57
1:A:206:ILE:HB	1:A:420:GLU:HA	1.87	0.57
1:C:68:ASP:O	1:C:81:ARG:NH2	2.38	0.57
1:C:206:ILE:HB	1:C:420:GLU:HA	1.87	0.57
2:D:126:LYS:HZ3	2:D:127:ASP:N	2.02	0.57
2:F:49:LYS:O	2:F:53:VAL:HG13	2.03	0.57
2:B:39:HIS:HA	2:B:65:THR:OG1	2.05	0.57
2:D:57:ARG:O	2:D:58:GLU:CD	2.47	0.57
1:E:206:ILE:CB	1:E:420:GLU:HA	2.35	0.57
1:G:27:LYS:HD3	2:H:66:ALA:CB	2.33	0.57
2:H:317:ALA:HB3	2:H:379:VAL:HG22	1.85	0.57
1:C:37:CYS:CB	1:C:155:GLY:CA	2.72	0.57
1:C:181:PRO:HD3	1:C:242:ARG:HG3	1.86	0.57
1:C:204:TYR:HA	1:C:229:ALA:O	2.05	0.57
1:E:67:TRP:C	1:E:67:TRP:CD1	2.82	0.57
2:F:8:ASN:O	2:F:9:LYS:CB	2.52	0.57
2:F:340:VAL:O	2:F:340:VAL:CG1	2.51	0.57
2:F:382:ASN:ND2	2:F:384:HIS:H	2.03	0.57
2:H:176:CYS:O	2:H:247:LEU:HD11	2.04	0.57
2:B:213:LEU:HG	2:B:223:THR:HG23	1.86	0.57
2:B:340:VAL:O	2:B:340:VAL:CG1	2.53	0.57
1:C:204:TYR:CE1	1:C:229:ALA:HB3	2.40	0.57
2:D:95:VAL:HG22	2:D:228:VAL:CG1	2.34	0.57
2:D:212:HIS:HB3	2:D:223:THR:HG21	1.85	0.57
2:D:340:VAL:O	2:D:340:VAL:HG12	2.04	0.57
1:E:301:GLU:O	1:E:304:ILE:HG13	2.05	0.57
2:B:27:ALA:HB2	2:B:146:PHE:CE1	2.40	0.57
2:B:93:PRO:HG3	2:B:96:ILE:CD1	2.34	0.57
1:C:373:ASP:CG	1:C:374:VAL:H	2.13	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:75:GLY:O	2:D:76:ALA:HB2	2.05	0.57
2:D:85:LYS:O	2:D:89:GLU:HG2	2.05	0.57
2:D:213:LEU:HD12	2:D:223:THR:OG1	2.05	0.57
1:E:199:ASN:ND2	1:E:225:LEU:HB2	2.14	0.57
2:H:173:ASN:HB2	2:H:240:THR:CG2	2.23	0.57
1:A:102:LEU:CD2	1:A:106:ILE:HD11	2.35	0.56
1:A:337:TRP:CE3	1:A:337:TRP:O	2.58	0.56
1:C:397:LEU:HD22	1:C:398:ILE:H	1.70	0.56
2:D:433:GLU:HG3	2:D:434:HIS:HD2	1.69	0.56
2:H:331:LEU:O	2:H:331:LEU:HD22	2.05	0.56
1:A:245:VAL:HG13	1:A:290:LEU:HD23	1.87	0.56
2:D:33:ARG:N	2:D:221:LEU:HD23	2.20	0.56
1:E:86:THR:O	1:E:86:THR:HG23	2.04	0.56
1:G:102:LEU:CD2	1:G:106:ILE:HD11	2.36	0.56
1:G:353:THR:HG22	1:G:377:LEU:HD23	1.85	0.56
2:H:57:ARG:O	2:H:58:GLU:CD	2.49	0.56
2:H:397:LEU:CD2	2:H:427:LEU:CD2	2.83	0.56
1:A:48:PRO:HG2	1:A:229:ALA:HB1	1.87	0.56
1:A:68:ASP:HB3	2:B:384:HIS:HE1	1.71	0.56
1:A:373:ASP:CG	1:A:374:VAL:N	2.64	0.56
2:B:34:SER:H	2:B:221:LEU:CD2	2.09	0.56
2:D:93:PRO:HG3	2:D:96:ILE:CD1	2.34	0.56
2:D:191:SER:CB	2:D:277:TRP:HZ3	2.16	0.56
2:D:433:GLU:HG3	2:D:434:HIS:CD2	2.39	0.56
1:E:207:ALA:HB2	1:E:421:ARG:O	2.05	0.56
2:F:31:LEU:O	2:F:221:LEU:HD21	2.05	0.56
2:F:34:SER:H	2:F:221:LEU:CD2	2.13	0.56
2:F:82:GLU:O	2:F:86:THR:OG1	2.16	0.56
1:G:67:TRP:HZ3	2:H:15:PRO:O	1.87	0.56
1:G:421:ARG:HH22	1:G:422:GLU:HB3	1.71	0.56
1:G:425:TYR:HD1	1:G:433:GLU:OE1	1.89	0.56
2:H:159:PRO:CG	2:H:257:ARG:NH1	2.67	0.56
2:H:383:SER:OG	2:H:403:GLN:HA	2.04	0.56
1:E:181:PRO:CD	1:E:242:ARG:HG3	2.36	0.56
1:E:404:MET:HE3	1:E:405:TYR:CE2	2.41	0.56
2:F:118:PHE:O	2:F:119:ARG:HD3	2.04	0.56
1:A:29:LYS:CB	1:A:30:PRO:HD2	2.28	0.56
2:B:433:GLU:HG3	2:B:434:HIS:CD2	2.41	0.56
1:C:362:ASP:C	1:C:366:ILE:HG13	2.31	0.56
2:D:126:LYS:HG3	2:D:127:ASP:N	2.20	0.56
1:G:356:LYS:HG2	1:G:376:MET:SD	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:213:LEU:HD12	2:H:223:THR:OG1	2.05	0.56
2:B:28:ILE:HG13	2:B:29:LEU:N	2.21	0.56
2:B:100:THR:HG22	2:B:134:ASN:HA	1.88	0.56
2:D:38:PHE:CD2	2:D:45:THR:HG22	2.41	0.56
2:D:173:ASN:HD22	2:D:240:THR:HG22	1.70	0.56
2:F:17:LYS:HG3	2:F:345:PRO:CB	2.33	0.56
1:G:27:LYS:HD2	1:G:27:LYS:O	2.04	0.56
1:G:67:TRP:O	1:G:81:ARG:NH2	2.39	0.56
2:B:158:VAL:N	2:B:159:PRO:CD	2.69	0.56
2:D:158:VAL:N	2:D:159:PRO:CD	2.69	0.56
2:D:213:LEU:CD2	2:D:214:ASP:H	2.16	0.56
1:E:287:PHE:O	1:E:291:LEU:HD23	2.05	0.56
2:F:100:THR:HG22	2:F:134:ASN:HA	1.88	0.56
1:G:337:TRP:CE3	1:G:337:TRP:O	2.58	0.56
1:G:355:THR:C	1:G:357:LYS:H	2.14	0.56
1:A:193:ILE:HD13	1:A:293:ASP:OD1	2.06	0.56
1:A:204:TYR:HB2	1:A:206:ILE:HD13	1.88	0.56
1:A:306:ARG:NH2	1:A:307:GLU:OE1	2.39	0.56
1:A:409:LYS:HB3	2:B:218:PHE:HZ	1.71	0.56
1:E:176:ILE:HG13	1:E:178:THR:HG23	1.88	0.56
2:H:185:LEU:HB2	2:H:206:SER:OG	2.06	0.56
1:A:193:ILE:C	1:A:195:VAL:N	2.61	0.56
2:B:397:LEU:HD23	2:B:427:LEU:HD21	1.86	0.56
1:E:337:TRP:O	1:E:337:TRP:CE3	2.59	0.56
2:D:173:ASN:HB2	2:D:240:THR:CG2	2.23	0.56
1:E:355:THR:C	1:E:357:LYS:H	2.15	0.56
2:F:68:ASP:CB	2:F:70:VAL:HG22	2.24	0.56
2:B:269:TYR:O	2:B:273:ALA:HB3	2.06	0.55
1:C:193:ILE:C	1:C:195:VAL:N	2.62	0.55
2:D:28:ILE:HD12	2:D:34:SER:OG	2.06	0.55
2:F:126:LYS:HG3	2:F:127:ASP:H	1.69	0.55
1:G:330:TYR:HB3	1:G:399:ALA:HB2	1.88	0.55
2:H:158:VAL:N	2:H:159:PRO:CD	2.69	0.55
1:A:67:TRP:CH2	2:B:15:PRO:O	2.60	0.55
1:A:197:ASP:OD2	1:A:223:ARG:HD3	2.06	0.55
1:C:275:TYR:CD2	1:C:338:SER:HB2	2.41	0.55
2:D:207:GLY:O	2:D:223:THR:O	2.25	0.55
1:E:174:TYR:CZ	1:E:234:TYR:CZ	2.94	0.55
1:E:421:ARG:NE	1:E:422:GLU:H	2.03	0.55
1:G:421:ARG:NH2	1:G:422:GLU:H	2.03	0.55
2:H:124:GLU:OE1	2:H:126:LYS:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:THR:O	1:A:126:PRO:HD2	2.06	0.55
1:A:287:PHE:O	1:A:291:LEU:HD23	2.06	0.55
2:B:75:GLY:O	2:B:76:ALA:HB2	2.06	0.55
1:C:370:MET:O	1:C:370:MET:HG2	2.05	0.55
1:C:439:CYS:O	1:C:440:ILE:C	2.49	0.55
2:D:185:LEU:HB2	2:D:206:SER:OG	2.06	0.55
1:E:226:CYS:HB3	1:E:240:MET:HE3	1.88	0.55
1:E:232:ALA:HA	1:E:236:GLU:OE1	2.05	0.55
2:F:26:LEU:HD21	2:F:401:PHE:CZ	2.42	0.55
2:F:95:VAL:HG22	2:F:228:VAL:CG1	2.37	0.55
2:F:213:LEU:CD2	2:F:214:ASP:H	2.16	0.55
2:H:191:SER:CB	2:H:277:TRP:HZ3	2.19	0.55
2:B:110:ASP:HB2	2:B:113:THR:HB	1.89	0.55
2:B:159:PRO:HB2	2:B:257:ARG:CG	2.37	0.55
2:B:433:GLU:HG3	2:B:434:HIS:HD2	1.71	0.55
1:C:92:ASP:HA	1:C:97:ARG:HB3	1.87	0.55
1:C:356:LYS:HG2	1:C:376:MET:SD	2.46	0.55
1:C:383:ARG:HE	2:D:90:ARG:HH12	1.54	0.55
2:D:188:ILE:HD11	2:D:268:LEU:HD12	1.87	0.55
1:E:204:TYR:CE1	1:E:229:ALA:HB3	2.41	0.55
2:F:20:GLN:HG2	2:F:135:THR:HB	1.87	0.55
2:F:93:PRO:HG3	2:F:96:ILE:HG13	1.87	0.55
2:F:158:VAL:N	2:F:159:PRO:CD	2.70	0.55
1:G:169:GLU:O	1:G:172:LEU:HG	2.05	0.55
2:H:93:PRO:HG3	2:H:96:ILE:HG13	1.88	0.55
2:B:185:LEU:HB2	2:B:206:SER:OG	2.06	0.55
2:B:212:HIS:NE2	2:D:295:ARG:NE	2.54	0.55
2:B:401:PHE:HD2	2:B:401:PHE:O	1.89	0.55
1:C:383:ARG:N	2:D:217:ARG:HH12	2.05	0.55
1:C:404:MET:HE3	1:C:405:TYR:CE2	2.41	0.55
1:E:383:ARG:HD2	2:F:217:ARG:HH22	1.72	0.55
1:G:190:ARG:HB3	1:G:191:PRO:HD2	0.74	0.55
2:H:118:PHE:O	2:H:119:ARG:HD3	2.06	0.55
2:B:164:GLN:O	2:B:167:LYS:HG2	2.06	0.55
1:C:355:THR:C	1:C:357:LYS:H	2.14	0.55
2:F:117:GLU:C	2:F:122:TYR:HH	2.14	0.55
2:F:385:ALA:O	2:F:386:LEU:C	2.50	0.55
1:G:137:CYS:SG	1:G:150:PRO:HB3	2.47	0.55
1:G:174:TYR:CZ	1:G:234:TYR:CE2	2.94	0.55
2:H:340:VAL:O	2:H:340:VAL:HG12	2.06	0.55
1:A:275:TYR:CD2	1:A:338:SER:HB2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:396:LEU:HD22	2:D:397:LEU:N	2.21	0.55
1:E:137:CYS:SG	1:E:150:PRO:HB3	2.47	0.55
1:E:193:ILE:C	1:E:195:VAL:N	2.62	0.55
2:H:246:SER:HB3	2:H:323:ASP:OD2	2.07	0.55
1:A:199:ASN:ND2	1:A:225:LEU:HB2	2.13	0.55
2:B:285:SER:HB3	2:B:287:ASN:HD21	1.72	0.55
2:B:395:PRO:HG3	2:B:434:HIS:CG	2.42	0.55
1:C:169:GLU:O	1:C:172:LEU:HG	2.07	0.55
1:E:206:ILE:HG13	1:E:419:GLN:HG3	1.88	0.55
1:E:275:TYR:CD2	1:E:338:SER:HB2	2.41	0.55
1:E:356:LYS:HG2	1:E:376:MET:SD	2.47	0.55
1:A:27:LYS:HD2	1:A:27:LYS:C	2.32	0.55
1:A:199:ASN:HB2	1:A:246:ASN:ND2	2.21	0.55
1:A:314:ALA:HB2	1:E:191:PRO:CG	2.37	0.55
1:A:383:ARG:HE	2:B:90:ARG:HH12	1.55	0.55
1:C:306:ARG:NH2	1:C:307:GLU:OE1	2.40	0.55
1:C:383:ARG:HD2	2:D:217:ARG:HH22	1.72	0.55
2:F:185:LEU:HB2	2:F:206:SER:OG	2.06	0.55
1:G:123:THR:O	1:G:126:PRO:HD2	2.06	0.55
1:G:302:ALA:O	1:G:305:ALA:HB3	2.07	0.55
1:C:40:ASP:O	1:C:44:ILE:HG12	2.06	0.55
1:C:199:ASN:HB2	1:C:246:ASN:ND2	2.22	0.55
1:E:52:VAL:C	1:E:79:LEU:HD23	2.32	0.55
2:F:213:LEU:HD12	2:F:223:THR:OG1	2.06	0.55
1:G:409:LYS:HB3	2:H:218:PHE:CZ	2.41	0.55
1:A:355:THR:O	1:A:357:LYS:N	2.37	0.54
1:C:67:TRP:O	1:C:81:ARG:NH2	2.39	0.54
1:C:133:VAL:HG23	1:C:134:ASP:OD1	2.07	0.54
1:E:424:GLY:O	1:E:433:GLU:OE2	2.23	0.54
2:F:191:SER:CB	2:F:277:TRP:HZ3	2.20	0.54
1:G:386:LEU:HD21	2:H:216:ASN:HB3	1.87	0.54
1:G:419:GLN:HE22	1:G:424:GLY:H	1.55	0.54
2:H:401:PHE:HD2	2:H:401:PHE:O	1.90	0.54
1:A:54:HIS:HD2	1:A:121:TYR:OH	1.90	0.54
1:C:48:PRO:HG2	1:C:229:ALA:HB1	1.89	0.54
1:C:67:TRP:CD1	1:C:67:TRP:C	2.84	0.54
2:D:228:VAL:HG23	2:D:229:ALA:N	2.21	0.54
1:E:68:ASP:HB3	2:F:384:HIS:CE1	2.43	0.54
2:F:4:ILE:N	2:F:353:ASP:OD2	2.41	0.54
2:F:124:GLU:O	2:F:125:TYR:C	2.50	0.54
1:G:165:ARG:NH1	4:G:502:CZL:S4B	2.77	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:204:TYR:HA	1:G:229:ALA:O	2.06	0.54
1:A:424:GLY:O	1:A:433:GLU:OE2	2.25	0.54
2:D:55:HIS:CE1	2:D:403:GLN:HG2	2.43	0.54
1:E:132:ASP:O	1:E:136:VAL:HG23	2.07	0.54
1:E:190:ARG:CB	1:E:191:PRO:CD	2.48	0.54
2:F:42:GLN:CA	2:F:64:THR:HG21	2.35	0.54
2:H:20:GLN:HG2	2:H:135:THR:CB	2.37	0.54
1:E:190:ARG:HB3	1:E:191:PRO:HD2	0.72	0.54
2:F:29:LEU:O	2:F:221:LEU:HD11	2.06	0.54
1:G:433:GLU:O	1:G:437:GLN:HG2	2.07	0.54
1:A:226:CYS:HB3	1:A:240:MET:HE3	1.90	0.54
1:A:421:ARG:NH2	1:A:422:GLU:H	2.06	0.54
2:D:354:SER:HB2	2:D:355:PRO:HD2	1.89	0.54
1:G:68:ASP:HB3	2:H:384:HIS:HE1	1.72	0.54
1:G:181:PRO:HD3	1:G:242:ARG:HG3	1.87	0.54
1:A:355:THR:C	1:A:357:LYS:H	2.14	0.54
1:C:86:THR:HG23	1:C:86:THR:O	2.07	0.54
2:D:126:LYS:HG3	2:D:127:ASP:H	1.72	0.54
2:D:159:PRO:HG3	2:D:257:ARG:NH1	2.18	0.54
1:E:71:GLY:HA2	1:E:420:GLU:CA	2.37	0.54
1:G:370:MET:O	1:G:370:MET:HG2	2.04	0.54
1:G:440:ILE:HG13	1:G:441:THR:N	2.22	0.54
2:H:397:LEU:HD22	2:H:427:LEU:HD23	1.89	0.54
2:B:420:SER:O	2:B:424:LEU:HD12	2.07	0.54
1:C:68:ASP:CA	1:C:81:ARG:HH22	2.21	0.54
1:C:237:VAL:O	1:C:238:GLN:C	2.50	0.54
1:E:57:HIS:O	1:E:126:PRO:HG2	2.08	0.54
1:G:68:ASP:O	1:G:81:ARG:NH2	2.40	0.54
1:G:206:ILE:HB	1:G:420:GLU:HA	1.88	0.54
1:G:209:GLU:HG2	1:G:210:PHE:N	2.15	0.54
2:H:64:THR:HG22	2:H:66:ALA:N	2.22	0.54
2:H:175:LEU:HB3	2:H:247:LEU:HD13	1.89	0.54
2:H:374:GLY:O	2:H:375:GLN:HB2	2.07	0.54
1:A:193:ILE:H	1:A:193:ILE:CD1	2.16	0.54
1:A:209:GLU:CD	1:A:419:GLN:OE1	2.50	0.54
2:B:173:ASN:HD22	2:B:240:THR:HG22	1.73	0.54
1:G:196:HIS:HB3	1:G:291:LEU:HD11	1.88	0.54
1:G:397:LEU:HD22	1:G:398:ILE:H	1.72	0.54
1:G:444:CYS:SG	1:G:446:VAL:HG23	2.47	0.54
1:A:206:ILE:HB	1:A:420:GLU:CA	2.37	0.54
1:C:359:THR:CG2	4:C:502:CZL:S2A	2.96	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:ILE:O	1:E:94:ILE:CD1	2.56	0.54
1:G:37:CYS:HB2	1:G:39:PHE:H	1.72	0.54
1:G:228:LEU:O	1:G:229:ALA:HB3	2.08	0.54
1:A:154:ALA:O	1:A:157:TYR:CD1	2.61	0.54
2:B:17:LYS:HG3	2:B:345:PRO:CB	2.35	0.54
2:B:89:GLU:OE2	2:B:124:GLU:HB2	2.07	0.54
1:C:29:LYS:CB	1:C:30:PRO:HD2	2.33	0.54
1:C:355:THR:O	1:C:357:LYS:N	2.37	0.54
2:F:24:ALA:HB1	2:F:149:ALA:HB2	1.90	0.54
1:G:199:ASN:HB2	1:G:246:ASN:ND2	2.22	0.54
1:G:373:ASP:CG	1:G:374:VAL:N	2.64	0.54
1:A:353:THR:HG22	1:A:377:LEU:HD23	1.90	0.53
2:D:26:LEU:HD21	2:D:401:PHE:CZ	2.43	0.53
1:A:196:HIS:ND1	1:A:291:LEU:HD12	2.23	0.53
2:D:191:SER:HG	2:D:277:TRP:HZ3	1.54	0.53
2:F:122:TYR:O	2:F:123:GLU:C	2.50	0.53
2:F:125:TYR:O	2:F:126:LYS:CB	2.56	0.53
1:G:206:ILE:HG13	1:G:419:GLN:HG3	1.89	0.53
1:G:421:ARG:NE	1:G:422:GLU:H	2.05	0.53
2:H:95:VAL:HG22	2:H:228:VAL:CG1	2.38	0.53
2:B:74:MET:O	2:B:75:GLY:C	2.50	0.53
2:B:160:GLU:O	2:B:161:ARG:C	2.52	0.53
2:B:354:SER:CB	2:B:355:PRO:HD2	2.38	0.53
2:D:256:GLU:HA	2:D:256:GLU:OE2	2.08	0.53
1:E:62:CYS:HA	3:E:501:SF4:S3	2.49	0.53
1:E:421:ARG:HH22	1:E:422:GLU:HB3	1.73	0.53
2:H:49:LYS:O	2:H:53:VAL:HG13	2.08	0.53
2:H:74:MET:O	2:H:75:GLY:C	2.51	0.53
2:H:186:GLU:O	2:H:190:GLU:HG2	2.08	0.53
2:H:420:SER:O	2:H:424:LEU:HD12	2.07	0.53
1:A:433:GLU:O	1:A:437:GLN:HG2	2.07	0.53
2:B:126:LYS:HG3	2:B:127:ASP:N	2.23	0.53
1:C:206:ILE:HB	1:C:420:GLU:CA	2.38	0.53
2:D:344:VAL:O	2:D:361:VAL:HA	2.08	0.53
2:F:173:ASN:HD22	2:F:240:THR:HG22	1.73	0.53
2:F:269:TYR:O	2:F:273:ALA:HB3	2.08	0.53
1:G:29:LYS:HG2	2:H:65:THR:O	2.09	0.53
1:G:380:GLY:HA2	1:G:383:ARG:HD3	1.90	0.53
1:G:383:ARG:H	2:H:217:ARG:HH22	1.56	0.53
2:H:110:ASP:HB2	2:H:113:THR:HB	1.89	0.53
2:H:315:ARG:HG3	2:H:340:VAL:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:HIS:ND1	1:A:241:HIS:N	2.52	0.53
2:B:33:ARG:N	2:B:221:LEU:HD23	2.22	0.53
1:C:54:HIS:HD2	1:C:121:TYR:OH	1.92	0.53
1:C:123:THR:CG2	3:C:501:SF4:S4	2.97	0.53
1:C:353:THR:HG22	1:C:377:LEU:HD23	1.89	0.53
2:D:333:ARG:NH1	2:D:333:ARG:HB2	2.23	0.53
1:G:61:ALA:HB2	2:H:137:ASP:CG	2.32	0.53
1:G:209:GLU:CD	1:G:419:GLN:OE1	2.51	0.53
2:H:85:LYS:O	2:H:89:GLU:HG2	2.08	0.53
2:H:275:ASP:OD1	2:H:297:ARG:NE	2.29	0.53
2:H:333:ARG:HB2	2:H:333:ARG:HH11	1.72	0.53
2:H:385:ALA:O	2:H:386:LEU:C	2.51	0.53
1:A:68:ASP:HB3	2:B:384:HIS:CE1	2.43	0.53
1:A:397:LEU:HD22	1:A:398:ILE:H	1.74	0.53
2:B:4:ILE:N	2:B:353:ASP:OD2	2.42	0.53
2:B:95:VAL:HG22	2:B:228:VAL:CG1	2.38	0.53
1:C:148:VAL:C	1:C:149:ILE:HD12	2.34	0.53
2:H:38:PHE:CD2	2:H:45:THR:HG22	2.44	0.53
1:A:307:GLU:O	1:A:311:VAL:CG2	2.54	0.53
2:B:85:LYS:O	2:B:89:GLU:HG2	2.09	0.53
1:C:337:TRP:CD1	1:C:365:ARG:HG2	2.44	0.53
2:D:28:ILE:HD11	2:D:36:PRO:N	2.23	0.53
2:D:351:LEU:O	2:D:353:ASP:N	2.42	0.53
1:E:102:LEU:HD23	1:E:102:LEU:O	2.09	0.53
1:G:327:VAL:HG23	1:G:327:VAL:O	2.09	0.53
1:A:335:LYS:O	1:A:338:SER:OG	2.27	0.53
1:A:380:GLY:HA2	1:A:383:ARG:HD3	1.90	0.53
2:D:38:PHE:HB2	2:D:45:THR:HG22	1.91	0.53
2:D:353:ASP:O	2:D:354:SER:OG	2.21	0.53
1:E:133:VAL:HG23	1:E:134:ASP:OD1	2.09	0.53
1:E:228:LEU:O	1:E:229:ALA:HB3	2.09	0.53
1:E:373:ASP:CG	1:E:374:VAL:N	2.66	0.53
2:F:252:ASP:O	2:F:256:GLU:HG2	2.09	0.53
2:F:333:ARG:HH11	2:F:333:ARG:CB	2.20	0.53
1:G:128:LEU:HD23	2:H:106:THR:HG21	1.90	0.53
2:H:75:GLY:O	2:H:76:ALA:CB	2.57	0.53
2:H:124:GLU:O	2:H:125:TYR:C	2.51	0.53
1:A:327:VAL:HG21	1:A:343:LEU:CD1	2.39	0.53
1:A:409:LYS:C	1:A:411:ARG:H	2.16	0.53
2:B:333:ARG:NH1	2:B:333:ARG:HB2	2.24	0.53
1:C:380:GLY:HA2	1:C:383:ARG:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:PHE:O	2:D:401:PHE:HD2	1.92	0.53
1:G:181:PRO:CD	1:G:242:ARG:HG3	2.39	0.53
1:G:300:THR:O	1:G:304:ILE:HG23	2.09	0.53
2:H:118:PHE:O	2:H:122:TYR:CE2	2.61	0.53
2:H:256:GLU:HA	2:H:256:GLU:OE2	2.09	0.53
1:A:57:HIS:HE1	1:A:131:ASP:OD1	1.92	0.53
1:A:191:PRO:HG2	1:E:310:LYS:HZ2	1.74	0.53
2:B:385:ALA:O	2:B:386:LEU:C	2.50	0.53
1:G:68:ASP:CA	1:G:81:ARG:HH22	2.22	0.53
1:G:173:LYS:HG3	1:G:173:LYS:O	2.05	0.53
1:G:440:ILE:HG13	1:G:441:THR:H	1.74	0.53
2:B:159:PRO:HG3	2:B:257:ARG:NH1	2.19	0.52
2:B:217:ARG:C	2:B:218:PHE:CD2	2.84	0.52
2:B:354:SER:HB2	2:B:355:PRO:HD2	1.92	0.52
1:C:241:HIS:ND1	1:C:241:HIS:N	2.49	0.52
1:C:337:TRP:CD1	1:C:365:ARG:HB3	2.43	0.52
1:C:409:LYS:C	1:C:411:ARG:H	2.17	0.52
2:D:110:ASP:HB2	2:D:113:THR:HB	1.91	0.52
1:E:40:ASP:O	1:E:44:ILE:HG12	2.10	0.52
2:F:105:GLU:HG2	2:F:136:PRO:HG3	1.91	0.52
2:F:433:GLU:HG3	2:F:434:HIS:HD2	1.74	0.52
1:G:67:TRP:CZ3	2:H:15:PRO:HG2	2.44	0.52
1:G:132:ASP:O	1:G:136:VAL:HG23	2.08	0.52
1:G:367:ARG:HH21	1:G:375:LYS:HD2	1.74	0.52
2:H:28:ILE:HD11	2:H:36:PRO:N	2.24	0.52
1:A:174:TYR:O	1:A:174:TYR:CD2	2.63	0.52
1:A:206:ILE:CB	1:A:420:GLU:HA	2.40	0.52
1:A:430:GLY:O	1:A:433:GLU:OE1	2.27	0.52
2:B:36:PRO:HB2	2:B:62:LEU:HD13	1.90	0.52
2:B:211:GLY:HA3	2:D:302:ASP:HB2	1.90	0.52
1:C:52:VAL:C	1:C:79:LEU:HD23	2.35	0.52
1:E:67:TRP:O	1:E:81:ARG:NH2	2.42	0.52
1:E:154:ALA:O	1:E:157:TYR:HD1	1.92	0.52
1:E:380:GLY:HA2	1:E:383:ARG:HD3	1.91	0.52
2:F:28:ILE:HG13	2:F:29:LEU:N	2.23	0.52
2:F:39:HIS:CD2	2:F:80:VAL:HG22	2.44	0.52
1:G:206:ILE:HG22	1:G:420:GLU:HA	1.90	0.52
2:H:31:LEU:HD12	2:H:226:LEU:HB2	1.91	0.52
2:H:354:SER:CB	2:H:355:PRO:HD2	2.39	0.52
2:H:396:LEU:HD22	2:H:397:LEU:N	2.24	0.52
1:A:199:ASN:OD1	1:A:240:MET:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:PHE:O	2:B:122:TYR:CE2	2.62	0.52
2:B:409:GLY:C	2:B:411:GLN:H	2.17	0.52
1:C:287:PHE:O	1:C:291:LEU:CD2	2.57	0.52
1:C:419:GLN:HE22	1:C:424:GLY:H	1.57	0.52
1:C:421:ARG:NH2	1:C:422:GLU:H	2.07	0.52
1:E:102:LEU:CD2	1:E:106:ILE:HD11	2.40	0.52
1:G:68:ASP:HB3	2:H:384:HIS:CE1	2.44	0.52
1:G:176:ILE:HG13	1:G:178:THR:HG23	1.91	0.52
2:H:348:ALA:O	2:H:349:ALA:O	2.27	0.52
1:A:172:LEU:CD1	1:A:173:LYS:N	2.64	0.52
1:C:108:GLN:NE2	2:D:11:LEU:H	2.07	0.52
1:C:327:VAL:HG21	1:C:343:LEU:CD1	2.39	0.52
2:D:159:PRO:CG	2:D:257:ARG:NH1	2.70	0.52
2:D:160:GLU:O	2:D:161:ARG:C	2.52	0.52
1:E:241:HIS:ND1	1:E:241:HIS:N	2.45	0.52
1:E:337:TRP:CD1	1:E:365:ARG:HB3	2.44	0.52
2:F:75:GLY:O	2:F:76:ALA:CB	2.57	0.52
1:G:253:ALA:HA	4:G:502:CZL:S5A	2.49	0.52
2:H:27:ALA:HB2	2:H:146:PHE:CD1	2.44	0.52
1:A:337:TRP:CD1	1:A:365:ARG:HB3	2.45	0.52
2:B:82:GLU:O	2:B:86:THR:OG1	2.20	0.52
2:B:116:HIS:C	2:B:119:ARG:H	2.17	0.52
2:B:124:GLU:O	2:B:125:TYR:C	2.52	0.52
1:C:228:LEU:O	1:C:229:ALA:HB3	2.09	0.52
2:D:74:MET:O	2:D:75:GLY:C	2.52	0.52
1:E:370:MET:O	1:E:370:MET:HG2	2.04	0.52
2:H:397:LEU:HD23	2:H:427:LEU:CD2	2.35	0.52
1:C:71:GLY:HA2	1:C:420:GLU:CA	2.40	0.52
1:C:206:ILE:CB	1:C:420:GLU:HA	2.40	0.52
1:E:61:ALA:HB2	2:F:137:ASP:CG	2.35	0.52
1:E:307:GLU:O	1:E:311:VAL:CG2	2.55	0.52
1:G:118:VAL:C	1:G:119:PHE:HD1	2.17	0.52
2:H:264:ARG:O	2:H:265:PHE:CB	2.54	0.52
2:B:20:GLN:HG2	2:B:135:THR:CB	2.39	0.52
1:C:206:ILE:HG22	1:C:420:GLU:HA	1.90	0.52
1:E:30:PRO:HD3	2:F:64:THR:O	2.10	0.52
1:E:173:LYS:HG3	1:E:173:LYS:O	2.04	0.52
1:G:27:LYS:HD2	1:G:27:LYS:C	2.34	0.52
1:G:322:LEU:HD22	1:G:322:LEU:N	2.25	0.52
1:G:336:SER:O	1:G:339:VAL:HG23	2.09	0.52
1:A:327:VAL:HG23	1:A:327:VAL:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:LEU:O	2:B:331:LEU:HD22	2.10	0.52
1:C:174:TYR:CZ	1:C:234:TYR:CZ	2.98	0.52
2:D:116:HIS:C	2:D:119:ARG:H	2.18	0.52
2:F:67:MET:HE2	2:F:71:SER:CB	2.37	0.52
2:F:159:PRO:HB2	2:F:257:ARG:CG	2.39	0.52
2:F:228:VAL:HG23	2:F:229:ALA:N	2.25	0.52
1:G:383:ARG:CA	2:H:217:ARG:HH12	2.22	0.52
2:H:118:PHE:HA	2:H:122:TYR:CE1	2.44	0.52
2:H:331:LEU:HD22	2:H:331:LEU:C	2.33	0.52
2:B:93:PRO:HG3	2:B:96:ILE:HG13	1.90	0.52
1:C:65:SER:O	1:C:68:ASP:OD1	2.28	0.52
1:C:206:ILE:CD1	1:C:419:GLN:HB3	2.40	0.52
1:E:409:LYS:C	1:E:411:ARG:H	2.18	0.52
2:F:74:MET:O	2:F:75:GLY:C	2.53	0.52
1:G:174:TYR:CD2	1:G:174:TYR:O	2.63	0.52
1:A:444:CYS:SG	1:A:446:VAL:HG23	2.50	0.52
2:B:51:PHE:CE1	2:B:402:PRO:HB3	2.46	0.52
1:C:421:ARG:NE	1:C:422:GLU:H	2.07	0.52
2:F:156:THR:HG22	2:F:157:LEU:HD13	1.92	0.52
2:F:317:ALA:HB3	2:F:379:VAL:HG22	1.91	0.52
1:G:143:ARG:HB3	1:G:143:ARG:NH1	2.25	0.52
1:G:316:GLU:C	1:G:316:GLU:CD	2.77	0.52
1:A:48:PRO:HG2	1:A:204:TYR:HD1	1.75	0.51
1:A:337:TRP:CD1	1:A:365:ARG:HG2	2.45	0.51
1:A:421:ARG:NE	1:A:422:GLU:H	2.07	0.51
2:F:348:ALA:O	2:F:349:ALA:O	2.27	0.51
1:G:337:TRP:CD1	1:G:365:ARG:HB3	2.44	0.51
1:A:86:THR:HG23	1:A:86:THR:O	2.09	0.51
1:A:252:LYS:CB	1:A:361:GLU:OE2	2.56	0.51
2:B:26:LEU:HD21	2:B:401:PHE:CZ	2.45	0.51
1:E:169:GLU:O	1:E:172:LEU:HG	2.10	0.51
1:E:181:PRO:HD3	1:E:242:ARG:HG3	1.91	0.51
1:E:353:THR:HG22	1:E:377:LEU:HD23	1.91	0.51
2:F:217:ARG:C	2:F:218:PHE:CD2	2.85	0.51
1:G:38:SER:O	1:G:163:GLY:HA3	2.10	0.51
1:G:179:ARG:NH2	1:G:239:THR:CG2	2.73	0.51
1:G:206:ILE:HB	1:G:420:GLU:CA	2.40	0.51
1:G:328:LEU:HD22	1:G:389:VAL:HG22	1.92	0.51
1:A:206:ILE:HG22	1:A:420:GLU:HA	1.91	0.51
1:A:245:VAL:CG1	1:A:290:LEU:HD23	2.39	0.51
1:C:30:PRO:HB3	2:D:63:GLN:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:PHE:O	2:D:119:ARG:HD3	2.10	0.51
2:D:228:VAL:CG2	2:D:229:ALA:N	2.73	0.51
2:D:325:LEU:HD11	2:D:342:ALA:HB1	1.92	0.51
1:E:306:ARG:NH2	1:E:307:GLU:OE1	2.43	0.51
2:F:85:LYS:O	2:F:89:GLU:HG2	2.10	0.51
2:F:110:ASP:HB2	2:F:113:THR:HB	1.92	0.51
1:G:40:ASP:O	1:G:44:ILE:HG12	2.10	0.51
1:C:196:HIS:ND1	1:C:291:LEU:HD12	2.26	0.51
1:E:227:THR:O	1:E:229:ALA:N	2.43	0.51
2:F:256:GLU:OE2	2:F:256:GLU:HA	2.10	0.51
2:H:354:SER:HB2	2:H:355:PRO:HD2	1.92	0.51
2:H:382:ASN:ND2	2:H:384:HIS:H	2.07	0.51
1:A:179:ARG:NH2	1:A:239:THR:CG2	2.73	0.51
1:A:204:TYR:CE1	1:A:229:ALA:CB	2.93	0.51
2:B:74:MET:O	2:B:76:ALA:N	2.44	0.51
2:B:228:VAL:HG23	2:B:229:ALA:N	2.24	0.51
1:C:67:TRP:HZ3	2:D:15:PRO:O	1.91	0.51
1:C:94:ILE:O	1:C:94:ILE:CD1	2.56	0.51
1:C:323:GLU:HA	1:C:323:GLU:OE2	2.09	0.51
2:D:124:GLU:OE1	2:D:126:LYS:N	2.42	0.51
2:D:340:VAL:O	2:D:340:VAL:CG1	2.59	0.51
