



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:54 AM UTC

PDB ID : 1I43 / pdb_00001i43
Title : CYSTATHIONINE GAMMA-SYNTHASE IN COMPLEX WITH THE INHIBITOR PPCA
Authors : Steegborn, C.; Laber, B.; Messerschmidt, A.; Huber, R.; Clausen, T.
Deposited on : 2001-02-19
Resolution : 3.10 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

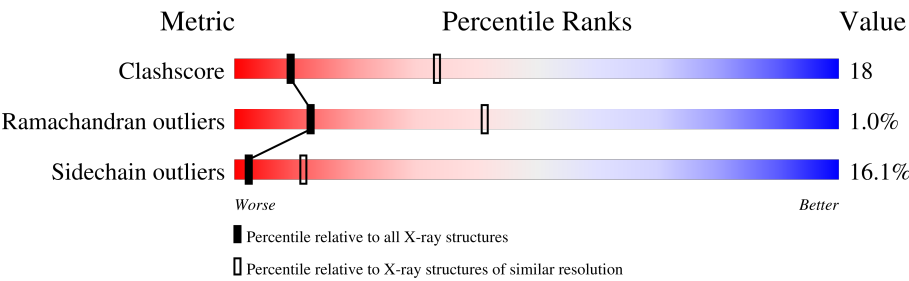
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	445	56% 29% • 11%
1	B	445	49% 34% 6% 11%
1	C	445	52% 32% 5% 11%
1	D	445	52% 31% 6% 11%
1	E	445	49% 34% 6% 11%
1	F	445	50% 33% 6% 11%
1	G	445	50% 35% • 11%
1	H	445	51% 32% 6% 11%

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Mol	Chain	Length	Quality of chain
1	I	445	
1	J	445	
1	K	445	
1	L	445	

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
2	PLP	C	500	-	X	-	-
2	PLP	D	500	-	X	-	-
2	PLP	F	500	-	X	-	-
2	PLP	H	500	-	X	-	-
3	PMC	F	605	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 36624 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 CYSTATHIONINE GAMMA-SYNTHASE.

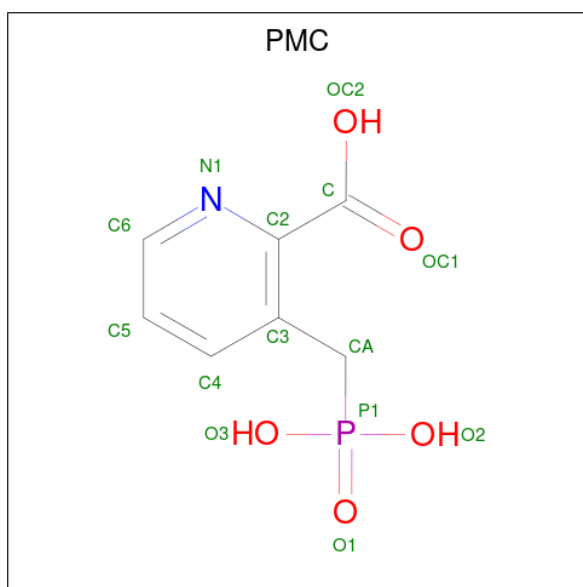
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	B	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	C	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	D	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	E	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	F	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	G	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	H	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	I	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	J	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	K	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	L	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	I	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	J	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	K	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	L	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is 3-(PHOSPHONOMETHYL)PYRIDINE-2-CARBOXYLIC ACID (CCD ID: PMC) (formula: C₇H₈NO₅P).

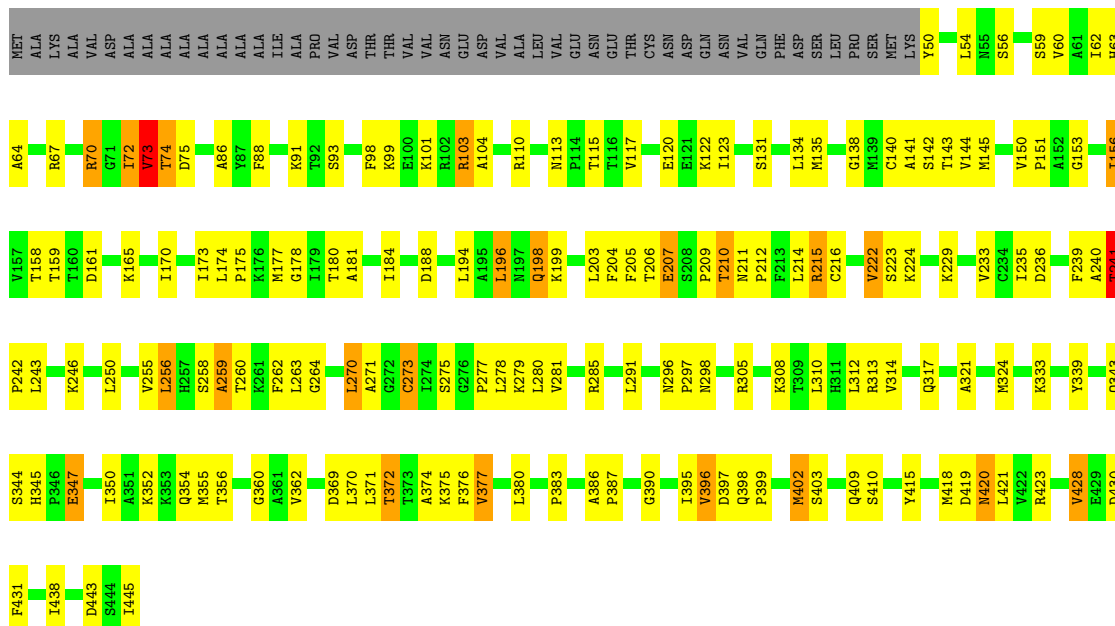


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	E	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	F	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	G	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	H	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	I	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	J	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	K	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	L	1	Total	C	N	O	P	0	0
			14	7	1	5	1		



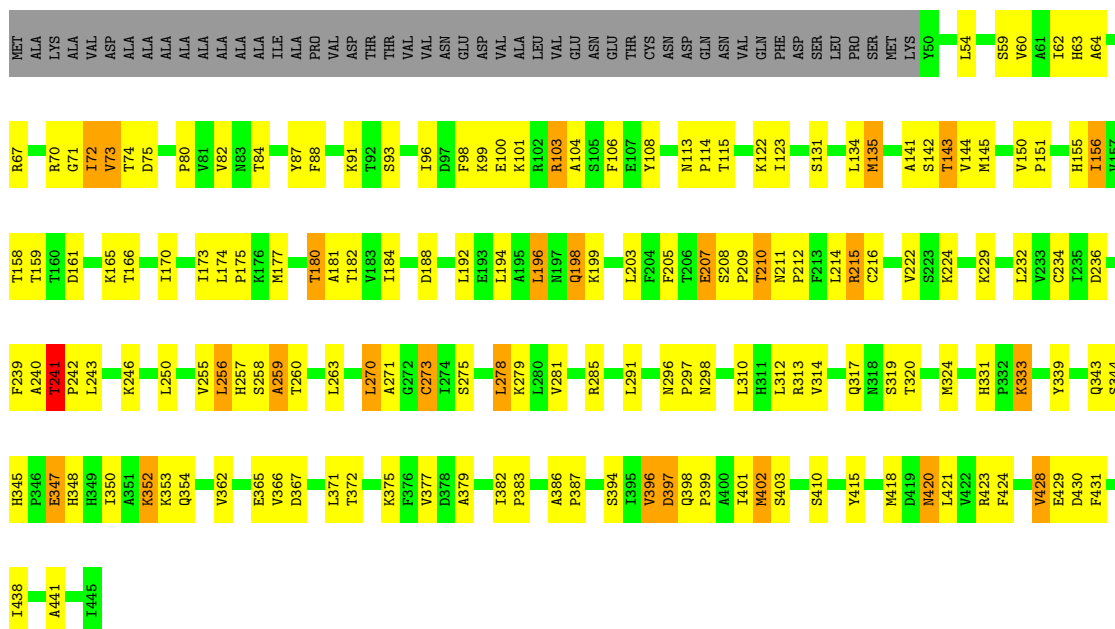
• Molecule 1: CYSTATHIONINE GAMMA-SYNTASE

Chain C:  52% 32% 5% 11%

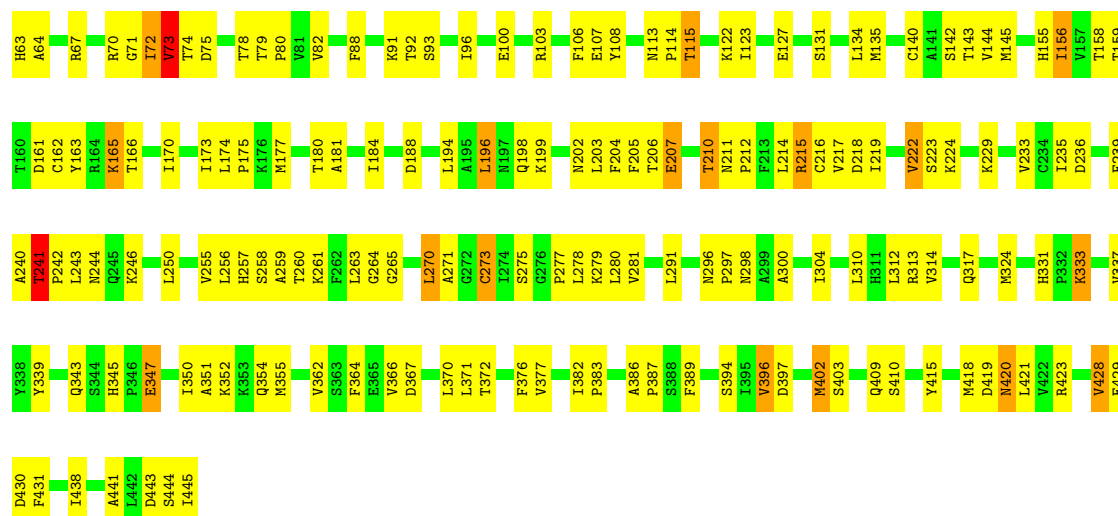


• Molecule 1: CYSTATHIONINE GAMMA-SYNTASE

Chain D:  52% 31% 6% 11%

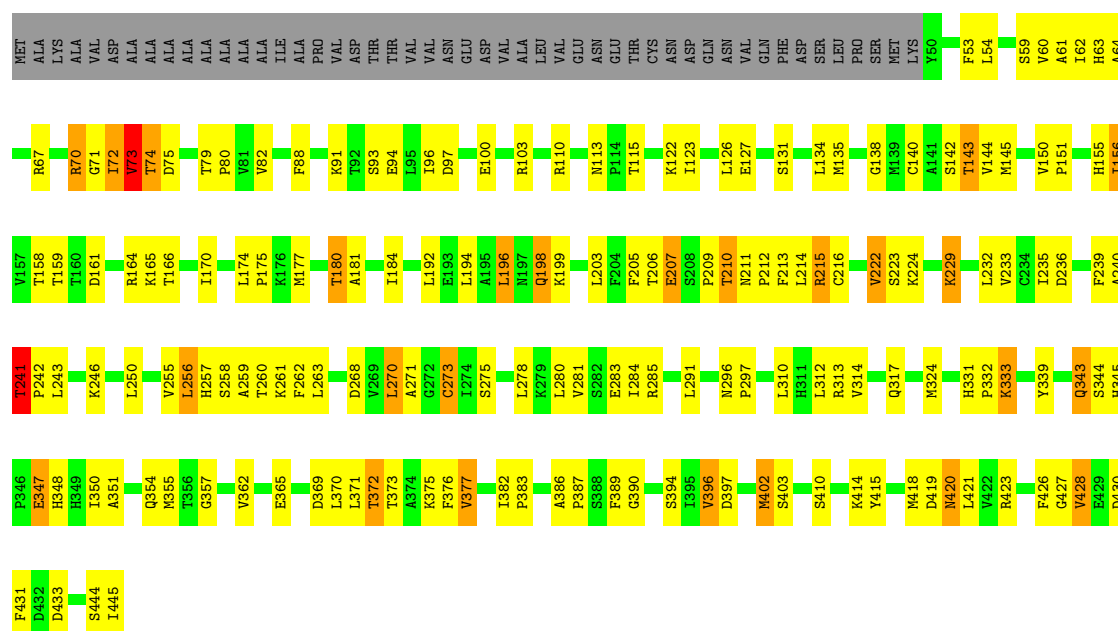


• Molecule 1: CYSTATHIONINE GAMMA-SYNTASE



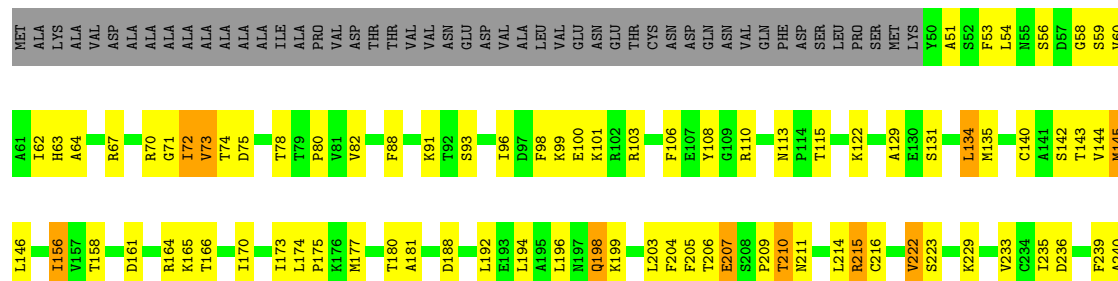
• Molecule 1: CYSTATHIONINE GAMMA-SYNTASE

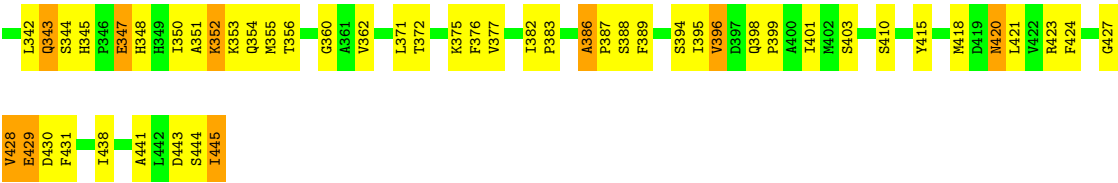
Chain H: 51% 32% 6% 11%



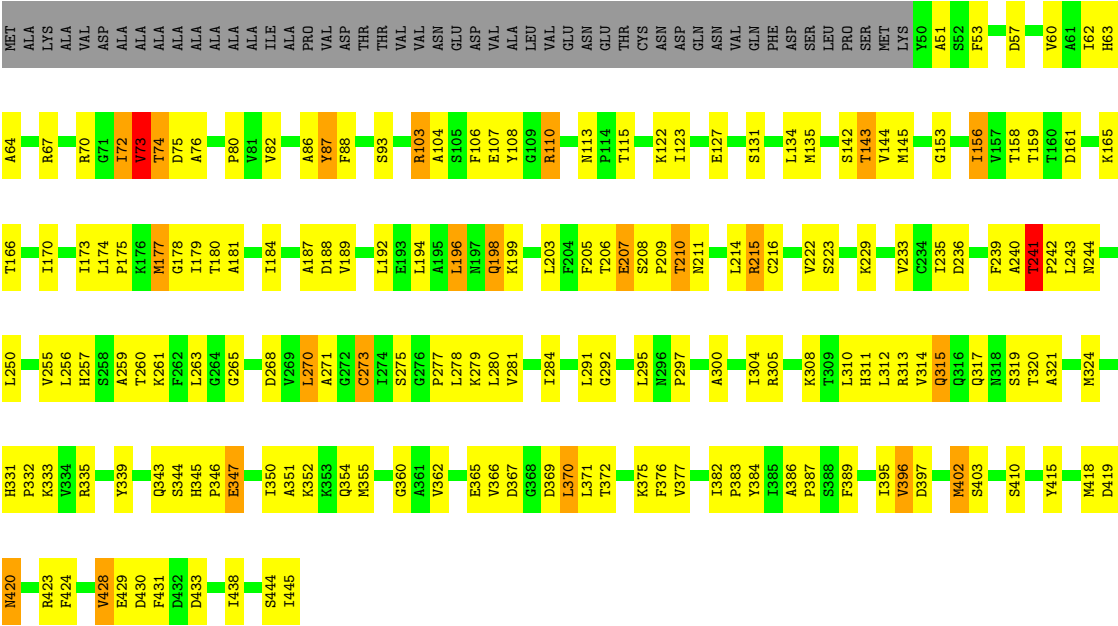
• Molecule 1: CYSTATHIONINE GAMMA-SYNTASE

