



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:00 PM GMT

PDB ID : 1I43  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

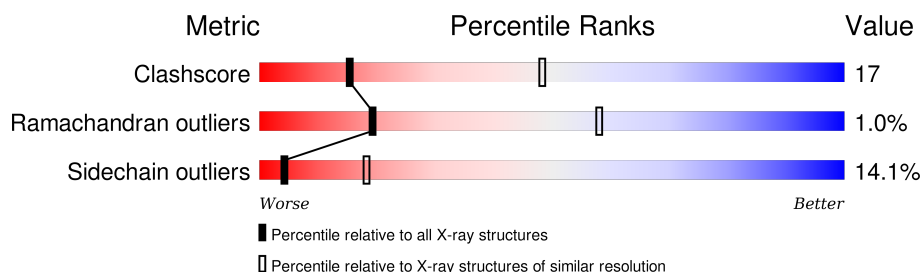
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	445	
1	B	445	
1	C	445	
1	D	445	
1	E	445	
1	F	445	
1	G	445	

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Mol	Chain	Length	Quality of chain
1	H	445	<div><div></div><div>52%</div><div>32%</div><div>5%</div><div>11%</div></div>
1	I	445	<div><div></div><div>52%</div><div>33%</div><div>•</div><div>11%</div></div>
1	J	445	<div><div></div><div>53%</div><div>31%</div><div>•</div><div>11%</div></div>
1	K	445	<div><div></div><div>52%</div><div>32%</div><div>5%</div><div>11%</div></div>
1	L	445	<div><div></div><div>51%</div><div>34%</div><div>•</div><div>11%</div></div>

## 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.

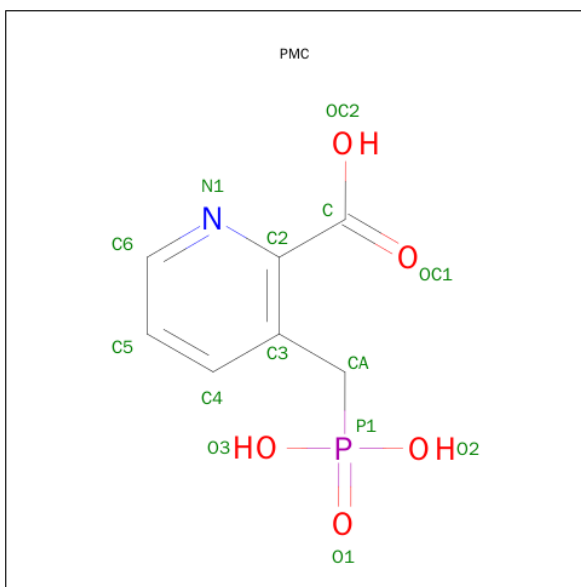
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	B	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	C	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	D	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	E	396	Total	C	N	O	S	0	0	0
			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 (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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 (three-letter code: PMC) (formula: C<sub>7</sub>H<sub>8</sub>NO<sub>5</sub>P).



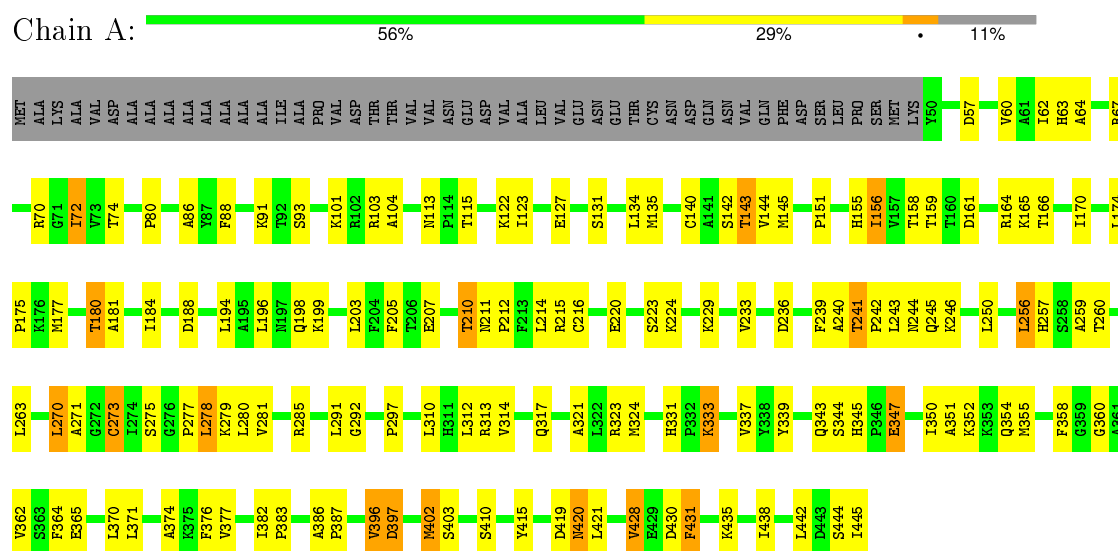
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	E	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	F	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	G	1	Total	C	N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