1:E:68:ASP:O	1:E:81:ARG:NH2	2.43	0.51
1:E:123:THR:C	1:E:126:PRO:HD2	2.36	0.51
2:F:89:GLU:OE2	2:F:124:GLU:HB2	2.11	0.51
2:F:213:LEU:HG	2:F:223:THR:HG23	1.93	0.51
1:G:424:GLY:C	1:G:433:GLU:OE2	2.54	0.51
1:A:421:ARG:HH22	1:A:422:GLU:HB3	1.74	0.51
1:A:439:CYS:O	1:A:440:ILE:C	2.53	0.51
2:B:191:SER:HB3	2:B:277:TRP:CZ3	2.43	0.51
1:E:57:HIS:HE1	1:E:131:ASP:OD1	1.94	0.51
1:E:357:LYS:N	1:E:357:LYS:HD2	2.25	0.51
2:F:396:LEU:HD22	2:F:397:LEU:N	2.25	0.51
1:G:323:GLU:HA	1:G:323:GLU:OE2	2.09	0.51
1:A:38:SER:O	1:A:163:GLY:HA3	2.10	0.51
1:A:339:VAL:O	1:A:342:ALA:HB3	2.11	0.51
2:B:125:TYR:O	2:B:126:LYS:CB	2.57	0.51
1:C:421:ARG:HH22	1:C:422:GLU:HB3	1.76	0.51
1:E:327:VAL:HG21	1:E:343:LEU:HD11	1.92	0.51
2:F:175:LEU:HB3	2:F:247:LEU:HD13	1.92	0.51
1:G:252:LYS:CB	1:G:361:GLU:OE2	2.57	0.51
2:H:160:GLU:CG	2:H:161:ARG:N	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:173:ASN:HD22	2:H:240:THR:HG22	1.76	0.51
1:A:336:SER:O	1:A:339:VAL:HG23	2.10	0.51
2:B:160:GLU:CG	2:B:161:ARG:N	2.74	0.51
1:C:316:GLU:C	1:C:316:GLU:CD	2.78	0.51
1:C:336:SER:O	1:C:339:VAL:HG23	2.11	0.51
1:C:373:ASP:CG	1:C:374:VAL:N	2.68	0.51
1:E:47:LEU:N	1:E:48:PRO:HD3	2.26	0.51
1:E:204:TYR:HB2	1:E:206:ILE:HD13	1.92	0.51
1:E:367:ARG:HH21	1:E:375:LYS:HD2	1.76	0.51
1:G:198:VAL:HG22	1:G:223:ARG:O	2.11	0.51
1:G:327:VAL:HG21	1:G:343:LEU:CD1	2.40	0.51
2:H:204:ASP:OD1	2:H:206:SER:HB2	2.11	0.51
2:H:269:TYR:O	2:H:273:ALA:HB3	2.10	0.51
1:A:169:GLU:O	1:A:172:LEU:HG	2.10	0.51
2:B:156:THR:HG22	2:B:157:LEU:HD13	1.92	0.51
2:B:354:SER:CB	2:B:355:PRO:CD	2.89	0.51
1:C:173:LYS:HG3	1:C:173:LYS:O	2.10	0.51
1:C:174:TYR:OH	1:C:238:GLN:CG	2.59	0.51
1:C:433:GLU:O	1:C:437:GLN:HG2	2.11	0.51
2:D:100:THR:HG22	2:D:135:THR:N	2.15	0.51
2:D:160:GLU:CG	2:D:161:ARG:N	2.73	0.51
1:E:204:TYR:CE1	1:E:229:ALA:CB	2.93	0.51
1:G:133:VAL:HG23	1:G:134:ASP:OD1	2.10	0.51
1:G:355:THR:O	1:G:357:LYS:N	2.39	0.51
1:A:61:ALA:HB2	2:B:137:ASP:CG	2.36	0.51
1:A:296:LEU:O	1:A:300:THR:HG23	2.11	0.51
1:A:330:TYR:HB3	1:A:399:ALA:CB	2.41	0.51
2:B:36:PRO:HB2	2:B:62:LEU:CD1	2.41	0.51
2:B:38:PHE:CD2	2:B:45:THR:HG22	2.46	0.51
2:B:221:LEU:C	2:B:223:THR:N	2.68	0.51
1:C:38:SER:O	1:C:163:GLY:HA3	2.11	0.51
1:C:204:TYR:CE1	1:C:229:ALA:CB	2.94	0.51
1:C:339:VAL:O	1:C:342:ALA:HB3	2.11	0.51
2:D:75:GLY:O	2:D:76:ALA:CB	2.59	0.51
1:E:204:TYR:HA	1:E:229:ALA:O	2.11	0.51
1:E:383:ARG:H	2:F:217:ARG:HH22	1.59	0.51
1:E:388:THR:O	1:E:392:TYR:HD2	1.94	0.51
2:F:55:HIS:CE1	2:F:403:GLN:HG2	2.46	0.51
2:F:160:GLU:CG	2:F:161:ARG:N	2.73	0.51
1:G:71:GLY:HA2	1:G:420:GLU:CA	2.41	0.51
1:G:206:ILE:CB	1:G:420:GLU:HA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASP:O	1:A:136:VAL:HG23	2.10	0.50
1:A:143:ARG:NH1	1:A:143:ARG:HB3	2.25	0.50
1:A:174:TYR:CZ	1:A:234:TYR:CZ	2.99	0.50
2:D:82:GLU:O	2:D:86:THR:OG1	2.18	0.50
2:D:118:PHE:O	2:D:118:PHE:CD2	2.64	0.50
1:G:171:MET:O	1:G:175:VAL:HB	2.11	0.50
1:A:323:GLU:OE2	1:A:347:GLY:O	2.30	0.50
2:B:39:HIS:CD2	2:B:80:VAL:HG22	2.46	0.50
2:B:124:GLU:OE1	2:B:126:LYS:N	2.43	0.50
1:C:29:LYS:CG	2:D:65:THR:O	2.60	0.50
1:C:327:VAL:HG23	1:C:327:VAL:O	2.11	0.50
2:D:126:LYS:NZ	2:D:127:ASP:N	2.55	0.50
2:H:28:ILE:HD12	2:H:34:SER:OG	2.11	0.50
2:H:67:MET:HE2	2:H:71:SER:CB	2.35	0.50
2:H:85:LYS:CD	2:H:118:PHE:HE1	2.22	0.50
1:A:68:ASP:CA	1:A:81:ARG:HH22	2.24	0.50
1:A:367:ARG:HH21	1:A:375:LYS:HD2	1.76	0.50
2:B:118:PHE:O	2:B:118:PHE:CD2	2.64	0.50
2:B:126:LYS:HG3	2:B:127:ASP:H	1.75	0.50
2:B:264:ARG:O	2:B:265:PHE:CB	2.55	0.50
1:E:226:CYS:SG	1:E:240:MET:HE3	2.51	0.50
1:G:154:ALA:O	1:G:157:TYR:CD1	2.64	0.50
1:A:67:TRP:HZ3	2:B:15:PRO:O	1.93	0.50
2:B:213:LEU:HD22	2:B:215:GLU:H	1.76	0.50
2:B:351:LEU:O	2:B:353:ASP:N	2.44	0.50
1:C:149:ILE:N	1:C:149:ILE:CD1	2.75	0.50
1:C:357:LYS:N	1:C:357:LYS:HD2	2.25	0.50
2:D:264:ARG:O	2:D:265:PHE:CB	2.55	0.50
1:E:143:ARG:HB3	1:E:143:ARG:NH1	2.27	0.50
1:E:355:THR:O	1:E:357:LYS:N	2.40	0.50
1:E:377:LEU:HD12	1:E:378:ASP:O	2.12	0.50
2:F:36:PRO:HB2	2:F:62:LEU:CD1	2.42	0.50
2:F:118:PHE:O	2:F:118:PHE:CD2	2.64	0.50
2:F:275:ASP:OD1	2:F:297:ARG:NE	2.33	0.50
2:F:401:PHE:HD2	2:F:401:PHE:O	1.94	0.50
1:G:190:ARG:CB	1:G:191:PRO:CD	2.49	0.50
1:A:37:CYS:HB2	1:A:39:PHE:H	1.76	0.50
1:A:57:HIS:O	1:A:126:PRO:HG2	2.11	0.50
1:A:322:LEU:HD22	1:A:322:LEU:N	2.26	0.50
1:E:37:CYS:CB	1:E:155:GLY:CA	2.73	0.50
1:E:65:SER:O	1:E:68:ASP:OD1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:SER:HB3	1:E:166:ILE:HG21	1.93	0.50
1:E:383:ARG:HE	2:F:90:ARG:HH12	1.58	0.50
2:F:31:LEU:HD23	2:F:95:VAL:HG11	1.92	0.50
1:G:57:HIS:O	1:G:126:PRO:HG2	2.12	0.50
1:G:66:SER:HB3	2:H:47:PHE:CZ	2.47	0.50
1:G:275:TYR:CD2	1:G:338:SER:HB2	2.45	0.50
2:H:311:LEU:HD23	2:H:431:LEU:HD12	1.93	0.50
1:A:357:LYS:N	1:A:357:LYS:HD2	2.26	0.50
2:B:252:ASP:O	2:B:256:GLU:HG2	2.11	0.50
1:C:94:ILE:O	1:C:94:ILE:CG1	2.60	0.50
1:C:367:ARG:HH21	1:C:375:LYS:HD2	1.75	0.50
2:D:374:GLY:O	2:D:375:GLN:HB2	2.11	0.50
1:E:37:CYS:HB3	1:E:155:GLY:HA3	1.86	0.50
1:E:52:VAL:O	1:E:79:LEU:HD23	2.12	0.50
1:E:199:ASN:OD1	1:E:240:MET:HG2	2.12	0.50
1:E:322:LEU:HD22	1:E:322:LEU:N	2.27	0.50
1:E:433:GLU:O	1:E:437:GLN:HG2	2.10	0.50
2:F:285:SER:HB3	2:F:287:ASN:HD21	1.75	0.50
2:F:410:PHE:CE2	2:F:411:GLN:HB2	2.47	0.50
1:G:204:TYR:CE1	1:G:229:ALA:HB3	2.47	0.50
1:G:382:ALA:HB3	2:H:217:ARG:HG3	1.93	0.50
2:H:156:THR:C	2:H:157:LEU:HD13	2.36	0.50
2:H:207:GLY:O	2:H:223:THR:O	2.29	0.50
2:H:213:LEU:HD22	2:H:215:GLU:H	1.76	0.50
1:C:29:LYS:HG2	2:D:65:THR:O	2.11	0.50
1:C:118:VAL:C	1:C:119:PHE:HD1	2.20	0.50
1:C:206:ILE:O	1:C:207:ALA:HB3	2.12	0.50
2:D:122:TYR:O	2:D:123:GLU:C	2.55	0.50
2:D:353:ASP:O	2:D:354:SER:CB	2.59	0.50
1:E:28:PRO:HD3	1:E:357:LYS:NZ	2.27	0.50
2:F:160:GLU:HG2	2:F:161:ARG:H	1.75	0.50
2:F:304:MET:O	2:F:308:HIS:HB3	2.12	0.50
1:G:339:VAL:O	1:G:342:ALA:HB3	2.11	0.50
2:H:116:HIS:C	2:H:119:ARG:H	2.20	0.50
2:H:228:VAL:HG23	2:H:229:ALA:N	2.27	0.50
2:H:340:VAL:O	2:H:340:VAL:CG1	2.58	0.50
1:A:227:THR:O	1:A:229:ALA:N	2.44	0.50
2:B:100:THR:HG22	2:B:135:THR:N	2.20	0.50
2:D:354:SER:CB	2:D:355:PRO:HD2	2.42	0.50
1:E:38:SER:O	1:E:163:GLY:HA3	2.11	0.50
1:E:296:LEU:O	1:E:300:THR:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:316:GLU:CD	1:E:316:GLU:C	2.80	0.50
1:E:404:MET:CB	1:E:414:PHE:CE1	2.95	0.50
2:F:160:GLU:O	2:F:161:ARG:C	2.54	0.50
1:G:335:LYS:O	1:G:338:SER:OG	2.29	0.50
2:H:39:HIS:CD2	2:H:80:VAL:HG22	2.47	0.50
1:A:174:TYR:OH	1:A:238:GLN:HG3	2.11	0.50
1:C:179:ARG:NH2	1:C:239:THR:CG2	2.75	0.50
1:C:312:ARG:HH11	1:C:312:ARG:HB2	1.77	0.50
2:D:26:LEU:CD1	2:D:146:PHE:CD1	2.94	0.50
2:D:93:PRO:HG3	2:D:96:ILE:HG13	1.94	0.50
2:D:126:LYS:C	2:D:128:VAL:H	2.20	0.50
1:E:228:LEU:HB2	1:E:240:MET:HE1	1.93	0.50
1:E:409:LYS:HB3	2:F:218:PHE:HZ	1.73	0.50
1:G:52:VAL:C	1:G:79:LEU:HD23	2.37	0.50
1:G:411:ARG:HH22	2:H:214:ASP:HA	1.77	0.50
1:A:440:ILE:HG13	1:A:441:THR:N	2.27	0.49
2:B:118:PHE:HA	2:B:122:TYR:CE1	2.46	0.49
1:C:123:THR:C	1:C:126:PRO:HD2	2.37	0.49
1:C:181:PRO:CD	1:C:242:ARG:HG3	2.42	0.49
1:C:383:ARG:N	2:D:217:ARG:NH1	2.59	0.49
2:F:121:GLN:CA	2:F:122:TYR:CD1	2.95	0.49
1:G:424:GLY:O	1:G:433:GLU:OE2	2.29	0.49
1:A:65:SER:O	1:A:68:ASP:OD1	2.30	0.49
1:A:133:VAL:HG23	1:A:134:ASP:OD1	2.12	0.49
1:A:149:ILE:N	1:A:149:ILE:HD12	2.27	0.49
1:A:177:GLY:HA3	1:A:241:HIS:CE1	2.41	0.49
1:E:383:ARG:HA	2:F:217:ARG:HH12	1.78	0.49
2:F:354:SER:CB	2:F:355:PRO:HD2	2.41	0.49
1:G:196:HIS:ND1	1:G:291:LEU:HD12	2.27	0.49
2:H:213:LEU:HD13	2:H:218:PHE:CG	2.47	0.49
2:B:156:THR:C	2:B:157:LEU:HD13	2.36	0.49
2:B:302:ASP:OD2	2:D:58:GLU:CD	2.55	0.49
1:C:57:HIS:HE1	1:C:131:ASP:OD1	1.96	0.49
1:C:190:ARG:CB	1:C:191:PRO:CD	2.48	0.49
1:C:226:CYS:HB3	1:C:240:MET:HE3	1.93	0.49
2:F:27:ALA:HB2	2:F:146:PHE:CD1	2.46	0.49
1:G:367:ARG:HD2	1:G:372:ASP:HA	1.94	0.49
2:B:159:PRO:CG	2:B:257:ARG:NH1	2.71	0.49
1:C:29:LYS:HG3	2:D:66:ALA:HB3	1.94	0.49
2:D:28:ILE:HG13	2:D:29:LEU:N	2.27	0.49
2:F:118:PHE:HA	2:F:122:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:183:GLY:O	2:F:413:CYS:HB2	2.12	0.49
1:G:204:TYR:HB2	1:G:206:ILE:HD13	1.94	0.49
1:G:337:TRP:CD1	1:G:365:ARG:HG2	2.48	0.49
1:G:380:GLY:HA3	1:G:384:VAL:CG2	2.42	0.49
2:B:160:GLU:CD	2:B:160:GLU:H	2.21	0.49
1:C:220:LEU:CD2	1:C:303:LEU:HD13	2.42	0.49
2:D:4:ILE:N	2:D:353:ASP:OD2	2.46	0.49
2:D:118:PHE:O	2:D:122:TYR:CE2	2.66	0.49
2:D:125:TYR:O	2:D:126:LYS:CB	2.58	0.49
1:E:68:ASP:CA	1:E:81:ARG:HH22	2.25	0.49
1:G:381:ASN:N	1:G:381:ASN:ND2	2.60	0.49
2:H:333:ARG:HH11	2:H:333:ARG:CB	2.25	0.49
1:A:204:TYR:HA	1:A:229:ALA:O	2.12	0.49
2:B:105:GLU:HG2	2:B:136:PRO:HG3	1.93	0.49
1:C:307:GLU:O	1:C:311:VAL:CG2	2.55	0.49
2:D:31:LEU:HD12	2:D:226:LEU:HB2	1.95	0.49
2:D:49:LYS:O	2:D:53:VAL:HG13	2.11	0.49
2:F:297:ARG:HG3	2:F:417:TYR:CE2	2.47	0.49
2:H:126:LYS:HZ3	2:H:127:ASP:N	2.09	0.49
2:B:85:LYS:CD	2:B:118:PHE:HE1	2.20	0.49
1:C:381:ASN:HB2	2:D:217:ARG:HH21	1.77	0.49
1:E:206:ILE:CD1	1:E:419:GLN:HB3	2.42	0.49
1:E:206:ILE:HG22	1:E:420:GLU:HA	1.95	0.49
1:E:425:TYR:HD1	1:E:433:GLU:OE1	1.96	0.49
2:F:74:MET:O	2:F:76:ALA:N	2.45	0.49
2:F:107:GLN:HE21	2:F:107:GLN:H	1.55	0.49
2:F:387:ALA:O	2:F:391:ARG:HB2	2.13	0.49
1:G:207:ALA:HB2	1:G:421:ARG:O	2.12	0.49
1:G:209:GLU:HG3	1:G:426:ALA:HB3	1.94	0.49
1:G:423:PHE:HD2	1:G:423:PHE:O	1.95	0.49
2:H:38:PHE:HB2	2:H:45:THR:HG22	1.93	0.49
2:H:297:ARG:HG3	2:H:417:TYR:CE2	2.47	0.49
1:A:302:ALA:O	1:A:305:ALA:HB3	2.12	0.49
2:B:188:ILE:HD11	2:B:268:LEU:HD12	1.94	0.49
1:C:383:ARG:CD	2:D:217:ARG:HH22	2.26	0.49
2:D:109:CYS:O	2:D:109:CYS:SG	2.70	0.49
2:D:124:GLU:O	2:D:125:TYR:C	2.55	0.49
2:F:57:ARG:O	2:F:58:GLU:CD	2.55	0.49
1:A:118:VAL:C	1:A:119:PHE:HD1	2.21	0.49
1:A:126:PRO:O	1:A:131:ASP:HB2	2.12	0.49
1:A:252:LYS:HD2	1:A:361:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:PHE:O	2:B:401:PHE:CD2	2.65	0.49
1:C:48:PRO:HB3	1:C:72:THR:CG2	2.43	0.49
1:C:204:TYR:HB2	1:C:206:ILE:HD13	1.95	0.49
2:D:160:GLU:HG2	2:D:161:ARG:H	1.77	0.49
2:D:168:ARG:CB	2:D:169:PRO:CD	2.90	0.49
1:E:179:ARG:NH2	1:E:239:THR:CG2	2.76	0.49
1:E:336:SER:O	1:E:339:VAL:HG23	2.12	0.49
2:F:344:VAL:HG13	2:F:346:ALA:H	1.78	0.49
1:G:108:GLN:HE22	2:H:11:LEU:N	2.00	0.49
1:A:214:LEU:N	1:A:215:PRO:CD	2.76	0.49
2:B:49:LYS:O	2:B:53:VAL:HG13	2.13	0.49
2:B:176:CYS:C	2:B:247:LEU:HD11	2.38	0.49
2:B:311:LEU:HD23	2:B:431:LEU:HD12	1.94	0.49
2:D:118:PHE:HA	2:D:122:TYR:CE1	2.48	0.49
2:D:333:ARG:CB	2:D:333:ARG:HH11	2.26	0.49
1:E:439:CYS:O	1:E:440:ILE:C	2.54	0.49
1:E:444:CYS:SG	1:E:446:VAL:HG23	2.52	0.49
1:G:28:PRO:HD3	1:G:357:LYS:NZ	2.28	0.49
1:G:48:PRO:HG2	1:G:204:TYR:HD1	1.77	0.49
1:G:247:MET:HE1	1:G:274:PHE:CE2	2.47	0.49
2:H:353:ASP:O	2:H:354:SER:OG	2.27	0.49
1:A:327:VAL:HG21	1:A:343:LEU:HD11	1.95	0.48
2:B:160:GLU:HG2	2:B:161:ARG:H	1.78	0.48
1:C:171:MET:O	1:C:175:VAL:HB	2.13	0.48
2:D:420:SER:O	2:D:424:LEU:HD12	2.12	0.48
1:E:149:ILE:HD12	1:E:149:ILE:N	2.28	0.48
2:F:126:LYS:HZ3	2:F:127:ASP:N	2.11	0.48
1:G:252:LYS:HD2	1:G:361:GLU:HG2	1.95	0.48
2:H:125:TYR:O	2:H:126:LYS:CB	2.57	0.48
1:C:425:TYR:HD1	1:C:433:GLU:OE1	1.96	0.48
1:C:431:MET:HB3	1:C:431:MET:HE2	1.72	0.48
2:D:105:GLU:HG2	2:D:136:PRO:HG3	1.95	0.48
2:D:378:LEU:HD13	2:D:379:VAL:N	2.28	0.48
1:E:337:TRP:CD1	1:E:365:ARG:HG2	2.48	0.48
1:G:226:CYS:HB3	1:G:240:MET:HE3	1.94	0.48
2:H:126:LYS:CG	2:H:127:ASP:H	2.26	0.48
1:A:27:LYS:CG	2:B:66:ALA:HB1	2.44	0.48
1:A:40:ASP:O	1:A:44:ILE:HG12	2.12	0.48
1:A:67:TRP:CZ3	2:B:15:PRO:HG2	2.47	0.48
1:A:228:LEU:O	1:A:229:ALA:HB3	2.14	0.48
2:B:122:TYR:O	2:B:123:GLU:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ASP:HB3	2:D:384:HIS:CE1	2.48	0.48
1:C:174:TYR:OH	1:C:238:GLN:HG3	2.12	0.48
2:D:115:LEU:O	2:D:119:ARG:N	2.47	0.48
1:E:359:THR:HG22	4:E:502:CZL:S2A	2.53	0.48
2:F:126:LYS:CG	2:F:127:ASP:H	2.26	0.48
2:F:162:ARG:NE	2:F:162:ARG:HA	2.28	0.48
2:F:374:GLY:O	2:F:375:GLN:HB2	2.12	0.48
2:H:159:PRO:HB2	2:H:257:ARG:CG	2.43	0.48
2:B:256:GLU:HA	2:B:256:GLU:OE2	2.13	0.48
2:B:315:ARG:HG3	2:B:340:VAL:HG21	1.94	0.48
2:F:200:LEU:HD22	2:F:200:LEU:C	2.38	0.48
1:G:343:LEU:HD23	1:G:343:LEU:H	1.77	0.48
2:H:74:MET:O	2:H:76:ALA:N	2.45	0.48
2:B:67:MET:HE2	2:B:71:SER:CB	2.40	0.48
1:C:64:GLY:O	1:C:67:TRP:HE3	1.95	0.48
1:C:330:TYR:HB3	1:C:399:ALA:CB	2.43	0.48
2:D:121:GLN:CA	2:D:122:TYR:CD1	2.97	0.48
2:D:397:LEU:CD2	2:D:427:LEU:HD21	2.43	0.48
1:E:67:TRP:HZ3	2:F:15:PRO:O	1.92	0.48
1:E:323:GLU:HA	1:E:323:GLU:OE2	2.13	0.48
1:G:65:SER:O	1:G:68:ASP:OD1	2.30	0.48
1:G:362:ASP:O	1:G:366:ILE:CG1	2.58	0.48
1:G:383:ARG:HA	2:H:217:ARG:HH12	1.79	0.48
1:G:423:PHE:O	1:G:423:PHE:CD2	2.67	0.48
2:B:206:SER:O	2:D:295:ARG:NH2	2.47	0.48
2:B:228:VAL:CG2	2:B:229:ALA:N	2.76	0.48
1:C:354:GLY:N	1:C:366:ILE:CD1	2.75	0.48
2:D:39:HIS:CD2	2:D:80:VAL:HG22	2.49	0.48
1:E:209:GLU:HG3	1:E:426:ALA:HB3	1.96	0.48
1:G:166:ILE:O	1:G:166:ILE:HG22	2.14	0.48
2:H:354:SER:CB	2:H:355:PRO:CD	2.91	0.48
1:A:187:GLY:O	1:A:188:SER:HB3	2.12	0.48
1:A:310:LYS:HZ2	1:E:191:PRO:HG2	1.78	0.48
2:B:31:LEU:HD12	2:B:226:LEU:HB2	1.96	0.48
2:B:160:GLU:O	2:B:162:ARG:O	2.32	0.48
1:C:57:HIS:O	1:C:126:PRO:HG2	2.14	0.48
1:C:296:LEU:O	1:C:300:THR:HG23	2.13	0.48
2:D:304:MET:O	2:D:308:HIS:HB3	2.13	0.48
1:E:304:ILE:HD12	1:E:305:ALA:N	2.28	0.48
1:E:367:ARG:HD2	1:E:372:ASP:HA	1.96	0.48
1:E:424:GLY:C	1:E:433:GLU:OE2	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:401:PHE:O	2:H:401:PHE:CD2	2.67	0.48
1:A:172:LEU:C	1:A:172:LEU:CD1	2.87	0.48
2:B:333:ARG:HB2	2:B:333:ARG:HH11	1.78	0.48
1:C:300:THR:O	1:C:304:ILE:HG23	2.13	0.48
1:C:328:LEU:HD22	1:C:389:VAL:HG22	1.95	0.48
1:A:171:MET:O	1:A:175:VAL:HB	2.14	0.48
1:A:429:ASP:O	1:A:432:LEU:HB2	2.13	0.48
2:B:28:ILE:HD12	2:B:34:SER:OG	2.14	0.48
2:B:75:GLY:O	2:B:76:ALA:CB	2.61	0.48
1:C:191:PRO:HG2	1:G:310:LYS:NZ	2.29	0.48
1:C:388:THR:O	1:C:392:TYR:HD2	1.96	0.48
2:D:237:SER:O	2:D:260:VAL:HG13	2.13	0.48
2:D:335:MET:SD	2:D:424:LEU:CD2	3.01	0.48
2:D:410:PHE:CD2	2:D:411:GLN:HB2	2.49	0.48
2:F:126:LYS:CG	2:F:127:ASP:N	2.76	0.48
2:F:191:SER:HB3	2:F:277:TRP:CZ3	2.43	0.48
2:F:331:LEU:HD22	2:F:331:LEU:C	2.38	0.48
2:F:351:LEU:O	2:F:353:ASP:N	2.46	0.48
1:G:214:LEU:N	1:G:215:PRO:CD	2.77	0.48
1:A:166:ILE:O	1:A:166:ILE:HG22	2.14	0.48
2:B:213:LEU:HD12	2:B:223:THR:OG1	2.13	0.48
2:D:67:MET:HE2	2:D:71:SER:CB	2.40	0.48
2:D:175:LEU:HB3	2:D:247:LEU:HD13	1.95	0.48
1:E:196:HIS:HB3	1:E:291:LEU:HD11	1.95	0.48
2:F:16:LEU:HD12	2:F:16:LEU:O	2.13	0.48
2:F:122:TYR:C	2:F:124:GLU:N	2.72	0.48
2:F:354:SER:CB	2:F:355:PRO:CD	2.91	0.48
1:G:172:LEU:C	1:G:172:LEU:CD1	2.86	0.48
1:G:220:LEU:CD2	1:G:303:LEU:HD13	2.44	0.48
1:G:353:THR:CG2	1:G:377:LEU:HD23	2.44	0.48
1:A:63:ALA:O	1:A:65:SER:N	2.47	0.47
1:A:66:SER:HB3	2:B:47:PHE:CZ	2.49	0.47
1:C:304:ILE:C	1:C:304:ILE:HD12	2.40	0.47
1:C:335:LYS:O	1:C:338:SER:OG	2.32	0.47
2:D:85:LYS:CD	2:D:118:PHE:HE1	2.23	0.47
2:D:95:VAL:CG2	2:D:228:VAL:CG1	2.92	0.47
2:D:397:LEU:CD2	2:D:427:LEU:CD2	2.92	0.47
1:E:99:GLU:O	1:E:100:LYS:C	2.57	0.47
1:E:118:VAL:C	1:E:119:PHE:CD1	2.92	0.47
1:E:174:TYR:OH	1:E:238:GLN:CG	2.62	0.47
1:E:248:MET:SD	1:E:258:ALA:HB2	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:20:GLN:HG2	2:F:135:THR:CB	2.44	0.47
2:F:93:PRO:CG	2:F:96:ILE:HG13	2.44	0.47
2:F:124:GLU:OE1	2:F:126:LYS:N	2.44	0.47
2:H:105:GLU:HG2	2:H:136:PRO:HG3	1.96	0.47
1:A:68:ASP:O	1:A:81:ARG:NH2	2.47	0.47
1:A:226:CYS:SG	1:A:240:MET:HE3	2.54	0.47
2:B:42:GLN:HA	2:B:64:THR:CG2	2.39	0.47
2:B:121:GLN:CA	2:B:122:TYR:CD1	2.97	0.47
2:B:173:ASN:HD22	2:B:240:THR:CG2	2.27	0.47
2:B:382:ASN:HD22	2:B:384:HIS:N	2.12	0.47
1:C:172:LEU:C	1:C:172:LEU:CD1	2.87	0.47
2:D:42:GLN:HA	2:D:64:THR:CG2	2.38	0.47
2:D:74:MET:O	2:D:76:ALA:N	2.47	0.47
1:E:209:GLU:CD	1:E:419:GLN:OE1	2.56	0.47
2:F:116:HIS:C	2:F:119:ARG:H	2.21	0.47
2:F:211:GLY:HA3	2:H:302:ASP:CB	2.44	0.47
2:F:397:LEU:CD2	2:F:427:LEU:CD2	2.92	0.47
1:G:172:LEU:CD1	1:G:173:LYS:N	2.65	0.47
1:G:383:ARG:HE	2:H:90:ARG:HH12	1.61	0.47
2:H:109:CYS:O	2:H:110:ASP:C	2.57	0.47
2:H:349:ALA:O	2:H:351:LEU:N	2.47	0.47
2:H:351:LEU:O	2:H:353:ASP:N	2.47	0.47
2:H:412:ARG:HB3	2:H:414:TRP:CZ3	2.49	0.47
1:A:137:CYS:SG	1:A:150:PRO:HB3	2.54	0.47
1:A:193:ILE:CD1	1:A:293:ASP:OD1	2.63	0.47
1:A:206:ILE:O	1:A:419:GLN:O	2.31	0.47
1:A:383:ARG:N	2:B:217:ARG:HH22	2.10	0.47
2:B:410:PHE:CE2	2:B:411:GLN:HB2	2.49	0.47
1:C:48:PRO:HG2	1:C:204:TYR:HD1	1.79	0.47
1:C:322:LEU:N	1:C:322:LEU:HD22	2.29	0.47
1:C:430:GLY:O	1:C:433:GLU:OE1	2.32	0.47
2:D:383:SER:OG	2:D:403:GLN:HA	2.15	0.47
2:D:397:LEU:HD23	2:D:427:LEU:CD2	2.43	0.47
2:F:38:PHE:CG	2:F:45:THR:HG22	2.48	0.47
1:G:204:TYR:CE1	1:G:229:ALA:CB	2.97	0.47
1:G:431:MET:HE2	1:G:431:MET:HB3	1.81	0.47
2:H:36:PRO:HB2	2:H:62:LEU:CD1	2.45	0.47
2:H:160:GLU:CD	2:H:160:GLU:H	2.22	0.47
1:A:380:GLY:HA3	1:A:384:VAL:CG2	2.44	0.47
1:C:383:ARG:HD2	2:D:217:ARG:NH2	2.29	0.47
2:D:21:THR:HG21	2:D:137:ASP:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:89:GLU:OE2	2:D:124:GLU:HB2	2.14	0.47
2:D:173:ASN:HD22	2:D:240:THR:CG2	2.26	0.47
2:D:186:GLU:O	2:D:190:GLU:HG2	2.14	0.47
1:E:343:LEU:HD23	1:E:343:LEU:H	1.79	0.47
2:F:213:LEU:HD22	2:F:215:GLU:H	1.79	0.47
2:F:397:LEU:HD23	2:F:427:LEU:CD2	2.40	0.47
1:G:174:TYR:CZ	1:G:234:TYR:CZ	3.02	0.47
1:G:357:LYS:N	1:G:357:LYS:HD2	2.29	0.47
2:H:285:SER:CB	2:H:287:ASN:HD21	2.27	0.47
1:A:323:GLU:OE2	1:A:323:GLU:HA	2.14	0.47
1:A:383:ARG:HD2	2:B:217:ARG:HH22	1.79	0.47
2:B:213:LEU:HD13	2:B:218:PHE:CG	2.50	0.47
1:E:47:LEU:N	1:E:48:PRO:CD	2.78	0.47
1:E:66:SER:HB3	2:F:47:PHE:CZ	2.50	0.47
2:F:325:LEU:HD11	2:F:342:ALA:HB1	1.97	0.47
2:H:126:LYS:CG	2:H:127:ASP:N	2.77	0.47
1:A:28:PRO:HD3	1:A:357:LYS:NZ	2.29	0.47
2:B:16:LEU:HD12	2:B:16:LEU:O	2.15	0.47
1:C:65:SER:C	1:C:67:TRP:H	2.22	0.47
1:C:322:LEU:CD2	1:C:439:CYS:SG	2.95	0.47
2:D:34:SER:N	2:D:221:LEU:HD22	2.11	0.47
2:D:168:ARG:HE	2:D:168:ARG:HB2	1.54	0.47
1:G:328:LEU:HD23	1:G:397:LEU:HD23	1.95	0.47
1:G:377:LEU:HD12	1:G:378:ASP:O	2.15	0.47
2:H:121:GLN:HB2	2:H:122:TYR:CE1	2.50	0.47
2:H:160:GLU:HG2	2:H:161:ARG:H	1.78	0.47
1:A:181:PRO:HD3	1:A:242:ARG:HG3	1.94	0.47
1:A:207:ALA:CB	1:A:421:ARG:O	2.63	0.47
1:C:28:PRO:HD3	1:C:357:LYS:NZ	2.30	0.47
1:E:27:LYS:C	1:E:27:LYS:CD	2.87	0.47
1:E:71:GLY:HA2	1:E:420:GLU:C	2.40	0.47
1:E:172:LEU:C	1:E:172:LEU:CD1	2.84	0.47
1:E:358:SER:HB2	1:E:363:LYS:HE3	1.97	0.47
2:F:168:ARG:HB2	2:F:169:PRO:CD	2.45	0.47
2:F:221:LEU:C	2:F:223:THR:N	2.73	0.47
2:F:349:ALA:O	2:F:351:LEU:N	2.48	0.47
1:G:64:GLY:O	1:G:67:TRP:HE3	1.97	0.47
1:G:206:ILE:O	1:G:207:ALA:HB3	2.13	0.47
1:G:322:LEU:CD2	1:G:439:CYS:SG	2.95	0.47
2:H:100:THR:HG22	2:H:134:ASN:HA	1.97	0.47
2:H:121:GLN:CA	2:H:122:TYR:CD1	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:159:PRO:HG3	2:H:257:ARG:NH1	2.21	0.47
2:H:200:LEU:C	2:H:200:LEU:HD22	2.39	0.47
2:H:428:ALA:O	2:H:432:VAL:HG23	2.15	0.47
1:A:27:LYS:HG3	2:B:66:ALA:HB1	1.97	0.47
1:A:29:LYS:CG	2:B:65:THR:O	2.62	0.47
1:A:71:GLY:HA2	1:A:420:GLU:CA	2.44	0.47
1:A:209:GLU:OE1	1:A:426:ALA:HB3	2.10	0.47
1:A:232:ALA:HA	1:A:236:GLU:OE1	2.14	0.47
1:A:304:ILE:HD12	1:A:305:ALA:N	2.30	0.47
2:B:412:ARG:HB3	2:B:414:TRP:CZ3	2.50	0.47
1:C:71:GLY:HA2	1:C:420:GLU:C	2.40	0.47
1:C:327:VAL:HG21	1:C:343:LEU:HD11	1.95	0.47
1:C:367:ARG:HD3	1:C:367:ARG:HA	1.40	0.47
1:C:396:ILE:HD11	1:C:442:LEU:HD23	1.95	0.47
2:D:159:PRO:HB2	2:D:257:ARG:CD	2.44	0.47
2:D:409:GLY:C	2:D:411:GLN:H	2.23	0.47
1:E:206:ILE:CB	1:E:419:GLN:O	2.58	0.47
1:G:421:ARG:NH2	1:G:422:GLU:CB	2.77	0.47
2:H:50:VAL:O	2:H:51:PHE:C	2.57	0.47
1:A:62:CYS:HA	3:A:501:SF4:S3	2.55	0.47
1:A:346:LEU:HD23	1:A:346:LEU:C	2.40	0.47
2:B:126:LYS:NZ	2:B:127:ASP:N	2.55	0.47
2:B:310:MET:HG3	2:B:428:ALA:HB1	1.97	0.47
1:C:30:PRO:HA	2:D:63:GLN:CD	2.38	0.47
2:D:401:PHE:O	2:D:401:PHE:CD2	2.68	0.47
1:E:37:CYS:HB2	1:E:39:PHE:H	1.80	0.47
1:E:323:GLU:OE2	1:E:347:GLY:O	2.33	0.47
1:E:335:LYS:O	1:E:338:SER:OG	2.32	0.47
1:G:323:GLU:OE2	1:G:347:GLY:O	2.33	0.47
1:G:404:MET:CB	1:G:414:PHE:CE1	2.97	0.47