Chain I: 50% 34% 11%





• Molecule 1: CYSTATIONINE GAMMA-SYNTHASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	309.60Å 170.10Å 162.10Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.10)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.236 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36624	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.36	0/3082	0.81	4/4179 (0.1%)
1	B	0.36	0/3082	0.81	4/4179 (0.1%)
1	C	0.37	0/3082	0.80	5/4179 (0.1%)
1	D	0.37	0/3082	0.80	4/4179 (0.1%)
1	E	0.36	0/3082	0.81	4/4179 (0.1%)
1	F	0.34	0/3082	0.80	5/4179 (0.1%)
1	G	0.36	0/3082	0.80	5/4179 (0.1%)
1	H	0.34	0/3082	0.81	4/4179 (0.1%)
1	I	0.37	0/3082	0.82	8/4179 (0.2%)
1	J	0.34	0/3082	0.80	4/4179 (0.1%)
1	K	0.35	0/3082	0.81	5/4179 (0.1%)
1	L	0.35	0/3082	0.79	3/4179 (0.1%)
All	All	0.36	0/36984	0.81	55/50148 (0.1%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	75	ASP	N-CA-C	-7.91	103.70	112.72
1	A	73	VAL	N-CA-C	7.79	119.50	109.30
1	B	75	ASP	N-CA-C	-7.33	104.36	112.72
1	E	73	VAL	N-CA-C	7.01	118.48	109.30
1	B	73	VAL	N-CA-C	6.98	118.80	109.37
1	J	75	ASP	N-CA-C	-6.93	104.82	112.72
1	H	73	VAL	N-CA-C	6.92	118.36	109.30
1	K	73	VAL	N-CA-C	6.76	118.16	109.30
1	L	73	VAL	N-CA-C	6.69	118.06	109.30
1	D	75	ASP	N-CA-C	-6.51	104.64	112.59
1	L	75	ASP	N-CA-C	-6.42	105.74	112.93
1	G	71	GLY	N-CA-C	-6.41	107.45	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	75	ASP	N-CA-C	-6.37	105.46	112.72
1	C	402	MET	N-CA-C	6.33	118.70	111.11
1	G	75	ASP	N-CA-C	-6.23	105.62	112.72
1	K	71	GLY	N-CA-C	-6.20	107.70	115.08
1	H	71	GLY	N-CA-C	-6.15	107.76	115.08
1	D	73	VAL	N-CA-C	6.10	118.23	109.51
1	H	402	MET	N-CA-C	6.06	117.88	111.28
1	D	71	GLY	N-CA-C	-6.00	107.95	115.08
1	D	402	MET	N-CA-C	5.99	117.81	111.28
1	F	73	VAL	N-CA-C	5.97	118.05	109.51
1	E	71	GLY	N-CA-C	-5.91	108.05	115.08
1	F	75	ASP	N-CA-C	-5.87	106.03	112.72
1	B	402	MET	N-CA-C	5.85	117.66	111.28
1	E	402	MET	N-CA-C	5.85	117.33	111.07
1	A	402	MET	N-CA-C	5.79	117.59	111.28
1	I	73	VAL	N-CA-C	5.79	117.79	109.51
1	C	73	VAL	N-CA-C	5.76	117.74	109.51
1	C	75	ASP	N-CA-C	-5.73	106.19	112.72
1	K	356	THR	N-CA-C	-5.70	106.31	113.72
1	F	402	MET	N-CA-C	5.69	117.48	111.28
1	G	73	VAL	N-CA-C	5.65	117.59	109.51
1	A	75	ASP	N-CA-C	-5.64	106.29	112.72
1	A	71	GLY	N-CA-C	-5.64	108.37	115.08
1	B	71	GLY	N-CA-C	-5.61	108.40	115.08
1	I	75	ASP	N-CA-C	-5.58	106.06	112.92
1	I	356	THR	N-CA-C	-5.45	107.00	113.97
1	J	73	VAL	N-CA-C	5.42	117.27	109.51
1	I	402	MET	N-CA-C	5.42	117.19	111.28
1	K	75	ASP	N-CA-C	-5.33	106.64	112.72
1	F	71	GLY	N-CA-C	-5.28	108.79	115.08
1	I	345	HIS	CA-C-N	5.27	124.72	119.24
1	I	345	HIS	C-N-CA	5.27	124.72	119.24
1	I	417	ILE	N-CA-C	5.25	115.15	108.12
1	G	264	GLY	N-CA-C	-5.22	106.18	112.49
1	G	402	MET	N-CA-C	5.21	116.96	111.28
1	J	356	THR	N-CA-C	-5.20	107.31	113.97
1	C	356	THR	N-CA-C	-5.19	107.33	113.97
1	K	386	ALA	N-CA-C	5.17	112.67	108.07
1	L	402	MET	N-CA-C	5.15	116.89	111.28
1	C	264	GLY	N-CA-C	-5.12	106.29	112.49
1	I	71	GLY	N-CA-C	-5.10	107.48	114.67
1	F	356	THR	N-CA-C	-5.08	107.11	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	402	MET	N-CA-C	5.05	116.87	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3023	0	3052	113	0
1	B	3023	0	3052	117	0
1	C	3023	0	3052	111	0
1	D	3023	0	3052	108	0
1	E	3023	0	3052	134	0
1	F	3023	0	3052	114	0
1	G	3023	0	3052	116	0
1	H	3023	0	3052	123	0
1	I	3023	0	3052	125	0
1	J	3023	0	3052	116	0
1	K	3023	0	3052	120	0
1	L	3023	0	3052	125	0
2	A	15	0	6	0	0
2	B	15	0	6	1	0
2	C	15	0	6	0	0
2	D	15	0	6	0	0
2	E	15	0	7	0	0
2	F	15	0	6	1	0
2	G	15	0	7	0	0
2	H	15	0	6	1	0
2	I	15	0	6	0	0
2	J	15	0	6	0	0
2	K	15	0	6	0	0
2	L	15	0	7	0	0
3	A	14	0	5	0	0
3	B	14	0	5	0	0
3	C	14	0	5	0	0
3	D	14	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	14	0	5	1	0
3	F	14	0	5	0	0
3	G	14	0	5	0	0
3	H	14	0	5	0	0
3	I	14	0	5	0	0
3	J	14	0	5	0	0
3	K	14	0	5	1	0
3	L	14	0	5	1	0
All	All	36624	0	36759	1328	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (1328) 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:I:376:PHE:HB2	1:I:445:ILE:HD11	1.21	1.12
1:C:376:PHE:HB2	1:C:445:ILE:HD11	1.40	1.03
1:F:241:THR:HG22	1:F:243:LEU:H	1.32	0.95
1:A:241:THR:HG22	1:A:243:LEU:H	1.32	0.94
1:K:241:THR:HG22	1:K:243:LEU:H	1.30	0.93
1:I:241:THR:HG22	1:I:243:LEU:H	1.31	0.93
1:I:428:VAL:HG12	1:L:62:ILE:HD11	1.50	0.93
1:D:241:THR:HG22	1:D:243:LEU:H	1.34	0.93
1:G:241:THR:HG22	1:G:243:LEU:H	1.34	0.92
1:B:376:PHE:HB2	1:B:445:ILE:HD11	1.50	0.91
1:E:241:THR:HG22	1:E:243:LEU:H	1.35	0.91
1:C:241:THR:HG22	1:C:243:LEU:H	1.31	0.91
1:H:241:THR:HG22	1:H:243:LEU:H	1.36	0.91
1:F:376:PHE:HB2	1:F:445:ILE:HD11	1.53	0.90
1:J:241:THR:HG22	1:J:243:LEU:H	1.37	0.90
1:J:376:PHE:HB2	1:J:445:ILE:HD11	1.52	0.89
1:C:240:ALA:O	1:C:241:THR:HB	1.71	0.88
1:B:241:THR:HG22	1:B:243:LEU:H	1.40	0.86
1:J:62:ILE:HD11	1:K:428:VAL:HG12	1.56	0.86
1:J:428:VAL:HG12	1:K:62:ILE:HD11	1.56	0.86
1:D:240:ALA:O	1:D:241:THR:HB	1.76	0.86
1:A:240:ALA:O	1:A:241:THR:HB	1.74	0.86
1:E:240:ALA:O	1:E:241:THR:HB	1.74	0.86
1:B:240:ALA:O	1:B:241:THR:HB	1.75	0.84
1:L:241:THR:HG22	1:L:243:LEU:H	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:240:ALA:O	1:L:241:THR:HB	1.78	0.84
1:F:62:ILE:HD11	1:G:428:VAL:HG12	1.58	0.83
1:H:240:ALA:O	1:H:241:THR:HB	1.77	0.83
1:I:62:ILE:HD11	1:L:428:VAL:HG12	1.58	0.83
1:J:240:ALA:O	1:J:241:THR:HB	1.77	0.81
1:A:431:PHE:HE1	1:A:435:LYS:HB2	1.44	0.81
1:I:376:PHE:HB2	1:I:445:ILE:CD1	2.10	0.81
1:F:240:ALA:O	1:F:241:THR:HB	1.81	0.81
1:H:313:ARG:O	1:H:317:GLN:HG3	1.79	0.80
1:K:240:ALA:O	1:K:241:THR:HB	1.79	0.80
1:E:259:ALA:HA	1:E:263:LEU:HB2	1.64	0.80
1:H:54:LEU:HD22	1:H:59:SER:HB3	1.63	0.80
1:A:113:ASN:OD1	1:A:115:THR:HG22	1.80	0.79
1:D:259:ALA:HB3	1:D:271:ALA:HB3	1.64	0.79
1:E:428:VAL:HG12	1:H:62:ILE:HD11	1.64	0.79
1:H:113:ASN:OD1	1:H:115:THR:HG22	1.83	0.79
1:B:324:MET:HE2	1:B:438:ILE:HD12	1.64	0.78
1:A:216:CYS:H	1:A:347:GLU:HG3	1.49	0.78
1:G:240:ALA:O	1:G:241:THR:HB	1.84	0.78
1:E:259:ALA:HB3	1:E:271:ALA:HB3	1.65	0.78
1:K:313:ARG:O	1:K:317:GLN:HG3	1.83	0.77
1:A:259:ALA:HB3	1:A:271:ALA:HB3	1.65	0.77
1:H:259:ALA:HB3	1:H:271:ALA:HB3	1.67	0.77
1:E:207:GLU:HB3	1:E:236:ASP:HB3	1.67	0.77
1:I:113:ASN:OD1	1:I:115:THR:HG22	1.85	0.77
1:H:207:GLU:HB3	1:H:236:ASP:HB3	1.66	0.76
1:G:207:GLU:HB3	1:G:236:ASP:HB3	1.67	0.75
1:E:62:ILE:HD11	1:H:428:VAL:HG12	1.67	0.75
1:L:113:ASN:OD1	1:L:115:THR:HG22	1.85	0.75
1:F:428:VAL:HG12	1:G:62:ILE:HD11	1.69	0.75
1:B:62:ILE:HD11	1:C:428:VAL:HG12	1.69	0.75
1:J:207:GLU:HB3	1:J:236:ASP:HB3	1.68	0.74
1:A:62:ILE:HD11	1:D:428:VAL:HG12	1.70	0.74
1:E:431:PHE:HE1	1:E:435:LYS:HB2	1.52	0.74
1:L:347:GLU:HB3	1:L:350:ILE:HD12	1.68	0.74
1:J:216:CYS:H	1:J:347:GLU:HG3	1.53	0.74
1:L:170:ILE:HG23	1:L:174:LEU:HD12	1.69	0.74
1:D:63:HIS:HB3	1:D:67:ARG:HB2	1.70	0.74
1:G:376:PHE:HB2	1:G:445:ILE:HD11	1.68	0.74
1:J:259:ALA:HA	1:J:263:LEU:HB2	1.70	0.74
1:I:240:ALA:O	1:I:241:THR:HB	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ALA:HA	1:B:263:LEU:HB2	1.71	0.73
1:H:72:ILE:HD12	1:H:80:PRO:HG2	1.70	0.73
1:K:216:CYS:H	1:K:347:GLU:HG3	1.52	0.73
1:I:207:GLU:HB3	1:I:236:ASP:HB3	1.71	0.72
1:C:72:ILE:HG23	1:C:72:ILE:O	1.89	0.72
1:L:259:ALA:HA	1:L:263:LEU:HB2	1.71	0.72
1:A:428:VAL:HG12	1:D:62:ILE:HD11	1.71	0.72
1:H:216:CYS:H	1:H:347:GLU:HG3	1.53	0.72
1:A:207:GLU:HB3	1:A:236:ASP:HB3	1.70	0.71
1:C:207:GLU:HB3	1:C:236:ASP:HB3	1.70	0.71
1:D:216:CYS:H	1:D:347:GLU:HG3	1.52	0.71
1:F:207:GLU:HB3	1:F:236:ASP:HB3	1.71	0.71
1:C:383:PRO:HB2	1:C:396:VAL:HG22	1.71	0.71
1:H:63:HIS:HB3	1:H:67:ARG:HB2	1.73	0.71
1:K:259:ALA:HA	1:K:263:LEU:HB2	1.72	0.71
1:K:260:THR:HG23	1:K:270:LEU:HD22	1.72	0.71
1:E:63:HIS:HB3	1:E:67:ARG:HB2	1.73	0.71
1:I:259:ALA:HA	1:I:263:LEU:HB2	1.71	0.71
1:D:259:ALA:HA	1:D:263:LEU:HB2	1.73	0.71
1:E:431:PHE:C	1:E:431:PHE:HD1	1.98	0.71
1:B:313:ARG:O	1:B:317:GLN:HG3	1.91	0.70
1:B:72:ILE:HG23	1:B:72:ILE:O	1.90	0.70
1:C:63:HIS:HB3	1:C:67:ARG:HB2	1.72	0.70
1:E:431:PHE:CE1	1:E:435:LYS:HB2	2.26	0.70
1:F:72:ILE:O	1:F:72:ILE:HG23	1.91	0.70
1:L:259:ALA:HB3	1:L:271:ALA:HB3	1.73	0.70
1:I:72:ILE:HG23	1:I:72:ILE:O	1.91	0.70
1:D:72:ILE:HD12	1:D:80:PRO:HG2	1.71	0.70
1:A:431:PHE:CE1	1:A:435:LYS:HB2	2.25	0.70
1:B:156:ILE:HG22	1:B:181:ALA:CB	2.22	0.70
1:J:347:GLU:HB3	1:J:350:ILE:HD12	1.72	0.70
1:G:313:ARG:O	1:G:317:GLN:HG3	1.91	0.70
1:G:383:PRO:HB2	1:G:396:VAL:HG22	1.72	0.70
1:J:313:ARG:O	1:J:317:GLN:HG3	1.91	0.70
1:C:259:ALA:HB3	1:C:271:ALA:HB3	1.73	0.69
1:K:72:ILE:HD12	1:K:80:PRO:HG2	1.72	0.69
1:G:170:ILE:HG23	1:G:174:LEU:HD12	1.74	0.69
1:C:259:ALA:HA	1:C:263:LEU:HB2	1.74	0.69
1:G:216:CYS:H	1:G:347:GLU:HG3	1.57	0.69
1:K:207:GLU:HB3	1:K:236:ASP:HB3	1.74	0.69
1:E:72:ILE:HG23	1:E:72:ILE:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:ILE:HG23	1:G:72:ILE:O	1.91	0.69
1:H:72:ILE:HG23	1:H:72:ILE:O	1.93	0.69
1:L:174:LEU:N	1:L:175:PRO:HD2	2.07	0.69
1:A:72:ILE:O	1:A:72:ILE:HG23	1.92	0.69
1:A:324:MET:HE2	1:A:438:ILE:HD12	1.75	0.69
1:H:115:THR:HG21	1:H:297:PRO:HB3	1.74	0.69
1:A:63:HIS:HB3	1:A:67:ARG:HB2	1.75	0.69
1:A:313:ARG:O	1:A:317:GLN:HG3	1.92	0.69
1:B:216:CYS:H	1:B:347:GLU:HG3	1.58	0.68
1:J:72:ILE:HG23	1:J:72:ILE:O	1.92	0.68
1:E:431:PHE:C	1:E:431:PHE:CD1	2.69	0.68
1:I:72:ILE:HD12	1:I:80:PRO:HG2	1.74	0.68
1:E:113:ASN:OD1	1:E:115:THR:HG22	1.94	0.68
1:B:428:VAL:HG12	1:C:62:ILE:HD11	1.74	0.68
1:I:259:ALA:HB3	1:I:271:ALA:HB3	1.75	0.68
1:J:88:PHE:HA	1:L:386:ALA:HB2	1.76	0.68
1:F:259:ALA:HA	1:F:263:LEU:HB2	1.75	0.68
1:A:72:ILE:HD12	1:A:80:PRO:HG2	1.74	0.67
1:C:243:LEU:HD12	1:C:314:VAL:HG21	1.77	0.67
1:A:123:ILE:HD13	1:A:273:CYS:SG	2.34	0.67
1:D:113:ASN:OD1	1:D:115:THR:HG22	1.94	0.67
1:E:216:CYS:H	1:E:347:GLU:HG3	1.59	0.67
1:G:242:PRO:O	1:G:246:LYS:HE2	1.95	0.67
1:K:72:ILE:O	1:K:72:ILE:HG23	1.92	0.67
1:A:431:PHE:CD1	1:A:431:PHE:C	2.73	0.67
1:H:53:PHE:CD1	1:H:54:LEU:HG	2.29	0.67
1:L:177:MET:HB2	1:L:179:ILE:HD12	1.75	0.67
1:A:431:PHE:C	1:A:431:PHE:HD1	2.02	0.67
1:I:63:HIS:HB3	1:I:67:ARG:HB2	1.77	0.66
1:L:72:ILE:HG23	1:L:72:ILE:O	1.94	0.66
1:K:347:GLU:HB3	1:K:350:ILE:HD12	1.76	0.66
1:C:113:ASN:OD1	1:C:115:THR:HG22	1.95	0.66
1:K:174:LEU:N	1:K:175:PRO:HD2	2.10	0.66
1:C:174:LEU:N	1:C:175:PRO:HD2	2.11	0.66
1:C:250:LEU:HD11	1:C:354:GLN:HB2	1.76	0.66
1:F:216:CYS:H	1:F:347:GLU:HG3	1.60	0.66
1:J:174:LEU:N	1:J:175:PRO:HD2	2.11	0.66
1:B:54:LEU:HD22	1:B:59:SER:HB3	1.76	0.66
1:D:313:ARG:O	1:D:317:GLN:HG3	1.96	0.66
1:H:259:ALA:HA	1:H:263:LEU:HB2	1.77	0.66
1:K:63:HIS:HB3	1:K:67:ARG:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:351:ALA:O	1:I:355:MET:HB2	1.96	0.66
1:C:210:THR:HG22	1:C:215:ARG:H	1.60	0.66
1:F:259:ALA:HB3	1:F:271:ALA:HB3	1.77	0.66
1:H:123:ILE:HD13	1:H:273:CYS:SG	2.36	0.66
1:H:383:PRO:HB2	1:H:396:VAL:HG22	1.77	0.66
1:I:260:THR:HG23	1:I:270:LEU:HD22	1.76	0.66
1:B:207:GLU:HB3	1:B:236:ASP:HB3	1.78	0.66
1:E:376:PHE:HB2	1:E:445:ILE:HD11	1.77	0.66
1:D:72:ILE:HG23	1:D:72:ILE:O	1.95	0.65
1:G:259:ALA:HA	1:G:263:LEU:HB2	1.78	0.65
1:J:63:HIS:HB3	1:J:67:ARG:HB2	1.78	0.65
1:J:159:THR:HA	1:J:184:ILE:O	1.97	0.65
1:L:216:CYS:H	1:L:347:GLU:HG3	1.62	0.65
1:D:156:ILE:HG22	1:D:181:ALA:CB	2.26	0.65
1:D:174:LEU:N	1:D:175:PRO:HD2	2.11	0.65
1:L:383:PRO:HB2	1:L:396:VAL:HG22	1.78	0.65
1:H:250:LEU:HD11	1:H:354:GLN:HB2	1.78	0.65
1:I:209:PRO:HG3	1:I:355:MET:HE1	1.78	0.65
1:A:115:THR:HG21	1:A:297:PRO:HB3	1.79	0.65
1:E:383:PRO:HB2	1:E:396:VAL:HG22	1.77	0.65
1:E:431:PHE:HD1	1:E:431:PHE:O	1.79	0.65
1:F:63:HIS:HB3	1:F:67:ARG:HB2	1.77	0.65
1:L:123:ILE:HD13	1:L:273:CYS:SG	2.37	0.65
1:B:174:LEU:N	1:B:175:PRO:HD2	2.12	0.65
1:D:207:GLU:HB3	1:D:236:ASP:HB3	1.78	0.65
1:J:170:ILE:HG23	1:J:174:LEU:HD12	1.79	0.65
1:K:242:PRO:O	1:K:246:LYS:HE2	1.96	0.65
1:A:383:PRO:HB2	1:A:396:VAL:HG22	1.78	0.65
1:B:277:PRO:HG2	1:B:280:LEU:HB2	1.79	0.65
1:F:113:ASN:OD1	1:F:115:THR:HG22	1.96	0.64
1:D:383:PRO:HB2	1:D:396:VAL:HG22	1.78	0.64
1:D:211:ASN:HB2	1:D:239:PHE:HE2	1.62	0.64
1:D:250:LEU:HD11	1:D:354:GLN:HB2	1.79	0.64
1:C:370:LEU:HD23	1:C:419:ASP:HB3	1.80	0.64
1:I:216:CYS:H	1:I:347:GLU:HG3	1.62	0.64
1:G:123:ILE:HD13	1:G:273:CYS:SG	2.38	0.64
1:A:170:ILE:HG23	1:A:174:LEU:HD12	1.80	0.64
1:D:324:MET:HE2	1:D:438:ILE:HD12	1.79	0.63
1:D:324:MET:HG2	1:D:431:PHE:HE1	1.63	0.63
1:J:72:ILE:HD12	1:J:80:PRO:HG2	1.80	0.63
1:J:383:PRO:HB2	1:J:396:VAL:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:THR:O	1:C:214:LEU:HA	1.98	0.63
1:D:123:ILE:HD13	1:D:273:CYS:SG	2.38	0.63
1:H:60:VAL:HG13	1:H:64:ALA:HB2	1.81	0.63
1:H:156:ILE:HG22	1:H:181:ALA:CB	2.29	0.63
1:J:173:ILE:C	1:J:175:PRO:HD2	2.22	0.63
1:I:386:ALA:HB2	1:K:88:PHE:HA	1.80	0.63
1:L:115:THR:CG2	1:L:297:PRO:HB3	2.27	0.63
1:H:159:THR:HA	1:H:184:ILE:O	1.98	0.63
1:H:174:LEU:N	1:H:175:PRO:HD2	2.13	0.63
1:F:88:PHE:HA	1:H:386:ALA:HB2	1.80	0.63
1:H:144:VAL:HG22	1:H:291:LEU:HD12	1.80	0.63
1:C:216:CYS:H	1:C:347:GLU:HG3	1.64	0.63
1:G:113:ASN:OD1	1:G:115:THR:HG22	1.99	0.63
1:F:51:ALA:HB1	1:F:53:PHE:CE2	2.34	0.63
1:H:260:THR:HG23	1:H:270:LEU:HD22	1.80	0.63
1:A:323:ARG:HD2	1:A:431:PHE:HE2	1.64	0.63
1:B:88:PHE:HA	1:D:386:ALA:HB2	1.79	0.63
1:D:194:LEU:O	1:D:198:GLN:HG3	1.98	0.62
1:K:243:LEU:HD12	1:K:314:VAL:HG21	1.79	0.62
1:F:292:GLY:O	1:H:140:CYS:HB2	1.99	0.62
1:F:170:ILE:HG23	1:F:174:LEU:HD12	1.81	0.62
1:C:54:LEU:HD22	1:C:59:SER:HB3	1.82	0.62
1:F:243:LEU:HD12	1:F:314:VAL:HG21	1.80	0.62
1:A:259:ALA:HA	1:A:263:LEU:HB2	1.81	0.62
1:C:156:ILE:HG22	1:C:181:ALA:CB	2.29	0.62
1:I:383:PRO:HB2	1:I:396:VAL:HG22	1.81	0.62
1:J:211:ASN:HB2	1:J:239:PHE:HE2	1.62	0.62
1:E:60:VAL:HG13	1:E:64:ALA:HB2	1.80	0.62
1:D:87:TYR:CE2	1:D:106:PHE:HB2	2.34	0.62
1:E:260:THR:HG23	1:E:270:LEU:HD22	1.79	0.62
1:H:211:ASN:HB2	1:H:239:PHE:HE2	1.65	0.62
1:A:174:LEU:N	1:A:175:PRO:HD2	2.14	0.62
1:B:63:HIS:HB3	1:B:67:ARG:HB2	1.82	0.62
1:L:207:GLU:HB3	1:L:236:ASP:HB3	1.82	0.62
1:A:211:ASN:HB2	1:A:239:PHE:HE2	1.65	0.62
1:F:115:THR:HG21	1:F:297:PRO:HB3	1.82	0.62
1:I:431:PHE:CE1	1:I:435:LYS:HB2	2.35	0.62
1:A:156:ILE:HG22	1:A:181:ALA:CB	2.29	0.61
1:K:113:ASN:OD1	1:K:115:THR:HG22	2.00	0.61
1:C:313:ARG:O	1:C:317:GLN:HG3	2.00	0.61
1:F:156:ILE:HG22	1:F:181:ALA:CB	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:442:LEU:HD23	1:F:445:ILE:HD12	1.82	0.61
1:I:174:LEU:N	1:I:175:PRO:HD2	2.15	0.61
1:L:115:THR:HG21	1:L:297:PRO:HB3	1.81	0.61
1:B:143:THR:HG21	1:D:291:LEU:HD22	1.82	0.61
1:D:310:LEU:O	1:D:314:VAL:HG23	1.99	0.61
1:G:156:ILE:HG22	1:G:181:ALA:CB	2.30	0.61
1:G:60:VAL:HG13	1:G:64:ALA:HB2	1.82	0.61
1:I:431:PHE:HE1	1:I:435:LYS:HB2	1.66	0.61
1:F:156:ILE:HG22	1:F:181:ALA:HB2	1.83	0.61
1:J:113:ASN:OD1	1:J:115:THR:HG22	2.00	0.61
1:K:54:LEU:HD22	1:K:59:SER:HB3	1.82	0.61
1:G:250:LEU:HD11	1:G:354:GLN:HB2	1.81	0.61
1:L:158:THR:HG22	1:L:205:PHE:O	2.00	0.61
1:J:243:LEU:HD12	1:J:314:VAL:HG21	1.83	0.61
1:E:88:PHE:HA	1:G:386:ALA:HB2	1.83	0.60
1:E:170:ILE:HG23	1:E:174:LEU:HD12	1.82	0.60
1:L:72:ILE:HD12	1:L:80:PRO:HG2	1.83	0.60
1:A:347:GLU:HB3	1:A:350:ILE:HD12	1.83	0.60
1:B:386:ALA:HB2	1:D:88:PHE:HA	1.82	0.60
1:J:156:ILE:HG22	1:J:181:ALA:CB	2.31	0.60
1:K:159:THR:HA	1:K:184:ILE:O	2.00	0.60
1:I:256:LEU:HB2	1:I:273:CYS:O	2.00	0.60
1:A:260:THR:HG23	1:A:270:LEU:HD22	1.81	0.60
1:I:347:GLU:HB3	1:I:350:ILE:HD12	1.83	0.60
1:B:260:THR:HG23	1:B:270:LEU:HD22	1.84	0.60
1:G:54:LEU:HD22	1:G:59:SER:HB3	1.84	0.60
1:J:140:CYS:HB2	1:L:292:GLY:O	2.00	0.60
1:I:60:VAL:HG13	1:I:64:ALA:HB2	1.84	0.60
1:E:174:LEU:N	1:E:175:PRO:HD2	2.17	0.60
1:J:62:ILE:CD1	1:K:428:VAL:HG12	2.30	0.60
1:G:210:THR:HG22	1:G:215:ARG:H	1.66	0.60
1:K:324:MET:HE2	1:K:438:ILE:HD12	1.84	0.60
1:F:115:THR:CG2	1:F:297:PRO:HB3	2.32	0.60
1:F:260:THR:HG23	1:F:270:LEU:HD22	1.84	0.60
1:K:156:ILE:HG22	1:K:181:ALA:CB	2.32	0.60