### 3 Residue-property plots

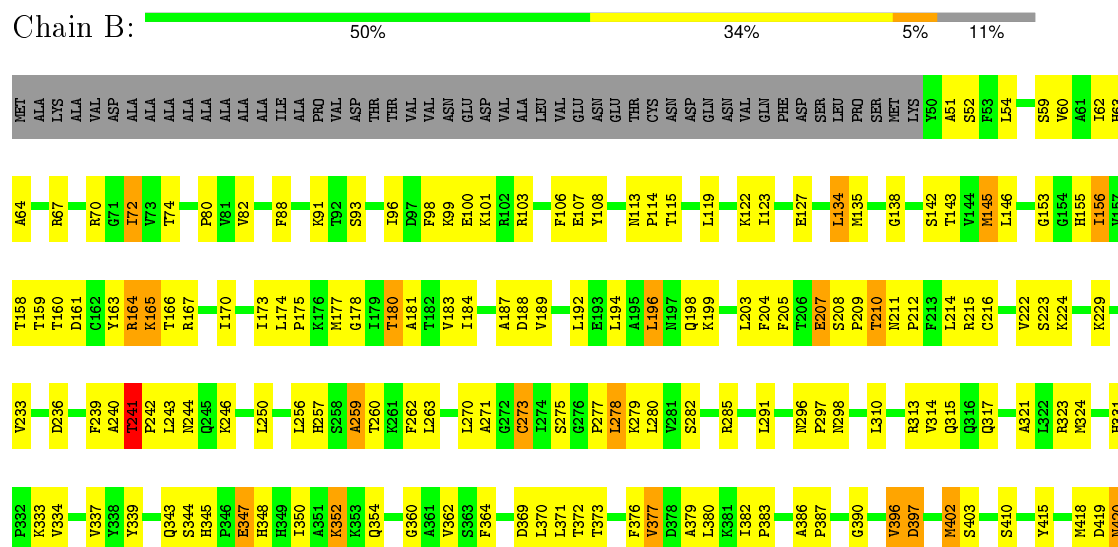
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

#### • Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

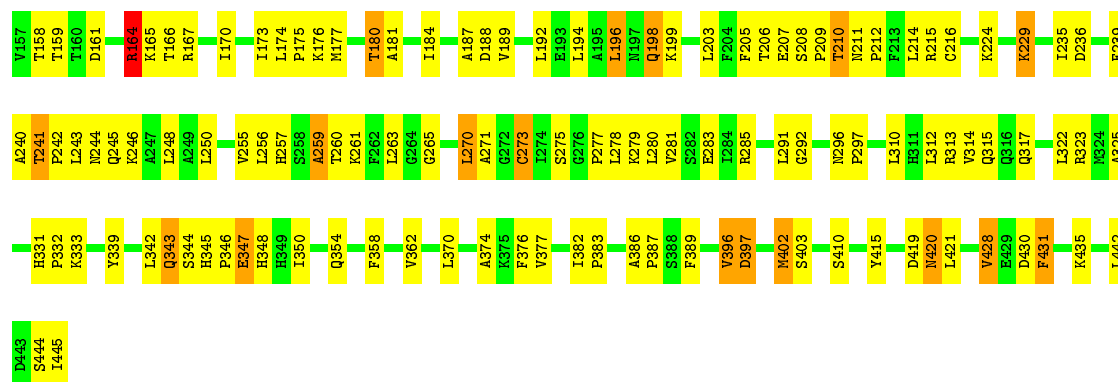


#### • Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

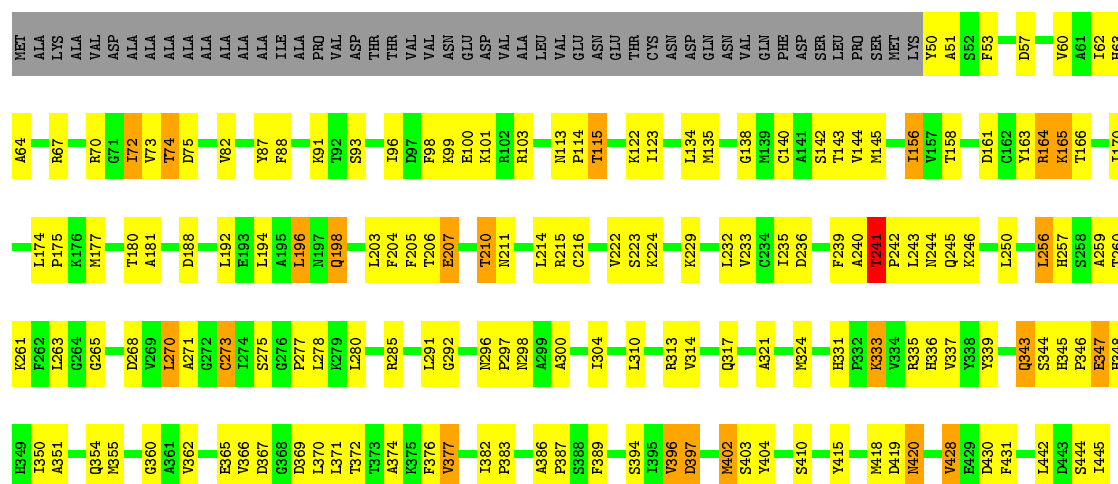




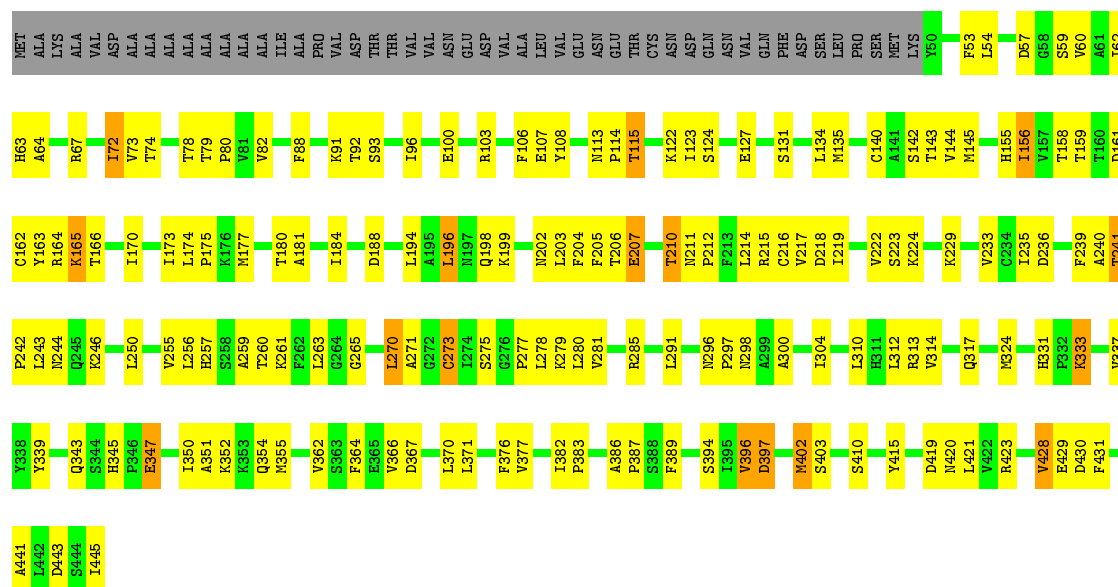