1:A:191:PRO:CG	1:E:314:ALA:HB2	2.44	0.47
2:B:29:LEU:O	2:B:221:LEU:HD11	2.14	0.47
2:B:55:HIS:CE1	2:B:403:GLN:HG2	2.50	0.47
2:D:269:TYR:O	2:D:273:ALA:HB3	2.15	0.47
1:E:346:LEU:HD23	1:E:346:LEU:C	2.39	0.47
1:G:304:ILE:HD12	1:G:304:ILE:C	2.40	0.47
1:A:48:PRO:HG2	1:A:204:TYR:CD1	2.50	0.46
1:C:31:GLY:N	1:C:33:THR:OG1	2.48	0.46
1:E:118:VAL:O	1:E:119:PHE:HD1	1.98	0.46
1:E:328:LEU:HD22	1:E:389:VAL:HG22	1.97	0.46
2:F:70:VAL:C	2:F:72:SER:H	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:109:CYS:O	2:F:110:ASP:C	2.59	0.46
2:F:113:THR:O	2:F:116:HIS:N	2.47	0.46
2:F:409:GLY:C	2:F:411:GLN:H	2.23	0.46
1:G:29:LYS:NZ	1:G:29:LYS:N	2.37	0.46
1:G:304:ILE:HD12	1:G:305:ALA:N	2.30	0.46
1:G:354:GLY:N	1:G:366:ILE:CD1	2.78	0.46
2:H:42:GLN:CA	2:H:64:THR:HG21	2.41	0.46
2:H:410:PHE:CD2	2:H:411:GLN:HB2	2.50	0.46
1:A:206:ILE:CB	1:A:419:GLN:O	2.59	0.46
1:C:367:ARG:HD2	1:C:372:ASP:HA	1.97	0.46
2:D:29:LEU:O	2:D:221:LEU:HD11	2.15	0.46
2:D:200:LEU:HD22	2:D:200:LEU:C	2.40	0.46
1:E:171:MET:O	1:E:175:VAL:HB	2.16	0.46
2:F:121:GLN:HB2	2:F:122:TYR:CE1	2.49	0.46
1:G:27:LYS:CD	2:H:66:ALA:HB1	2.43	0.46
1:G:58:GLY:O	1:G:86:THR:O	2.33	0.46
1:G:307:GLU:O	1:G:311:VAL:CG2	2.60	0.46
2:H:171:GLN:O	2:H:237:SER:HB2	2.16	0.46
2:H:285:SER:HB3	2:H:287:ASN:HD21	1.79	0.46
1:A:47:LEU:C	1:A:49:VAL:H	2.23	0.46
1:A:94:ILE:O	1:A:94:ILE:CG1	2.63	0.46
1:A:209:GLU:HG3	1:A:426:ALA:HB3	1.96	0.46
1:A:343:LEU:HD23	1:A:343:LEU:H	1.80	0.46
1:A:367:ARG:HD2	1:A:372:ASP:HA	1.98	0.46
2:B:295:ARG:NE	2:D:212:HIS:NE2	2.63	0.46
1:C:214:LEU:N	1:C:215:PRO:CD	2.78	0.46
1:C:228:LEU:HB2	1:C:240:MET:HE1	1.97	0.46
2:D:159:PRO:CB	2:D:257:ARG:CD	2.90	0.46
2:F:311:LEU:HD23	2:F:431:LEU:HD12	1.97	0.46
1:G:388:THR:O	1:G:392:TYR:HD2	1.97	0.46
2:H:89:GLU:OE2	2:H:124:GLU:HB2	2.14	0.46
2:H:93:PRO:CG	2:H:96:ILE:HG13	2.46	0.46
2:H:122:TYR:O	2:H:123:GLU:C	2.57	0.46
2:H:168:ARG:CB	2:H:169:PRO:CD	2.92	0.46
1:A:381:ASN:HB2	2:B:217:ARG:HH21	1.80	0.46
2:B:168:ARG:HB2	2:B:169:PRO:CD	2.44	0.46
2:B:212:HIS:CE1	2:D:295:ARG:NE	2.83	0.46
2:D:213:LEU:HD22	2:D:215:GLU:H	1.80	0.46
2:D:311:LEU:HD23	2:D:431:LEU:HD12	1.97	0.46
1:E:48:PRO:HG2	1:E:204:TYR:HD1	1.81	0.46
2:F:33:ARG:N	2:F:221:LEU:HD23	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:409:LYS:HD2	2:H:218:PHE:CZ	2.50	0.46
2:H:27:ALA:HB2	2:H:146:PHE:CE1	2.50	0.46
2:H:228:VAL:CG2	2:H:229:ALA:N	2.78	0.46
1:A:24:GLY:O	1:A:25:CYS:HB3	2.16	0.46
1:A:206:ILE:H	1:A:206:ILE:HG12	1.33	0.46
1:A:404:MET:CB	1:A:414:PHE:CE1	2.99	0.46
2:B:36:PRO:HD2	2:B:61:PRO:O	2.16	0.46
2:B:218:PHE:O	2:B:220:ALA:N	2.49	0.46
1:E:304:ILE:HD12	1:E:304:ILE:C	2.40	0.46
1:G:52:VAL:O	1:G:79:LEU:HD23	2.16	0.46
1:G:65:SER:C	1:G:67:TRP:H	2.22	0.46
1:G:346:LEU:HD23	1:G:346:LEU:C	2.40	0.46
2:H:136:PRO:O	2:H:137:ASP:C	2.56	0.46
2:H:378:LEU:HD13	2:H:379:VAL:N	2.30	0.46
1:A:78:ASP:O	1:A:81:ARG:HB2	2.16	0.46
1:A:214:LEU:HB3	1:A:215:PRO:HD3	1.97	0.46
1:A:228:LEU:HB2	1:A:240:MET:HE1	1.97	0.46
2:B:95:VAL:HG22	2:B:228:VAL:HG11	1.97	0.46
1:C:346:LEU:HD23	1:C:346:LEU:C	2.41	0.46
1:E:174:TYR:CD2	1:E:174:TYR:O	2.68	0.46
1:E:328:LEU:HD23	1:E:397:LEU:HD23	1.98	0.46
1:E:440:ILE:HG13	1:E:441:THR:N	2.31	0.46
2:F:354:SER:HB2	2:F:355:PRO:HD2	1.97	0.46
1:G:47:LEU:C	1:G:49:VAL:H	2.24	0.46
1:G:71:GLY:HA2	1:G:420:GLU:C	2.40	0.46
1:G:206:ILE:CD1	1:G:419:GLN:HB3	2.45	0.46
2:H:221:LEU:C	2:H:223:THR:N	2.74	0.46
2:B:269:TYR:O	2:B:273:ALA:CB	2.64	0.46
2:B:383:SER:OG	2:B:403:GLN:HA	2.16	0.46
1:C:68:ASP:HB3	2:D:384:HIS:HE1	1.81	0.46
1:C:252:LYS:HD2	1:C:361:GLU:HG2	1.97	0.46
1:C:440:ILE:HG13	1:C:441:THR:N	2.30	0.46
2:D:285:SER:HB3	2:D:287:ASN:HD21	1.81	0.46
1:E:354:GLY:N	1:E:366:ILE:CD1	2.78	0.46
1:E:383:ARG:CD	2:F:217:ARG:HH22	2.29	0.46
1:E:421:ARG:CZ	1:E:422:GLU:N	2.75	0.46
2:F:116:HIS:HA	2:F:119:ARG:HB2	1.98	0.46
1:G:179:ARG:HB3	1:G:238:GLN:CB	2.46	0.46
2:H:36:PRO:HB2	2:H:62:LEU:HD13	1.98	0.46
2:H:226:LEU:HD22	2:H:226:LEU:HA	1.67	0.46
2:H:236:GLN:O	2:H:236:GLN:HG2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ALA:O	1:A:386:LEU:N	2.48	0.46
2:B:179:ASN:HB3	2:B:324:LEU:HD11	1.98	0.46
2:B:212:HIS:CE1	2:D:295:ARG:HG3	2.51	0.46
1:C:196:HIS:HB3	1:C:291:LEU:HD11	1.97	0.46
2:D:38:PHE:CG	2:D:45:THR:HG22	2.51	0.46
2:F:36:PRO:HB2	2:F:62:LEU:HD13	1.98	0.46
2:F:156:THR:C	2:F:157:LEU:HD13	2.41	0.46
2:F:401:PHE:O	2:F:401:PHE:CD2	2.69	0.46
1:G:155:GLY:HA3	3:G:501:SF4:S4	2.56	0.46
1:G:286:ASP:O	1:G:290:LEU:HB2	2.15	0.46
1:G:439:CYS:O	1:G:440:ILE:C	2.57	0.46
2:H:55:HIS:CE1	2:H:403:GLN:HG2	2.51	0.46
1:A:316:GLU:C	1:A:316:GLU:CD	2.84	0.46
2:B:167:LYS:O	2:B:167:LYS:HG3	2.15	0.46
2:B:175:LEU:HB3	2:B:247:LEU:HD13	1.98	0.46
1:C:339:VAL:HG11	1:C:417:ILE:HD11	1.98	0.46
1:C:343:LEU:HD23	1:C:343:LEU:H	1.81	0.46
2:D:100:THR:HG22	2:D:134:ASN:HA	1.98	0.46
2:D:159:PRO:CB	2:D:257:ARG:CG	2.93	0.46
1:E:339:VAL:O	1:E:342:ALA:HB3	2.16	0.46
2:F:42:GLN:HA	2:F:64:THR:CG2	2.41	0.46
2:H:162:ARG:NE	2:H:162:ARG:HA	2.31	0.46
2:H:257:ARG:CZ	2:H:257:ARG:HB3	2.45	0.46
2:H:310:MET:N	2:H:310:MET:HE3	2.31	0.46
1:A:328:LEU:HD22	1:A:389:VAL:HG22	1.96	0.46
1:A:377:LEU:HD12	1:A:378:ASP:O	2.15	0.46
2:B:121:GLN:HB2	2:B:122:TYR:CE1	2.51	0.46
2:B:126:LYS:C	2:B:128:VAL:H	2.24	0.46
2:D:91:GLN:HE21	2:D:91:GLN:HB2	1.63	0.46
2:F:302:ASP:OD2	2:H:58:GLU:CD	2.59	0.46
1:G:128:LEU:C	1:G:130:GLY:H	2.23	0.46
1:G:174:TYR:OH	1:G:238:GLN:CG	2.64	0.46
2:H:33:ARG:N	2:H:221:LEU:CD2	2.79	0.46
2:H:160:GLU:O	2:H:162:ARG:O	2.34	0.46
1:A:148:VAL:C	1:A:149:ILE:HD12	2.40	0.45
1:A:310:LYS:HZ3	1:E:191:PRO:HG2	1.81	0.45
1:A:362:ASP:O	1:A:366:ILE:CG1	2.61	0.45
1:A:383:ARG:N	2:B:217:ARG:NH2	2.63	0.45
2:B:300:LEU:HD12	2:B:300:LEU:O	2.16	0.45
1:C:61:ALA:HB2	2:D:137:ASP:CG	2.42	0.45
1:C:174:TYR:CD2	1:C:174:TYR:O	2.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:GLU:OE2	1:C:347:GLY:O	2.34	0.45
1:C:404:MET:CB	1:C:414:PHE:CE1	2.99	0.45
2:D:176:CYS:C	2:D:247:LEU:HD11	2.41	0.45
1:E:24:GLY:O	1:E:25:CYS:HB3	2.16	0.45
1:E:29:LYS:HG3	2:F:66:ALA:HB3	1.98	0.45
1:E:341:SER:HA	1:E:344:GLN:HE21	1.80	0.45
1:G:316:GLU:HA	1:G:319:ARG:HG3	1.98	0.45
1:G:409:LYS:C	1:G:411:ARG:H	2.24	0.45
2:H:29:LEU:O	2:H:221:LEU:HD11	2.16	0.45
1:C:46:LEU:HB2	1:C:121:TYR:OH	2.16	0.45
1:C:179:ARG:HB3	1:C:238:GLN:CB	2.46	0.45
1:E:189:GLU:O	1:E:190:ARG:O	2.34	0.45
1:E:196:HIS:ND1	1:E:291:LEU:HD12	2.31	0.45
2:H:213:LEU:HD13	2:H:218:PHE:CB	2.45	0.45
1:A:94:ILE:O	1:A:94:ILE:CD1	2.62	0.45
1:A:181:PRO:CD	1:A:242:ARG:HG3	2.47	0.45
1:C:99:GLU:O	1:C:100:LYS:C	2.58	0.45
2:D:160:GLU:O	2:D:162:ARG:O	2.34	0.45
2:H:33:ARG:H	2:H:221:LEU:HD23	1.80	0.45
2:H:188:ILE:HD11	2:H:268:LEU:CD1	2.44	0.45
1:A:341:SER:HA	1:A:344:GLN:HE21	1.81	0.45
2:B:91:GLN:HE21	2:B:91:GLN:HB2	1.56	0.45
1:C:190:ARG:CG	1:C:191:PRO:HD2	2.42	0.45
1:C:383:ARG:HG2	1:C:384:VAL:N	2.28	0.45
2:D:16:LEU:HB2	2:D:363:ASP:HA	1.98	0.45
2:F:26:LEU:CD1	2:F:146:PHE:CD1	2.99	0.45
2:F:113:THR:O	2:F:117:GLU:N	2.47	0.45
1:G:62:CYS:HA	3:G:501:SF4:S3	2.56	0.45
1:G:126:PRO:O	1:G:131:ASP:HB2	2.16	0.45
1:G:328:LEU:HD22	1:G:389:VAL:CG2	2.46	0.45
2:H:299:GLN:OE1	2:H:418:ARG:NH2	2.45	0.45
2:B:271:LEU:O	2:B:272:ASP:C	2.57	0.45
1:C:295:ASP:O	1:C:299:ARG:HG3	2.17	0.45
1:C:337:TRP:O	1:C:337:TRP:HE3	1.98	0.45
2:D:159:PRO:HB2	2:D:257:ARG:HD3	1.97	0.45
1:E:382:ALA:CB	2:F:217:ARG:HG3	2.45	0.45
2:F:102:GLY:HA2	2:F:138:PHE:CE1	2.52	0.45
2:F:315:ARG:HG3	2:F:340:VAL:HG21	1.94	0.45
1:G:421:ARG:HE	1:G:421:ARG:HB3	1.15	0.45
1:A:174:TYR:OH	1:A:238:GLN:CG	2.64	0.45
1:A:328:LEU:HD22	1:A:389:VAL:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:GLY:C	1:A:433:GLU:OE2	2.60	0.45
2:B:197:LEU:HD12	2:B:281:LEU:HD22	1.98	0.45
1:E:140:ALA:O	1:E:141:ALA:C	2.60	0.45
1:E:396:ILE:HG23	1:E:413:PRO:HB2	1.98	0.45
1:A:191:PRO:HB2	1:E:310:LYS:HG2	1.98	0.45
1:A:220:LEU:CD2	1:A:303:LEU:HD13	2.46	0.45
1:A:381:ASN:N	1:A:381:ASN:ND2	2.60	0.45
1:A:425:TYR:HD1	1:A:433:GLU:OE1	1.99	0.45
2:B:317:ALA:HB3	2:B:379:VAL:HG22	1.97	0.45
1:C:203:GLU:HB3	1:C:227:THR:HG23	1.99	0.45
1:C:316:GLU:HA	1:C:319:ARG:HG3	1.99	0.45
1:C:444:CYS:SG	1:C:446:VAL:HG23	2.57	0.45
2:D:122:TYR:C	2:D:124:GLU:N	2.72	0.45
2:D:382:ASN:HD22	2:D:384:HIS:N	2.14	0.45
1:E:78:ASP:O	1:E:81:ARG:HB2	2.17	0.45
1:E:94:ILE:O	1:E:94:ILE:CG1	2.65	0.45
1:E:417:ILE:HD13	1:E:417:ILE:HA	1.63	0.45
1:E:419:GLN:HE22	1:E:424:GLY:H	1.65	0.45
1:G:340:VAL:O	1:G:344:GLN:HB3	2.17	0.45
1:A:27:LYS:HD3	2:B:66:ALA:HB3	1.95	0.45
1:A:190:ARG:CB	1:A:191:PRO:CD	2.41	0.45
1:A:312:ARG:HB2	1:A:312:ARG:HH11	1.81	0.45
2:B:64:THR:HG22	2:B:66:ALA:N	2.26	0.45
2:B:221:LEU:C	2:B:223:THR:H	2.25	0.45
1:C:314:ALA:HB2	1:G:191:PRO:CG	2.46	0.45
2:D:382:ASN:ND2	2:D:384:HIS:N	2.64	0.45
1:G:203:GLU:HB3	1:G:227:THR:HG23	1.99	0.45
1:G:419:GLN:NE2	1:G:424:GLY:H	2.15	0.45
2:H:16:LEU:HD12	2:H:16:LEU:O	2.17	0.45
2:H:113:THR:O	2:H:117:GLU:N	2.48	0.45
2:H:316:THR:OG1	2:H:339:THR:HA	2.17	0.45
2:H:353:ASP:O	2:H:354:SER:CB	2.64	0.45
2:H:433:GLU:HG3	2:H:434:HIS:CD2	2.51	0.45
1:A:60:ILE:H	1:A:60:ILE:HG12	1.44	0.45
2:B:38:PHE:CG	2:B:45:THR:HG22	2.51	0.45
2:B:76:ALA:HA	2:B:79:ASN:OD1	2.17	0.45
2:B:295:ARG:HG3	2:D:212:HIS:CE1	2.52	0.45
2:B:435:HIS:CD2	1:C:422:GLU:HG2	2.51	0.45
1:C:132:ASP:O	1:C:136:VAL:HG23	2.15	0.45
1:C:209:GLU:HG3	1:C:426:ALA:HB3	1.98	0.45
2:D:382:ASN:HD22	2:D:384:HIS:H	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:LEU:HD23	1:E:102:LEU:C	2.42	0.45
1:E:126:PRO:O	1:E:131:ASP:HB2	2.17	0.45
1:E:252:LYS:HD2	1:E:361:GLU:HG2	1.99	0.45
1:E:341:SER:HA	1:E:344:GLN:NE2	2.32	0.45
1:E:381:ASN:HB2	2:F:217:ARG:HH21	1.81	0.45
2:F:204:ASP:OD1	2:F:206:SER:HB2	2.17	0.45
1:A:209:GLU:HG3	1:A:209:GLU:O	2.16	0.45
1:A:423:PHE:O	1:A:423:PHE:HD2	1.99	0.45
2:B:58:GLU:CD	2:D:302:ASP:OD2	2.59	0.45
1:C:47:LEU:C	1:C:49:VAL:H	2.24	0.45
2:F:121:GLN:HB2	2:F:122:TYR:HE1	1.82	0.45
1:G:354:GLY:O	1:G:375:LYS:O	2.35	0.45
1:A:249:VAL:O	1:A:251:SER:N	2.50	0.44
1:A:423:PHE:O	1:A:423:PHE:CD2	2.70	0.44
2:D:315:ARG:HG3	2:D:340:VAL:HG21	1.96	0.44
2:F:363:ASP:O	2:F:366:ASP:HB2	2.17	0.44
1:G:209:GLU:OE1	1:G:426:ALA:HB3	2.13	0.44
1:G:245:VAL:HG11	1:G:290:LEU:HD23	1.99	0.44
2:H:304:MET:O	2:H:308:HIS:HB3	2.17	0.44
1:A:123:THR:C	1:A:126:PRO:HD2	2.43	0.44
2:B:113:THR:O	2:B:116:HIS:N	2.47	0.44
2:B:126:LYS:CG	2:B:127:ASP:H	2.31	0.44
2:B:175:LEU:HD23	2:B:175:LEU:HA	1.81	0.44
1:C:27:LYS:C	1:C:27:LYS:CD	2.87	0.44
2:D:168:ARG:CG	2:D:169:PRO:HD3	2.47	0.44
2:D:265:PHE:HB3	2:D:266:GLY:H	1.56	0.44
1:E:108:GLN:NE2	2:F:11:LEU:N	2.55	0.44
1:E:187:GLY:O	1:E:188:SER:HB3	2.16	0.44
2:F:228:VAL:CG2	2:F:229:ALA:N	2.80	0.44
2:H:26:LEU:HD21	2:H:401:PHE:CZ	2.53	0.44
1:A:176:ILE:HG13	1:A:178:THR:HG23	2.00	0.44
1:A:316:GLU:HA	1:A:319:ARG:HG3	2.00	0.44
1:A:421:ARG:CZ	1:A:422:GLU:N	2.80	0.44
2:B:168:ARG:HE	2:B:168:ARG:HB2	1.64	0.44
2:B:316:THR:OG1	2:B:339:THR:HA	2.17	0.44
2:B:344:VAL:HG13	2:B:346:ALA:H	1.83	0.44
2:B:382:ASN:HD22	2:B:384:HIS:H	1.63	0.44
1:C:31:GLY:C	1:C:33:THR:N	2.73	0.44
1:C:60:ILE:H	1:C:60:ILE:HG12	1.50	0.44
1:C:187:GLY:O	1:C:188:SER:HB3	2.16	0.44
1:C:286:ASP:O	1:C:290:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:LEU:HD12	1:C:378:ASP:O	2.16	0.44
2:D:95:VAL:HG22	2:D:228:VAL:HG11	1.98	0.44
2:D:162:ARG:HA	2:D:162:ARG:NE	2.31	0.44
2:D:344:VAL:HG13	2:D:346:ALA:H	1.83	0.44
1:E:404:MET:HB2	1:E:414:PHE:HE1	1.77	0.44
1:E:421:ARG:NH2	1:E:422:GLU:CB	2.80	0.44
2:F:257:ARG:CZ	2:F:257:ARG:HB3	2.47	0.44
1:G:190:ARG:CG	1:G:191:PRO:HD2	2.41	0.44
1:G:383:ARG:H	2:H:217:ARG:NH2	2.14	0.44
2:H:18:ALA:HB1	2:H:22:MET:CE	2.47	0.44
2:H:122:TYR:C	2:H:124:GLU:N	2.74	0.44
1:A:179:ARG:NH2	1:A:235:ARG:O	2.50	0.44
1:A:388:THR:O	1:A:392:TYR:HD2	2.00	0.44
2:B:349:ALA:O	2:B:351:LEU:N	2.51	0.44
2:D:221:LEU:C	2:D:223:THR:N	2.75	0.44
1:E:64:GLY:O	1:E:67:TRP:HE3	1.99	0.44
1:E:102:LEU:CD2	1:E:102:LEU:C	2.90	0.44
1:E:190:ARG:CG	1:E:191:PRO:HD2	2.41	0.44
1:E:247:MET:HE1	1:E:274:PHE:CE2	2.53	0.44
2:F:218:PHE:O	2:F:220:ALA:N	2.50	0.44
1:G:379:GLU:H	1:G:379:GLU:HG2	1.53	0.44
2:H:168:ARG:HB2	2:H:169:PRO:CD	2.37	0.44
2:B:20:GLN:HG2	2:B:135:THR:CG2	2.47	0.44
2:B:362:GLY:HA3	2:B:366:ASP:OD1	2.16	0.44
1:C:316:GLU:N	1:C:317:PRO:CD	2.80	0.44
2:D:19:SER:O	2:D:20:GLN:C	2.60	0.44
2:D:109:CYS:O	2:D:110:ASP:C	2.61	0.44
2:D:157:LEU:C	2:D:159:PRO:HD3	2.43	0.44
2:D:271:LEU:HD23	2:D:271:LEU:HA	1.83	0.44
1:E:175:VAL:O	1:E:177:GLY:N	2.50	0.44
2:F:94:SER:O	2:F:129:PRO:HD2	2.17	0.44
2:F:271:LEU:O	2:F:272:ASP:C	2.61	0.44
1:G:417:ILE:O	1:G:417:ILE:CG2	2.65	0.44
1:A:30:PRO:HA	2:B:63:GLN:CD	2.42	0.44
1:A:103:PHE:HZ	1:A:143:ARG:HD3	1.83	0.44
1:A:198:VAL:HG22	1:A:223:ARG:O	2.18	0.44
2:D:121:GLN:HB2	2:D:122:TYR:CE1	2.52	0.44
2:D:354:SER:CB	2:D:355:PRO:CD	2.96	0.44
1:E:184:LEU:H	1:E:184:LEU:HG	1.67	0.44
2:F:271:LEU:HD23	2:F:271:LEU:HA	1.83	0.44
1:G:322:LEU:O	1:G:325:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:TYR:CE2	1:A:234:TYR:CE2	3.05	0.44
1:A:340:VAL:O	1:A:344:GLN:HB3	2.17	0.44
2:B:382:ASN:ND2	2:B:384:HIS:N	2.64	0.44
1:C:31:GLY:C	1:C:33:THR:H	2.26	0.44
1:C:302:ALA:O	1:C:305:ALA:HB3	2.17	0.44
2:D:191:SER:HB3	2:D:277:TRP:CZ3	2.48	0.44
1:E:166:ILE:O	1:E:166:ILE:HG22	2.18	0.44
1:E:220:LEU:CD2	1:E:303:LEU:HD13	2.47	0.44
1:E:383:ARG:NE	2:F:90:ARG:HH12	2.16	0.44
2:F:23:GLY:HA3	2:F:142:PHE:O	2.18	0.44
2:F:28:ILE:HD11	2:F:36:PRO:N	2.33	0.44
2:F:395:PRO:HG3	2:F:434:HIS:CG	2.53	0.44
1:G:179:ARG:NH2	1:G:235:ARG:O	2.50	0.44
1:G:231:ASP:OD1	1:G:233:ARG:NH2	2.50	0.44
2:H:185:LEU:CB	2:H:206:SER:OG	2.66	0.44
1:A:29:LYS:HG2	2:B:65:THR:O	2.18	0.44
1:A:164:ASN:O	1:A:254:MET:HE2	2.17	0.44
1:A:209:GLU:CD	1:A:426:ALA:HB3	2.42	0.44
2:B:89:GLU:OE2	2:B:124:GLU:CB	2.66	0.44
2:B:102:GLY:HA2	2:B:138:PHE:CE1	2.53	0.44
1:C:24:GLY:O	1:C:25:CYS:HB3	2.17	0.44
1:C:177:GLY:C	1:C:179:ARG:H	2.24	0.44
1:C:380:GLY:HA3	1:C:384:VAL:CG2	2.46	0.44
2:D:126:LYS:CG	2:D:127:ASP:H	2.31	0.44
1:E:249:VAL:O	1:E:251:SER:N	2.49	0.44
2:F:226:LEU:HD22	2:F:226:LEU:HA	1.67	0.44
2:F:255:ALA:O	2:F:258:THR:O	2.36	0.44
2:F:295:ARG:NE	2:H:212:HIS:NE2	2.66	0.44
2:F:410:PHE:CD2	2:F:410:PHE:C	2.95	0.44
1:G:68:ASP:OD1	1:G:68:ASP:N	2.51	0.44
2:H:118:PHE:O	2:H:118:PHE:CD2	2.71	0.44
2:H:191:SER:HB3	2:H:277:TRP:CZ3	2.47	0.44
2:H:275:ASP:CG	2:H:297:ARG:HE	2.20	0.44
2:H:409:GLY:C	2:H:411:GLN:H	2.26	0.44
1:A:64:GLY:O	1:A:67:TRP:HE3	2.00	0.44
1:A:155:GLY:N	3:A:501:SF4:S4	2.90	0.44
2:B:113:THR:O	2:B:117:GLU:N	2.50	0.44
1:C:209:GLU:CD	1:C:419:GLN:OE1	2.60	0.44
1:E:149:ILE:N	1:E:149:ILE:CD1	2.81	0.44
1:E:152:ASP:O	1:E:166:ILE:HG21	2.18	0.44
1:G:285:ARG:O	1:G:288:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:287:PHE:O	1:G:291:LEU:CD2	2.65	0.44
1:G:307:GLU:HG2	1:G:428:TYR:CG	2.52	0.44
1:G:429:ASP:O	1:G:432:LEU:HB2	2.17	0.44
2:H:23:GLY:HA3	2:H:142:PHE:O	2.18	0.44
2:H:38:PHE:CG	2:H:45:THR:HG22	2.52	0.44
1:A:108:GLN:NE2	2:B:11:LEU:H	2.12	0.43
1:A:310:LYS:HG2	1:E:191:PRO:HB2	2.00	0.43
1:A:353:THR:CG2	1:A:377:LEU:HD23	2.48	0.43
2:B:93:PRO:CG	2:B:96:ILE:HG13	2.47	0.43
2:B:95:VAL:CG2	2:B:228:VAL:CG1	2.96	0.43
2:B:122:TYR:C	2:B:124:GLU:N	2.74	0.43
2:B:271:LEU:HD23	2:B:271:LEU:HA	1.73	0.43
2:B:378:LEU:CD1	2:B:378:LEU:C	2.92	0.43
1:C:193:ILE:HD13	1:C:293:ASP:OD1	2.18	0.43
1:C:231:ASP:OD1	1:C:233:ARG:NH2	2.51	0.43
2:D:99:LEU:HD23	2:D:133:VAL:HB	2.00	0.43
2:D:105:GLU:O	2:D:105:GLU:HG3	2.18	0.43
2:D:136:PRO:O	2:D:137:ASP:C	2.60	0.43
2:D:351:LEU:H	2:D:351:LEU:HG	1.54	0.43
1:E:27:LYS:CD	2:F:66:ALA:HB1	2.48	0.43
1:E:125:VAL:CB	1:E:126:PRO:HD3	2.47	0.43
1:E:148:VAL:C	1:E:149:ILE:HD12	2.42	0.43
1:E:275:TYR:HD2	1:E:338:SER:HB2	1.81	0.43
1:G:327:VAL:HG21	1:G:343:LEU:HD11	1.98	0.43
1:G:404:MET:HB2	1:G:414:PHE:HE1	1.81	0.43
2:H:175:LEU:HD23	2:H:175:LEU:HA	1.88	0.43
2:H:315:ARG:HG3	2:H:340:VAL:CG2	2.48	0.43
1:A:396:ILE:HG23	1:A:413:PRO:HB2	2.00	0.43
2:B:226:LEU:HD22	2:B:226:LEU:HA	1.69	0.43
2:D:218:PHE:O	2:D:220:ALA:N	2.51	0.43
1:E:397:LEU:O	1:E:414:PHE:HD2	2.01	0.43
2:F:125:TYR:N	2:F:125:TYR:CD1	2.84	0.43
2:F:173:ASN:HD22	2:F:240:THR:CG2	2.30	0.43
1:G:54:HIS:CD2	1:G:121:TYR:OH	2.69	0.43
1:G:102:LEU:HD23	1:G:102:LEU:O	2.17	0.43
1:G:355:THR:N	1:G:358:SER:OG	2.45	0.43
2:H:329:ASP:OD2	2:H:333:ARG:NH1	2.41	0.43
2:H:329:ASP:CG	2:H:333:ARG:HH12	2.26	0.43
1:A:102:LEU:O	1:A:102:LEU:HD23	2.17	0.43
1:A:189:GLU:O	1:A:190:ARG:O	2.35	0.43
1:A:383:ARG:N	2:B:217:ARG:HH12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:VAL:HG12	2:B:96:ILE:N	2.32	0.43
2:B:301:GLN:HB3	1:C:450:VAL:HG11	1.99	0.43
1:C:189:GLU:O	1:C:190:ARG:O	2.36	0.43
1:C:307:GLU:HG2	1:C:428:TYR:CG	2.53	0.43
1:C:358:SER:HB2	1:C:363:LYS:HE3	1.99	0.43
2:D:76:ALA:HA	2:D:79:ASN:OD1	2.18	0.43
2:D:228:VAL:O	2:D:229:ALA:C	2.61	0.43
2:D:310:MET:HE2	2:D:310:MET:HB3	1.92	0.43
1:E:330:TYR:HB3	1:E:399:ALA:CB	2.47	0.43
2:F:76:ALA:HA	2:F:79:ASN:OD1	2.19	0.43
2:F:315:ARG:HG3	2:F:340:VAL:CG2	2.49	0.43
1:G:39:PHE:O	1:G:40:ASP:C	2.61	0.43
1:G:164:ASN:O	1:G:254:MET:HE2	2.18	0.43
1:G:377:LEU:O	1:G:384:VAL:HG11	2.17	0.43
2:H:126:LYS:NZ	2:H:127:ASP:N	2.56	0.43
1:A:65:SER:C	1:A:67:TRP:H	2.26	0.43
1:A:174:TYR:CD2	1:A:174:TYR:C	2.94	0.43
1:A:286:ASP:O	1:A:290:LEU:HB2	2.18	0.43
1:A:287:PHE:O	1:A:291:LEU:CD2	2.66	0.43
2:B:20:GLN:HG2	2:B:135:THR:HG22	2.01	0.43
2:B:24:ALA:HB1	2:B:149:ALA:HB2	1.99	0.43
2:B:26:LEU:CD1	2:B:146:PHE:CD1	3.01	0.43
2:B:168:ARG:CB	2:B:169:PRO:CD	2.97	0.43
2:B:314:ALA:HA	2:B:377:GLN:OE1	2.17	0.43
1:C:409:LYS:HD2	2:D:218:PHE:CZ	2.52	0.43
2:F:118:PHE:O	2:F:122:TYR:CE2	2.70	0.43
1:G:48:PRO:HG2	1:G:204:TYR:CD1	2.52	0.43
1:G:312:ARG:HB2	1:G:312:ARG:HH11	1.84	0.43
2:H:26:LEU:CD1	2:H:146:PHE:CD1	3.01	0.43
1:A:382:ALA:CB	2:B:217:ARG:HG3	2.46	0.43
2:B:94:SER:O	2:B:129:PRO:HD2	2.19	0.43
1:C:126:PRO:O	1:C:131:ASP:HB2	2.19	0.43
1:C:137:CYS:SG	1:C:150:PRO:HB3	2.58	0.43
1:C:204:TYR:CD1	1:C:229:ALA:O	2.71	0.43
1:C:340:VAL:O	1:C:344:GLN:HB3	2.18	0.43
1:C:382:ALA:O	1:C:386:LEU:N	2.50	0.43
2:D:16:LEU:H	2:D:363:ASP:CG	2.26	0.43
1:E:157:TYR:HD1	1:E:157:TYR:H	1.67	0.43
1:E:362:ASP:O	1:E:366:ILE:CG1	2.63	0.43
2:F:168:ARG:H	2:F:236:GLN:HB2	1.84	0.43
2:F:312:SER:O	2:F:313:SER:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:347:ARG:O	2:F:348:ALA:O	2.36	0.43
1:G:94:ILE:O	1:G:94:ILE:CD1	2.66	0.43
1:G:94:ILE:O	1:G:94:ILE:CG1	2.66	0.43
1:G:123:THR:C	1:G:126:PRO:HD2	2.43	0.43
2:H:16:LEU:HB2	2:H:363:ASP:HA	2.01	0.43
2:H:213:LEU:CD1	2:H:218:PHE:HB3	2.46	0.43
1:A:71:GLY:HA2	1:A:420:GLU:C	2.42	0.43
1:A:168:GLY:O	1:A:169:GLU:C	2.60	0.43
1:A:207:ALA:HB2	1:A:421:ARG:C	2.44	0.43
1:A:322:LEU:O	1:A:325:LYS:HG2	2.18	0.43
1:A:341:SER:HA	1:A:344:GLN:NE2	2.32	0.43
2:B:183:GLY:O	2:B:413:CYS:HB2	2.19	0.43
2:B:236:GLN:O	2:B:236:GLN:HG2	2.18	0.43
2:B:395:PRO:HG3	2:B:434:HIS:ND1	2.33	0.43
1:C:164:ASN:O	1:C:254:MET:HE2	2.19	0.43
1:C:179:ARG:NH2	1:C:235:ARG:O	2.51	0.43
1:C:328:LEU:HD22	1:C:389:VAL:CG2	2.49	0.43
1:C:440:ILE:HG13	1:C:441:THR:H	1.83	0.43
2:D:116:HIS:HA	2:D:119:ARG:HB2	2.00	0.43
1:E:174:TYR:OH	1:E:234:TYR:CD1	2.72	0.43
1:G:155:GLY:CA	3:G:501:SF4:S4	3.05	0.43
2:H:105:GLU:HG3	2:H:105:GLU:O	2.19	0.43
2:H:136:PRO:C	2:H:138:PHE:N	2.76	0.43
1:A:71:GLY:O	1:A:72:THR:O	2.36	0.43
1:A:204:TYR:CD1	1:A:229:ALA:O	2.72	0.43
1:C:47:LEU:N	1:C:48:PRO:HD3	2.34	0.43
1:C:304:ILE:HD12	1:C:305:ALA:N	2.34	0.43
1:C:304:ILE:O	1:C:308:GLU:HG3	2.18	0.43
2:D:26:LEU:HD13	2:D:146:PHE:CE1	2.54	0.43
2:D:260:VAL:HA	2:D:261:PRO:HD3	1.88	0.43
1:E:47:LEU:C	1:E:49:VAL:H	2.27	0.43
1:E:286:ASP:O	1:E:290:LEU:HB2	2.18	0.43
2:F:91:GLN:HE21	2:F:91:GLN:HB2	1.61	0.43
2:F:176:CYS:C	2:F:247:LEU:HD11	2.43	0.43
2:H:21:THR:HG21	2:H:137:ASP:OD1	2.18	0.43
2:H:39:HIS:HD2	2:H:65:THR:OG1	2.01	0.43
2:H:299:GLN:OE1	2:H:418:ARG:NE	2.48	0.43
1:A:31:GLY:C	1:A:33:THR:N	2.76	0.43
1:A:345:ASP:OD1	1:A:346:LEU:N	2.52	0.43
1:A:383:ARG:CG	1:A:384:VAL:H	2.30	0.43