1:G:240:ALA:O	1:G:244:ASN:HB2	2.02	0.59
1:H:243:LEU:HD12	1:H:314:VAL:HG21	1.84	0.59
1:K:60:VAL:HG13	1:K:64:ALA:HB2	1.83	0.59
1:D:158:THR:HG22	1:D:205:PHE:O	2.02	0.59
1:I:242:PRO:O	1:I:246:LYS:HE2	2.01	0.59
1:L:387:PRO:HB3	3:L:611:PMC:HCA2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:ASN:HB2	1:D:239:PHE:CE2	2.37	0.59
1:E:156:ILE:HG22	1:E:181:ALA:CB	2.32	0.59
1:C:194:LEU:O	1:C:198:GLN:HG3	2.03	0.59
1:J:386:ALA:HB2	1:L:88:PHE:HA	1.84	0.59
1:K:339:TYR:CD1	1:K:362:VAL:HG22	2.37	0.59
1:F:250:LEU:HD11	1:F:354:GLN:HB2	1.83	0.59
1:H:345:HIS:CE1	1:H:347:GLU:HG2	2.37	0.59
1:I:260:THR:CG2	1:I:270:LEU:HD22	2.32	0.59
1:F:277:PRO:HG2	1:F:280:LEU:HB2	1.85	0.59
1:G:53:PHE:CD1	1:G:54:LEU:HG	2.37	0.59
1:F:260:THR:CG2	1:F:270:LEU:HD22	2.33	0.59
1:G:63:HIS:HB3	1:G:67:ARG:HB2	1.85	0.59
1:G:174:LEU:N	1:G:175:PRO:HD2	2.18	0.59
1:B:259:ALA:HB3	1:B:271:ALA:HB3	1.84	0.58
1:F:174:LEU:N	1:F:175:PRO:HD2	2.18	0.58
1:I:210:THR:HG23	1:I:211:ASN:N	2.18	0.58
1:J:250:LEU:HD11	1:J:354:GLN:HB2	1.85	0.58
1:A:397:ASP:HB2	1:A:402:MET:HG3	1.85	0.58
1:G:331:HIS:CE1	1:G:333:LYS:HB2	2.38	0.58
1:B:158:THR:HG22	1:B:205:PHE:O	2.02	0.58
1:C:260:THR:HG23	1:C:270:LEU:HD22	1.84	0.58
1:J:259:ALA:HB3	1:J:271:ALA:HB3	1.85	0.58
1:K:260:THR:CG2	1:K:270:LEU:HD22	2.32	0.58
1:A:345:HIS:CE1	1:A:347:GLU:HG2	2.38	0.58
1:D:260:THR:HG23	1:D:270:LEU:HD22	1.85	0.58
1:E:211:ASN:HB2	1:E:239:PHE:HE2	1.67	0.58
1:L:156:ILE:HG22	1:L:181:ALA:CB	2.33	0.58
1:A:158:THR:HG22	1:A:205:PHE:O	2.04	0.58
1:I:428:VAL:HG12	1:L:62:ILE:CD1	2.28	0.58
1:K:259:ALA:HB3	1:K:271:ALA:HB3	1.84	0.58
1:E:64:ALA:O	1:E:122:LYS:HE2	2.03	0.58
1:J:115:THR:CG2	1:J:297:PRO:HB3	2.34	0.58
1:A:211:ASN:HB2	1:A:239:PHE:CE2	2.39	0.58
1:B:383:PRO:HB2	1:B:396:VAL:HG22	1.85	0.58
1:F:82:VAL:HG21	1:F:114:PRO:HG2	1.86	0.58
1:F:383:PRO:HB2	1:F:396:VAL:HG22	1.84	0.58
1:I:211:ASN:HB2	1:I:239:PHE:HE2	1.69	0.58
1:B:170:ILE:HG23	1:B:174:LEU:HD12	1.85	0.58
1:B:211:ASN:HB2	1:B:239:PHE:HE2	1.69	0.58
1:B:113:ASN:OD1	1:B:115:THR:HG22	2.04	0.57
1:H:376:PHE:HB2	1:H:445:ILE:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:VAL:HG13	1:F:64:ALA:HB2	1.86	0.57
1:F:62:ILE:CD1	1:G:428:VAL:HG12	2.31	0.57
1:G:115:THR:HG21	1:G:297:PRO:HB3	1.85	0.57
1:J:433:ASP:OD2	1:K:56:SER:HB3	2.04	0.57
1:C:347:GLU:HB3	1:C:350:ILE:HD12	1.85	0.57
1:E:313:ARG:O	1:E:317:GLN:HG3	2.03	0.57
1:H:260:THR:CG2	1:H:270:LEU:HD22	2.34	0.57
1:I:131:SER:HB3	1:I:281:VAL:HG11	1.86	0.57
1:D:64:ALA:O	1:D:122:LYS:HE2	2.04	0.57
1:E:428:VAL:HG13	1:E:428:VAL:O	2.03	0.57
1:G:210:THR:O	1:G:214:LEU:HA	2.05	0.57
1:I:211:ASN:HB2	1:I:239:PHE:CE2	2.39	0.57
1:C:60:VAL:HG13	1:C:64:ALA:HB2	1.86	0.57
1:E:347:GLU:HB3	1:E:350:ILE:HD12	1.85	0.57
1:I:115:THR:HG21	1:I:297:PRO:HB3	1.86	0.57
1:K:324:MET:HG2	1:K:431:PHE:HE1	1.70	0.57
1:G:256:LEU:HB2	1:G:273:CYS:O	2.05	0.57
1:H:115:THR:CG2	1:H:297:PRO:HB3	2.34	0.57
1:H:207:GLU:CB	1:H:236:ASP:HB3	2.33	0.57
1:J:260:THR:HG23	1:J:270:LEU:HD22	1.85	0.57
1:L:159:THR:HA	1:L:184:ILE:O	2.05	0.57
1:C:324:MET:HE2	1:C:438:ILE:HD12	1.87	0.57
1:E:207:GLU:CB	1:E:236:ASP:HB3	2.33	0.57
1:E:345:HIS:CE1	1:E:347:GLU:HG2	2.40	0.57
1:L:63:HIS:HB3	1:L:67:ARG:HB2	1.87	0.57
1:D:397:ASP:HB2	1:D:402:MET:HG3	1.86	0.57
1:F:242:PRO:HD3	1:F:257:HIS:CE1	2.40	0.57
1:I:431:PHE:CD1	1:I:431:PHE:C	2.82	0.57
1:B:60:VAL:HG13	1:B:64:ALA:HB2	1.87	0.57
1:H:210:THR:O	1:H:214:LEU:HA	2.05	0.57
1:K:324:MET:HE2	1:K:438:ILE:CD1	2.35	0.57
1:A:323:ARG:CZ	1:A:431:PHE:HD2	2.17	0.56
1:F:73:VAL:O	1:F:74:THR:HG23	2.05	0.56
1:K:194:LEU:O	1:K:198:GLN:HG3	2.05	0.56
1:K:383:PRO:HB2	1:K:396:VAL:HG22	1.87	0.56
1:A:207:GLU:CB	1:A:236:ASP:HB3	2.34	0.56
1:C:73:VAL:O	1:C:74:THR:HG23	2.05	0.56
1:D:113:ASN:ND2	1:D:297:PRO:HG3	2.20	0.56
1:J:207:GLU:CB	1:J:236:ASP:HB3	2.33	0.56
1:K:64:ALA:O	1:K:122:LYS:HE2	2.05	0.56
1:B:242:PRO:O	1:B:246:LYS:HE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:386:ALA:HB2	1:H:88:PHE:HA	1.87	0.56
1:J:428:VAL:O	1:J:428:VAL:HG13	2.04	0.56
1:D:156:ILE:HG22	1:D:181:ALA:HB2	1.88	0.56
1:I:88:PHE:HA	1:K:386:ALA:HB2	1.88	0.56
1:B:194:LEU:O	1:B:198:GLN:HG3	2.06	0.56
1:G:260:THR:HG23	1:G:270:LEU:HD22	1.87	0.56
1:I:428:VAL:O	1:I:428:VAL:HG13	2.06	0.56
1:E:250:LEU:HD11	1:E:354:GLN:HB2	1.86	0.56
1:G:370:LEU:HD23	1:G:419:ASP:HB3	1.87	0.56
1:H:96:ILE:O	1:H:100:GLU:HG3	2.06	0.56
1:I:210:THR:O	1:I:214:LEU:HA	2.04	0.56
1:B:291:LEU:HD22	1:D:143:THR:HG21	1.88	0.56
1:E:82:VAL:HG21	1:E:114:PRO:HG2	1.86	0.56
1:E:194:LEU:O	1:E:198:GLN:HG3	2.05	0.56
1:K:300:ALA:O	1:K:304:ILE:HG13	2.06	0.56
1:E:51:ALA:HB1	1:E:53:PHE:CE2	2.41	0.56
1:F:324:MET:HG2	1:F:431:PHE:HE1	1.71	0.56
1:J:351:ALA:O	1:J:355:MET:HB2	2.06	0.56
1:L:376:PHE:HB2	1:L:445:ILE:HD11	1.87	0.56
1:A:143:THR:HG21	1:C:291:LEU:HD22	1.88	0.56
1:A:323:ARG:CZ	1:A:431:PHE:CD2	2.89	0.56
1:E:386:ALA:HB2	1:G:88:PHE:HA	1.88	0.56
1:L:207:GLU:HG3	1:L:210:THR:HA	1.88	0.56
1:L:313:ARG:O	1:L:317:GLN:HG3	2.06	0.56
1:A:115:THR:CG2	1:A:297:PRO:HB3	2.36	0.55
1:A:210:THR:HG23	1:A:211:ASN:N	2.19	0.55
1:C:242:PRO:O	1:C:246:LYS:HE2	2.05	0.55
1:G:156:ILE:HG22	1:G:181:ALA:HB2	1.87	0.55
1:C:260:THR:CG2	1:C:270:LEU:HD22	2.36	0.55
1:I:170:ILE:HG23	1:I:174:LEU:HD12	1.88	0.55
1:J:210:THR:O	1:J:214:LEU:HA	2.07	0.55
1:C:383:PRO:HB2	1:C:396:VAL:CG2	2.35	0.55
1:D:347:GLU:HB3	1:D:350:ILE:HD12	1.89	0.55
1:J:156:ILE:HG22	1:J:181:ALA:HB2	1.87	0.55
1:F:50:TYR:CE2	1:F:64:ALA:HA	2.41	0.55
1:I:429:GLU:OE2	1:L:63:HIS:HE1	1.90	0.55
1:K:351:ALA:O	1:K:355:MET:HB2	2.05	0.55
1:L:173:ILE:C	1:L:175:PRO:HD2	2.31	0.55
1:L:194:LEU:O	1:L:198:GLN:HG3	2.07	0.55
1:E:260:THR:CG2	1:E:270:LEU:HD22	2.37	0.55
1:I:215:ARG:HD2	1:I:347:GLU:OE2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:211:ASN:HB2	1:J:239:PHE:CE2	2.41	0.55
1:J:428:VAL:HG12	1:K:62:ILE:CD1	2.33	0.55
1:K:204:PHE:CE2	1:K:222:VAL:HG11	2.40	0.55
1:D:170:ILE:HG23	1:D:174:LEU:HD12	1.89	0.55
1:J:123:ILE:HD13	1:J:273:CYS:SG	2.47	0.55
1:L:260:THR:HG23	1:L:270:LEU:HD22	1.87	0.55
1:K:376:PHE:HB2	1:K:445:ILE:HD11	1.88	0.55
1:E:296:ASN:ND2	1:E:297:PRO:HD2	2.22	0.55
1:L:324:MET:HE2	1:L:438:ILE:HD12	1.89	0.55
1:A:156:ILE:HG22	1:A:181:ALA:HB2	1.89	0.55
1:A:310:LEU:O	1:A:314:VAL:HG23	2.07	0.55
1:G:339:TYR:CD1	1:G:362:VAL:HG22	2.41	0.55
1:A:223:SER:HA	1:A:233:VAL:HG21	1.89	0.54
1:A:382:ILE:HG12	1:D:54:LEU:HD21	1.89	0.54
1:D:96:ILE:O	1:D:100:GLU:HG3	2.07	0.54
1:D:115:THR:HG21	1:D:297:PRO:HB3	1.89	0.54
1:J:155:HIS:O	1:J:202:ASN:HB2	2.07	0.54
1:B:173:ILE:C	1:B:175:PRO:HD2	2.32	0.54
1:G:441:ALA:C	1:G:443:ASP:H	2.15	0.54
1:E:159:THR:HA	1:E:184:ILE:O	2.07	0.54
1:G:115:THR:CG2	1:G:297:PRO:HB3	2.37	0.54
1:J:241:THR:HG23	1:J:242:PRO:HD2	1.89	0.54
1:K:207:GLU:CB	1:K:236:ASP:HB3	2.37	0.54
1:A:241:THR:HG22	1:A:243:LEU:N	2.14	0.54
1:L:87:TYR:N	1:L:87:TYR:CD2	2.76	0.54
1:L:256:LEU:HB2	1:L:273:CYS:O	2.07	0.54
1:F:143:THR:HG21	1:H:291:LEU:HD22	1.89	0.54
1:I:242:PRO:HD3	1:I:257:HIS:CE1	2.43	0.54
1:C:262:PHE:CE1	1:C:390:GLY:HA2	2.43	0.54
1:E:158:THR:HG22	1:E:205:PHE:O	2.07	0.54
1:F:211:ASN:HB2	1:F:239:PHE:CE2	2.42	0.54
1:F:346:PRO:HB2	1:F:347:GLU:OE2	2.08	0.54
1:J:260:THR:CG2	1:J:270:LEU:HD22	2.37	0.54
1:D:379:ALA:HB3	1:D:441:ALA:HB1	1.89	0.54
1:E:166:THR:O	1:E:170:ILE:HG13	2.08	0.54
1:C:428:VAL:O	1:C:428:VAL:HG13	2.07	0.54
1:D:243:LEU:HD12	1:D:314:VAL:HG21	1.89	0.54
1:F:158:THR:HG22	1:F:205:PHE:O	2.07	0.54
1:B:156:ILE:HG22	1:B:181:ALA:HB2	1.90	0.54
1:E:428:VAL:HG12	1:H:62:ILE:CD1	2.36	0.54
1:H:166:THR:O	1:H:170:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:291:LEU:HD22	1:L:143:THR:HG21	1.90	0.54
1:K:170:ILE:HG23	1:K:174:LEU:HD12	1.89	0.54
1:L:144:VAL:HG22	1:L:291:LEU:HD12	1.89	0.54
1:A:428:VAL:O	1:A:428:VAL:HG13	2.07	0.53
1:D:242:PRO:HD3	1:D:257:HIS:CE1	2.42	0.53
1:F:365:GLU:HB3	1:F:420:ASN:HB3	1.90	0.53
1:H:156:ILE:HG22	1:H:181:ALA:HB2	1.88	0.53
1:K:73:VAL:O	1:K:74:THR:HG23	2.08	0.53
1:B:156:ILE:HG22	1:B:181:ALA:HB1	1.90	0.53
1:I:323:ARG:HD2	1:I:431:PHE:HE2	1.74	0.53
1:L:51:ALA:HB1	1:L:53:PHE:CE2	2.43	0.53
1:B:260:THR:HG21	1:D:108:TYR:OH	2.08	0.53
1:C:241:THR:HG22	1:C:243:LEU:N	2.14	0.53
1:H:347:GLU:HB3	1:H:350:ILE:HD12	1.89	0.53
1:C:156:ILE:HG22	1:C:181:ALA:HB2	1.89	0.53
1:D:260:THR:CG2	1:D:270:LEU:HD22	2.38	0.53
1:K:123:ILE:HD13	1:K:273:CYS:SG	2.48	0.53
1:B:345:HIS:CE1	1:B:347:GLU:HG2	2.43	0.53
1:C:115:THR:HG21	1:C:297:PRO:HB3	1.90	0.53
1:D:215:ARG:NH1	1:D:347:GLU:OE2	2.41	0.53
1:F:313:ARG:O	1:F:317:GLN:HG3	2.08	0.53
1:I:345:HIS:CE1	1:I:347:GLU:HG2	2.43	0.53
1:K:158:THR:HG22	1:K:205:PHE:O	2.08	0.53
1:E:310:LEU:O	1:E:314:VAL:HG23	2.08	0.53
1:G:73:VAL:O	1:G:74:THR:HG23	2.07	0.53
1:B:210:THR:O	1:B:214:LEU:HA	2.08	0.53
1:B:370:LEU:HD23	1:B:419:ASP:HB3	1.91	0.53
1:D:242:PRO:O	1:D:246:LYS:HE2	2.09	0.53
1:D:428:VAL:O	1:D:428:VAL:HG13	2.07	0.53
1:G:324:MET:HE2	1:G:438:ILE:HD12	1.91	0.53
1:I:78:THR:HG21	1:L:268:ASP:HB3	1.89	0.53
1:K:321:ALA:HB2	1:K:360:GLY:HA2	1.90	0.53
1:B:428:VAL:HG13	1:B:428:VAL:O	2.09	0.53
1:C:207:GLU:CB	1:C:236:ASP:HB3	2.39	0.53
1:G:243:LEU:HD12	1:G:314:VAL:HG21	1.91	0.53
1:L:215:ARG:HD2	1:L:347:GLU:OE2	2.09	0.53
1:F:397:ASP:HB2	1:F:402:MET:HG3	1.91	0.52
1:H:64:ALA:O	1:H:122:LYS:HE2	2.09	0.52
1:I:194:LEU:O	1:I:198:GLN:HG3	2.09	0.52
1:C:211:ASN:HB2	1:C:239:PHE:HE2	1.73	0.52
1:I:158:THR:HG22	1:I:205:PHE:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:250:LEU:HD11	1:K:354:GLN:HB2	1.92	0.52
1:A:62:ILE:CD1	1:D:428:VAL:HG12	2.40	0.52
1:G:310:LEU:O	1:G:314:VAL:HG23	2.10	0.52
1:C:211:ASN:HB2	1:C:239:PHE:CE2	2.45	0.52
1:J:115:THR:HG21	1:J:297:PRO:HB3	1.90	0.52
1:L:156:ILE:HG22	1:L:181:ALA:HB2	1.91	0.52
1:B:242:PRO:HD3	1:B:257:HIS:CE1	2.43	0.52
1:K:80:PRO:HB3	1:L:82:VAL:HG22	1.91	0.52
1:G:207:GLU:CB	1:G:236:ASP:HB3	2.36	0.52
1:A:60:VAL:HG13	1:A:64:ALA:HB2	1.92	0.52
1:D:166:THR:O	1:D:170:ILE:HG13	2.10	0.52
1:K:211:ASN:HB2	1:K:239:PHE:HE2	1.75	0.52
1:L:153:GLY:HA2	1:L:178:GLY:O	2.09	0.52
1:B:115:THR:HG21	1:B:297:PRO:HB3	1.91	0.52
1:B:347:GLU:HB3	1:B:350:ILE:HD12	1.92	0.52
1:C:173:ILE:C	1:C:175:PRO:HD2	2.35	0.52
1:L:210:THR:HG22	1:L:215:ARG:H	1.75	0.52
1:L:261:LYS:HD2	1:L:389:PHE:CZ	2.44	0.52
1:A:428:VAL:CG2	1:D:312:LEU:HD11	2.40	0.52
1:B:386:ALA:HB1	1:B:387:PRO:CD	2.40	0.52
1:E:63:HIS:CD2	1:E:67:ARG:HD3	2.45	0.52
1:F:64:ALA:O	1:F:122:LYS:HE2	2.10	0.52
1:H:345:HIS:HE1	1:H:347:GLU:HG2	1.75	0.52
1:K:256:LEU:HB2	1:K:273:CYS:O	2.10	0.52
1:J:163:TYR:CE2	1:J:165:LYS:HB2	2.45	0.51
1:B:250:LEU:HD11	1:B:354:GLN:HB2	1.92	0.51
1:F:210:THR:O	1:F:214:LEU:HA	2.10	0.51
1:G:351:ALA:O	1:G:355:MET:HB2	2.10	0.51
1:I:313:ARG:O	1:I:317:GLN:HG3	2.10	0.51
1:J:60:VAL:HG13	1:J:64:ALA:HB2	1.92	0.51
1:J:144:VAL:HG22	1:J:291:LEU:HD12	1.92	0.51
1:K:240:ALA:O	1:K:244:ASN:HB2	2.09	0.51
1:L:428:VAL:O	1:L:428:VAL:HG13	2.09	0.51
1:A:131:SER:HB3	1:A:281:VAL:HG11	1.93	0.51
1:F:386:ALA:HB1	1:F:387:PRO:CD	2.41	0.51
1:H:250:LEU:CD1	1:H:354:GLN:HB2	2.39	0.51
1:A:260:THR:CG2	1:A:270:LEU:HD22	2.39	0.51
1:C:115:THR:CG2	1:C:297:PRO:HB3	2.39	0.51
1:H:158:THR:HG22	1:H:205:PHE:O	2.10	0.51
1:L:250:LEU:HD11	1:L:354:GLN:HB2	1.93	0.51
1:A:323:ARG:NH1	1:A:431:PHE:CD2	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:THR:HG23	1:F:242:PRO:HD2	1.92	0.51
1:F:324:MET:HE2	1:F:438:ILE:HD12	1.93	0.51
1:G:63:HIS:CD2	1:G:67:ARG:HD3	2.45	0.51
1:L:210:THR:O	1:L:214:LEU:HA	2.10	0.51
1:E:123:ILE:HD13	1:E:273:CYS:SG	2.51	0.51
1:F:194:LEU:O	1:F:198:GLN:HG3	2.11	0.51
1:F:418:MET:C	1:F:420:ASN:H	2.17	0.51
1:G:277:PRO:HG2	1:G:280:LEU:HB2	1.93	0.51
1:B:418:MET:C	1:B:420:ASN:H	2.18	0.51
1:E:211:ASN:HB2	1:E:239:PHE:CE2	2.45	0.51
1:E:323:ARG:HD2	1:E:431:PHE:HE2	1.76	0.51
1:F:291:LEU:HD22	1:H:143:THR:HG21	1.93	0.51
1:H:324:MET:HG2	1:H:431:PHE:HE1	1.76	0.51
1:I:250:LEU:HD11	1:I:354:GLN:HB2	1.91	0.51
1:I:365:GLU:HB3	1:I:420:ASN:HB3	1.93	0.51
1:L:310:LEU:O	1:L:314:VAL:HG23	2.11	0.51
1:C:339:TYR:CD1	1:C:362:VAL:HG22	2.46	0.51
1:I:96:ILE:O	1:I:100:GLU:HG3	2.11	0.51
1:B:51:ALA:HB3	1:B:54:LEU:HB2	1.92	0.51
1:D:339:TYR:CD1	1:D:362:VAL:HG22	2.45	0.51
1:G:260:THR:CG2	1:G:270:LEU:HD22	2.40	0.51
1:I:310:LEU:O	1:I:314:VAL:HG23	2.11	0.51
1:J:170:ILE:HA	1:J:174:LEU:HD12	1.93	0.51
1:A:351:ALA:O	1:A:355:MET:HB2	2.11	0.50
1:A:365:GLU:HB3	1:A:420:ASN:HB3	1.92	0.50
1:E:131:SER:OG	1:E:281:VAL:HG11	2.11	0.50
1:G:64:ALA:O	1:G:122:LYS:HE2	2.10	0.50
1:A:166:THR:O	1:A:170:ILE:HG13	2.10	0.50
1:B:324:MET:HE2	1:B:438:ILE:CD1	2.40	0.50
1:B:386:ALA:HB1	1:B:387:PRO:HD2	1.93	0.50
1:K:331:HIS:CE1	1:K:333:LYS:HB2	2.46	0.50
1:B:369:ASP:H	1:B:372:THR:HB	1.75	0.50
1:E:143:THR:HG21	1:G:291:LEU:HD22	1.92	0.50
1:H:261:LYS:HD2	1:H:389:PHE:CZ	2.46	0.50
1:B:397:ASP:HB2	1:B:402:MET:HG3	1.94	0.50
1:D:60:VAL:HG13	1:D:64:ALA:HB2	1.93	0.50
1:H:397:ASP:HB2	1:H:402:MET:HG3	1.92	0.50
1:B:210:THR:HG23	1:B:211:ASN:N	2.26	0.50
1:D:331:HIS:CE1	1:D:333:LYS:HB2	2.46	0.50
1:E:323:ARG:CZ	1:E:431:PHE:HD2	2.25	0.50
1:A:88:PHE:HA	1:C:386:ALA:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ILE:HA	1:B:174:LEU:HD12	1.94	0.50
1:D:210:THR:O	1:D:214:LEU:HA	2.11	0.50
1:E:387:PRO:HB3	3:E:604:PMC:HCA2	1.93	0.50
1:H:131:SER:HB3	1:H:281:VAL:HG11	1.94	0.50
1:F:207:GLU:CB	1:F:236:ASP:HB3	2.38	0.50
1:G:324:MET:HG2	1:G:431:PHE:HE1	1.76	0.50
1:J:324:MET:HG2	1:J:431:PHE:HE1	1.76	0.50
1:L:211:ASN:HB2	1:L:239:PHE:CE2	2.46	0.50
1:C:277:PRO:HG2	1:C:280:LEU:HB2	1.93	0.50
1:C:72:ILE:O	1:C:72:ILE:CG2	2.58	0.50
1:D:115:THR:CG2	1:D:297:PRO:HB3	2.41	0.50
1:E:243:LEU:HD12	1:E:314:VAL:HG21	1.94	0.50
1:F:123:ILE:HD13	1:F:273:CYS:SG	2.52	0.50
1:H:256:LEU:HB2	1:H:273:CYS:O	2.12	0.50
1:A:127:GLU:CD	1:A:242:PRO:HB3	2.37	0.49
1:B:241:THR:CG2	1:B:243:LEU:H	2.18	0.49
1:E:242:PRO:HD3	1:E:257:HIS:CE1	2.47	0.49
1:F:138:GLY:N	2:F:500:PLP:O2P	2.46	0.49
1:K:127:GLU:OE2	1:K:257:HIS:NE2	2.42	0.49
1:B:260:THR:CG2	1:B:270:LEU:HD22	2.42	0.49
1:J:194:LEU:O	1:J:198:GLN:HG3	2.12	0.49
1:B:379:ALA:HB3	1:B:441:ALA:HB1	1.92	0.49
1:F:428:VAL:HG13	1:F:428:VAL:O	2.12	0.49
1:G:397:ASP:HB2	1:G:402:MET:HG3	1.94	0.49
1:I:311:HIS:HE2	1:L:428:VAL:HG13	1.77	0.49
1:A:277:PRO:HG2	1:A:280:LEU:HB2	1.94	0.49
1:B:72:ILE:O	1:B:72:ILE:CG2	2.59	0.49
1:H:215:ARG:HD2	1:H:347:GLU:OE2	2.13	0.49
1:J:321:ALA:HB2	1:J:360:GLY:HA2	1.95	0.49
1:A:345:HIS:HE1	1:A:347:GLU:HG2	1.75	0.49
1:B:256:LEU:HB2	1:B:273:CYS:O	2.11	0.49
1:C:223:SER:HA	1:C:233:VAL:HG21	1.94	0.49
1:G:345:HIS:CE1	1:G:347:GLU:HG2	2.48	0.49
1:H:54:LEU:HD22	1:H:59:SER:CB	2.40	0.49
1:J:174:LEU:N	1:J:175:PRO:CD	2.76	0.49
1:J:397:ASP:HB2	1:J:402:MET:HG3	1.93	0.49
1:B:82:VAL:HG21	1:B:114:PRO:HG2	1.95	0.49
1:B:115:THR:CG2	1:B:297:PRO:HB3	2.43	0.49
1:F:210:THR:HG23	1:F:211:ASN:N	2.27	0.49
1:G:140:CYS:O	1:G:144:VAL:HG23	2.13	0.49
1:H:351:ALA:O	1:H:355:MET:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:204:PHE:CE2	1:I:222:VAL:HG11	2.48	0.49
1:K:82:VAL:HG21	1:K:114:PRO:HG2	1.94	0.49
1:L:60:VAL:HG13	1:L:64:ALA:HB2	1.94	0.49
1:D:278:LEU:HA	1:D:281:VAL:HG12	1.95	0.49
1:F:331:HIS:CE1	1:F:333:LYS:HB2	2.47	0.49
1:K:210:THR:HG23	1:K:211:ASN:N	2.27	0.49
1:F:63:HIS:HE1	1:G:429:GLU:OE2	1.95	0.49
1:G:80:PRO:HB3	1:H:82:VAL:HG22	1.95	0.49
1:H:331:HIS:CE1	1:H:333:LYS:HB2	2.48	0.49
1:H:365:GLU:HB3	1:H:420:ASN:HB3	1.95	0.49
1:C:386:ALA:HB1	1:C:387:PRO:CD	2.41	0.49
1:D:386:ALA:HB1	1:D:387:PRO:CD	2.43	0.49
1:E:210:THR:HG23	1:E:211:ASN:N	2.27	0.49
1:J:223:SER:HA	1:J:233:VAL:HG21	1.95	0.49
1:J:250:LEU:CD1	1:J:354:GLN:HB2	2.42	0.49
1:C:158:THR:HG22	1:C:205:PHE:O	2.13	0.49
1:E:386:ALA:HB1	1:E:387:PRO:CD	2.43	0.49
1:F:163:TYR:CE2	1:F:165:LYS:HB2	2.47	0.49
1:G:131:SER:HB3	1:G:281:VAL:HG11	1.94	0.49
1:G:194:LEU:O	1:G:198:GLN:HG3	2.13	0.49
1:H:255:VAL:O	1:H:255:VAL:HG13	2.13	0.49
1:K:174:LEU:N	1:K:175:PRO:CD	2.75	0.49