1:A:383:ARG:CD	2:B:217:ARG:HH22	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:LEU:O	2:B:221:LEU:HG	2.19	0.43
2:B:221:LEU:O	2:B:222:THR:C	2.62	0.43
2:B:299:GLN:OE1	2:B:418:ARG:NH2	2.49	0.43
2:B:329:ASP:OD2	2:B:333:ARG:NH1	2.47	0.43
1:C:57:HIS:O	1:C:123:THR:OG1	2.33	0.43
1:C:191:PRO:HG2	1:G:310:LYS:HZ2	1.82	0.43
1:C:382:ALA:CB	2:D:217:ARG:HG3	2.42	0.43
1:E:179:ARG:HB3	1:E:238:GLN:CB	2.49	0.43
1:E:409:LYS:HD2	2:F:218:PHE:CZ	2.53	0.43
2:F:185:LEU:CB	2:F:206:SER:OG	2.67	0.43
2:F:378:LEU:CD1	2:F:378:LEU:C	2.92	0.43
1:G:103:PHE:HZ	1:G:143:ARG:HD3	1.84	0.43
1:G:152:ASP:O	1:G:166:ILE:HG21	2.18	0.43
2:H:173:ASN:HD22	2:H:240:THR:CG2	2.31	0.43
2:B:39:HIS:HD2	2:B:65:THR:CB	2.32	0.43
2:B:100:THR:CG2	2:B:134:ASN:HA	2.49	0.43
1:C:252:LYS:CB	1:C:361:GLU:OE2	2.64	0.43
1:C:353:THR:CG2	1:C:377:LEU:HD23	2.48	0.43
2:D:158:VAL:N	2:D:159:PRO:HD2	2.34	0.43
1:E:58:GLY:O	1:E:86:THR:O	2.36	0.43
1:E:65:SER:C	1:E:67:TRP:H	2.26	0.43
1:E:383:ARG:H	2:F:217:ARG:NH2	2.16	0.43
2:F:245:GLN:C	2:F:247:LEU:H	2.27	0.43
1:G:47:LEU:N	1:G:48:PRO:HD3	2.34	0.43
1:G:149:ILE:N	1:G:149:ILE:HD12	2.34	0.43
1:G:293:ASP:OD2	1:G:294:PRO:HD2	2.19	0.43
2:H:329:ASP:OD1	2:H:356:LEU:HD22	2.19	0.43
2:H:352:VAL:CG1	2:H:354:SER:H	2.32	0.43
1:A:27:LYS:CD	1:A:27:LYS:C	2.92	0.43
1:A:206:ILE:CD1	1:A:419:GLN:HB3	2.48	0.43
1:C:166:ILE:O	1:C:166:ILE:HG22	2.19	0.43
1:E:68:ASP:OD1	1:E:68:ASP:N	2.51	0.43
1:E:340:VAL:O	1:E:344:GLN:HB3	2.19	0.43
2:F:126:LYS:O	2:F:127:ASP:CB	2.65	0.43
2:F:344:VAL:O	2:F:361:VAL:HA	2.18	0.43
1:G:384:VAL:O	1:G:387:LYS:HG2	2.19	0.43
2:H:91:GLN:HE21	2:H:91:GLN:HB2	1.58	0.43
2:H:126:LYS:HZ2	2:H:127:ASP:H	1.61	0.43
2:H:325:LEU:HD11	2:H:342:ALA:HB1	2.00	0.43
1:A:304:ILE:O	1:A:308:GLU:HG3	2.19	0.42
1:C:47:LEU:N	1:C:48:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ALA:O	1:C:157:TYR:HD1	2.01	0.42
1:C:198:VAL:HG22	1:C:223:ARG:O	2.19	0.42
1:C:289:ARG:HE	1:C:289:ARG:HB3	1.70	0.42
1:C:322:LEU:O	1:C:325:LYS:HG2	2.19	0.42
2:D:70:VAL:C	2:D:72:SER:H	2.26	0.42
2:D:126:LYS:CG	2:D:127:ASP:N	2.82	0.42
2:D:173:ASN:ND2	2:D:240:THR:HG22	2.34	0.42
1:E:46:LEU:HB2	1:E:121:TYR:OH	2.19	0.42
1:E:128:LEU:HD23	2:F:106:THR:HG21	2.00	0.42
1:E:237:VAL:O	1:E:238:GLN:C	2.61	0.42
2:F:173:ASN:HB2	2:F:240:THR:CG2	2.24	0.42
2:F:221:LEU:O	2:F:221:LEU:HG	2.19	0.42
1:G:78:ASP:O	1:G:81:ARG:HB2	2.18	0.42
1:G:209:GLU:CD	1:G:426:ALA:HB3	2.44	0.42
1:G:228:LEU:HB2	1:G:240:MET:HE1	2.01	0.42
2:H:125:TYR:HB2	2:H:126:LYS:O	2.18	0.42
1:A:63:ALA:O	1:A:64:GLY:C	2.62	0.42
1:A:337:TRP:O	1:A:337:TRP:HE3	2.01	0.42
1:A:421:ARG:NH2	1:A:422:GLU:CB	2.80	0.42
2:B:331:LEU:HD22	2:B:331:LEU:C	2.45	0.42
2:B:391:ARG:HE	2:B:391:ARG:HB2	1.61	0.42
1:C:415:LEU:C	1:C:415:LEU:HD23	2.45	0.42
1:E:379:GLU:H	1:E:379:GLU:HG2	1.56	0.42
1:E:383:ARG:N	2:F:217:ARG:HH12	2.17	0.42
2:F:168:ARG:CB	2:F:169:PRO:CD	2.97	0.42
2:F:213:LEU:HD13	2:F:218:PHE:CG	2.54	0.42
2:F:285:SER:CB	2:F:287:ASN:HD21	2.31	0.42
1:G:179:ARG:HB3	1:G:238:GLN:HB2	2.00	0.42
2:H:113:THR:O	2:H:116:HIS:N	2.49	0.42
2:H:347:ARG:O	2:H:348:ALA:O	2.37	0.42
1:A:383:ARG:HD2	2:B:217:ARG:NH2	2.34	0.42
2:B:304:MET:O	2:B:308:HIS:HB3	2.19	0.42
1:C:247:MET:HE1	1:C:274:PHE:CE2	2.54	0.42
2:D:126:LYS:O	2:D:127:ASP:CB	2.63	0.42
2:D:291:ASP:HA	2:D:294:LYS:HG3	2.01	0.42
1:E:48:PRO:HG2	1:E:204:TYR:CD1	2.55	0.42
2:F:159:PRO:CB	2:F:257:ARG:CD	2.93	0.42
1:G:174:TYR:OH	1:G:234:TYR:C	2.62	0.42
1:G:248:MET:SD	1:G:258:ALA:HB2	2.59	0.42
2:H:149:ALA:O	2:H:153:ILE:CG1	2.62	0.42
2:H:386:LEU:HD23	2:H:386:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:LYS:CG	2:B:127:ASP:N	2.82	0.42
1:C:179:ARG:HB3	1:C:238:GLN:HB3	2.01	0.42
1:C:207:ALA:CB	1:C:421:ARG:O	2.67	0.42
2:D:16:LEU:O	2:D:16:LEU:HD12	2.18	0.42
1:E:174:TYR:CE2	1:E:234:TYR:CE2	3.07	0.42
1:E:287:PHE:O	1:E:291:LEU:CD2	2.66	0.42
1:E:308:GLU:O	1:E:312:ARG:HD3	2.18	0.42
1:E:431:MET:HE2	1:E:431:MET:HB3	1.81	0.42
1:E:440:ILE:HG13	1:E:441:THR:H	1.85	0.42
2:F:265:PHE:HB3	2:F:266:GLY:H	1.56	0.42
1:G:31:GLY:N	1:G:33:THR:OG1	2.52	0.42
1:G:184:LEU:HA	1:G:185:PRO:HD3	1.82	0.42
1:G:210:PHE:C	1:G:212:HIS:N	2.78	0.42
2:B:167:LYS:HA	2:B:237:SER:H	1.84	0.42
2:B:295:ARG:NE	2:D:212:HIS:CE1	2.87	0.42
1:C:341:SER:HA	1:C:344:GLN:HE21	1.84	0.42
2:D:26:LEU:HD12	2:D:146:PHE:CD1	2.55	0.42
2:D:175:LEU:HD23	2:D:175:LEU:HA	1.86	0.42
2:D:322:PRO:HG2	2:D:348:ALA:CB	2.49	0.42
2:D:335:MET:SD	2:D:424:LEU:HD21	2.59	0.42
1:E:220:LEU:HD21	1:E:303:LEU:HD13	2.01	0.42
2:F:89:GLU:OE2	2:F:124:GLU:CB	2.67	0.42
2:F:100:THR:CG2	2:F:134:ASN:HA	2.49	0.42
2:F:105:GLU:HG2	2:F:136:PRO:CG	2.50	0.42
2:F:126:LYS:C	2:F:128:VAL:H	2.27	0.42
1:G:433:GLU:HA	1:G:436:ARG:HD2	2.01	0.42
1:A:26:ALA:O	1:A:27:LYS:CB	2.63	0.42
1:A:174:TYR:CZ	1:A:234:TYR:CD2	3.08	0.42
1:C:312:ARG:HB2	1:C:312:ARG:NH1	2.35	0.42
1:C:383:ARG:NE	2:D:90:ARG:HH12	2.16	0.42
1:C:397:LEU:O	1:C:414:PHE:HD2	2.02	0.42
2:D:213:LEU:HD13	2:D:218:PHE:CG	2.55	0.42
2:D:352:VAL:CG1	2:D:354:SER:H	2.33	0.42
1:E:103:PHE:HZ	1:E:143:ARG:HD3	1.84	0.42
2:H:70:VAL:C	2:H:72:SER:H	2.27	0.42
1:A:71:GLY:O	1:A:72:THR:C	2.63	0.42
2:B:168:ARG:HG3	2:B:236:GLN:CB	2.44	0.42
2:B:335:MET:SD	2:B:424:LEU:CD2	3.08	0.42
1:C:184:LEU:HA	1:C:185:PRO:HD3	1.80	0.42
1:C:220:LEU:HD21	1:C:303:LEU:HD13	2.00	0.42
1:C:316:GLU:CD	1:C:317:PRO:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:MET:SD	2:D:48:ALA:HA	2.60	0.42
2:D:55:HIS:HE1	2:D:403:GLN:HG2	1.83	0.42
1:E:174:TYR:OH	1:E:238:GLN:HG2	2.20	0.42
1:E:174:TYR:OH	1:E:238:GLN:HG3	2.20	0.42
1:E:312:ARG:HB2	1:E:312:ARG:HH11	1.85	0.42
2:F:158:VAL:N	2:F:159:PRO:HD2	2.34	0.42
2:H:39:HIS:HD2	2:H:65:THR:CB	2.32	0.42
2:H:398:ARG:NH1	2:H:405:ASP:OD1	2.52	0.42
2:B:116:HIS:HA	2:B:119:ARG:HB2	2.02	0.42
2:B:117:GLU:O	2:B:122:TYR:OH	2.32	0.42
2:B:162:ARG:NE	2:B:162:ARG:HA	2.34	0.42
1:C:68:ASP:OD1	1:C:68:ASP:N	2.53	0.42
1:C:128:LEU:C	1:C:130:GLY:H	2.26	0.42
1:C:191:PRO:HG3	1:G:314:ALA:HB2	2.00	0.42
1:C:417:ILE:HD13	1:C:417:ILE:HA	1.64	0.42
1:E:62:CYS:SG	1:E:123:THR:HG21	2.60	0.42
1:E:246:ASN:HD22	1:E:246:ASN:HA	1.69	0.42
1:E:327:VAL:O	1:E:327:VAL:HG23	2.20	0.42
1:E:367:ARG:HD3	1:E:367:ARG:HA	1.43	0.42
2:F:353:ASP:O	2:F:354:SER:OG	2.35	0.42
1:G:417:ILE:HD13	1:G:417:ILE:HA	1.62	0.42
1:A:304:ILE:HD12	1:A:304:ILE:C	2.44	0.42
1:A:417:ILE:HD13	1:A:417:ILE:HA	1.66	0.42
2:B:121:GLN:HB2	2:B:122:TYR:HE1	1.85	0.42
2:B:213:LEU:CD1	2:B:218:PHE:HB3	2.48	0.42
2:B:329:ASP:OD1	2:B:356:LEU:HD22	2.19	0.42
1:C:66:SER:HB3	2:D:47:PHE:CZ	2.54	0.42
1:C:293:ASP:OD2	1:C:294:PRO:HD2	2.19	0.42
1:C:355:THR:N	1:C:358:SER:OG	2.46	0.42
2:D:160:GLU:CD	2:D:160:GLU:H	2.28	0.42
2:D:185:LEU:CB	2:D:206:SER:OG	2.67	0.42
2:D:395:PRO:HG3	2:D:434:HIS:CG	2.55	0.42
1:E:201:ILE:HA	1:E:228:LEU:HB3	2.01	0.42
1:E:209:GLU:OE1	1:E:426:ALA:HB3	2.19	0.42
1:E:270:PHE:CD2	1:E:286:ASP:OD2	2.73	0.42
1:E:322:LEU:CD2	1:E:439:CYS:SG	2.95	0.42
2:F:99:LEU:HD23	2:F:133:VAL:HB	2.02	0.42
1:G:29:LYS:CG	2:H:65:THR:O	2.68	0.42
2:H:131:VAL:HA	2:H:132:PRO:HD3	1.90	0.42
2:H:168:ARG:HE	2:H:168:ARG:HB2	1.58	0.42
2:H:218:PHE:C	2:H:219:ASN:OD1	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ILE:HA	1:A:228:LEU:HB3	2.02	0.42
2:B:33:ARG:N	2:B:221:LEU:CD2	2.83	0.42
2:B:66:ALA:O	2:B:67:MET:C	2.63	0.42
2:B:265:PHE:HB3	2:B:266:GLY:H	1.61	0.42
1:C:29:LYS:HZ2	1:C:29:LYS:HB2	1.84	0.42
1:C:206:ILE:O	1:C:419:GLN:O	2.38	0.42
1:C:323:GLU:OE2	1:C:324:GLY:N	2.53	0.42
1:C:377:LEU:O	1:C:384:VAL:HG11	2.19	0.42
2:D:236:GLN:HG2	2:D:236:GLN:O	2.19	0.42
2:D:333:ARG:HB2	2:D:333:ARG:HH11	1.83	0.42
2:D:362:GLY:HA3	2:D:366:ASP:OD1	2.20	0.42
1:E:353:THR:CG2	1:E:377:LEU:HD23	2.50	0.42
2:F:64:THR:HG22	2:F:66:ALA:N	2.25	0.42
2:F:70:VAL:C	2:F:72:SER:N	2.78	0.42
2:F:397:LEU:HD22	2:F:427:LEU:HD23	2.01	0.42
1:G:339:VAL:HG11	1:G:417:ILE:HD11	2.02	0.42
2:H:68:ASP:CB	2:H:70:VAL:HG22	2.25	0.42
2:H:168:ARG:CG	2:H:169:PRO:HD3	2.50	0.42
1:A:203:GLU:HB3	1:A:227:THR:HG23	2.02	0.41
1:A:359:THR:CG2	4:A:502:CZL:S2A	3.07	0.41
1:A:440:ILE:HG13	1:A:441:THR:H	1.85	0.41
2:B:218:PHE:C	2:B:219:ASN:OD1	2.63	0.41
1:C:48:PRO:CB	1:C:72:THR:HG21	2.48	0.41
1:C:102:LEU:O	1:C:102:LEU:HD23	2.20	0.41
1:C:270:PHE:CD2	1:C:286:ASP:OD2	2.73	0.41
2:D:113:THR:O	2:D:117:GLU:N	2.52	0.41
2:D:349:ALA:O	2:D:351:LEU:N	2.53	0.41
2:F:159:PRO:CB	2:F:257:ARG:HH11	2.32	0.41
2:F:215:GLU:O	2:F:218:PHE:CE2	2.73	0.41
1:G:148:VAL:C	1:G:149:ILE:HD12	2.45	0.41
1:G:174:TYR:OH	1:G:238:GLN:HG2	2.19	0.41
1:G:174:TYR:CD2	1:G:174:TYR:C	2.90	0.41
1:G:187:GLY:O	1:G:188:SER:HB3	2.19	0.41
1:G:341:SER:HA	1:G:344:GLN:HE21	1.85	0.41
1:G:421:ARG:CZ	1:G:422:GLU:N	2.78	0.41
2:H:160:GLU:HG2	2:H:161:ARG:N	2.35	0.41
1:A:248:MET:SD	1:A:258:ALA:HB2	2.59	0.41
1:A:355:THR:C	1:A:357:LYS:N	2.78	0.41
1:A:383:ARG:N	2:B:217:ARG:NH1	2.68	0.41
1:A:419:GLN:NE2	1:A:424:GLY:H	2.15	0.41
2:B:33:ARG:H	2:B:221:LEU:HD23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:GLU:HG2	2:B:136:PRO:CG	2.51	0.41
2:B:295:ARG:HH22	2:D:206:SER:HB3	1.85	0.41
1:C:63:ALA:O	1:C:65:SER:N	2.53	0.41
1:C:205:ASN:CG	1:C:205:ASN:O	2.61	0.41
1:C:206:ILE:H	1:C:206:ILE:HG12	1.35	0.41
1:C:341:SER:HA	1:C:344:GLN:NE2	2.34	0.41
2:D:33:ARG:H	2:D:221:LEU:HD23	1.86	0.41
1:E:30:PRO:HA	2:F:63:GLN:CD	2.43	0.41
1:E:210:PHE:C	1:E:212:HIS:N	2.78	0.41
1:G:47:LEU:N	1:G:48:PRO:CD	2.83	0.41
1:G:175:VAL:O	1:G:177:GLY:N	2.52	0.41
2:H:183:GLY:O	2:H:413:CYS:HB2	2.20	0.41
2:H:382:ASN:CB	2:H:402:PRO:HD2	2.50	0.41
1:A:193:ILE:O	1:A:195:VAL:N	2.52	0.41
2:B:109:CYS:O	2:B:110:ASP:C	2.64	0.41
2:B:340:VAL:CG1	2:B:374:GLY:HA3	2.50	0.41
2:B:344:VAL:O	2:B:361:VAL:HA	2.21	0.41
2:B:374:GLY:O	2:B:375:GLN:HB2	2.19	0.41
1:C:201:ILE:HA	1:C:228:LEU:HB3	2.01	0.41
1:C:246:ASN:O	1:C:269:TRP:HA	2.20	0.41
1:C:345:ASP:OD1	1:C:346:LEU:N	2.54	0.41
2:D:346:ALA:O	2:D:347:ARG:C	2.63	0.41
1:E:354:GLY:O	1:E:375:LYS:O	2.38	0.41
2:F:131:VAL:HA	2:F:132:PRO:HD3	1.86	0.41
2:F:171:GLN:O	2:F:237:SER:HB2	2.20	0.41
2:F:218:PHE:C	2:F:219:ASN:OD1	2.64	0.41
2:F:314:ALA:HA	2:F:377:GLN:OE1	2.19	0.41
1:G:356:LYS:HD3	1:G:378:ASP:HA	2.00	0.41
2:H:31:LEU:HD23	2:H:95:VAL:HG11	2.01	0.41
2:H:121:GLN:N	2:H:122:TYR:CD1	2.89	0.41
1:A:154:ALA:O	1:A:157:TYR:HD1	2.03	0.41
1:A:174:TYR:OH	1:A:234:TYR:C	2.62	0.41
2:B:149:ALA:O	2:B:153:ILE:CG1	2.66	0.41
2:B:332:LEU:HB3	2:B:337:ALA:HB3	2.01	0.41
2:B:333:ARG:HH11	2:B:333:ARG:CB	2.32	0.41
1:C:48:PRO:HG2	1:C:204:TYR:CD1	2.55	0.41
1:C:293:ASP:OD2	1:C:294:PRO:CD	2.69	0.41
1:C:433:GLU:HA	1:C:436:ARG:HD2	2.02	0.41
2:D:159:PRO:CB	2:D:257:ARG:HG3	2.51	0.41
2:D:218:PHE:C	2:D:219:ASN:OD1	2.63	0.41
2:D:329:ASP:CG	2:D:333:ARG:HH12	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:397:LEU:HD22	2:D:427:LEU:HD23	2.02	0.41
2:F:38:PHE:CB	2:F:45:THR:HG22	2.50	0.41
2:F:107:GLN:NE2	2:F:107:GLN:H	2.16	0.41
2:F:125:TYR:HB2	2:F:126:LYS:O	2.20	0.41
2:F:291:ASP:HA	2:F:294:LYS:HG3	2.03	0.41
2:H:291:ASP:HA	2:H:294:LYS:HG3	2.03	0.41
2:H:335:MET:SD	2:H:424:LEU:CD2	3.09	0.41
1:A:220:LEU:HD21	1:A:303:LEU:HD13	2.03	0.41
1:A:246:ASN:HD22	1:A:246:ASN:HA	1.70	0.41
1:C:143:ARG:NH1	1:C:143:ARG:HB3	2.35	0.41
1:C:199:ASN:OD1	1:C:240:MET:HG2	2.21	0.41
1:C:249:VAL:O	1:C:251:SER:N	2.53	0.41
2:D:160:GLU:HG2	2:D:161:ARG:N	2.35	0.41
1:E:67:TRP:CZ3	2:F:15:PRO:HG2	2.56	0.41
1:E:380:GLY:HA3	1:E:384:VAL:CG2	2.47	0.41
1:E:381:ASN:HB2	2:F:217:ARG:NH2	2.36	0.41
1:E:421:ARG:HE	1:E:421:ARG:HB3	1.15	0.41
2:F:20:GLN:HA	2:F:141:CYS:O	2.20	0.41
2:F:51:PHE:CE1	2:F:402:PRO:HB3	2.54	0.41
2:F:55:HIS:HE1	2:F:403:GLN:HG2	1.85	0.41
2:F:329:ASP:OD1	2:F:356:LEU:HD22	2.21	0.41
1:G:316:GLU:CD	1:G:317:PRO:N	2.79	0.41
2:H:95:VAL:HG22	2:H:228:VAL:HG11	2.02	0.41
1:A:50:ALA:HB3	1:A:77:PRO:HG2	2.01	0.41
2:B:125:TYR:N	2:B:125:TYR:CD1	2.83	0.41
2:B:396:LEU:HD22	2:B:397:LEU:N	2.36	0.41
2:D:93:PRO:CG	2:D:96:ILE:HG13	2.50	0.41
2:D:347:ARG:O	2:D:348:ALA:O	2.38	0.41
1:E:304:ILE:O	1:E:308:GLU:HG3	2.20	0.41
2:F:160:GLU:CD	2:F:160:GLU:H	2.28	0.41
2:F:168:ARG:CG	2:F:169:PRO:HD3	2.50	0.41
2:F:351:LEU:H	2:F:351:LEU:HG	1.54	0.41
1:G:24:GLY:O	1:G:25:CYS:HB3	2.21	0.41
1:G:29:LYS:CB	1:G:30:PRO:HD2	2.32	0.41
1:G:182:ASP:HA	1:G:183:PRO:HD3	1.91	0.41
1:G:316:GLU:N	1:G:317:PRO:CD	2.84	0.41
1:G:322:LEU:N	1:G:322:LEU:CD2	2.83	0.41
2:H:66:ALA:O	2:H:67:MET:C	2.64	0.41
2:H:344:VAL:HG13	2:H:346:ALA:H	1.86	0.41
2:H:395:PRO:HG3	2:H:434:HIS:CG	2.55	0.41
1:A:322:LEU:CD2	1:A:322:LEU:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LEU:HD23	1:A:397:LEU:HD23	2.03	0.41
2:B:125:TYR:HB2	2:B:126:LYS:O	2.20	0.41
2:B:168:ARG:H	2:B:236:GLN:HB2	1.85	0.41
1:C:247:MET:HB2	1:C:270:PHE:CE1	2.55	0.41
2:D:156:THR:C	2:D:157:LEU:HD13	2.44	0.41
2:D:271:LEU:O	2:D:272:ASP:C	2.64	0.41
1:E:355:THR:C	1:E:357:LYS:N	2.78	0.41
1:E:383:ARG:HD2	2:F:217:ARG:NH2	2.34	0.41
2:F:53:VAL:O	2:F:57:ARG:HA	2.21	0.41
2:F:263:ARG:HE	2:F:263:ARG:HB2	1.60	0.41
1:G:193:ILE:O	1:G:195:VAL:N	2.53	0.41
1:G:304:ILE:O	1:G:308:GLU:HG3	2.20	0.41
1:G:355:THR:C	1:G:357:LYS:N	2.78	0.41
1:G:358:SER:HB2	1:G:363:LYS:HE3	2.03	0.41
2:H:159:PRO:HB2	2:H:257:ARG:HD3	2.01	0.41
2:H:166:GLY:O	2:H:236:GLN:HA	2.21	0.41
2:H:256:GLU:OE2	2:H:256:GLU:CA	2.68	0.41
1:A:209:GLU:O	1:A:212:HIS:HB2	2.21	0.41
2:B:100:THR:HG21	2:B:134:ASN:OD1	2.20	0.41
2:B:329:ASP:CG	2:B:333:ARG:HH12	2.28	0.41
2:B:354:SER:HB2	2:B:355:PRO:CD	2.50	0.41
1:C:227:THR:O	1:C:229:ALA:N	2.54	0.41
1:C:245:VAL:HG11	1:C:290:LEU:HD23	2.00	0.41
1:C:247:MET:HB2	1:C:270:PHE:CZ	2.56	0.41
1:C:429:ASP:O	1:C:432:LEU:HB2	2.20	0.41
2:D:102:GLY:HA2	2:D:138:PHE:CE1	2.55	0.41
2:D:410:PHE:CD2	2:D:410:PHE:C	2.99	0.41
1:E:31:GLY:C	1:E:33:THR:N	2.78	0.41
1:E:174:TYR:CZ	1:E:234:TYR:CD2	3.08	0.41
1:E:328:LEU:HD22	1:E:389:VAL:CG2	2.50	0.41
1:G:250:CYS:O	1:G:251:SER:C	2.64	0.41
1:A:29:LYS:HG3	2:B:66:ALA:HB3	2.02	0.41
1:A:149:ILE:N	1:A:149:ILE:CD1	2.84	0.41
2:B:28:ILE:HD11	2:B:36:PRO:N	2.36	0.41
2:B:257:ARG:CZ	2:B:257:ARG:HB3	2.51	0.41
2:B:291:ASP:HA	2:B:294:LYS:HG3	2.03	0.41
2:B:352:VAL:CG1	2:B:354:SER:H	2.34	0.41
2:B:353:ASP:O	2:B:354:SER:CB	2.69	0.41
1:C:27:LYS:CG	2:D:66:ALA:HB1	2.50	0.41
1:C:174:TYR:CZ	1:C:234:TYR:CD2	3.09	0.41
1:C:421:ARG:NH2	1:C:422:GLU:CB	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:GLY:O	1:C:433:GLU:OE2	2.39	0.41
2:D:51:PHE:CE1	2:D:402:PRO:HB3	2.56	0.41
2:D:329:ASP:OD1	2:D:356:LEU:HD22	2.20	0.41
2:D:435:HIS:CD2	2:D:435:HIS:C	2.99	0.41
1:E:63:ALA:O	1:E:65:SER:N	2.54	0.41
1:E:146:THR:O	1:E:148:VAL:HG23	2.21	0.41
1:E:322:LEU:N	1:E:322:LEU:CD2	2.84	0.41
2:F:16:LEU:HB2	2:F:363:ASP:HA	2.02	0.41
2:F:27:ALA:HB2	2:F:146:PHE:CE1	2.56	0.41
2:F:31:LEU:HD12	2:F:226:LEU:HB2	2.03	0.41
2:F:85:LYS:CD	2:F:118:PHE:HE1	2.23	0.41
2:F:161:ARG:C	2:F:161:ARG:HD3	2.45	0.41
2:F:175:LEU:HD23	2:F:175:LEU:HA	1.87	0.41
2:F:211:GLY:HA3	2:H:302:ASP:HB2	2.03	0.41
2:F:269:TYR:O	2:F:273:ALA:CB	2.69	0.41
2:F:335:MET:SD	2:F:424:LEU:CD2	3.09	0.41
1:G:48:PRO:HB3	1:G:72:THR:CG2	2.51	0.41
1:G:57:HIS:HE1	1:G:131:ASP:OD1	2.04	0.41
1:G:60:ILE:H	1:G:60:ILE:HG12	1.45	0.41
1:G:193:ILE:HD13	1:G:293:ASP:OD1	2.20	0.41
1:G:249:VAL:O	1:G:251:SER:N	2.53	0.41
1:G:337:TRP:O	1:G:337:TRP:HE3	2.02	0.41
1:G:355:THR:CB	1:G:377:LEU:HD11	2.50	0.41
2:H:42:GLN:HA	2:H:64:THR:CG2	2.47	0.41
2:H:95:VAL:CG2	2:H:228:VAL:CG1	2.99	0.41
2:H:159:PRO:CB	2:H:257:ARG:HH11	2.31	0.41
2:H:176:CYS:C	2:H:247:LEU:HD11	2.45	0.41
2:H:382:ASN:ND2	2:H:384:HIS:N	2.69	0.41
2:B:326:LEU:HD23	2:B:326:LEU:N	2.35	0.41
1:C:356:LYS:HD3	1:C:378:ASP:HA	2.02	0.41
1:C:381:ASN:HB2	2:D:217:ARG:NH2	2.36	0.41
1:C:405:TYR:CE1	2:D:57:ARG:O	2.74	0.41
1:C:419:GLN:NE2	1:C:424:GLY:H	2.19	0.41
2:D:33:ARG:N	2:D:221:LEU:CD2	2.84	0.41
2:D:297:ARG:HG3	2:D:417:TYR:CE2	2.56	0.41
1:E:52:VAL:CG1	1:E:53:ALA:N	2.84	0.41
1:E:60:ILE:H	1:E:60:ILE:HG12	1.40	0.41
1:E:316:GLU:OE1	1:E:317:PRO:HD3	2.21	0.41
1:E:316:GLU:N	1:E:317:PRO:CD	2.84	0.41
1:E:335:LYS:H	1:E:335:LYS:HG3	1.64	0.41
1:E:381:ASN:H	1:E:381:ASN:ND2	2.10	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:384:VAL:O	1:E:387:LYS:HG2	2.21	0.41
1:E:430:GLY:O	1:E:433:GLU:OE1	2.39	0.41
2:F:119:ARG:HG2	2:F:119:ARG:HH11	1.86	0.41
2:F:245:GLN:C	2:F:247:LEU:N	2.79	0.41
1:G:27:LYS:C	1:G:27:LYS:CD	2.93	0.41
2:H:76:ALA:HA	2:H:79:ASN:OD1	2.21	0.41
1:A:30:PRO:HB3	2:B:63:GLN:HG3	2.02	0.40
1:A:304:ILE:O	1:A:305:ALA:C	2.61	0.40
2:B:109:CYS:O	2:B:109:CYS:SG	2.80	0.40
2:B:118:PHE:O	2:B:119:ARG:HD3	2.15	0.40
1:C:125:VAL:CB	1:C:126:PRO:HD3	2.50	0.40
2:F:126:LYS:NZ	2:F:127:ASP:N	2.59	0.40
2:F:200:LEU:C	2:F:200:LEU:CD2	2.92	0.40
2:F:329:ASP:OD2	2:F:333:ARG:NH1	2.44	0.40
1:G:52:VAL:CG1	1:G:53:ALA:N	2.83	0.40
2:H:240:THR:HG23	2:H:260:VAL:HG11	2.03	0.40
2:B:159:PRO:CB	2:B:257:ARG:CD	2.94	0.40
1:C:355:THR:C	1:C:357:LYS:N	2.78	0.40
2:D:125:TYR:HB2	2:D:126:LYS:O	2.22	0.40
2:D:144:SER:O	2:D:145:GLY:C	2.64	0.40
1:E:134:ASP:OD1	1:E:134:ASP:N	2.54	0.40
1:E:304:ILE:O	1:E:305:ALA:C	2.65	0.40
1:E:382:ALA:O	1:E:386:LEU:N	2.48	0.40
2:F:352:VAL:CG1	2:F:354:SER:H	2.35	0.40
2:F:423:VAL:O	2:F:423:VAL:HG12	2.21	0.40
1:G:99:GLU:O	1:G:100:LYS:C	2.63	0.40
1:G:373:ASP:OD2	1:G:374:VAL:N	2.55	0.40
2:H:121:GLN:HB2	2:H:122:TYR:HE1	1.85	0.40
2:H:126:LYS:O	2:H:127:ASP:CB	2.63	0.40
1:A:354:GLY:N	1:A:366:ILE:CD1	2.83	0.40
1:C:310:LYS:HZ2	1:G:191:PRO:HG2	1.84	0.40
1:C:311:VAL:CG2	1:C:428:TYR:HB3	2.51	0.40
2:D:23:GLY:HA3	2:D:142:PHE:O	2.21	0.40
2:D:221:LEU:O	2:D:221:LEU:HG	2.22	0.40
2:D:226:LEU:HD22	2:D:226:LEU:HA	1.65	0.40
2:F:105:GLU:O	2:F:105:GLU:HG3	2.22	0.40
2:F:159:PRO:CB	2:F:257:ARG:CG	2.99	0.40
1:G:63:ALA:O	1:G:64:GLY:C	2.64	0.40
1:G:102:LEU:CD2	1:G:102:LEU:C	2.94	0.40
1:G:199:ASN:OD1	1:G:240:MET:HG2	2.21	0.40
1:G:322:LEU:HD11	1:G:439:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:LYS:HB3	2:H:17:LYS:HE3	1.90	0.40
2:H:281:LEU:HD23	2:H:281:LEU:HA	1.92	0.40
1:A:303:LEU:C	1:A:303:LEU:HD23	2.47	0.40
1:A:383:ARG:HG2	1:A:384:VAL:N	2.31	0.40
2:B:159:PRO:HB2	2:B:257:ARG:CD	2.52	0.40
2:B:287:ASN:ND2	2:B:287:ASN:N	2.69	0.40
2:B:410:PHE:CD2	2:B:410:PHE:C	3.00	0.40
1:C:174:TYR:OH	1:C:238:GLN:HG2	2.21	0.40
1:C:174:TYR:OH	1:C:234:TYR:CD1	2.74	0.40
1:C:214:LEU:HD12	1:C:214:LEU:HA	1.83	0.40
1:C:375:LYS:O	1:C:375:LYS:HG2	2.21	0.40
2:D:39:HIS:HD2	2:D:65:THR:CB	2.34	0.40
2:D:121:GLN:N	2:D:122:TYR:CD1	2.88	0.40
2:D:256:GLU:OE2	2:D:256:GLU:CA	2.68	0.40
2:D:386:LEU:HD23	2:D:386:LEU:HA	1.86	0.40
2:D:428:ALA:O	2:D:432:VAL:HG23	2.21	0.40
1:E:193:ILE:O	1:E:195:VAL:N	2.53	0.40
1:E:206:ILE:O	1:E:207:ALA:HB3	2.21	0.40
2:F:117:GLU:O	2:F:121:GLN:OE1	2.39	0.40
2:F:167:LYS:HA	2:F:237:SER:H	1.85	0.40
2:F:200:LEU:HA	2:F:200:LEU:HD23	1.78	0.40
2:F:295:ARG:NE	2:H:212:HIS:CE1	2.90	0.40
1:G:153:SER:HB3	1:G:166:ILE:HG21	2.04	0.40
2:H:202:ILE:HA	2:H:203:PRO:HA	1.70	0.40
2:H:228:VAL:O	2:H:229:ALA:C	2.63	0.40
2:H:245:GLN:C	2:H:247:LEU:N	2.78	0.40
2:H:271:LEU:HD23	2:H:271:LEU:HA	1.70	0.40
2:D:121:GLN:HB2	2:D:122:TYR:HE1	1.86	0.40
2:D:213:LEU:CG	2:D:223:THR:HG23	2.51	0.40
2:D:275:ASP:OD1	2:D:297:ARG:NE	2.37	0.40
2:D:363:ASP:O	2:D:366:ASP:HB2	2.21	0.40
1:E:119:PHE:CD1	1:E:119:PHE:N	2.89	0.40
1:E:206:ILE:O	1:E:419:GLN:O	2.39	0.40
2:F:168:ARG:HE	2:F:168:ARG:HB2	1.61	0.40
2:F:285:SER:HB3	2:F:287:ASN:ND2	2.37	0.40
2:F:375:GLN:O	2:F:376:ALA:C	2.65	0.40
1:G:206:ILE:H	1:G:206:ILE:HG12	1.33	0.40
1:G:382:ALA:O	1:G:386:LEU:N	2.51	0.40
2:H:32:ALA:N	2:H:226:LEU:O	2.44	0.40
2:H:159:PRO:CB	2:H:257:ARG:CD	2.96	0.40
2:H:221:LEU:O	2:H:221:LEU:HG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:351:LEU:O	2:H:352:VAL:CG1	2.60	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:ARG:NH1	2:H:161:ARG:NH1[1_455]	1.89	0.31
2:B:170:ARG:NH1	2:H:161:ARG:O[1_455]	2.03	0.17
2:B:170:ARG:CZ	2:H:161:ARG:CZ[1_455]	2.04	0.16
2:D:169:PRO:CA	2:H:170:ARG:NH1[1_455]	2.09	0.11
2:B:170:ARG:NE	2:H:161:ARG:NE[1_455]	2.10	0.10
2:D:169:PRO:C	2:H:170:ARG:NH1[1_455]	2.11	0.09
2:B:170:ARG:NH1	2:H:161:ARG:CZ[1_455]	2.18	0.02

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	425/483 (88%)	348 (82%)	54 (13%)	23 (5%)	1	1
1	C	425/483 (88%)	350 (82%)	50 (12%)	25 (6%)	1	0
1	E	425/483 (88%)	355 (84%)	47 (11%)	23 (5%)	1	1
1	G	425/483 (88%)	347 (82%)	53 (12%)	25 (6%)	1	0
2	B	430/458 (94%)	361 (84%)	46 (11%)	23 (5%)	1	1
2	D	430/458 (94%)	359 (84%)	48 (11%)	23 (5%)	1	1
2	F	430/458 (94%)	359 (84%)	47 (11%)	24 (6%)	1	1
2	H	430/458 (94%)	356 (83%)	49 (11%)	25 (6%)	1	0
All	All	3420/3764 (91%)	2835 (83%)	394 (12%)	191 (6%)	1	1

All (191) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	64	GLY
1	A	95	MET
1	A	177	GLY
1	A	190	ARG
1	A	191	PRO
1	A	381	ASN
2	B	9	LYS
2	B	76	ALA
2	B	121	GLN
2	B	158	VAL
2	B	164	GLN
2	B	169	PRO
2	B	219	ASN
2	B	222	THR
2	B	265	PHE
2	B	348	ALA
2	B	349	ALA
2	B	352	VAL
2	B	354	SER
1	C	30	PRO
1	C	64	GLY
1	C	95	MET
1	C	190	ARG
1	C	191	PRO
1	C	381	ASN
1	C	421	ARG
2	D	9	LYS
2	D	73	VAL
2	D	76	ALA
2	D	121	GLN
2	D	158	VAL
2	D	164	GLN
2	D	169	PRO
2	D	219	ASN
2	D	222	THR
2	D	265	PHE
2	D	348	ALA
2	D	349	ALA
2	D	352	VAL
2	D	354	SER
1	E	30	PRO
1	E	64	GLY