1:K:418:MET:C	1:K:420:ASN:H	2.20	0.49
1:E:208:SER:HA	1:E:209:PRO:C	2.37	0.48
1:F:296:ASN:OD1	1:F:298:ASN:HB2	2.13	0.48
1:G:242:PRO:HD3	1:G:257:HIS:CE1	2.48	0.48
1:I:73:VAL:O	1:I:74:THR:HG23	2.13	0.48
1:I:223:SER:HA	1:I:233:VAL:HG21	1.94	0.48
1:K:210:THR:O	1:K:214:LEU:HA	2.13	0.48
1:D:210:THR:HG23	1:D:211:ASN:N	2.27	0.48
1:I:386:ALA:HB1	1:I:387:PRO:CD	2.43	0.48
1:I:386:ALA:HB1	1:I:387:PRO:HD2	1.94	0.48
1:K:211:ASN:HB2	1:K:239:PHE:CE2	2.48	0.48
1:K:242:PRO:HD3	1:K:257:HIS:CE1	2.47	0.48
1:B:96:ILE:O	1:B:100:GLU:HG3	2.13	0.48
1:E:323:ARG:CZ	1:E:431:PHE:CD2	2.96	0.48
1:F:300:ALA:O	1:F:304:ILE:HG13	2.13	0.48
1:K:343:GLN:HA	1:K:348:HIS:CD2	2.48	0.48
1:C:241:THR:HG23	1:C:242:PRO:HD2	1.95	0.48
1:C:310:LEU:O	1:C:314:VAL:HG23	2.11	0.48
1:D:87:TYR:CD2	1:D:106:PHE:HB2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:THR:O	1:E:235:ILE:HA	2.13	0.48
1:G:113:ASN:ND2	1:G:297:PRO:HG3	2.29	0.48
1:J:73:VAL:O	1:J:74:THR:HG23	2.13	0.48
1:A:321:ALA:HB2	1:A:360:GLY:HA2	1.95	0.48
1:C:324:MET:HG2	1:C:431:PHE:HE1	1.78	0.48
1:G:170:ILE:HA	1:G:174:LEU:HD12	1.96	0.48
1:I:156:ILE:HG22	1:I:181:ALA:CB	2.43	0.48
1:I:215:ARG:NH1	1:I:347:GLU:OE2	2.44	0.48
1:I:324:MET:HE2	1:I:438:ILE:HD12	1.94	0.48
1:K:156:ILE:HG22	1:K:181:ALA:HB2	1.94	0.48
1:K:261:LYS:HD2	1:K:389:PHE:CZ	2.49	0.48
1:K:387:PRO:HB3	3:K:610:PMC:HCA2	1.94	0.48
1:L:86:ALA:C	1:L:87:TYR:CD2	2.92	0.48
1:A:370:LEU:HD23	1:A:419:ASP:HB3	1.94	0.48
1:E:72:ILE:O	1:E:72:ILE:CG2	2.59	0.48
1:H:211:ASN:HB2	1:H:239:PHE:CE2	2.46	0.48
1:I:62:ILE:CD1	1:L:428:VAL:HG12	2.36	0.48
1:K:113:ASN:ND2	1:K:297:PRO:HG3	2.29	0.48
1:K:382:ILE:HB	1:K:383:PRO:HD3	1.94	0.48
1:F:347:GLU:HB3	1:F:350:ILE:HD12	1.95	0.48
1:G:158:THR:HG22	1:G:205:PHE:O	2.14	0.48
1:L:127:GLU:CD	1:L:242:PRO:HB3	2.39	0.48
1:A:140:CYS:O	1:A:144:VAL:HG23	2.14	0.48
1:B:382:ILE:HB	1:B:383:PRO:HD3	1.96	0.48
1:E:173:ILE:O	1:E:176:LYS:HB2	2.14	0.48
1:F:428:VAL:CG2	1:G:312:LEU:HD11	2.44	0.48
1:I:140:CYS:HB2	1:K:292:GLY:O	2.14	0.48
1:J:261:LYS:HD2	1:J:389:PHE:CZ	2.49	0.48
1:K:70:ARG:HD3	1:K:79:THR:OG1	2.14	0.48
1:K:265:GLY:HA3	1:K:313:ARG:NH1	2.28	0.48
1:D:159:THR:HA	1:D:184:ILE:O	2.14	0.48
1:D:387:PRO:HB3	3:D:603:PMC:HCA2	1.95	0.48
1:E:292:GLY:O	1:G:140:CYS:HB2	2.14	0.48
1:F:339:TYR:CD1	1:F:362:VAL:HG22	2.49	0.48
1:I:115:THR:CG2	1:I:297:PRO:HB3	2.42	0.48
1:C:206:THR:O	1:C:235:ILE:HA	2.14	0.48
1:D:54:LEU:HD22	1:D:59:SER:HB3	1.96	0.48
1:F:351:ALA:O	1:F:355:MET:HB2	2.13	0.48
1:G:82:VAL:HG21	1:G:114:PRO:HG2	1.96	0.48
1:H:194:LEU:O	1:H:198:GLN:HG3	2.14	0.48
1:I:54:LEU:HD22	1:I:59:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:143:THR:HG21	1:K:291:LEU:HD22	1.95	0.48
1:K:441:ALA:C	1:K:443:ASP:H	2.22	0.48
1:L:208:SER:HA	1:L:209:PRO:C	2.39	0.48
1:L:346:PRO:HB2	1:L:347:GLU:OE2	2.14	0.48
1:A:113:ASN:ND2	1:A:297:PRO:HG3	2.28	0.47
1:B:159:THR:HA	1:B:184:ILE:O	2.14	0.47
1:C:70:ARG:C	1:C:72:ILE:H	2.21	0.47
1:I:156:ILE:HG22	1:I:181:ALA:HB2	1.96	0.47
1:L:365:GLU:HB3	1:L:420:ASN:HB3	1.96	0.47
1:A:155:HIS:HA	1:A:180:THR:O	2.14	0.47
1:B:337:VAL:HG22	1:B:364:PHE:HB3	1.95	0.47
1:B:348:HIS:O	1:B:352:LYS:HB2	2.15	0.47
1:D:98:PHE:HE2	1:D:99:LYS:HE2	1.79	0.47
1:F:113:ASN:OD1	1:F:115:THR:CG2	2.61	0.47
1:F:166:THR:O	1:F:170:ILE:HG13	2.14	0.47
1:I:56:SER:HB3	1:L:433:ASP:OD2	2.13	0.47
1:K:204:PHE:HE2	1:K:222:VAL:HG11	1.78	0.47
1:A:291:LEU:HD22	1:C:143:THR:HG21	1.96	0.47
1:B:211:ASN:HB2	1:B:239:PHE:CE2	2.50	0.47
1:C:296:ASN:OD1	1:C:298:ASN:HB2	2.15	0.47
1:E:256:LEU:HB2	1:E:273:CYS:O	2.13	0.47
1:A:242:PRO:O	1:A:246:LYS:HE2	2.14	0.47
1:F:72:ILE:O	1:F:72:ILE:CG2	2.62	0.47
1:F:374:ALA:O	1:F:377:VAL:HG22	2.15	0.47
1:G:106:PHE:O	1:G:108:TYR:N	2.47	0.47
1:J:382:ILE:HB	1:J:383:PRO:HD3	1.97	0.47
1:A:159:THR:HA	1:A:184:ILE:O	2.15	0.47
1:B:166:THR:O	1:B:170:ILE:HG13	2.13	0.47
1:B:212:PRO:HG2	1:B:421:LEU:HD21	1.96	0.47
1:B:278:LEU:O	1:B:282:SER:HB3	2.14	0.47
1:C:256:LEU:HB2	1:C:273:CYS:O	2.14	0.47
1:C:374:ALA:O	1:C:377:VAL:HG22	2.15	0.47
1:E:127:GLU:OE2	1:E:257:HIS:NE2	2.45	0.47
1:F:57:ASP:HB3	1:F:243:LEU:CD2	2.44	0.47
1:H:343:GLN:HA	1:H:348:HIS:CD2	2.49	0.47
1:D:173:ILE:C	1:D:175:PRO:HD2	2.39	0.47
1:E:115:THR:HG21	1:E:297:PRO:HB3	1.97	0.47
1:E:339:TYR:CD1	1:E:362:VAL:HG22	2.49	0.47
1:F:382:ILE:HB	1:F:383:PRO:HD3	1.97	0.47
1:K:82:VAL:HG12	1:K:84:THR:HG22	1.97	0.47
1:K:173:ILE:C	1:K:175:PRO:HD2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:428:VAL:O	1:K:428:VAL:HG13	2.15	0.47
1:A:131:SER:CB	1:A:281:VAL:HG11	2.45	0.47
1:B:145:MET:HE2	1:B:146:LEU:HA	1.95	0.47
1:B:174:LEU:N	1:B:175:PRO:CD	2.77	0.47
1:B:428:VAL:CG2	1:C:312:LEU:HD11	2.45	0.47
1:D:103:ARG:HG2	1:D:104:ALA:N	2.30	0.47
1:E:210:THR:O	1:E:214:LEU:HA	2.15	0.47
1:E:265:GLY:HA3	1:E:313:ARG:NH1	2.29	0.47
1:F:98:PHE:HE2	1:F:99:LYS:HE2	1.79	0.47
1:G:166:THR:O	1:G:170:ILE:HG13	2.14	0.47
1:G:300:ALA:O	1:G:304:ILE:HG13	2.15	0.47
1:I:266:HIS:CD2	1:L:305:ARG:HG2	2.49	0.47
1:K:115:THR:HG21	1:K:297:PRO:HB3	1.95	0.47
1:K:345:HIS:CE1	1:K:347:GLU:HG2	2.49	0.47
1:L:127:GLU:OE2	1:L:242:PRO:HB3	2.15	0.47
1:L:211:ASN:HB2	1:L:239:PHE:HE2	1.80	0.47
1:L:223:SER:HA	1:L:233:VAL:HG21	1.97	0.47
1:L:366:VAL:HG12	1:L:367:ASP:N	2.30	0.47
1:L:386:ALA:HB1	1:L:387:PRO:CD	2.44	0.47
1:A:103:ARG:HG2	1:A:104:ALA:N	2.30	0.47
1:E:57:ASP:HB3	1:E:243:LEU:CD2	2.45	0.47
1:F:75:ASP:OD1	1:F:75:ASP:N	2.47	0.47
1:G:173:ILE:C	1:G:175:PRO:HD2	2.39	0.47
1:H:373:THR:O	1:H:377:VAL:HG13	2.15	0.47
1:I:240:ALA:O	1:I:244:ASN:HB2	2.15	0.47
1:I:387:PRO:O	1:I:388:SER:HB3	2.14	0.47
1:B:428:VAL:HG12	1:C:62:ILE:CD1	2.45	0.47
1:E:78:THR:HG21	1:H:268:ASP:HB3	1.96	0.47
1:B:72:ILE:HD12	1:B:80:PRO:HG2	1.97	0.47
1:B:215:ARG:HD2	1:B:347:GLU:OE2	2.15	0.47
1:B:240:ALA:O	1:B:244:ASN:HB2	2.15	0.47
1:C:210:THR:HG23	1:C:211:ASN:N	2.29	0.47
1:C:258:SER:C	1:C:260:THR:N	2.71	0.47
1:J:396:VAL:HG13	1:J:424:PHE:CD2	2.50	0.47
1:K:223:SER:HA	1:K:233:VAL:HG21	1.96	0.47
1:F:242:PRO:O	1:F:246:LYS:HE2	2.15	0.46
1:F:369:ASP:H	1:F:372:THR:HB	1.79	0.46
1:G:159:THR:HA	1:G:184:ILE:O	2.15	0.46
1:H:428:VAL:HG13	1:H:428:VAL:O	2.14	0.46
1:J:343:GLN:HA	1:J:348:HIS:CD2	2.50	0.46
1:F:310:LEU:O	1:F:314:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:72:ILE:O	1:I:72:ILE:CG2	2.62	0.46
1:I:207:GLU:CB	1:I:236:ASP:HB3	2.43	0.46
1:J:261:LYS:HD2	1:J:389:PHE:CE2	2.51	0.46
1:K:277:PRO:HG2	1:K:280:LEU:HB2	1.97	0.46
1:L:300:ALA:O	1:L:304:ILE:HG13	2.15	0.46
1:A:386:ALA:HB2	1:C:88:PHE:HA	1.97	0.46
1:B:98:PHE:HE2	1:B:99:LYS:HE2	1.79	0.46
1:B:127:GLU:OE2	1:B:257:HIS:NE2	2.46	0.46
1:C:153:GLY:HA2	1:C:178:GLY:O	2.15	0.46
1:D:345:HIS:CE1	1:D:347:GLU:HG2	2.50	0.46
1:I:82:VAL:HG22	1:J:80:PRO:HB3	1.96	0.46
1:I:173:ILE:C	1:I:175:PRO:HD2	2.39	0.46
1:I:291:LEU:HD22	1:K:143:THR:HG21	1.97	0.46
1:D:210:THR:HG22	1:D:215:ARG:H	1.80	0.46
1:E:96:ILE:O	1:E:100:GLU:HG3	2.16	0.46
1:G:383:PRO:HA	1:G:394:SER:O	2.16	0.46
1:K:63:HIS:HB3	1:K:67:ARG:CB	2.45	0.46
1:L:72:ILE:O	1:L:72:ILE:CG2	2.64	0.46
1:L:240:ALA:O	1:L:244:ASN:HB2	2.16	0.46
1:A:215:ARG:HD2	1:A:347:GLU:OE2	2.16	0.46
1:C:103:ARG:HG2	1:C:104:ALA:N	2.30	0.46
1:C:174:LEU:N	1:C:175:PRO:CD	2.77	0.46
1:E:156:ILE:HG22	1:E:181:ALA:HB2	1.96	0.46
1:F:211:ASN:HB2	1:F:239:PHE:HE2	1.80	0.46
1:H:210:THR:HG23	1:H:211:ASN:N	2.30	0.46
1:L:174:LEU:N	1:L:175:PRO:CD	2.75	0.46
1:C:418:MET:C	1:C:420:ASN:H	2.23	0.46
1:E:397:ASP:HB2	1:E:402:MET:HG3	1.98	0.46
1:H:223:SER:HA	1:H:233:VAL:HG21	1.97	0.46
1:D:418:MET:C	1:D:420:ASN:H	2.22	0.46
1:E:255:VAL:O	1:E:255:VAL:HG13	2.15	0.46
1:E:370:LEU:HD23	1:E:419:ASP:HB3	1.98	0.46
1:G:428:VAL:HG13	1:G:428:VAL:O	2.15	0.46
1:H:53:PHE:CE1	1:H:54:LEU:HG	2.50	0.46
1:I:166:THR:O	1:I:170:ILE:HG13	2.16	0.46
1:I:418:MET:C	1:I:420:ASN:H	2.23	0.46
1:K:72:ILE:O	1:K:72:ILE:CG2	2.63	0.46
1:B:396:VAL:HG13	1:B:424:PHE:CD2	2.50	0.46
1:G:72:ILE:O	1:G:72:ILE:CG2	2.61	0.46
1:G:261:LYS:HD2	1:G:389:PHE:CZ	2.50	0.46
1:I:321:ALA:HB2	1:I:360:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:63:HIS:HE1	1:K:429:GLU:OE2	1.99	0.46
1:J:255:VAL:HG13	1:J:255:VAL:O	2.15	0.46
1:L:277:PRO:HG2	1:L:280:LEU:HB2	1.98	0.46
1:A:431:PHE:HD1	1:A:431:PHE:O	1.99	0.46
1:B:54:LEU:HD22	1:B:59:SER:CB	2.44	0.46
1:C:215:ARG:HD2	1:C:347:GLU:OE2	2.15	0.46
1:C:398:GLN:O	1:C:399:PRO:C	2.58	0.46
1:E:240:ALA:O	1:E:244:ASN:HB2	2.16	0.46
1:F:370:LEU:HD23	1:F:419:ASP:HB3	1.97	0.46
1:H:53:PHE:HD1	1:H:54:LEU:HG	1.80	0.46
1:H:386:ALA:HB1	1:H:387:PRO:CD	2.46	0.46
1:J:331:HIS:ND1	1:J:332:PRO:HD2	2.31	0.46
1:K:250:LEU:CD1	1:K:354:GLN:HB2	2.46	0.46
1:L:166:THR:O	1:L:170:ILE:HG13	2.15	0.46
1:C:345:HIS:CE1	1:C:347:GLU:HG2	2.51	0.46
1:D:131:SER:OG	1:D:281:VAL:HG11	2.16	0.46
1:D:174:LEU:N	1:D:175:PRO:CD	2.78	0.46
1:F:250:LEU:CD1	1:F:354:GLN:HB2	2.46	0.46
1:F:343:GLN:HA	1:F:348:HIS:CD2	2.50	0.46
1:H:192:LEU:HD22	1:H:222:VAL:HG22	1.98	0.46
1:K:386:ALA:HB1	1:K:387:PRO:CD	2.46	0.46
1:A:337:VAL:HG22	1:A:364:PHE:HB3	1.98	0.45
1:F:383:PRO:HB3	1:F:394:SER:HB3	1.97	0.45
1:G:206:THR:O	1:G:235:ILE:HA	2.16	0.45
1:G:212:PRO:HG2	1:G:421:LEU:HD21	1.98	0.45
1:G:250:LEU:CD1	1:G:354:GLN:HB2	2.45	0.45
1:J:64:ALA:O	1:J:122:LYS:HE2	2.16	0.45
1:K:53:PHE:CD1	1:K:54:LEU:HG	2.51	0.45
1:E:72:ILE:HD12	1:E:80:PRO:HG2	1.97	0.45
1:E:170:ILE:HA	1:E:174:LEU:HD12	1.98	0.45
1:E:312:LEU:HD11	1:H:428:VAL:CG2	2.46	0.45
1:F:82:VAL:HG21	1:F:114:PRO:CG	2.46	0.45
1:F:206:THR:O	1:F:235:ILE:HA	2.16	0.45
1:F:321:ALA:HB2	1:F:360:GLY:HA2	1.97	0.45
1:G:53:PHE:CE1	1:G:54:LEU:HG	2.51	0.45
1:L:57:ASP:HB3	1:L:243:LEU:CD2	2.46	0.45
1:B:207:GLU:CB	1:B:236:ASP:HB3	2.45	0.45
1:K:215:ARG:HD2	1:K:347:GLU:OE2	2.16	0.45
1:L:192:LEU:HG	1:L:196:LEU:HD23	1.97	0.45
1:C:98:PHE:HE2	1:C:99:LYS:HE2	1.81	0.45
1:C:241:THR:CG2	1:C:243:LEU:H	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:335:ARG:HH21	1:F:367:ASP:HA	1.81	0.45
1:H:206:THR:O	1:H:235:ILE:HA	2.16	0.45
1:H:212:PRO:HG2	1:H:421:LEU:HD21	1.99	0.45
1:I:72:ILE:HD11	1:J:72:ILE:HD11	1.97	0.45
1:I:131:SER:CB	1:I:281:VAL:HG11	2.46	0.45
1:J:346:PRO:HB2	1:J:347:GLU:OE2	2.17	0.45
1:J:370:LEU:HD23	1:J:419:ASP:HB3	1.98	0.45
1:J:379:ALA:HB3	1:J:441:ALA:HB1	1.98	0.45
1:J:386:ALA:HB1	1:J:387:PRO:CD	2.46	0.45
1:K:206:THR:O	1:K:235:ILE:HA	2.15	0.45
1:K:241:THR:HG22	1:K:243:LEU:N	2.14	0.45
1:L:351:ALA:O	1:L:355:MET:HB2	2.16	0.45
1:L:428:VAL:O	1:L:428:VAL:CG1	2.63	0.45
1:E:241:THR:HG23	1:E:242:PRO:HD2	1.98	0.45
1:F:418:MET:C	1:F:420:ASN:N	2.75	0.45
1:I:63:HIS:HE1	1:L:429:GLU:OE2	1.99	0.45
1:I:243:LEU:HD12	1:I:314:VAL:HG21	1.98	0.45
1:I:343:GLN:HA	1:I:348:HIS:CD2	2.51	0.45
1:J:242:PRO:O	1:J:246:LYS:HE2	2.17	0.45
1:L:241:THR:HG23	1:L:242:PRO:HD2	1.99	0.45
1:A:383:PRO:HB2	1:A:396:VAL:CG2	2.45	0.45
1:B:187:ALA:O	1:B:189:VAL:HG23	2.16	0.45
1:B:208:SER:HA	1:B:209:PRO:C	2.41	0.45
1:A:215:ARG:NH1	1:A:347:GLU:OE2	2.50	0.45
1:B:163:TYR:CE2	1:B:165:LYS:HB2	2.52	0.45
1:B:418:MET:C	1:B:420:ASN:N	2.71	0.45
1:D:256:LEU:HB2	1:D:273:CYS:O	2.17	0.45
1:D:365:GLU:HB3	1:D:420:ASN:HB3	1.97	0.45
1:F:210:THR:HG22	1:F:215:ARG:H	1.81	0.45
1:H:209:PRO:HG3	1:H:355:MET:HE1	1.98	0.45
1:I:323:ARG:CZ	1:I:431:PHE:HD2	2.30	0.45
1:C:428:VAL:O	1:C:428:VAL:CG1	2.64	0.45
1:D:192:LEU:HG	1:D:196:LEU:HD23	1.99	0.45
1:E:250:LEU:CD1	1:E:354:GLN:HB2	2.46	0.45
1:E:261:LYS:HD2	1:E:389:PHE:CZ	2.52	0.45
1:G:259:ALA:HB3	1:G:271:ALA:HB3	1.98	0.45
1:H:310:LEU:O	1:H:314:VAL:HG23	2.16	0.45
1:J:98:PHE:HE2	1:J:99:LYS:HE2	1.81	0.45
1:J:240:ALA:O	1:J:244:ASN:HB2	2.16	0.45
1:A:386:ALA:HB1	1:A:387:PRO:CD	2.46	0.45
1:B:62:ILE:CD1	1:C:428:VAL:HG12	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:PHE:O	1:B:108:TYR:N	2.49	0.45
1:C:397:ASP:HB2	1:C:402:MET:HG3	1.99	0.45
1:E:345:HIS:HE1	1:E:347:GLU:HG2	1.81	0.45
1:E:382:ILE:HB	1:E:383:PRO:HD3	1.99	0.45
1:F:256:LEU:HB2	1:F:273:CYS:O	2.17	0.45
1:G:441:ALA:C	1:G:443:ASP:N	2.74	0.45
1:I:379:ALA:HB3	1:I:441:ALA:HB1	1.99	0.45
1:K:396:VAL:HG13	1:K:424:PHE:CD2	2.51	0.45
1:B:324:MET:HG2	1:B:431:PHE:HE1	1.82	0.45
1:E:140:CYS:O	1:E:144:VAL:HG23	2.16	0.45
1:E:428:VAL:CG2	1:H:312:LEU:HD11	2.47	0.45
1:H:63:HIS:HB3	1:H:67:ARG:CB	2.46	0.45
1:I:64:ALA:O	1:I:122:LYS:HE2	2.17	0.45
1:L:122:LYS:NZ	1:L:308:LYS:HE2	2.31	0.45
1:A:127:GLU:OE2	1:A:257:HIS:NE2	2.49	0.44
1:D:144:VAL:HG22	1:D:291:LEU:HD12	1.99	0.44
1:E:194:LEU:HG	1:E:198:GLN:CD	2.42	0.44
1:H:144:VAL:HG12	1:H:284:ILE:HG23	2.00	0.44
1:H:242:PRO:HD3	1:H:257:HIS:CE1	2.51	0.44
1:I:250:LEU:CD1	1:I:354:GLN:HB2	2.47	0.44
1:I:277:PRO:HG2	1:I:280:LEU:HB2	1.98	0.44
1:A:382:ILE:HB	1:A:383:PRO:HD3	1.99	0.44
1:C:258:SER:O	1:C:260:THR:N	2.51	0.44
1:H:174:LEU:N	1:H:175:PRO:CD	2.81	0.44
1:H:192:LEU:HG	1:H:196:LEU:HD23	1.99	0.44
1:H:196:LEU:HD12	1:H:229:LYS:HB2	1.97	0.44
1:H:369:ASP:H	1:H:372:THR:HB	1.82	0.44
1:I:192:LEU:HD22	1:I:222:VAL:HG22	1.98	0.44
1:K:106:PHE:O	1:K:108:TYR:N	2.50	0.44
1:K:398:GLN:O	1:K:399:PRO:C	2.61	0.44
1:L:106:PHE:O	1:L:108:TYR:N	2.50	0.44
1:C:122:LYS:NZ	1:C:308:LYS:HE2	2.32	0.44
1:E:185:ASP:CG	1:E:186:PRO:HD2	2.42	0.44
1:I:382:ILE:HB	1:I:383:PRO:HD3	1.99	0.44
1:I:431:PHE:C	1:I:431:PHE:HD1	2.23	0.44
1:J:420:ASN:HD22	1:J:420:ASN:HA	1.58	0.44
1:K:418:MET:C	1:K:420:ASN:N	2.73	0.44
1:H:331:HIS:ND1	1:H:332:PRO:HD2	2.32	0.44
1:H:418:MET:C	1:H:420:ASN:H	2.26	0.44
1:L:64:ALA:O	1:L:122:LYS:HE2	2.17	0.44
1:E:245:GLN:OE1	1:E:355:MET:HE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:212:PRO:HD2	1:H:213:PHE:CD2	2.53	0.44
1:L:207:GLU:CB	1:L:236:ASP:HB3	2.46	0.44
1:L:324:MET:HG2	1:L:431:PHE:HE1	1.83	0.44
1:L:345:HIS:CE1	1:L:347:GLU:HG2	2.53	0.44
1:A:428:VAL:O	1:A:428:VAL:CG1	2.65	0.44
1:C:170:ILE:HG23	1:C:174:LEU:HD12	2.00	0.44
1:C:196:LEU:HD13	1:C:196:LEU:HA	1.87	0.44
1:C:395:ILE:HG22	1:C:396:VAL:N	2.33	0.44
1:E:215:ARG:NH1	1:E:347:GLU:OE2	2.50	0.44
1:E:242:PRO:O	1:E:246:LYS:HE2	2.18	0.44
1:F:82:VAL:CG2	1:F:114:PRO:HG2	2.48	0.44
1:I:428:VAL:HG22	1:L:312:LEU:HD11	2.00	0.44
1:A:420:ASN:HD22	1:A:420:ASN:HA	1.56	0.44
1:B:258:SER:C	1:B:260:THR:N	2.75	0.44
1:C:376:PHE:CB	1:C:445:ILE:HD11	2.29	0.44
1:D:348:HIS:O	1:D:352:LYS:HB2	2.18	0.44
1:E:277:PRO:HG2	1:E:280:LEU:HB2	1.99	0.44
1:F:428:VAL:HG12	1:G:62:ILE:CD1	2.40	0.44
1:G:217:VAL:O	1:G:219:ILE:N	2.51	0.44
1:I:143:THR:HG22	1:I:144:VAL:N	2.33	0.44
1:I:331:HIS:CE1	1:I:333:LYS:HB2	2.52	0.44
1:K:155:HIS:ND1	1:K:180:THR:HG23	2.33	0.44
1:A:376:PHE:HB2	1:A:445:ILE:HD11	2.00	0.44
1:D:82:VAL:HG21	1:D:114:PRO:HG2	2.00	0.44
1:D:258:SER:C	1:D:260:THR:N	2.74	0.44
1:D:383:PRO:HB2	1:D:396:VAL:CG2	2.48	0.44
1:G:241:THR:HG23	1:G:242:PRO:HD2	2.00	0.44
1:G:296:ASN:OD1	1:G:298:ASN:HB2	2.18	0.44
1:I:339:TYR:CD1	1:I:362:VAL:HG22	2.52	0.44
1:J:129:ALA:HB2	1:J:248:LEU:CD1	2.48	0.44
1:J:210:THR:HG22	1:J:215:ARG:H	1.82	0.44
1:J:383:PRO:HB3	1:J:394:SER:HB3	1.99	0.44
1:K:131:SER:OG	1:K:281:VAL:HG11	2.17	0.44
1:B:262:PHE:CE1	1:B:390:GLY:HA2	2.52	0.44
1:E:346:PRO:HB2	1:E:347:GLU:OE2	2.18	0.44
1:G:382:ILE:HB	1:G:383:PRO:HD3	1.99	0.44
1:H:192:LEU:O	1:H:196:LEU:HB2	2.17	0.44
1:I:261:LYS:HD2	1:I:389:PHE:CZ	2.53	0.44
1:J:212:PRO:HG2	1:J:421:LEU:HD21	1.99	0.44
1:C:138:GLY:O	1:C:141:ALA:HB3	2.18	0.43
1:D:255:VAL:HG13	1:D:255:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:VAL:HG13	1:D:424:PHE:CD2	2.53	0.43
1:E:207:GLU:HG3	1:E:210:THR:HA	1.99	0.43
1:G:174:LEU:N	1:G:175:PRO:CD	2.81	0.43
1:I:255:VAL:O	1:I:255:VAL:HG13	2.18	0.43
1:J:268:ASP:HB3	1:K:78:THR:HG21	1.99	0.43
1:K:115:THR:CG2	1:K:297:PRO:HB3	2.48	0.43
1:L:321:ALA:HB2	1:L:360:GLY:HA2	1.99	0.43
1:L:347:GLU:CB	1:L:350:ILE:HD12	2.41	0.43
1:C:255:VAL:HG13	1:C:255:VAL:O	2.17	0.43
1:E:65:GLY:O	1:E:118:VAL:HG13	2.18	0.43
1:I:134:LEU:HD22	1:I:295:LEU:HD22	1.99	0.43
1:L:144:VAL:HG12	1:L:284:ILE:HG23	1.99	0.43
1:C:369:ASP:H	1:C:372:THR:HB	1.82	0.43
1:C:418:MET:C	1:C:420:ASN:N	2.76	0.43