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Mol	Chain	Res	Type
1	E	95	MET
1	E	177	GLY
1	E	190	ARG
1	E	191	PRO
1	E	381	ASN
1	E	421	ARG
2	F	76	ALA
2	F	121	GLN
2	F	158	VAL
2	F	164	GLN
2	F	169	PRO
2	F	219	ASN
2	F	222	THR
2	F	265	PHE
2	F	348	ALA
2	F	349	ALA
2	F	352	VAL
2	F	354	SER
1	G	30	PRO
1	G	64	GLY
1	G	95	MET
1	G	177	GLY
1	G	190	ARG
1	G	191	PRO
1	G	381	ASN
2	H	73	VAL
2	H	76	ALA
2	H	121	GLN
2	H	158	VAL
2	H	164	GLN
2	H	169	PRO
2	H	219	ASN
2	H	222	THR
2	H	265	PHE
2	H	348	ALA
2	H	349	ALA
2	H	352	VAL
2	H	354	SER
1	A	25	CYS
1	A	27	LYS
1	A	229	ALA
1	A	421	ARG

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Mol	Chain	Res	Type
2	B	73	VAL
2	B	75	GLY
2	B	77	ASP
1	C	27	LYS
1	C	63	ALA
1	C	177	GLY
1	C	229	ALA
2	D	75	GLY
2	D	77	ASP
2	D	237	SER
1	E	25	CYS
1	E	27	LYS
1	E	63	ALA
1	E	211	TRP
1	E	229	ALA
2	F	9	LYS
2	F	73	VAL
2	F	75	GLY
2	F	77	ASP
1	G	25	CYS
1	G	27	LYS
1	G	63	ALA
1	G	176	ILE
1	G	211	TRP
1	G	342	ALA
1	G	421	ARG
2	H	9	LYS
2	H	75	GLY
2	H	77	ASP
1	A	28	PRO
1	A	63	ALA
1	A	188	SER
1	A	211	TRP
1	A	342	ALA
2	B	111	LEU
2	B	237	SER
1	C	25	CYS
1	C	28	PRO
1	C	69	ASN
1	C	176	ILE
1	C	211	TRP
1	C	228	LEU

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Mol	Chain	Res	Type
1	C	342	ALA
1	E	28	PRO
1	E	69	ASN
1	E	176	ILE
1	E	188	SER
1	E	342	ALA
1	E	371	GLY
2	F	111	LEU
1	G	28	PRO
1	G	69	ASN
1	G	229	ALA
2	H	111	LEU
2	H	237	SER
1	A	69	ASN
1	A	176	ILE
1	A	238	GLN
2	B	350	ALA
2	B	362	GLY
2	B	402	PRO
2	D	111	LEU
2	D	362	GLY
2	D	402	PRO
1	E	228	LEU
1	E	250	CYS
2	F	237	SER
2	F	350	ALA
2	F	362	GLY
1	G	72	THR
1	G	188	SER
2	H	29	LEU
2	H	161	ARG
2	H	362	GLY
2	H	402	PRO
1	A	72	THR
1	A	228	LEU
1	A	371	GLY
2	B	168	ARG
1	C	188	SER
1	C	238	GLN
1	C	250	CYS
1	C	371	GLY
1	C	399	ALA

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Mol	Chain	Res	Type
2	D	168	ARG
2	D	341	ALA
2	D	375	GLN
1	E	399	ALA
2	F	168	ARG
2	F	402	PRO
1	G	371	GLY
2	H	168	ARG
2	B	271	LEU
2	F	161	ARG
1	G	141	ALA
1	G	228	LEU
1	G	250	CYS
2	H	110	ASP
2	H	350	ALA
1	G	129	ILE
1	A	195	VAL
1	C	129	ILE
1	C	195	VAL
1	E	195	VAL
1	G	195	VAL
2	F	132	PRO