1:J:82:VAL:HG21	1:J:114:PRO:HG2	1.99	0.43
1:K:63:HIS:CD2	1:K:67:ARG:HD3	2.54	0.43
1:K:140:CYS:O	1:K:144:VAL:HG23	2.19	0.43
1:L:131:SER:HB3	1:L:281:VAL:HG11	2.00	0.43
1:A:241:THR:HG23	1:A:242:PRO:HD2	2.00	0.43
1:B:223:SER:HA	1:B:233:VAL:HG21	2.00	0.43
1:B:323:ARG:NH1	1:B:431:PHE:CD2	2.86	0.43
1:D:383:PRO:HA	1:D:394:SER:O	2.18	0.43
1:E:331:HIS:CE1	1:E:333:LYS:HB2	2.54	0.43
1:E:339:TYR:HB3	1:E:342:LEU:HG	2.00	0.43
1:E:428:VAL:O	1:E:428:VAL:CG1	2.64	0.43
1:F:428:VAL:HG21	1:G:312:LEU:HD11	2.00	0.43
1:G:347:GLU:HB3	1:G:350:ILE:HD12	1.99	0.43
1:H:383:PRO:HA	1:H:394:SER:O	2.18	0.43
1:I:428:VAL:CG2	1:L:312:LEU:HD11	2.47	0.43
1:J:339:TYR:CZ	1:J:358:PHE:HB2	2.53	0.43
1:K:232:LEU:HD23	1:K:232:LEU:HA	1.89	0.43
1:L:383:PRO:HB2	1:L:396:VAL:CG2	2.48	0.43
1:A:143:THR:HG22	1:A:144:VAL:N	2.33	0.43
1:A:428:VAL:HG21	1:D:312:LEU:HD11	2.00	0.43
1:E:396:VAL:O	1:E:397:ASP:HB3	2.19	0.43
1:E:431:PHE:CE1	1:E:435:LYS:HD3	2.53	0.43
1:G:210:THR:HG23	1:G:211:ASN:N	2.33	0.43
1:J:206:THR:O	1:J:235:ILE:HA	2.19	0.43
1:J:418:MET:C	1:J:420:ASN:N	2.76	0.43
1:K:150:VAL:HA	1:K:151:PRO:HD3	1.87	0.43
1:B:63:HIS:CD2	1:B:67:ARG:HD3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:LEU:HD13	1:E:196:LEU:HA	1.86	0.43
1:F:208:SER:HA	1:F:209:PRO:C	2.44	0.43
1:G:215:ARG:NH1	1:G:347:GLU:OE2	2.52	0.43
1:G:383:PRO:HB3	1:G:394:SER:HB3	1.99	0.43
1:H:370:LEU:HD23	1:H:419:ASP:HB3	2.01	0.43
1:H:382:ILE:HB	1:H:383:PRO:HD3	1.99	0.43
1:I:324:MET:HE2	1:I:438:ILE:CD1	2.48	0.43
1:A:86:ALA:HB1	1:C:387:PRO:HD2	1.99	0.43
1:B:243:LEU:HD12	1:B:314:VAL:HG21	1.99	0.43
1:E:343:GLN:HA	1:E:348:HIS:CD2	2.53	0.43
1:G:113:ASN:OD1	1:G:115:THR:CG2	2.67	0.43
1:I:174:LEU:N	1:I:175:PRO:CD	2.80	0.43
1:K:57:ASP:HB3	1:K:243:LEU:CD2	2.48	0.43
1:K:187:ALA:O	1:K:189:VAL:HG23	2.19	0.43
1:L:242:PRO:HD3	1:L:257:HIS:CE1	2.54	0.43
1:A:174:LEU:N	1:A:175:PRO:CD	2.80	0.43
1:A:212:PRO:HG2	1:A:421:LEU:HD21	2.01	0.43
1:D:208:SER:HA	1:D:209:PRO:C	2.44	0.43
1:D:428:VAL:O	1:D:428:VAL:CG1	2.67	0.43
1:F:240:ALA:O	1:F:244:ASN:HB2	2.18	0.43
1:F:345:HIS:CE1	1:F:347:GLU:HG2	2.54	0.43
1:I:145:MET:HE2	1:I:146:LEU:HA	2.01	0.43
1:J:122:LYS:NZ	1:J:308:LYS:HE2	2.33	0.43
1:J:127:GLU:OE2	1:J:242:PRO:HB3	2.18	0.43
1:L:319:SER:O	1:L:320:THR:C	2.62	0.43
1:A:438:ILE:O	1:A:442:LEU:HD12	2.18	0.43
1:B:296:ASN:OD1	1:B:298:ASN:HB2	2.18	0.43
1:C:310:LEU:HA	1:C:313:ARG:NH2	2.34	0.43
1:F:232:LEU:HD23	1:F:232:LEU:HA	1.92	0.43
1:H:150:VAL:HA	1:H:151:PRO:HD3	1.89	0.43
1:I:129:ALA:HB2	1:I:248:LEU:CD1	2.49	0.43
1:J:339:TYR:OH	1:J:358:PHE:HB2	2.19	0.43
1:D:258:SER:O	1:D:260:THR:N	2.52	0.43
1:H:258:SER:C	1:H:260:THR:N	2.76	0.43
1:I:258:SER:C	1:I:260:THR:N	2.75	0.43
1:L:73:VAL:O	1:L:74:THR:HG23	2.19	0.43
1:B:215:ARG:NH1	1:B:347:GLU:OE2	2.52	0.42
1:B:380:LEU:HD13	1:B:396:VAL:HG21	2.00	0.42
1:B:428:VAL:HG22	1:C:312:LEU:HD11	2.01	0.42
1:C:144:VAL:HG22	1:C:291:LEU:HD12	2.00	0.42
1:E:331:HIS:CG	1:E:332:PRO:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:ARG:HD2	1:F:404:TYR:CE2	2.53	0.42
1:H:73:VAL:O	1:H:74:THR:HG23	2.18	0.42
1:H:79:THR:HA	1:H:80:PRO:HD3	1.88	0.42
1:J:103:ARG:HG2	1:J:104:ALA:N	2.34	0.42
1:J:155:HIS:HA	1:J:180:THR:O	2.19	0.42
1:K:208:SER:HA	1:K:209:PRO:C	2.44	0.42
1:L:265:GLY:HA3	1:L:313:ARG:NH1	2.34	0.42
1:A:240:ALA:O	1:A:244:ASN:HB2	2.19	0.42
1:B:123:ILE:HD13	1:B:273:CYS:SG	2.59	0.42
1:C:131:SER:HB3	1:C:281:VAL:HG11	2.00	0.42
1:C:215:ARG:NH1	1:C:347:GLU:OE2	2.49	0.42
1:C:258:SER:C	1:C:260:THR:H	2.27	0.42
1:D:250:LEU:CD1	1:D:354:GLN:HB2	2.45	0.42
1:E:79:THR:HA	1:E:80:PRO:HD3	1.90	0.42
1:E:312:LEU:HD11	1:H:428:VAL:HG22	2.01	0.42
1:H:70:ARG:HD3	1:H:79:THR:OG1	2.19	0.42
1:I:106:PHE:O	1:I:108:TYR:N	2.50	0.42
1:I:113:ASN:ND2	1:I:297:PRO:HG3	2.34	0.42
1:J:383:PRO:HA	1:J:394:SER:O	2.19	0.42
1:L:324:MET:HE2	1:L:438:ILE:CD1	2.49	0.42
1:A:64:ALA:O	1:A:122:LYS:HE2	2.18	0.42
1:A:339:TYR:CZ	1:A:358:PHE:HB2	2.54	0.42
1:A:428:VAL:HG22	1:D:312:LEU:HD11	2.01	0.42
1:B:339:TYR:CD1	1:B:362:VAL:HG22	2.54	0.42
1:C:372:THR:CG2	1:C:445:ILE:HG23	2.49	0.42
1:C:376:PHE:HB2	1:C:445:ILE:CD1	2.29	0.42
1:E:82:VAL:CG2	1:E:114:PRO:HG2	2.50	0.42
1:E:215:ARG:HD2	1:E:347:GLU:OE2	2.20	0.42
1:L:206:THR:O	1:L:235:ILE:HA	2.19	0.42
1:A:374:ALA:O	1:A:377:VAL:HG22	2.19	0.42
1:D:398:GLN:O	1:D:399:PRO:C	2.62	0.42
1:E:57:ASP:HB3	1:E:243:LEU:HD22	2.01	0.42
1:E:258:SER:C	1:E:260:THR:N	2.77	0.42
1:E:339:TYR:OH	1:E:358:PHE:HB2	2.20	0.42
1:G:255:VAL:O	1:G:255:VAL:HG13	2.19	0.42
1:G:366:VAL:HG11	1:G:445:ILE:HD13	2.02	0.42
1:H:232:LEU:HD23	1:H:232:LEU:HA	1.92	0.42
1:J:209:PRO:HD3	1:J:240:ALA:HB2	2.01	0.42
1:L:63:HIS:CD2	1:L:67:ARG:HD3	2.54	0.42
1:L:331:HIS:CG	1:L:332:PRO:HD2	2.54	0.42
1:L:384:TYR:O	1:L:395:ILE:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLY:O	1:C:140:CYS:HB2	2.18	0.42
1:C:420:ASN:HD22	1:C:420:ASN:HA	1.56	0.42
1:D:150:VAL:HA	1:D:151:PRO:HD3	1.86	0.42
1:E:322:LEU:O	1:E:325:ALA:HB3	2.19	0.42
1:F:261:LYS:HD2	1:F:389:PHE:CZ	2.55	0.42
1:G:72:ILE:HD12	1:G:80:PRO:HG2	2.00	0.42
1:H:60:VAL:C	1:H:62:ILE:N	2.76	0.42
1:I:58:GLY:O	1:I:62:ILE:HG13	2.19	0.42
1:J:256:LEU:HB2	1:J:273:CYS:O	2.18	0.42
1:K:72:ILE:HD11	1:L:72:ILE:HD11	2.01	0.42
1:L:57:ASP:HB3	1:L:243:LEU:HD22	2.01	0.42
1:L:210:THR:HG23	1:L:211:ASN:N	2.34	0.42
1:A:210:THR:O	1:A:214:LEU:HA	2.19	0.42
1:A:241:THR:C	1:A:243:LEU:H	2.27	0.42
1:E:80:PRO:O	1:E:115:THR:HB	2.20	0.42
1:H:113:ASN:ND2	1:H:297:PRO:HG3	2.33	0.42
1:H:339:TYR:CD1	1:H:362:VAL:HG22	2.54	0.42
1:I:396:VAL:HG13	1:I:424:PHE:CD2	2.53	0.42
1:J:57:ASP:HB3	1:J:243:LEU:CD2	2.50	0.42
1:J:265:GLY:O	1:J:391:GLY:HA2	2.20	0.42
1:K:196:LEU:HD13	1:K:196:LEU:HA	1.93	0.42
1:A:173:ILE:C	1:A:175:PRO:HD2	2.44	0.42
1:D:82:VAL:HG12	1:D:84:THR:HG22	2.02	0.42
1:D:211:ASN:HA	1:D:212:PRO:HA	1.86	0.42
1:E:155:HIS:HA	1:E:180:THR:O	2.20	0.42
1:F:70:ARG:C	1:F:72:ILE:H	2.28	0.42
1:G:366:VAL:HG12	1:G:367:ASP:N	2.34	0.42
1:I:280:LEU:O	1:I:283:GLU:HB2	2.20	0.42
1:J:312:LEU:HD11	1:K:428:VAL:CG2	2.49	0.42
1:J:331:HIS:CE1	1:J:333:LYS:HB2	2.55	0.42
1:A:323:ARG:NH1	1:A:431:PHE:CE2	2.88	0.42
1:D:398:GLN:O	1:D:401:ILE:N	2.53	0.42
1:E:374:ALA:HB1	1:G:92:THR:HG21	2.02	0.42
1:F:223:SER:HA	1:F:233:VAL:HG21	2.01	0.42
1:G:258:SER:C	1:G:260:THR:N	2.78	0.42
1:G:383:PRO:HB2	1:G:396:VAL:CG2	2.46	0.42
1:I:383:PRO:HA	1:I:394:SER:O	2.19	0.42
1:K:258:SER:C	1:K:260:THR:N	2.77	0.42
1:E:53:PHE:CE1	1:E:54:LEU:HG	2.55	0.42
1:H:155:HIS:HA	1:H:180:THR:O	2.20	0.42
1:I:429:GLU:OE2	1:L:63:HIS:CE1	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:212:PRO:HG2	1:K:421:LEU:HD21	2.01	0.42
1:A:57:ASP:HB3	1:A:243:LEU:CD2	2.50	0.42
1:A:312:LEU:HD11	1:D:428:VAL:CG2	2.50	0.42
1:C:159:THR:HA	1:C:184:ILE:O	2.20	0.42
1:C:321:ALA:HB2	1:C:360:GLY:HA2	2.01	0.42
1:E:291:LEU:HD22	1:G:143:THR:HG21	2.01	0.42
1:E:413:ALA:C	1:E:415:TYR:N	2.78	0.42
1:I:206:THR:O	1:I:235:ILE:HA	2.20	0.42
1:I:210:THR:HG22	1:I:215:ARG:H	1.85	0.42
1:K:192:LEU:HG	1:K:196:LEU:HD23	2.02	0.42
1:L:369:ASP:O	1:L:370:LEU:C	2.62	0.42
1:A:194:LEU:O	1:A:198:GLN:HG3	2.19	0.41
1:A:339:TYR:CD1	1:A:362:VAL:HG22	2.55	0.41
1:B:145:MET:CE	1:B:146:LEU:HD23	2.50	0.41
1:C:383:PRO:CB	1:C:396:VAL:HG22	2.46	0.41
1:E:324:MET:HE2	1:E:438:ILE:HD12	2.02	0.41
1:F:265:GLY:HA3	1:F:313:ARG:NH1	2.35	0.41
1:H:296:ASN:HA	1:H:297:PRO:HD3	1.94	0.41
1:J:331:HIS:CG	1:J:332:PRO:HD2	2.54	0.41
1:K:60:VAL:C	1:K:62:ILE:N	2.76	0.41
1:K:395:ILE:HG22	1:K:396:VAL:N	2.34	0.41
1:K:398:GLN:O	1:K:401:ILE:N	2.53	0.41
1:L:255:VAL:O	1:L:255:VAL:HG13	2.20	0.41
1:L:331:HIS:ND1	1:L:332:PRO:HD2	2.35	0.41
1:B:138:GLY:N	2:B:500:PLP:O2P	2.53	0.41
1:B:310:LEU:O	1:B:314:VAL:HG23	2.20	0.41
1:D:258:SER:C	1:D:260:THR:H	2.28	0.41
1:E:115:THR:CG2	1:E:297:PRO:HB3	2.50	0.41
1:F:366:VAL:HG12	1:F:367:ASP:N	2.34	0.41
1:G:211:ASN:HB2	1:G:239:PHE:HE2	1.85	0.41
1:I:418:MET:C	1:I:420:ASN:N	2.76	0.41
1:J:211:ASN:HA	1:J:212:PRO:HA	1.91	0.41
1:B:373:THR:O	1:B:377:VAL:HG13	2.20	0.41
1:B:419:ASP:OD1	1:B:419:ASP:N	2.52	0.41
1:E:82:VAL:HG21	1:E:114:PRO:CG	2.50	0.41
1:E:269:VAL:C	1:E:270:LEU:HD23	2.45	0.41
1:E:270:LEU:HD23	1:E:270:LEU:N	2.36	0.41
1:E:280:LEU:O	1:E:283:GLU:HB2	2.20	0.41
1:G:127:GLU:CD	1:G:242:PRO:HB3	2.45	0.41
1:H:126:LEU:HD23	1:H:126:LEU:HA	1.86	0.41
1:H:127:GLU:OE2	1:H:257:HIS:NE2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:394:SER:OG	1:H:427:GLY:N	2.43	0.41
1:I:312:LEU:HD11	1:L:428:VAL:CG2	2.51	0.41
1:I:404:TYR:O	1:I:412:ARG:HD3	2.20	0.41
1:J:208:SER:HA	1:J:209:PRO:C	2.45	0.41
1:A:250:LEU:HD11	1:A:354:GLN:HB2	2.03	0.41
1:A:256:LEU:HB2	1:A:273:CYS:O	2.20	0.41
1:A:278:LEU:O	1:A:279:LYS:C	2.62	0.41
1:B:160:THR:HG23	1:B:183:VAL:HG12	2.03	0.41
1:E:187:ALA:O	1:E:189:VAL:HG23	2.20	0.41
1:G:57:ASP:HB3	1:G:243:LEU:CD2	2.51	0.41
1:G:79:THR:HA	1:G:80:PRO:HD3	1.90	0.41
1:G:127:GLU:OE2	1:G:257:HIS:NE2	2.53	0.41
1:G:337:VAL:HG22	1:G:364:PHE:HB3	2.02	0.41
1:G:386:ALA:HB1	1:G:387:PRO:CD	2.50	0.41
1:H:131:SER:CB	1:H:281:VAL:HG11	2.51	0.41
1:K:270:LEU:N	1:K:270:LEU:HD23	2.35	0.41
1:L:87:TYR:N	1:L:87:TYR:HD2	2.16	0.41
1:L:339:TYR:CD1	1:L:362:VAL:HG22	2.55	0.41
1:L:370:LEU:HD23	1:L:419:ASP:HB3	2.01	0.41
1:L:382:ILE:HB	1:L:383:PRO:HD3	2.03	0.41
1:B:331:HIS:CE1	1:B:333:LYS:HB2	2.55	0.41
1:C:150:VAL:HA	1:C:151:PRO:HD3	1.90	0.41
1:D:72:ILE:O	1:D:72:ILE:CG2	2.66	0.41
1:D:382:ILE:HB	1:D:383:PRO:HD3	2.01	0.41
1:F:319:SER:O	1:F:320:THR:C	2.62	0.41
1:G:207:GLU:H	1:G:207:GLU:HG2	1.75	0.41
1:H:241:THR:C	1:H:243:LEU:H	2.29	0.41
1:H:280:LEU:O	1:H:283:GLU:HB2	2.20	0.41
1:I:241:THR:HG22	1:I:243:LEU:N	2.15	0.41
1:L:260:THR:CG2	1:L:270:LEU:HD22	2.49	0.41
1:C:212:PRO:HG2	1:C:421:LEU:HD21	2.02	0.41
1:E:56:SER:HB3	1:H:433:ASP:OD2	2.20	0.41
1:E:129:ALA:HB2	1:E:248:LEU:CD1	2.50	0.41
1:F:173:ILE:C	1:F:175:PRO:HD2	2.45	0.41
1:F:324:MET:HE2	1:F:438:ILE:CD1	2.49	0.41
1:G:196:LEU:HD13	1:G:196:LEU:HA	1.85	0.41
1:G:418:MET:C	1:G:420:ASN:H	2.27	0.41
1:H:241:THR:HG23	1:H:242:PRO:HD2	2.01	0.41
1:H:262:PHE:CE1	1:H:390:GLY:HA2	2.56	0.41
1:H:324:MET:HG3	1:H:426:PHE:CE1	2.56	0.41
1:J:217:VAL:O	1:J:219:ILE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:339:TYR:HB3	1:K:342:LEU:HG	2.02	0.41
1:A:63:HIS:HE1	1:D:429:GLU:OE2	2.04	0.41
1:A:123:ILE:HG21	1:A:273:CYS:SG	2.61	0.41
1:A:278:LEU:HA	1:A:281:VAL:HG12	2.02	0.41
1:B:64:ALA:O	1:B:122:LYS:HE2	2.20	0.41
1:C:209:PRO:HG3	1:C:355:MET:HE1	2.01	0.41
1:C:377:VAL:HA	1:C:380:LEU:HD12	2.02	0.41
1:E:420:ASN:HD22	1:E:420:ASN:HA	1.58	0.41
1:F:215:ARG:NH1	1:F:347:GLU:OE2	2.54	0.41
1:F:419:ASP:OD1	1:F:419:ASP:N	2.54	0.41
1:I:265:GLY:HA3	1:I:313:ARG:NH1	2.36	0.41
1:J:145:MET:HE2	1:J:146:LEU:HA	2.03	0.41
1:J:156:ILE:CG1	1:J:203:LEU:HD23	2.51	0.41
1:J:210:THR:HG23	1:J:211:ASN:N	2.35	0.41
1:J:347:GLU:CB	1:J:350:ILE:HD12	2.46	0.41
1:K:240:ALA:O	1:K:241:THR:CB	2.59	0.41
1:L:187:ALA:O	1:L:189:VAL:HG23	2.21	0.41
1:A:72:ILE:O	1:A:72:ILE:CG2	2.63	0.41
1:A:220:GLU:HA	1:A:250:LEU:O	2.20	0.41
1:B:192:LEU:HG	1:B:196:LEU:HD23	2.02	0.41
1:D:135:MET:SD	1:D:141:ALA:HA	2.61	0.41
1:E:212:PRO:HG2	1:E:421:LEU:HD21	2.03	0.41
1:F:140:CYS:O	1:F:144:VAL:HG23	2.20	0.41
1:G:96:ILE:O	1:G:100:GLU:HG3	2.21	0.41
1:G:265:GLY:HA3	1:G:313:ARG:NH1	2.36	0.41
1:J:426:PHE:HE1	1:J:438:ILE:HD11	1.86	0.41
1:L:311:HIS:O	1:L:315:GLN:HB2	2.20	0.41
1:L:418:MET:C	1:L:420:ASN:H	2.28	0.41
1:A:243:LEU:HD12	1:A:314:VAL:HG21	2.03	0.41
1:A:331:HIS:CE1	1:A:333:LYS:HB2	2.55	0.41
1:A:387:PRO:HD2	1:C:86:ALA:HB1	2.02	0.41
1:B:119:LEU:HG	1:B:134:LEU:HD11	2.03	0.41
1:B:196:LEU:HD13	1:B:196:LEU:HA	1.85	0.41
1:C:56:SER:O	1:C:60:VAL:HG23	2.20	0.41
1:D:207:GLU:H	1:D:207:GLU:HG2	1.77	0.41
1:D:232:LEU:HD23	1:D:232:LEU:HA	1.94	0.41
1:D:234:CYS:SG	1:D:256:LEU:HD23	2.61	0.41
1:E:60:VAL:C	1:E:62:ILE:N	2.79	0.41
1:E:75:ASP:O	1:F:87:TYR:HA	2.20	0.41
1:E:196:LEU:HD12	1:E:229:LYS:HB2	2.03	0.41
1:G:366:VAL:CG1	1:G:445:ILE:HD13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:420:ASN:HD22	1:H:420:ASN:HA	1.55	0.41
1:I:241:THR:HG23	1:I:242:PRO:HD2	2.03	0.41
1:I:248:LEU:HD23	1:I:248:LEU:HA	1.87	0.41
1:J:65:GLY:O	1:J:118:VAL:HG13	2.21	0.41
1:J:145:MET:HE2	1:J:146:LEU:N	2.36	0.41
1:K:255:VAL:O	1:K:255:VAL:HG13	2.21	0.41
1:L:243:LEU:CD1	1:L:311:HIS:HA	2.51	0.41
1:C:117:VAL:HA	1:C:120:GLU:HB2	2.03	0.41
1:C:123:ILE:HD13	1:C:273:CYS:SG	2.60	0.41
1:D:319:SER:O	1:D:320:THR:C	2.64	0.41
1:D:418:MET:C	1:D:420:ASN:N	2.76	0.41
1:E:164:ARG:O	1:E:167:ARG:HB3	2.20	0.41
1:E:192:LEU:HG	1:E:196:LEU:HD23	2.03	0.41
1:G:155:HIS:O	1:G:202:ASN:HB2	2.20	0.41
1:G:163:TYR:CE2	1:G:165:LYS:HB2	2.56	0.41
1:I:54:LEU:HD22	1:I:59:SER:CB	2.51	0.41
1:L:127:GLU:OE2	1:L:257:HIS:NE2	2.53	0.41
1:L:335:ARG:HH21	1:L:367:ASP:HA	1.85	0.41
1:A:131:SER:OG	1:A:281:VAL:HG11	2.21	0.40
1:B:321:ALA:HB2	1:B:360:GLY:HA2	2.03	0.40
1:D:296:ASN:OD1	1:D:298:ASN:HB2	2.22	0.40
1:F:196:LEU:HD13	1:F:196:LEU:HA	1.87	0.40
1:F:336:HIS:ND1	1:F:337:VAL:N	2.70	0.40
1:H:94:GLU:O	1:H:97:ASP:HB2	2.21	0.40
1:H:355:MET:HB3	1:H:357:GLY:O	2.21	0.40
1:I:51:ALA:HB1	1:I:53:PHE:CE2	2.56	0.40
1:J:270:LEU:HD23	1:J:270:LEU:N	2.36	0.40
1:J:314:VAL:O	1:J:315:GLN:C	2.64	0.40
1:J:324:MET:HE2	1:J:438:ILE:CD1	2.50	0.40
1:J:366:VAL:HG12	1:J:367:ASP:N	2.35	0.40
1:K:155:HIS:HA	1:K:180:THR:O	2.21	0.40
1:K:241:THR:HG23	1:K:242:PRO:HD2	2.04	0.40
1:L:74:THR:C	1:L:76:ALA:H	2.28	0.40
1:D:212:PRO:HG2	1:D:421:LEU:HD21	2.03	0.40
1:F:96:ILE:O	1:F:100:GLU:HG3	2.21	0.40
1:G:204:PHE:CE2	1:G:222:VAL:HG11	2.56	0.40
1:G:223:SER:HA	1:G:233:VAL:HG21	2.02	0.40
1:H:63:HIS:CD2	1:H:67:ARG:HD3	2.57	0.40
1:J:140:CYS:O	1:J:144:VAL:HG23	2.22	0.40
1:K:394:SER:OG	1:K:427:GLY:N	2.40	0.40
1:A:140:CYS:HA	1:C:291:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ARG:O	1:B:167:ARG:HB3	2.22	0.40
1:C:50:TYR:CE2	1:C:64:ALA:HA	2.56	0.40
1:F:204:PHE:CE2	1:F:222:VAL:HG11	2.57	0.40
1:H:138:GLY:N	2:H:500:PLP:O2P	2.54	0.40
1:H:242:PRO:O	1:H:246:LYS:HE2	2.21	0.40
1:J:418:MET:C	1:J:420:ASN:H	2.28	0.40
1:K:348:HIS:O	1:K:352:LYS:HB2	2.22	0.40
1:L:103:ARG:HG2	1:L:104:ALA:N	2.36	0.40
1:B:153:GLY:HA2	1:B:178:GLY:O	2.22	0.40
1:B:319:SER:O	1:B:320:THR:C	2.63	0.40
1:B:334:VAL:HG11	1:B:337:VAL:HG23	2.04	0.40
1:C:204:PHE:CE2	1:C:222:VAL:HG11	2.57	0.40
1:D:155:HIS:HA	1:D:180:THR:O	2.21	0.40
1:E:339:TYR:CZ	1:E:358:PHE:HB2	2.57	0.40
1:F:192:LEU:HG	1:F:196:LEU:HD23	2.04	0.40
1:H:60:VAL:O	1:H:62:ILE:N	2.54	0.40
1:H:143:THR:HG22	1:H:144:VAL:N	2.37	0.40
1:I:164:ARG:HD2	1:I:404:TYR:CE2	2.56	0.40
1:I:428:VAL:O	1:I:428:VAL:CG1	2.67	0.40
1:J:153:GLY:HA2	1:J:178:GLY:O	2.21	0.40
1:J:280:LEU:HD23	1:J:280:LEU:HA	1.92	0.40
1:L:108:TYR:CD2	1:L:110:ARG:HB2	2.55	0.40
1:L:396:VAL:HG13	1:L:424:PHE:CD2	2.57	0.40
1:B:204:PHE:CE2	1:B:222:VAL:HG11	2.56	0.40
1:B:268:ASP:CG	1:C:305:ARG:HH21	2.30	0.40
1:B:420:ASN:HD22	1:B:420:ASN:HA	1.53	0.40
1:D:366:VAL:HG12	1:D:367:ASP:N	2.36	0.40
1:E:62:ILE:CD1	1:H:428:VAL:HG12	2.45	0.40
1:F:268:ASP:HB3	1:G:78:THR:HG21	2.04	0.40
1:H:170:ILE:HG23	1:H:174:LEU:HD12	2.03	0.40
1:I:98:PHE:HE2	1:I:99:LYS:HE2	1.86	0.40
1:J:324:MET:HE2	1:J:438:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	394/445 (88%)	355 (90%)	37 (9%)	2 (0%)	24	57
1	B	394/445 (88%)	364 (92%)	25 (6%)	5 (1%)	9	35
1	C	394/445 (88%)	353 (90%)	37 (9%)	4 (1%)	12	41
1	D	394/445 (88%)	363 (92%)	27 (7%)	4 (1%)	12	41
1	E	394/445 (88%)	354 (90%)	35 (9%)	5 (1%)	9	35
1	F	394/445 (88%)	356 (90%)	35 (9%)	3 (1%)	16	47
1	G	394/445 (88%)	357 (91%)	33 (8%)	4 (1%)	12	41
1	H	394/445 (88%)	363 (92%)	28 (7%)	3 (1%)	16	47
1	I	394/445 (88%)	354 (90%)	37 (9%)	3 (1%)	16	47
1	J	394/445 (88%)	354 (90%)	37 (9%)	3 (1%)	16	47
1	K	394/445 (88%)	359 (91%)	30 (8%)	5 (1%)	9	35
1	L	394/445 (88%)	356 (90%)	34 (9%)	4 (1%)	12	41
All	All	4728/5340 (88%)	4288 (91%)	395 (8%)	45 (1%)	12	41