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	343/388 (88%)	260 (76%)	83 (24%)	1	1
1	C	343/388 (88%)	254 (74%)	89 (26%)	0	0
1	E	343/388 (88%)	257 (75%)	86 (25%)	0	1
1	G	343/388 (88%)	257 (75%)	86 (25%)	0	1
2	B	335/363 (92%)	258 (77%)	77 (23%)	1	1
2	D	335/363 (92%)	262 (78%)	73 (22%)	1	1
2	F	335/363 (92%)	257 (77%)	78 (23%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	335/363 (92%)	261 (78%)	74 (22%)	1	1
All	All	2712/3004 (90%)	2066 (76%)	646 (24%)	1	1

All (646) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	29	LYS
1	A	33	THR
1	A	34	ASP
1	A	37	CYS
1	A	52	VAL
1	A	60	ILE
1	A	62	CYS
1	A	67	TRP
1	A	68	ASP
1	A	69	ASN
1	A	70	ARG
1	A	72	THR
1	A	73	ARG
1	A	81	ARG
1	A	102	LEU
1	A	111	GLU
1	A	123	THR
1	A	157	TYR
1	A	160	LYS
1	A	164	ASN
1	A	172	LEU
1	A	184	LEU
1	A	186	VAL
1	A	190	ARG
1	A	193	ILE
1	A	195	VAL
1	A	203	GLU
1	A	206	ILE
1	A	209	GLU
1	A	216	LEU
1	A	220	LEU
1	A	233	ARG
1	A	235	ARG
1	A	256	ASN
1	A	257	VAL

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Mol	Chain	Res	Type
1	A	259	ARG
1	A	261	LEU
1	A	262	GLN
1	A	271	GLU
1	A	273	SER
1	A	279	ASP
1	A	285	ARG
1	A	287	PHE
1	A	292	ASP
1	A	307	GLU
1	A	311	VAL
1	A	315	LEU
1	A	322	LEU
1	A	323	GLU
1	A	329	LEU
1	A	335	LYS
1	A	338	SER
1	A	339	VAL
1	A	341	SER
1	A	344	GLN
1	A	353	THR
1	A	359	THR
1	A	365	ARG
1	A	366	ILE
1	A	367	ARG
1	A	370	MET
1	A	376	MET
1	A	379	GLU
1	A	381	ASN
1	A	383	ARG
1	A	393	GLN
1	A	396	ILE
1	A	397	LEU
1	A	402	ARG
1	A	403	ASN
1	A	406	THR
1	A	408	LEU
1	A	417	ILE
1	A	419	GLN
1	A	420	GLU
1	A	421	ARG
1	A	422	GLU

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Mol	Chain	Res	Type
1	A	423	PHE
1	A	433	GLU
1	A	440	ILE
1	A	442	LEU
1	A	448	GLU
2	B	17	LYS
2	B	21	THR
2	B	26	LEU
2	B	28	ILE
2	B	31	LEU
2	B	41	SER
2	B	53	VAL
2	B	58	GLU
2	B	62	LEU
2	B	69	GLN
2	B	74	MET
2	B	77	ASP
2	B	85	LYS
2	B	91	GLN
2	B	94	SER
2	B	99	LEU
2	B	103	LEU
2	B	107	GLN
2	B	115	LEU
2	B	122	TYR
2	B	123	GLU
2	B	137	ASP
2	B	157	LEU
2	B	158	VAL
2	B	160	GLU
2	B	161	ARG
2	B	165	VAL
2	B	168	ARG
2	B	170	ARG
2	B	172	VAL
2	B	180	LEU
2	B	188	ILE
2	B	190	GLU
2	B	194	SER
2	B	198	ARG
2	B	200	LEU
2	B	210	ASP

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Mol	Chain	Res	Type
2	B	212	HIS
2	B	213	LEU
2	B	215	GLU
2	B	217	ARG
2	B	218	PHE
2	B	221	LEU
2	B	222	THR
2	B	223	THR
2	B	226	LEU
2	B	227	SER
2	B	257	ARG
2	B	260	VAL
2	B	262	ASP
2	B	263	ARG
2	B	264	ARG
2	B	265	PHE
2	B	274	VAL
2	B	277	TRP
2	B	284	ILE
2	B	287	ASN
2	B	308	HIS
2	B	310	MET
2	B	331	LEU
2	B	339	THR
2	B	344	VAL
2	B	351	LEU
2	B	352	VAL
2	B	356	LEU
2	B	359	VAL
2	B	361	VAL
2	B	363	ASP
2	B	378	LEU
2	B	379	VAL
2	B	382	ASN
2	B	386	LEU
2	B	391	ARG
2	B	394	VAL
2	B	396	LEU
2	B	398	ARG
2	B	401	PHE
1	C	27	LYS
1	C	29	LYS

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Mol	Chain	Res	Type
1	C	33	THR
1	C	34	ASP
1	C	37	CYS
1	C	55	ILE
1	C	60	ILE
1	C	62	CYS
1	C	67	TRP
1	C	68	ASP
1	C	69	ASN
1	C	70	ARG
1	C	72	THR
1	C	73	ARG
1	C	86	THR
1	C	102	LEU
1	C	111	GLU
1	C	123	THR
1	C	149	ILE
1	C	157	TYR
1	C	159	THR
1	C	160	LYS
1	C	164	ASN
1	C	166	ILE
1	C	172	LEU
1	C	178	THR
1	C	184	LEU
1	C	186	VAL
1	C	190	ARG
1	C	193	ILE
1	C	195	VAL
1	C	203	GLU
1	C	206	ILE
1	C	209	GLU
1	C	216	LEU
1	C	220	LEU
1	C	233	ARG
1	C	235	ARG
1	C	241	HIS
1	C	256	ASN
1	C	257	VAL
1	C	259	ARG
1	C	261	LEU
1	C	262	GLN

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Mol	Chain	Res	Type
1	C	269	TRP
1	C	271	GLU
1	C	273	SER
1	C	279	ASP
1	C	285	ARG
1	C	287	PHE
1	C	292	ASP
1	C	307	GLU
1	C	311	VAL
1	C	315	LEU
1	C	322	LEU
1	C	323	GLU
1	C	329	LEU
1	C	335	LYS
1	C	338	SER
1	C	339	VAL
1	C	341	SER
1	C	344	GLN
1	C	351	VAL
1	C	353	THR
1	C	359	THR
1	C	365	ARG
1	C	366	ILE
1	C	367	ARG
1	C	370	MET
1	C	376	MET
1	C	379	GLU
1	C	381	ASN
1	C	383	ARG
1	C	393	GLN
1	C	396	ILE
1	C	397	LEU
1	C	402	ARG
1	C	403	ASN
1	C	408	LEU
1	C	417	ILE
1	C	419	GLN
1	C	420	GLU
1	C	421	ARG
1	C	422	GLU
1	C	423	PHE
1	C	433	GLU

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Mol	Chain	Res	Type
1	C	440	ILE
1	C	442	LEU
1	C	448	GLU
2	D	17	LYS
2	D	21	THR
2	D	26	LEU
2	D	28	ILE
2	D	31	LEU
2	D	53	VAL
2	D	58	GLU
2	D	62	LEU
2	D	69	GLN
2	D	74	MET
2	D	77	ASP
2	D	85	LYS
2	D	91	GLN
2	D	94	SER
2	D	99	LEU
2	D	103	LEU
2	D	107	GLN
2	D	109	CYS
2	D	115	LEU
2	D	122	TYR
2	D	123	GLU
2	D	137	ASP
2	D	157	LEU
2	D	158	VAL
2	D	160	GLU
2	D	161	ARG
2	D	165	VAL
2	D	168	ARG
2	D	170	ARG
2	D	172	VAL
2	D	180	LEU
2	D	188	ILE
2	D	190	GLU
2	D	198	ARG
2	D	200	LEU
2	D	210	ASP
2	D	212	HIS
2	D	213	LEU
2	D	215	GLU

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Mol	Chain	Res	Type
2	D	217	ARG
2	D	218	PHE
2	D	221	LEU
2	D	222	THR
2	D	223	THR
2	D	226	LEU
2	D	227	SER
2	D	257	ARG
2	D	260	VAL
2	D	262	ASP
2	D	263	ARG
2	D	264	ARG
2	D	265	PHE
2	D	277	TRP
2	D	287	ASN
2	D	308	HIS
2	D	310	MET
2	D	331	LEU
2	D	339	THR
2	D	344	VAL
2	D	351	LEU
2	D	352	VAL
2	D	356	LEU
2	D	359	VAL
2	D	361	VAL
2	D	363	ASP
2	D	378	LEU
2	D	382	ASN
2	D	386	LEU
2	D	391	ARG
2	D	394	VAL
2	D	396	LEU
2	D	398	ARG
2	D	401	PHE
1	E	27	LYS
1	E	29	LYS
1	E	33	THR
1	E	34	ASP
1	E	37	CYS
1	E	52	VAL
1	E	60	ILE
1	E	62	CYS

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Mol	Chain	Res	Type
1	E	67	TRP
1	E	68	ASP
1	E	69	ASN
1	E	70	ARG
1	E	72	THR
1	E	73	ARG
1	E	81	ARG
1	E	86	THR
1	E	102	LEU
1	E	111	GLU
1	E	123	THR
1	E	134	ASP
1	E	149	ILE
1	E	157	TYR
1	E	159	THR
1	E	160	LYS
1	E	164	ASN
1	E	172	LEU
1	E	178	THR
1	E	184	LEU
1	E	190	ARG
1	E	193	ILE
1	E	195	VAL
1	E	203	GLU
1	E	206	ILE
1	E	209	GLU
1	E	216	LEU
1	E	220	LEU
1	E	233	ARG
1	E	235	ARG
1	E	241	HIS
1	E	256	ASN
1	E	257	VAL
1	E	259	ARG
1	E	261	LEU
1	E	262	GLN
1	E	271	GLU
1	E	273	SER
1	E	279	ASP
1	E	285	ARG
1	E	287	PHE
1	E	292	ASP

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Mol	Chain	Res	Type
1	E	307	GLU
1	E	311	VAL
1	E	315	LEU
1	E	322	LEU
1	E	323	GLU
1	E	329	LEU
1	E	338	SER
1	E	339	VAL
1	E	341	SER
1	E	344	GLN
1	E	353	THR
1	E	359	THR
1	E	365	ARG
1	E	366	ILE
1	E	367	ARG
1	E	370	MET
1	E	376	MET
1	E	379	GLU
1	E	381	ASN
1	E	383	ARG
1	E	393	GLN
1	E	396	ILE
1	E	397	LEU
1	E	402	ARG
1	E	403	ASN
1	E	408	LEU
1	E	417	ILE
1	E	419	GLN
1	E	420	GLU
1	E	421	ARG
1	E	422	GLU
1	E	423	PHE
1	E	433	GLU
1	E	440	ILE
1	E	442	LEU
1	E	448	GLU
2	F	14	SER
2	F	17	LYS
2	F	21	THR
2	F	26	LEU
2	F	28	ILE
2	F	31	LEU

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Mol	Chain	Res	Type
2	F	41	SER
2	F	53	VAL
2	F	58	GLU
2	F	62	LEU
2	F	69	GLN
2	F	74	MET
2	F	77	ASP
2	F	85	LYS
2	F	91	GLN
2	F	94	SER
2	F	99	LEU
2	F	103	LEU
2	F	107	GLN
2	F	115	LEU
2	F	122	TYR
2	F	123	GLU
2	F	137	ASP
2	F	157	LEU
2	F	158	VAL
2	F	160	GLU
2	F	161	ARG
2	F	165	VAL
2	F	168	ARG
2	F	170	ARG
2	F	172	VAL
2	F	180	LEU
2	F	188	ILE
2	F	190	GLU
2	F	194	SER
2	F	198	ARG
2	F	200	LEU
2	F	210	ASP
2	F	212	HIS
2	F	213	LEU
2	F	215	GLU
2	F	217	ARG
2	F	218	PHE
2	F	221	LEU
2	F	222	THR
2	F	223	THR
2	F	226	LEU
2	F	227	SER

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Mol	Chain	Res	Type
2	F	257	ARG
2	F	260	VAL
2	F	262	ASP
2	F	263	ARG
2	F	264	ARG
2	F	265	PHE
2	F	274	VAL
2	F	277	TRP
2	F	287	ASN
2	F	308	HIS
2	F	310	MET
2	F	313	SER
2	F	331	LEU
2	F	339	THR
2	F	344	VAL
2	F	351	LEU
2	F	352	VAL
2	F	356	LEU
2	F	359	VAL
2	F	361	VAL
2	F	363	ASP
2	F	378	LEU
2	F	379	VAL
2	F	382	ASN
2	F	386	LEU
2	F	391	ARG
2	F	394	VAL
2	F	396	LEU
2	F	398	ARG
2	F	401	PHE
1	G	27	LYS
1	G	29	LYS
1	G	33	THR
1	G	34	ASP
1	G	37	CYS
1	G	52	VAL
1	G	60	ILE
1	G	67	TRP
1	G	68	ASP
1	G	69	ASN
1	G	70	ARG
1	G	72	THR

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Mol	Chain	Res	Type
1	G	73	ARG
1	G	86	THR
1	G	102	LEU
1	G	111	GLU
1	G	123	THR
1	G	134	ASP
1	G	149	ILE
1	G	157	TYR
1	G	159	THR
1	G	160	LYS
1	G	164	ASN
1	G	172	LEU
1	G	184	LEU
1	G	190	ARG
1	G	193	ILE
1	G	195	VAL
1	G	203	GLU
1	G	206	ILE
1	G	209	GLU
1	G	216	LEU
1	G	220	LEU
1	G	233	ARG
1	G	235	ARG
1	G	240	MET
1	G	256	ASN
1	G	257	VAL
1	G	259	ARG
1	G	261	LEU
1	G	262	GLN
1	G	271	GLU
1	G	273	SER
1	G	279	ASP
1	G	285	ARG
1	G	287	PHE
1	G	292	ASP
1	G	307	GLU
1	G	311	VAL
1	G	315	LEU
1	G	322	LEU
1	G	323	GLU
1	G	329	LEU
1	G	335	LYS

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Mol	Chain	Res	Type
1	G	338	SER
1	G	339	VAL
1	G	341	SER
1	G	344	GLN
1	G	351	VAL
1	G	353	THR
1	G	359	THR
1	G	365	ARG
1	G	366	ILE
1	G	367	ARG
1	G	370	MET
1	G	376	MET
1	G	379	GLU
1	G	381	ASN
1	G	383	ARG
1	G	393	GLN
1	G	396	ILE
1	G	397	LEU
1	G	402	ARG
1	G	403	ASN
1	G	406	THR
1	G	408	LEU
1	G	417	ILE
1	G	419	GLN
1	G	420	GLU
1	G	421	ARG
1	G	422	GLU
1	G	423	PHE
1	G	433	GLU
1	G	440	ILE
1	G	442	LEU
1	G	448	GLU
2	H	11	LEU
2	H	14	SER
2	H	17	LYS
2	H	21	THR
2	H	26	LEU
2	H	28	ILE
2	H	31	LEU
2	H	53	VAL
2	H	58	GLU
2	H	62	LEU

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Mol	Chain	Res	Type
2	H	69	GLN
2	H	74	MET
2	H	77	ASP
2	H	85	LYS
2	H	91	GLN
2	H	94	SER
2	H	103	LEU
2	H	107	GLN
2	H	109	CYS
2	H	115	LEU
2	H	122	TYR
2	H	123	GLU
2	H	137	ASP
2	H	157	LEU
2	H	158	VAL
2	H	160	GLU
2	H	161	ARG
2	H	165	VAL
2	H	168	ARG
2	H	170	ARG
2	H	172	VAL
2	H	180	LEU
2	H	188	ILE
2	H	190	GLU
2	H	194	SER
2	H	198	ARG
2	H	200	LEU
2	H	210	ASP
2	H	212	HIS
2	H	213	LEU
2	H	215	GLU
2	H	217	ARG
2	H	218	PHE
2	H	221	LEU
2	H	222	THR
2	H	223	THR
2	H	226	LEU
2	H	227	SER
2	H	257	ARG
2	H	260	VAL
2	H	262	ASP
2	H	264	ARG

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Mol	Chain	Res	Type
2	H	265	PHE
2	H	274	VAL
2	H	287	ASN
2	H	308	HIS
2	H	310	MET
2	H	331	LEU
2	H	339	THR
2	H	344	VAL
2	H	351	LEU
2	H	352	VAL
2	H	356	LEU
2	H	359	VAL
2	H	361	VAL
2	H	363	ASP
2	H	378	LEU
2	H	382	ASN
2	H	386	LEU
2	H	391	ARG
2	H	394	VAL
2	H	396	LEU
2	H	398	ARG
2	H	401	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	57	HIS
1	A	108	GLN
1	A	199	ASN
1	A	246	ASN
1	A	344	GLN
1	A	381	ASN
1	A	393	GLN
1	A	419	GLN
2	B	39	HIS
2	B	91	GLN
2	B	107	GLN
2	B	112	HIS
2	B	173	ASN
2	B	287	ASN
2	B	301	GLN

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Mol	Chain	Res	Type
2	B	308	HIS
2	B	382	ASN
2	B	411	GLN
2	B	435	HIS
1	C	54	HIS
1	C	57	HIS
1	C	69	ASN
1	C	108	GLN
1	C	199	ASN
1	C	246	ASN
1	C	344	GLN
1	C	381	ASN
1	C	393	GLN
1	C	419	GLN
2	D	91	GLN
2	D	107	GLN
2	D	112	HIS
2	D	173	ASN
2	D	287	ASN
2	D	296	GLN
2	D	301	GLN
2	D	308	HIS
2	D	382	ASN
2	D	434	HIS
2	D	435	HIS
1	E	54	HIS
1	E	57	HIS
1	E	108	GLN
1	E	199	ASN
1	E	246	ASN
1	E	344	GLN
1	E	381	ASN
1	E	393	GLN
1	E	419	GLN
2	F	91	GLN
2	F	107	GLN
2	F	112	HIS
2	F	287	ASN
2	F	301	GLN
2	F	308	HIS
2	F	382	ASN
2	F	384	HIS

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Mol	Chain	Res	Type
2	F	411	GLN
2	F	434	HIS
1	G	54	HIS
1	G	57	HIS
1	G	69	ASN
1	G	104	HIS
1	G	108	GLN
1	G	161	ASN
1	G	199	ASN
1	G	246	ASN
1	G	344	GLN
1	G	381	ASN
1	G	393	GLN
1	G	419	GLN
2	H	91	GLN
2	H	107	GLN
2	H	112	HIS
2	H	287	ASN
2	H	301	GLN
2	H	308	HIS
2	H	382	ASN
2	H	411	GLN
2	H	434	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 ⓘ

8 ligands are modelled in this entry.

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	$\# Z > 2$
3	SF4	A	501	1,2	0,12,12	-	-	-		
4	CZL	G	502	-	0,24,24	-	-	-		
3	SF4	C	501	1,2	0,12,12	-	-	-		
4	CZL	C	502	-	0,24,24	-	-	-		
4	CZL	A	502	-	0,24,24	-	-	-		
3	SF4	G	501	1,2	0,12,12	-	-	-		
3	SF4	E	501	1,2	0,12,12	-	-	-		
4	CZL	E	502	-	0,24,24	-	-	-		

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
3	SF4	A	501	1,2	-	-	0/6/5/5
3	SF4	G	501	1,2	-	-	0/6/5/5
3	SF4	E	501	1,2	-	-	0/6/5/5
3	SF4	C	501	1,2	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	SF4	2	0
4	G	502	CZL	4	0
3	C	501	SF4	2	0
4	C	502	CZL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	CZL	3	0
3	G	501	SF4	4	0
3	E	501	SF4	3	0
4	E	502	CZL	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	427/483 (88%)	-0.80	0 100 100	14, 42, 91, 112	0
1	C	427/483 (88%)	-0.76	2 (0%) 87 85	17, 44, 91, 116	0
1	E	427/483 (88%)	-0.77	1 (0%) 91 89	15, 43, 91, 117	0
1	G	427/483 (88%)	-0.75	0 100 100	17, 44, 93, 114	0
2	B	432/458 (94%)	-0.95	0 100 100	14, 35, 72, 89	0
2	D	432/458 (94%)	-0.90	0 100 100	12, 36, 75, 91	0
2	F	432/458 (94%)	-0.84	1 (0%) 91 89	14, 37, 73, 90	0
2	H	432/458 (94%)	-0.88	0 100 100	13, 37, 74, 89	0
All	All	3436/3764 (91%)	-0.83	4 (0%) 92 90	12, 40, 82, 117	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	104	SER	3.0
1	C	376	MET	2.2
1	E	420	GLU	2.1
1	C	229	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SF4	C	501	8/8	0.99	0.03	16,26,34,53	0
3	SF4	G	501	8/8	0.99	0.03	25,29,31,44	0
4	CZL	A	502	17/17	0.99	0.03	26,47,58,62	0
4	CZL	C	502	17/17	0.99	0.03	59,81,108,114	0
4	CZL	E	502	17/17	0.99	0.04	74,89,128,134	0
4	CZL	G	502	17/17	0.99	0.03	55,87,123,129	0
3	SF4	E	501	8/8	1.00	0.03	14,32,40,43	0
3	SF4	A	501	8/8	1.00	0.02	17,21,23,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.