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	188	ASP
1	C	188	ASP
1	D	188	ASP
1	E	188	ASP
1	F	188	ASP
1	G	188	ASP
1	J	188	ASP
1	J	198	GLN
1	K	188	ASP
1	L	188	ASP
1	A	188	ASP
1	C	259	ALA
1	D	198	GLN
1	D	259	ALA
1	H	198	GLN
1	I	198	GLN
1	K	198	GLN
1	L	198	GLN

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Mol	Chain	Res	Type
1	C	198	GLN
1	E	198	GLN
1	F	198	GLN
1	G	107	GLU
1	H	61	ALA
1	I	188	ASP
1	K	429	GLU
1	A	241	THR
1	B	107	GLU
1	B	259	ALA
1	B	427	GLY
1	C	241	THR
1	E	164	ARG
1	E	259	ALA
1	G	218	ASP
1	L	107	GLU
1	B	241	THR
1	D	241	THR
1	E	241	THR
1	H	241	THR
1	K	241	THR
1	K	388	SER
1	I	241	THR
1	L	241	THR
1	F	241	THR
1	J	241	THR
1	G	241	THR

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	327/364 (90%)	276 (84%)	51 (16%)	2	12
1	B	327/364 (90%)	271 (83%)	56 (17%)	2	10
1	C	327/364 (90%)	273 (84%)	54 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	327/364 (90%)	272 (83%)	55 (17%)	2	10
1	E	327/364 (90%)	276 (84%)	51 (16%)	2	12
1	F	327/364 (90%)	272 (83%)	55 (17%)	2	10
1	G	327/364 (90%)	278 (85%)	49 (15%)	3	13
1	H	327/364 (90%)	274 (84%)	53 (16%)	2	11
1	I	327/364 (90%)	278 (85%)	49 (15%)	3	13
1	J	327/364 (90%)	276 (84%)	51 (16%)	2	12
1	K	327/364 (90%)	274 (84%)	53 (16%)	2	11
1	L	327/364 (90%)	272 (83%)	55 (17%)	2	10
All	All	3924/4368 (90%)	3292 (84%)	632 (16%)	2	11

All (632) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	72	ILE
1	A	73	VAL
1	A	74	THR
1	A	91	LYS
1	A	93	SER
1	A	134	LEU
1	A	135	MET
1	A	142	SER
1	A	143	THR
1	A	145	MET
1	A	156	ILE
1	A	161	ASP
1	A	165	LYS
1	A	177	MET
1	A	180	THR
1	A	196	LEU
1	A	199	LYS
1	A	203	LEU
1	A	207	GLU
1	A	210	THR
1	A	215	ARG
1	A	222	VAL
1	A	224	LYS
1	A	229	LYS

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Mol	Chain	Res	Type
1	A	241	THR
1	A	245	GLN
1	A	256	LEU
1	A	270	LEU
1	A	273	CYS
1	A	275	SER
1	A	278	LEU
1	A	285	ARG
1	A	333	LYS
1	A	343	GLN
1	A	344	SER
1	A	347	GLU
1	A	371	LEU
1	A	372	THR
1	A	375	LYS
1	A	377	VAL
1	A	396	VAL
1	A	403	SER
1	A	410	SER
1	A	415	TYR
1	A	420	ASN
1	A	423	ARG
1	A	428	VAL
1	A	430	ASP
1	A	431	PHE
1	A	444	SER
1	B	70	ARG
1	B	72	ILE
1	B	73	VAL
1	B	74	THR
1	B	91	LYS
1	B	93	SER
1	B	101	LYS
1	B	103	ARG
1	B	134	LEU
1	B	135	MET
1	B	142	SER
1	B	145	MET
1	B	156	ILE
1	B	161	ASP
1	B	165	LYS
1	B	177	MET

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Mol	Chain	Res	Type
1	B	180	THR
1	B	196	LEU
1	B	199	LYS
1	B	203	LEU
1	B	207	GLU
1	B	210	THR
1	B	215	ARG
1	B	222	VAL
1	B	224	LYS
1	B	229	LYS
1	B	241	THR
1	B	270	LEU
1	B	273	CYS
1	B	275	SER
1	B	278	LEU
1	B	279	LYS
1	B	295	LEU
1	B	333	LYS
1	B	343	GLN
1	B	344	SER
1	B	347	GLU
1	B	352	LYS
1	B	371	LEU
1	B	372	THR
1	B	375	LYS
1	B	377	VAL
1	B	396	VAL
1	B	397	ASP
1	B	402	MET
1	B	403	SER
1	B	410	SER
1	B	415	TYR
1	B	419	ASP
1	B	420	ASN
1	B	423	ARG
1	B	428	VAL
1	B	430	ASP
1	B	440	GLN
1	B	444	SER
1	B	445	ILE
1	C	70	ARG
1	C	72	ILE

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Mol	Chain	Res	Type
1	C	73	VAL
1	C	74	THR
1	C	91	LYS
1	C	93	SER
1	C	101	LYS
1	C	103	ARG
1	C	110	ARG
1	C	134	LEU
1	C	135	MET
1	C	142	SER
1	C	145	MET
1	C	156	ILE
1	C	161	ASP
1	C	165	LYS
1	C	177	MET
1	C	180	THR
1	C	196	LEU
1	C	199	LYS
1	C	203	LEU
1	C	207	GLU
1	C	210	THR
1	C	215	ARG
1	C	222	VAL
1	C	224	LYS
1	C	229	LYS
1	C	241	THR
1	C	256	LEU
1	C	270	LEU
1	C	273	CYS
1	C	275	SER
1	C	278	LEU
1	C	279	LYS
1	C	285	ARG
1	C	333	LYS
1	C	343	GLN
1	C	344	SER
1	C	347	GLU
1	C	352	LYS
1	C	371	LEU
1	C	372	THR
1	C	375	LYS
1	C	377	VAL

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Mol	Chain	Res	Type
1	C	396	VAL
1	C	403	SER
1	C	409	GLN
1	C	410	SER
1	C	415	TYR
1	C	420	ASN
1	C	423	ARG
1	C	428	VAL
1	C	430	ASP
1	C	443	ASP
1	D	70	ARG
1	D	72	ILE
1	D	73	VAL
1	D	74	THR
1	D	91	LYS
1	D	93	SER
1	D	101	LYS
1	D	103	ARG
1	D	134	LEU
1	D	135	MET
1	D	142	SER
1	D	143	THR
1	D	145	MET
1	D	156	ILE
1	D	161	ASP
1	D	165	LYS
1	D	177	MET
1	D	180	THR
1	D	182	THR
1	D	196	LEU
1	D	199	LYS
1	D	203	LEU
1	D	207	GLU
1	D	210	THR
1	D	215	ARG
1	D	222	VAL
1	D	224	LYS
1	D	229	LYS
1	D	241	THR
1	D	256	LEU
1	D	270	LEU
1	D	273	CYS

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Mol	Chain	Res	Type
1	D	275	SER
1	D	278	LEU
1	D	279	LYS
1	D	285	ARG
1	D	333	LYS
1	D	343	GLN
1	D	344	SER
1	D	347	GLU
1	D	352	LYS
1	D	353	LYS
1	D	371	LEU
1	D	372	THR
1	D	375	LYS
1	D	377	VAL
1	D	396	VAL
1	D	397	ASP
1	D	403	SER
1	D	410	SER
1	D	415	TYR
1	D	420	ASN
1	D	423	ARG
1	D	428	VAL
1	D	430	ASP
1	E	70	ARG
1	E	72	ILE
1	E	73	VAL
1	E	74	THR
1	E	91	LYS
1	E	93	SER
1	E	101	LYS
1	E	103	ARG
1	E	134	LEU
1	E	135	MET
1	E	142	SER
1	E	145	MET
1	E	156	ILE
1	E	165	LYS
1	E	177	MET
1	E	180	THR
1	E	196	LEU
1	E	199	LYS
1	E	203	LEU

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Mol	Chain	Res	Type
1	E	207	GLU
1	E	210	THR
1	E	215	ARG
1	E	222	VAL
1	E	224	LYS
1	E	229	LYS
1	E	241	THR
1	E	245	GLN
1	E	270	LEU
1	E	275	SER
1	E	278	LEU
1	E	279	LYS
1	E	285	ARG
1	E	308	LYS
1	E	333	LYS
1	E	343	GLN
1	E	344	SER
1	E	347	GLU
1	E	372	THR
1	E	377	VAL
1	E	396	VAL
1	E	397	ASP
1	E	403	SER
1	E	410	SER
1	E	415	TYR
1	E	420	ASN
1	E	423	ARG
1	E	428	VAL
1	E	430	ASP
1	E	431	PHE
1	E	442	LEU
1	E	444	SER
1	F	70	ARG
1	F	72	ILE
1	F	74	THR
1	F	93	SER
1	F	101	LYS
1	F	103	ARG
1	F	110	ARG
1	F	115	THR
1	F	134	LEU
1	F	135	MET

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Mol	Chain	Res	Type
1	F	142	SER
1	F	143	THR
1	F	145	MET
1	F	156	ILE
1	F	161	ASP
1	F	165	LYS
1	F	177	MET
1	F	180	THR
1	F	196	LEU
1	F	199	LYS
1	F	203	LEU
1	F	207	GLU
1	F	210	THR
1	F	215	ARG
1	F	222	VAL
1	F	224	LYS
1	F	229	LYS
1	F	241	THR
1	F	245	GLN
1	F	256	LEU
1	F	270	LEU
1	F	273	CYS
1	F	275	SER
1	F	278	LEU
1	F	279	LYS
1	F	285	ARG
1	F	312	LEU
1	F	333	LYS
1	F	343	GLN
1	F	344	SER
1	F	347	GLU
1	F	371	LEU
1	F	372	THR
1	F	375	LYS
1	F	377	VAL
1	F	396	VAL
1	F	403	SER
1	F	410	SER
1	F	415	TYR
1	F	419	ASP
1	F	420	ASN
1	F	423	ARG

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Mol	Chain	Res	Type
1	F	428	VAL
1	F	430	ASP
1	F	444	SER
1	G	70	ARG
1	G	72	ILE
1	G	73	VAL
1	G	91	LYS
1	G	93	SER
1	G	103	ARG
1	G	115	THR
1	G	134	LEU
1	G	135	MET
1	G	142	SER
1	G	145	MET
1	G	156	ILE
1	G	161	ASP
1	G	162	CYS
1	G	165	LYS
1	G	177	MET
1	G	180	THR
1	G	196	LEU
1	G	199	LYS
1	G	203	LEU
1	G	207	GLU
1	G	210	THR
1	G	215	ARG
1	G	222	VAL
1	G	224	LYS
1	G	229	LYS
1	G	241	THR
1	G	270	LEU
1	G	273	CYS
1	G	275	SER
1	G	278	LEU
1	G	279	LYS
1	G	333	LYS
1	G	343	GLN
1	G	347	GLU
1	G	352	LYS
1	G	371	LEU
1	G	372	THR
1	G	377	VAL

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Mol	Chain	Res	Type
1	G	396	VAL
1	G	403	SER
1	G	409	GLN
1	G	410	SER
1	G	415	TYR
1	G	420	ASN
1	G	423	ARG
1	G	428	VAL
1	G	430	ASP
1	G	444	SER
1	H	70	ARG
1	H	72	ILE
1	H	73	VAL
1	H	74	THR
1	H	91	LYS
1	H	93	SER
1	H	103	ARG
1	H	110	ARG
1	H	134	LEU
1	H	135	MET
1	H	142	SER
1	H	143	THR
1	H	145	MET
1	H	156	ILE
1	H	161	ASP
1	H	164	ARG
1	H	165	LYS
1	H	177	MET
1	H	180	THR
1	H	196	LEU
1	H	199	LYS
1	H	203	LEU
1	H	207	GLU
1	H	210	THR
1	H	215	ARG
1	H	222	VAL
1	H	224	LYS
1	H	229	LYS
1	H	241	THR
1	H	256	LEU
1	H	270	LEU
1	H	273	CYS

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Mol	Chain	Res	Type
1	H	275	SER
1	H	278	LEU
1	H	285	ARG
1	H	333	LYS
1	H	343	GLN
1	H	344	SER
1	H	347	GLU
1	H	371	LEU
1	H	372	THR
1	H	375	LYS
1	H	377	VAL
1	H	396	VAL
1	H	403	SER
1	H	410	SER
1	H	414	LYS
1	H	415	TYR
1	H	420	ASN
1	H	423	ARG
1	H	428	VAL
1	H	430	ASP
1	H	444	SER
1	I	70	ARG
1	I	72	ILE
1	I	91	LYS
1	I	93	SER
1	I	101	LYS
1	I	103	ARG
1	I	110	ARG
1	I	134	LEU
1	I	135	MET
1	I	142	SER
1	I	145	MET
1	I	156	ILE
1	I	161	ASP
1	I	165	LYS
1	I	177	MET
1	I	180	THR
1	I	196	LEU
1	I	199	LYS
1	I	203	LEU
1	I	207	GLU
1	I	210	THR

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Mol	Chain	Res	Type
1	I	215	ARG
1	I	222	VAL
1	I	229	LYS
1	I	241	THR
1	I	256	LEU
1	I	270	LEU
1	I	273	CYS
1	I	275	SER
1	I	278	LEU
1	I	279	LYS
1	I	333	LYS
1	I	343	GLN
1	I	347	GLU
1	I	353	LYS
1	I	371	LEU
1	I	372	THR
1	I	375	LYS
1	I	377	VAL
1	I	396	VAL
1	I	397	ASP
1	I	403	SER
1	I	410	SER
1	I	415	TYR
1	I	420	ASN
1	I	423	ARG
1	I	428	VAL
1	I	430	ASP
1	I	444	SER
1	J	70	ARG
1	J	72	ILE
1	J	74	THR
1	J	93	SER
1	J	101	LYS
1	J	103	ARG
1	J	134	LEU
1	J	135	MET
1	J	142	SER
1	J	145	MET
1	J	156	ILE
1	J	161	ASP
1	J	165	LYS
1	J	177	MET

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Mol	Chain	Res	Type
1	J	180	THR
1	J	196	LEU
1	J	199	LYS
1	J	203	LEU
1	J	207	GLU
1	J	210	THR
1	J	215	ARG
1	J	222	VAL
1	J	224	LYS
1	J	229	LYS
1	J	241	THR
1	J	256	LEU
1	J	270	LEU
1	J	273	CYS
1	J	275	SER
1	J	278	LEU
1	J	279	LYS
1	J	282	SER
1	J	285	ARG
1	J	333	LYS
1	J	343	GLN
1	J	344	SER
1	J	347	GLU
1	J	352	LYS
1	J	370	LEU
1	J	371	LEU
1	J	372	THR
1	J	375	LYS
1	J	377	VAL
1	J	396	VAL
1	J	403	SER
1	J	410	SER
1	J	415	TYR
1	J	420	ASN
1	J	423	ARG
1	J	428	VAL
1	J	430	ASP
1	K	70	ARG
1	K	72	ILE
1	K	74	THR
1	K	93	SER
1	K	101	LYS

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Mol	Chain	Res	Type
1	K	103	ARG
1	K	132	THR
1	K	134	LEU
1	K	135	MET
1	K	142	SER
1	K	143	THR
1	K	145	MET
1	K	156	ILE
1	K	161	ASP
1	K	165	LYS
1	K	177	MET
1	K	180	THR
1	K	196	LEU
1	K	199	LYS
1	K	203	LEU
1	K	207	GLU
1	K	210	THR
1	K	215	ARG
1	K	222	VAL
1	K	224	LYS
1	K	229	LYS
1	K	241	THR
1	K	256	LEU
1	K	270	LEU
1	K	273	CYS
1	K	275	SER
1	K	278	LEU
1	K	279	LYS
1	K	333	LYS
1	K	343	GLN
1	K	344	SER
1	K	347	GLU
1	K	352	LYS
1	K	353	LYS
1	K	371	LEU
1	K	372	THR
1	K	375	LYS
1	K	377	VAL
1	K	396	VAL
1	K	403	SER
1	K	410	SER
1	K	415	TYR

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Mol	Chain	Res	Type
1	K	420	ASN
1	K	423	ARG
1	K	428	VAL
1	K	430	ASP
1	K	444	SER
1	K	445	ILE
1	L	70	ARG
1	L	72	ILE
1	L	73	VAL
1	L	74	THR
1	L	87	TYR
1	L	93	SER
1	L	103	ARG
1	L	110	ARG
1	L	134	LEU
1	L	135	MET
1	L	142	SER
1	L	143	THR
1	L	145	MET
1	L	156	ILE
1	L	161	ASP
1	L	165	LYS
1	L	177	MET
1	L	180	THR
1	L	196	LEU
1	L	199	LYS
1	L	203	LEU
1	L	207	GLU
1	L	210	THR
1	L	215	ARG
1	L	222	VAL
1	L	229	LYS
1	L	241	THR
1	L	270	LEU
1	L	273	CYS
1	L	275	SER
1	L	278	LEU
1	L	279	LYS
1	L	295	LEU
1	L	315	GLN
1	L	333	LYS
1	L	343	GLN

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Mol	Chain	Res	Type
1	L	344	SER
1	L	347	GLU
1	L	352	LYS
1	L	370	LEU
1	L	371	LEU
1	L	372	THR
1	L	375	LYS
1	L	377	VAL
1	L	396	VAL
1	L	397	ASP
1	L	402	MET
1	L	403	SER
1	L	410	SER
1	L	415	TYR
1	L	420	ASN
1	L	423	ARG
1	L	428	VAL
1	L	430	ASP
1	L	444	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	83	ASN
1	A	211	ASN
1	A	298	ASN
1	A	343	GLN
1	A	420	ASN
1	B	55	ASN
1	B	63	HIS
1	B	317	GLN
1	B	343	GLN
1	B	420	ASN
1	C	63	HIS
1	C	317	GLN
1	C	343	GLN
1	C	420	ASN
1	D	63	HIS
1	D	83	ASN
1	D	298	ASN
1	D	343	GLN

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Mol	Chain	Res	Type
1	D	345	HIS
1	D	420	ASN
1	E	63	HIS
1	E	288	HIS
1	E	343	GLN
1	E	420	ASN
1	F	63	HIS
1	F	211	ASN
1	F	317	GLN
1	F	343	GLN
1	F	345	HIS
1	F	420	ASN
1	G	63	HIS
1	G	211	ASN
1	G	343	GLN
1	G	420	ASN
1	H	63	HIS
1	H	211	ASN
1	H	288	HIS
1	H	317	GLN
1	H	343	GLN
1	H	345	HIS
1	H	420	ASN
1	I	63	HIS
1	I	83	ASN
1	I	211	ASN
1	I	288	HIS
1	I	343	GLN
1	I	348	HIS
1	I	420	ASN
1	J	63	HIS
1	J	211	ASN
1	J	317	GLN
1	J	343	GLN
1	J	345	HIS
1	J	348	HIS
1	J	420	ASN
1	K	63	HIS
1	K	211	ASN
1	K	343	GLN
1	L	63	HIS
1	L	211	ASN

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Mol	Chain	Res	Type
1	L	317	GLN
1	L	343	GLN
1	L	345	HIS
1	L	420	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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	PMC	C	602	-	14,14,14	2.82	8 (57%)	20,20,20	1.74	5 (25%)
2	PLP	J	500	1	15,15,16	3.66	6 (40%)	21,22,23	2.33	8 (38%)
2	PLP	L	500	1	15,15,16	3.33	6 (40%)	21,22,23	2.43	8 (38%)
3	PMC	G	606	-	14,14,14	2.53	8 (57%)	20,20,20	1.67	5 (25%)
3	PMC	A	600	-	14,14,14	2.73	9 (64%)	20,20,20	1.75	5 (25%)
3	PMC	E	604	-	14,14,14	2.80	7 (50%)	20,20,20	1.80	5 (25%)
3	PMC	I	608	-	14,14,14	2.57	8 (57%)	20,20,20	1.66	5 (25%)
2	PLP	D	500	1	15,15,16	4.42	6 (40%)	21,22,23	2.62	10 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PMC	J	609	-	14,14,14	2.54	9 (64%)	20,20,20	1.67	5 (25%)
3	PMC	K	610	-	14,14,14	2.67	8 (57%)	20,20,20	1.73	5 (25%)
2	PLP	F	500	1	15,15,16	4.20	6 (40%)	21,22,23	2.44	10 (47%)
3	PMC	L	611	-	14,14,14	2.59	8 (57%)	20,20,20	1.67	5 (25%)
2	PLP	A	500	1	15,15,16	3.91	5 (33%)	21,22,23	2.50	10 (47%)
2	PLP	G	500	1	15,15,16	3.68	6 (40%)	21,22,23	2.40	9 (42%)
3	PMC	B	601	-	14,14,14	2.67	8 (57%)	20,20,20	1.70	5 (25%)
2	PLP	K	500	1	15,15,16	4.16	5 (33%)	21,22,23	2.62	10 (47%)
3	PMC	F	605	-	14,14,14	2.66	9 (64%)	20,20,20	1.74	6 (30%)
2	PLP	I	500	1	15,15,16	3.95	5 (33%)	21,22,23	2.38	10 (47%)
2	PLP	E	500	1	15,15,16	3.59	6 (40%)	21,22,23	2.41	9 (42%)
2	PLP	H	500	1	15,15,16	4.29	7 (46%)	21,22,23	2.51	10 (47%)
2	PLP	B	500	1	15,15,16	4.29	5 (33%)	21,22,23	2.53	10 (47%)
3	PMC	H	607	-	14,14,14	2.63	8 (57%)	20,20,20	1.72	5 (25%)
2	PLP	C	500	1	15,15,16	3.68	6 (40%)	21,22,23	2.48	11 (52%)
3	PMC	D	603	-	14,14,14	2.49	7 (50%)	20,20,20	1.67	5 (25%)

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	PMC	C	602	-	-	3/9/9/9	0/1/1/1
2	PLP	J	500	1	-	2/6/6/8	0/1/1/1
2	PLP	L	500	1	-	2/6/6/8	0/1/1/1
3	PMC	G	606	-	-	3/9/9/9	0/1/1/1
3	PMC	A	600	-	-	3/9/9/9	0/1/1/1
3	PMC	E	604	-	-	5/9/9/9	0/1/1/1
3	PMC	I	608	-	-	3/9/9/9	0/1/1/1
2	PLP	D	500	1	-	2/6/6/8	0/1/1/1
3	PMC	J	609	-	-	3/9/9/9	0/1/1/1
3	PMC	K	610	-	-	3/9/9/9	0/1/1/1
2	PLP	F	500	1	-	2/6/6/8	0/1/1/1
3	PMC	L	611	-	-	4/9/9/9	0/1/1/1
2	PLP	A	500	1	-	2/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	G	500	1	-	2/6/6/8	0/1/1/1
3	PMC	B	601	-	-	3/9/9/9	0/1/1/1
2	PLP	K	500	1	-	2/6/6/8	0/1/1/1
3	PMC	F	605	-	-	3/9/9/9	0/1/1/1
2	PLP	I	500	1	-	2/6/6/8	0/1/1/1
2	PLP	E	500	1	-	2/6/6/8	0/1/1/1
2	PLP	H	500	1	-	2/6/6/8	0/1/1/1
2	PLP	B	500	1	-	2/6/6/8	0/1/1/1
3	PMC	H	607	-	-	3/9/9/9	0/1/1/1
2	PLP	C	500	1	-	2/6/6/8	0/1/1/1
3	PMC	D	603	-	-	4/9/9/9	0/1/1/1

All (166) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	PLP	C5-C4	13.67	1.55	1.40
2	D	500	PLP	C5-C4	13.30	1.55	1.40
2	F	500	PLP	C5-C4	13.21	1.55	1.40
2	I	500	PLP	C5-C4	13.16	1.55	1.40
2	H	500	PLP	C5-C4	13.03	1.55	1.40
2	A	500	PLP	C5-C4	12.55	1.54	1.40
2	K	500	PLP	C5-C4	12.16	1.54	1.40
2	C	500	PLP	C5-C4	11.97	1.54	1.40
2	J	500	PLP	C5-C4	11.83	1.53	1.40
2	G	500	PLP	C5-C4	11.73	1.53	1.40
2	E	500	PLP	C5-C4	11.12	1.53	1.40
2	L	500	PLP	C5-C4	10.89	1.52	1.40
2	D	500	PLP	C3-C2	8.95	1.50	1.41
2	K	500	PLP	C3-C2	8.90	1.50	1.41
2	H	500	PLP	C3-C2	7.56	1.48	1.41
2	B	500	PLP	C3-C2	7.22	1.48	1.41
2	F	500	PLP	C3-C2	7.08	1.48	1.41
2	A	500	PLP	C3-C2	6.30	1.47	1.41
2	E	500	PLP	C3-C2	6.15	1.47	1.41
3	E	604	PMC	C2-C3	5.98	1.46	1.40
3	C	602	PMC	C2-C3	5.86	1.46	1.40
2	G	500	PLP	C3-C2	5.71	1.46	1.41
3	L	611	PMC	C2-C3	5.54	1.46	1.40
3	A	600	PMC	C2-C3	5.24	1.45	1.40
2	J	500	PLP	C3-C2	5.05	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	607	PMC	C2-C3	5.01	1.45	1.40
3	B	601	PMC	C2-C3	4.97	1.45	1.40
2	C	500	PLP	C3-C2	4.96	1.46	1.41
3	K	610	PMC	C2-C3	4.94	1.45	1.40
2	I	500	PLP	C3-C2	4.89	1.46	1.41
3	J	609	PMC	C2-C3	4.88	1.45	1.40
3	G	606	PMC	C2-C3	4.83	1.45	1.40
3	D	603	PMC	C2-C3	4.83	1.45	1.40
3	F	605	PMC	C2-C3	4.71	1.45	1.40
3	I	608	PMC	C2-C3	4.59	1.45	1.40
2	H	500	PLP	C2-N1	4.23	1.41	1.33
3	I	608	PMC	OC1-C	4.13	1.34	1.22
3	F	605	PMC	OC1-C	4.13	1.34	1.22
2	I	500	PLP	C2-N1	4.13	1.41	1.33
3	B	601	PMC	OC1-C	4.11	1.34	1.22
2	F	500	PLP	C2-N1	4.10	1.41	1.33
3	H	607	PMC	OC1-C	4.10	1.34	1.22
3	K	610	PMC	OC1-C	4.08	1.34	1.22
3	G	606	PMC	OC1-C	4.06	1.34	1.22
3	C	602	PMC	OC1-C	4.05	1.34	1.22
3	C	602	PMC	CA-C3	3.97	1.56	1.51
3	E	604	PMC	OC1-C	3.94	1.34	1.22
3	J	609	PMC	OC1-C	3.92	1.34	1.22
3	E	604	PMC	CA-C3	3.91	1.56	1.51
3	A	600	PMC	P1-CA	3.87	1.85	1.79
3	L	611	PMC	OC1-C	3.83	1.33	1.22
2	B	500	PLP	C2-N1	3.83	1.40	1.33
3	A	600	PMC	OC1-C	3.82	1.33	1.22
3	K	610	PMC	CA-C3	3.79	1.56	1.51
2	L	500	PLP	C3-C2	3.77	1.44	1.41
3	A	600	PMC	CA-C3	3.74	1.56	1.51
3	F	605	PMC	P1-CA	3.73	1.85	1.79
3	F	605	PMC	CA-C3	3.72	1.56	1.51
3	D	603	PMC	OC1-C	3.68	1.33	1.22
2	C	500	PLP	C2-N1	3.67	1.40	1.33
2	J	500	PLP	C2-N1	3.67	1.40	1.33
3	C	602	PMC	P1-CA	3.67	1.85	1.79
3	K	610	PMC	P1-CA	3.63	1.85	1.79
3	E	604	PMC	P1-CA	3.61	1.85	1.79
2	D	500	PLP	C2-N1	3.57	1.40	1.33
3	B	601	PMC	P1-CA	3.56	1.85	1.79
3	I	608	PMC	P1-CA	3.51	1.85	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	PMC	CA-C3	3.48	1.55	1.51
2	A	500	PLP	C2-N1	3.47	1.40	1.33
3	H	607	PMC	CA-C3	3.39	1.55	1.51
3	H	607	PMC	P1-CA	3.38	1.84	1.79
2	K	500	PLP	C2-N1	3.32	1.39	1.33
3	D	603	PMC	CA-C3	3.32	1.55	1.51
3	J	609	PMC	P1-CA	3.28	1.84	1.79
2	G	500	PLP	C2-N1	3.26	1.39	1.33
3	L	611	PMC	CA-C3	3.24	1.55	1.51
3	I	608	PMC	CA-C3	3.19	1.55	1.51
2	E	500	PLP	C2-N1	3.17	1.39	1.33
2	L	500	PLP	C2-N1	3.16	1.39	1.33
3	D	603	PMC	P1-CA	3.14	1.84	1.79
3	G	606	PMC	P1-CA	3.12	1.84	1.79
3	G	606	PMC	CA-C3	3.09	1.55	1.51
3	J	609	PMC	CA-C3	2.98	1.55	1.51
3	L	611	PMC	P1-CA	2.90	1.84	1.79
3	F	605	PMC	OC2-C	-2.78	1.22	1.30
2	E	500	PLP	P-O2P	-2.68	1.44	1.54
2	F	500	PLP	P-O2P	-2.66	1.44	1.54
3	B	601	PMC	OC2-C	-2.65	1.22	1.30
2	H	500	PLP	P-O2P	-2.64	1.45	1.54
3	I	608	PMC	OC2-C	-2.64	1.22	1.30
2	B	500	PLP	P-O2P	-2.62	1.45	1.54
2	G	500	PLP	P-O2P	-2.61	1.45	1.54
3	L	611	PMC	P1-O3	-2.60	1.49	1.55
3	E	604	PMC	OC2-C	-2.58	1.22	1.30
3	D	603	PMC	OC2-C	-2.58	1.22	1.30
3	K	610	PMC	OC2-C	-2.57	1.22	1.30
3	H	607	PMC	OC2-C	-2.56	1.22	1.30
3	G	606	PMC	OC2-C	-2.54	1.23	1.30
2	J	500	PLP	P-O2P	-2.54	1.45	1.54
2	C	500	PLP	P-O2P	-2.53	1.45	1.54
3	A	600	PMC	OC2-C	-2.51	1.23	1.30
3	C	602	PMC	OC2-C	-2.50	1.23	1.30
2	H	500	PLP	C5A-C5	2.49	1.57	1.50
2	I	500	PLP	P-O2P	-2.48	1.45	1.54
3	J	609	PMC	OC2-C	-2.47	1.23	1.30
3	D	603	PMC	P1-O3	-2.44	1.49	1.55
2	L	500	PLP	P-O2P	-2.43	1.45	1.54
3	A	600	PMC	P1-O3	-2.41	1.49	1.55
2	H	500	PLP	C2A-C2	2.40	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	PMC	P1-O3	-2.39	1.49	1.55
3	L	611	PMC	OC2-C	-2.38	1.23	1.30
2	A	500	PLP	P-O2P	-2.37	1.46	1.54
2	K	500	PLP	P-O2P	-2.35	1.46	1.54
3	J	609	PMC	P1-O3	-2.35	1.49	1.55
2	L	500	PLP	P-O3P	-2.32	1.46	1.54
3	B	601	PMC	P1-O3	-2.31	1.49	1.55
3	I	608	PMC	P1-O3	-2.30	1.49	1.55
3	E	604	PMC	P1-O3	-2.30	1.49	1.55
3	H	607	PMC	P1-O3	-2.30	1.49	1.55
3	A	600	PMC	P1-O2	-2.30	1.49	1.55
2	G	500	PLP	C2A-C2	2.29	1.54	1.50
3	F	605	PMC	P1-O3	-2.29	1.49	1.55
2	D	500	PLP	P-O2P	-2.28	1.46	1.54
2	D	500	PLP	C2A-C2	2.28	1.54	1.50
3	D	603	PMC	P1-O2	-2.27	1.49	1.55
2	C	500	PLP	C2A-C2	2.25	1.53	1.50
3	K	610	PMC	P1-O3	-2.24	1.49	1.55
3	B	601	PMC	C4-C3	2.23	1.43	1.39
2	F	500	PLP	P-O3P	-2.23	1.46	1.54
3	K	610	PMC	P1-O2	-2.22	1.50	1.55
3	B	601	PMC	P1-O2	-2.20	1.50	1.55
2	E	500	PLP	P-O3P	-2.19	1.46	1.54
3	G	606	PMC	P1-O2	-2.19	1.50	1.55
3	H	607	PMC	C4-C3	2.18	1.43	1.39
2	I	500	PLP	P-O3P	-2.18	1.46	1.54
3	I	608	PMC	C4-C3	2.18	1.43	1.39
3	G	606	PMC	P1-O3	-2.18	1.50	1.55
3	C	602	PMC	P1-O2	-2.17	1.50	1.55
3	J	609	PMC	C4-C3	2.17	1.43	1.39
3	A	600	PMC	C5-C4	2.14	1.42	1.38
3	L	611	PMC	P1-O2	-2.14	1.50	1.55
3	L	611	PMC	C5-C4	2.13	1.42	1.38
3	H	607	PMC	P1-O2	-2.13	1.50	1.55
2	A	500	PLP	P-O3P	-2.12	1.46	1.54
2	E	500	PLP	C2A-C2	2.10	1.53	1.50
3	F	605	PMC	P1-O2	-2.10	1.50	1.55
2	J	500	PLP	P-O3P	-2.09	1.47	1.54
2	G	500	PLP	P-O3P	-2.09	1.47	1.54
2	H	500	PLP	P-O3P	-2.09	1.47	1.54
3	K	610	PMC	C4-C3	2.07	1.43	1.39
2	L	500	PLP	C2A-C2	2.07	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	PLP	C5A-C5	2.06	1.56	1.50
3	A	600	PMC	C4-C3	2.06	1.43	1.39
3	F	605	PMC	C4-C3	2.06	1.43	1.39
2	C	500	PLP	P-O3P	-2.05	1.47	1.54
3	F	605	PMC	C5-C4	2.05	1.42	1.38
3	I	608	PMC	C5-C4	2.04	1.42	1.38
3	E	604	PMC	P1-O2	-2.04	1.50	1.55
2	J	500	PLP	C2A-C2	2.04	1.53	1.50
2	K	500	PLP	P-O3P	-2.03	1.47	1.54
3	J	609	PMC	P1-O2	-2.03	1.50	1.55
3	J	609	PMC	C5-C4	2.03	1.42	1.38
3	C	602	PMC	C5-C4	2.01	1.42	1.38
2	D	500	PLP	P-O3P	-2.01	1.47	1.54
2	B	500	PLP	P-O3P	-2.00	1.47	1.54
3	G	606	PMC	C4-C3	2.00	1.42	1.39

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	500	PLP	C2A-C2-C3	6.34	128.22	120.80
2	L	500	PLP	C2A-C2-C3	6.24	128.10	120.80
2	E	500	PLP	C2A-C2-C3	6.22	128.08	120.80
2	F	500	PLP	C2A-C2-C3	6.21	128.07	120.80
2	A	500	PLP	C2A-C2-C3	6.21	128.06	120.80
2	B	500	PLP	C2A-C2-C3	6.01	127.84	120.80
2	D	500	PLP	C2A-C2-C3	5.94	127.75	120.80
2	C	500	PLP	C2A-C2-C3	5.88	127.68	120.80
2	H	500	PLP	C2A-C2-C3	5.86	127.66	120.80
2	I	500	PLP	C2A-C2-C3	5.85	127.65	120.80
2	G	500	PLP	C2A-C2-C3	5.76	127.54	120.80
2	J	500	PLP	C2A-C2-C3	5.50	127.24	120.80
2	D	500	PLP	C4A-C4-C5	4.25	125.32	120.94
2	L	500	PLP	C6-N1-C2	4.19	126.80	119.20
2	A	500	PLP	O4P-C5A-C5	4.09	117.03	109.36
2	I	500	PLP	C6-N1-C2	3.93	126.33	119.20
2	C	500	PLP	C6-N1-C2	3.93	126.32	119.20
2	K	500	PLP	C4A-C4-C5	3.91	124.97	120.94
2	J	500	PLP	O4P-C5A-C5	3.86	116.58	109.36
2	D	500	PLP	C6-C5-C4	3.85	121.25	118.10
2	L	500	PLP	O4P-C5A-C5	3.79	116.45	109.36
3	E	604	PMC	P1-CA-C3	3.79	121.04	114.06
2	A	500	PLP	C6-N1-C2	3.76	126.02	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	PLP	O3-C3-C4	3.76	127.90	118.10
2	F	500	PLP	C6-N1-C2	3.75	126.00	119.20
2	H	500	PLP	O3-C3-C4	3.72	127.80	118.10
2	J	500	PLP	C6-N1-C2	3.70	125.91	119.20
2	B	500	PLP	C6-N1-C2	3.69	125.90	119.20
2	E	500	PLP	C6-N1-C2	3.69	125.89	119.20
2	G	500	PLP	O3-C3-C4	3.69	127.72	118.10
2	E	500	PLP	O3-C3-C4	3.68	127.71	118.10
2	K	500	PLP	C6-C5-C4	3.66	121.10	118.10
2	G	500	PLP	C6-N1-C2	3.65	125.81	119.20
2	L	500	PLP	O3-C3-C4	3.64	127.61	118.10
2	E	500	PLP	O4P-C5A-C5	3.63	116.16	109.36
2	J	500	PLP	O3-C3-C4	3.60	127.50	118.10
2	B	500	PLP	C4A-C4-C5	3.57	124.62	120.94
2	K	500	PLP	O3-C3-C4	3.56	127.40	118.10
3	C	602	PMC	P1-CA-C3	3.55	120.61	114.06
2	A	500	PLP	O3-C3-C4	3.51	127.25	118.10
2	F	500	PLP	O3-C3-C4	3.50	127.24	118.10
2	H	500	PLP	C6-N1-C2	3.50	125.54	119.20
2	H	500	PLP	O4P-C5A-C5	3.48	115.88	109.36
2	B	500	PLP	O3-C3-C4	3.41	127.01	118.10
2	I	500	PLP	O3-C3-C4	3.34	126.83	118.10
2	D	500	PLP	O3-C3-C4	3.33	126.80	118.10
3	K	610	PMC	P1-CA-C3	3.32	120.18	114.06
3	F	605	PMC	C6-N1-C2	3.31	123.24	116.80
3	A	600	PMC	P1-CA-C3	3.30	120.16	114.06
2	F	500	PLP	C3-C2-N1	-3.29	116.81	120.96
2	K	500	PLP	C6-N1-C2	3.29	125.17	119.20
3	K	610	PMC	C6-N1-C2	3.26	123.14	116.80
3	H	607	PMC	C6-N1-C2	3.24	123.10	116.80
3	G	606	PMC	C6-N1-C2	3.22	123.07	116.80
3	A	600	PMC	C6-N1-C2	3.22	123.06	116.80
3	E	604	PMC	C6-N1-C2	3.22	123.06	116.80
3	C	602	PMC	C6-N1-C2	3.22	123.06	116.80
3	B	601	PMC	C6-N1-C2	3.21	123.04	116.80
3	J	609	PMC	C6-N1-C2	3.20	123.03	116.80
3	D	603	PMC	C6-N1-C2	3.20	123.03	116.80
3	I	608	PMC	C6-N1-C2	3.19	123.01	116.80
2	C	500	PLP	O4P-C5A-C5	3.19	115.34	109.36
2	D	500	PLP	C3-C4-C5	-3.18	114.77	118.59
2	B	500	PLP	C3-C2-N1	-3.18	116.95	120.96
3	F	605	PMC	P1-CA-C3	3.17	119.91	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	PLP	C6-N1-C2	3.16	124.92	119.20
2	H	500	PLP	O3-C3-C2	-3.13	111.09	117.58
2	D	500	PLP	O4P-C5A-C5	3.13	115.22	109.36
2	L	500	PLP	C5-C6-N1	-3.13	118.74	123.83
2	B	500	PLP	O4P-C5A-C5	3.13	115.21	109.36
3	L	611	PMC	C6-N1-C2	3.12	122.88	116.80
3	H	607	PMC	P1-CA-C3	3.11	119.80	114.06
2	I	500	PLP	C5-C6-N1	-3.10	118.79	123.83
2	L	500	PLP	C3-C2-N1	-3.09	117.06	120.96
2	H	500	PLP	C3-C2-N1	-3.06	117.09	120.96
2	I	500	PLP	C3-C2-N1	-3.06	117.10	120.96
2	A	500	PLP	C3-C2-N1	-3.05	117.11	120.96
3	L	611	PMC	P1-CA-C3	3.04	119.66	114.06
2	C	500	PLP	C3-C2-N1	-3.02	117.15	120.96
3	L	611	PMC	OC2-C-C2	3.00	123.96	114.39
3	A	600	PMC	OC2-C-C2	2.99	123.92	114.39
3	D	603	PMC	OC2-C-C2	2.98	123.89	114.39
3	E	604	PMC	OC2-C-C2	2.96	123.83	114.39
2	I	500	PLP	O4P-C5A-C5	2.95	114.88	109.36
2	K	500	PLP	O3-C3-C2	-2.93	111.51	117.58
2	E	500	PLP	C3-C2-N1	-2.92	117.27	120.96
2	B	500	PLP	C6-C5-C4	2.92	120.49	118.10
2	C	500	PLP	C5-C6-N1	-2.92	119.09	123.83
2	K	500	PLP	C3-C2-N1	-2.91	117.29	120.96
3	J	609	PMC	OC2-C-C2	2.91	123.65	114.39
2	J	500	PLP	C3-C2-N1	-2.89	117.31	120.96
2	B	500	PLP	O3-C3-C2	-2.89	111.59	117.58
2	F	500	PLP	C6-C5-C4	2.89	120.47	118.10
3	B	601	PMC	P1-CA-C3	2.88	119.38	114.06
2	G	500	PLP	C4A-C4-C5	2.88	123.91	120.94
2	K	500	PLP	C3-C4-C5	-2.88	115.13	118.59
2	G	500	PLP	O4P-C5A-C5	2.88	114.76	109.36
2	G	500	PLP	C3-C2-N1	-2.86	117.35	120.96
2	G	500	PLP	O3-C3-C2	-2.83	111.72	117.58
2	D	500	PLP	O3-C3-C2	-2.82	111.73	117.58
3	K	610	PMC	OC2-C-C2	2.82	123.38	114.39
3	C	602	PMC	OC2-C-C2	2.82	123.37	114.39
2	C	500	PLP	O3-C3-C2	-2.80	111.78	117.58
2	C	500	PLP	O3P-P-O2P	2.80	118.29	107.80
2	F	500	PLP	O3-C3-C2	-2.79	111.79	117.58
3	F	605	PMC	OC2-C-C2	2.79	123.27	114.39
3	G	606	PMC	OC2-C-C2	2.76	123.19	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	608	PMC	P1-CA-C3	2.75	119.14	114.06
2	J	500	PLP	C5-C6-N1	-2.74	119.38	123.83
3	B	601	PMC	OC2-C-C2	2.73	123.08	114.39
3	H	607	PMC	OC2-C-C2	2.71	123.04	114.39
2	K	500	PLP	O4P-C5A-C5	2.71	114.44	109.36
2	D	500	PLP	C3-C2-N1	-2.70	117.55	120.96
3	I	608	PMC	OC2-C-C2	2.67	122.89	114.39
2	J	500	PLP	O3-C3-C2	-2.66	112.07	117.58
2	H	500	PLP	C6-C5-C4	2.65	120.27	118.10
3	G	606	PMC	C3-C2-N1	-2.65	119.23	122.40
2	E	500	PLP	C5-C6-N1	-2.64	119.54	123.83
3	D	603	PMC	P1-CA-C3	2.64	118.92	114.06
2	H	500	PLP	C4A-C4-C5	2.64	123.66	120.94
2	F	500	PLP	C5-C6-N1	-2.63	119.55	123.83
2	G	500	PLP	C5-C6-N1	-2.62	119.57	123.83
3	H	607	PMC	C3-C2-N1	-2.62	119.27	122.40
2	H	500	PLP	O4P-P-O1P	-2.61	99.38	106.44
3	D	603	PMC	C3-C2-N1	-2.61	119.28	122.40
3	J	609	PMC	P1-CA-C3	2.60	118.86	114.06
3	J	609	PMC	C3-C2-N1	-2.60	119.29	122.40
3	E	604	PMC	C3-C2-N1	-2.60	119.29	122.40
2	F	500	PLP	C4A-C4-C5	2.59	123.61	120.94
3	B	601	PMC	C3-C2-N1	-2.58	119.31	122.40
3	K	610	PMC	C3-C2-N1	-2.56	119.34	122.40
3	C	602	PMC	C3-C2-N1	-2.55	119.36	122.40
2	E	500	PLP	O3-C3-C2	-2.54	112.31	117.58
3	A	600	PMC	C3-C2-N1	-2.54	119.36	122.40
2	A	500	PLP	O3-C3-C2	-2.54	112.31	117.58
2	C	500	PLP	C6-C5-C4	2.54	120.18	118.10
3	J	609	PMC	OC2-C-OC1	-2.53	117.92	123.35
2	B	500	PLP	C5-C6-N1	-2.52	119.72	123.83
3	B	601	PMC	OC2-C-OC1	-2.51	117.96	123.35
3	F	605	PMC	C3-C2-N1	-2.51	119.40	122.40
2	H	500	PLP	C5-C6-N1	-2.50	119.76	123.83
2	I	500	PLP	C4A-C4-C5	2.49	123.51	120.94
3	E	604	PMC	OC2-C-OC1	-2.48	118.01	123.35
3	G	606	PMC	P1-CA-C3	2.47	118.62	114.06
3	H	607	PMC	OC2-C-OC1	-2.47	118.04	123.35
3	G	606	PMC	OC2-C-OC1	-2.47	118.05	123.35
3	F	605	PMC	OC2-C-OC1	-2.47	118.05	123.35
2	A	500	PLP	C5-C6-N1	-2.46	119.83	123.83
3	A	600	PMC	OC2-C-OC1	-2.46	118.06	123.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	603	PMC	OC2-C-OC1	-2.46	118.07	123.35
3	I	608	PMC	C3-C2-N1	-2.45	119.47	122.40
3	C	602	PMC	OC2-C-OC1	-2.44	118.10	123.35
3	L	611	PMC	C3-C2-N1	-2.43	119.50	122.40
3	I	608	PMC	OC2-C-OC1	-2.43	118.14	123.35
2	E	500	PLP	C6-C5-C4	2.42	120.08	118.10
2	I	500	PLP	O3-C3-C2	-2.42	112.57	117.58
2	C	500	PLP	O3P-P-O4P	-2.41	100.38	106.67
3	L	611	PMC	OC2-C-OC1	-2.41	118.17	123.35
2	G	500	PLP	C6-C5-C4	2.38	120.05	118.10
2	B	500	PLP	C3-C4-C5	-2.37	115.74	118.59
3	K	610	PMC	OC2-C-OC1	-2.35	118.31	123.35
2	F	500	PLP	O4P-C5A-C5	2.33	113.72	109.36
2	D	500	PLP	C5-C6-N1	-2.32	120.07	123.83
2	F	500	PLP	O3P-P-O2P	2.29	116.39	107.80
2	A	500	PLP	O2P-P-O4P	2.28	112.63	106.67
2	L	500	PLP	O3-C3-C2	-2.25	112.92	117.58
2	A	500	PLP	C4A-C4-C5	2.22	123.22	120.94
2	K	500	PLP	C5-C6-N1	-2.20	120.25	123.83
2	C	500	PLP	C4A-C4-C5	2.19	123.20	120.94
2	L	500	PLP	O3P-P-O2P	2.18	115.97	107.80
3	F	605	PMC	C3-C2-C	2.18	126.53	122.66
2	E	500	PLP	O3P-P-O2P	2.17	115.94	107.80
2	A	500	PLP	O3P-P-O2P	2.12	115.75	107.80
2	I	500	PLP	C6-C5-C4	2.10	119.81	118.10
2	J	500	PLP	C6-C5-C4	2.06	119.79	118.10
2	I	500	PLP	O4P-P-O1P	-2.03	100.96	106.44

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	PLP	C4-C5-C5A-O4P
2	A	500	PLP	C6-C5-C5A-O4P
2	B	500	PLP	C4-C5-C5A-O4P
2	B	500	PLP	C6-C5-C5A-O4P
2	C	500	PLP	C4-C5-C5A-O4P
2	C	500	PLP	C6-C5-C5A-O4P
2	D	500	PLP	C4-C5-C5A-O4P
2	D	500	PLP	C6-C5-C5A-O4P
2	E	500	PLP	C4-C5-C5A-O4P
2	E	500	PLP	C6-C5-C5A-O4P

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Mol	Chain	Res	Type	Atoms
2	F	500	PLP	C4-C5-C5A-O4P
2	F	500	PLP	C6-C5-C5A-O4P
2	G	500	PLP	C4-C5-C5A-O4P
2	G	500	PLP	C6-C5-C5A-O4P
2	H	500	PLP	C4-C5-C5A-O4P
2	H	500	PLP	C6-C5-C5A-O4P
2	I	500	PLP	C4-C5-C5A-O4P
2	I	500	PLP	C6-C5-C5A-O4P
2	J	500	PLP	C4-C5-C5A-O4P
2	J	500	PLP	C6-C5-C5A-O4P
2	K	500	PLP	C4-C5-C5A-O4P
2	K	500	PLP	C6-C5-C5A-O4P
2	L	500	PLP	C4-C5-C5A-O4P
2	L	500	PLP	C6-C5-C5A-O4P
3	A	600	PMC	C3-CA-P1-O3
3	A	600	PMC	C3-CA-P1-O2
3	A	600	PMC	C3-CA-P1-O1
3	B	601	PMC	C3-CA-P1-O3
3	B	601	PMC	C3-CA-P1-O2
3	B	601	PMC	C3-CA-P1-O1
3	C	602	PMC	C3-CA-P1-O3
3	C	602	PMC	C3-CA-P1-O2
3	C	602	PMC	C3-CA-P1-O1
3	D	603	PMC	C3-CA-P1-O3
3	D	603	PMC	C3-CA-P1-O2
3	D	603	PMC	C3-CA-P1-O1
3	E	604	PMC	C3-CA-P1-O3
3	E	604	PMC	C3-CA-P1-O1
3	F	605	PMC	C3-CA-P1-O3
3	F	605	PMC	C3-CA-P1-O2
3	F	605	PMC	C3-CA-P1-O1
3	G	606	PMC	C3-CA-P1-O3
3	G	606	PMC	C3-CA-P1-O2
3	G	606	PMC	C3-CA-P1-O1
3	H	607	PMC	C3-CA-P1-O3
3	H	607	PMC	C3-CA-P1-O2
3	H	607	PMC	C3-CA-P1-O1
3	I	608	PMC	C3-CA-P1-O3
3	I	608	PMC	C3-CA-P1-O2
3	I	608	PMC	C3-CA-P1-O1
3	J	609	PMC	C3-CA-P1-O3
3	J	609	PMC	C3-CA-P1-O2

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Mol	Chain	Res	Type	Atoms
3	J	609	PMC	C3-CA-P1-O1
3	K	610	PMC	C3-CA-P1-O3
3	K	610	PMC	C3-CA-P1-O2
3	K	610	PMC	C3-CA-P1-O1
3	L	611	PMC	C3-CA-P1-O3
3	L	611	PMC	C3-CA-P1-O2
3	L	611	PMC	C3-CA-P1-O1
3	E	604	PMC	C3-CA-P1-O2
3	D	603	PMC	C2-C3-CA-P1
3	E	604	PMC	OC2-C-C2-C3
3	E	604	PMC	OC1-C-C2-C3
3	L	611	PMC	OC2-C-C2-C3

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	604	PMC	1	0
3	K	610	PMC	1	0
2	F	500	PLP	1	0
3	L	611	PMC	1	0
2	H	500	PLP	1	0
2	B	500	PLP	1	0
3	D	603	PMC	1	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.