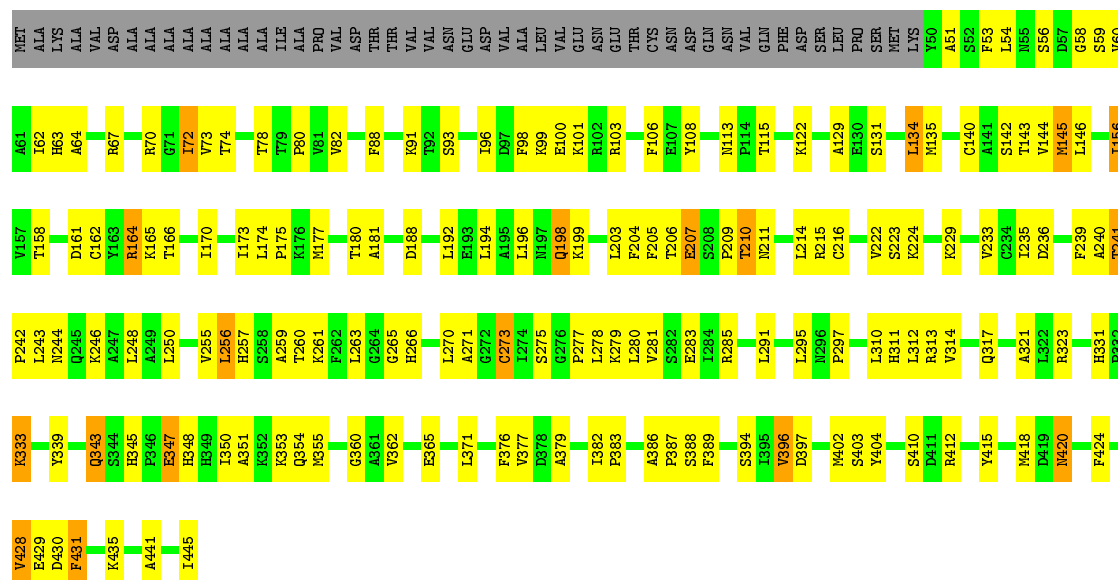
• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE



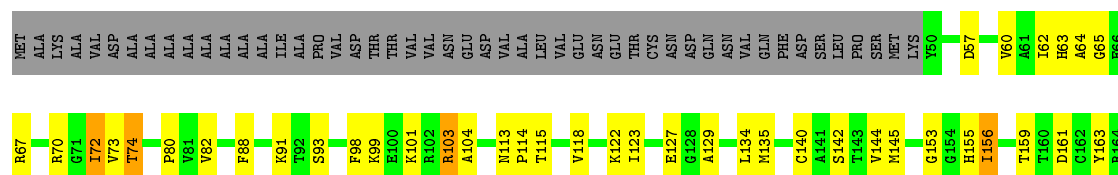
• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

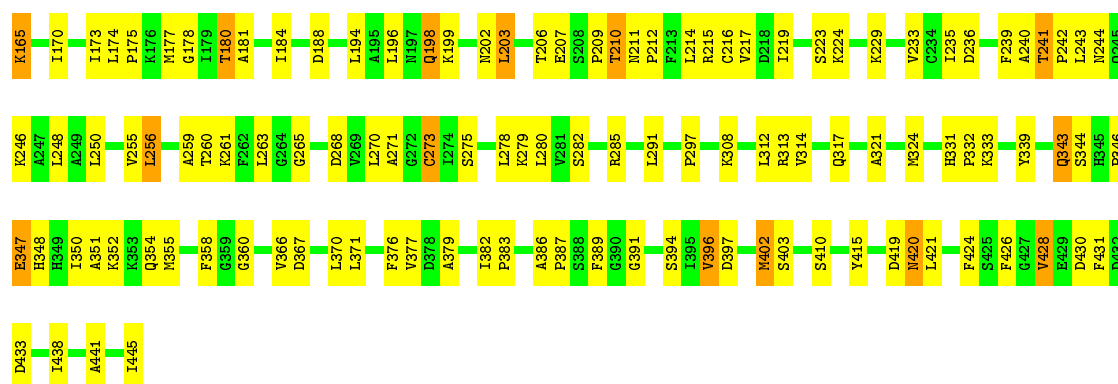


Chain H:  52% 32% 5% 11%



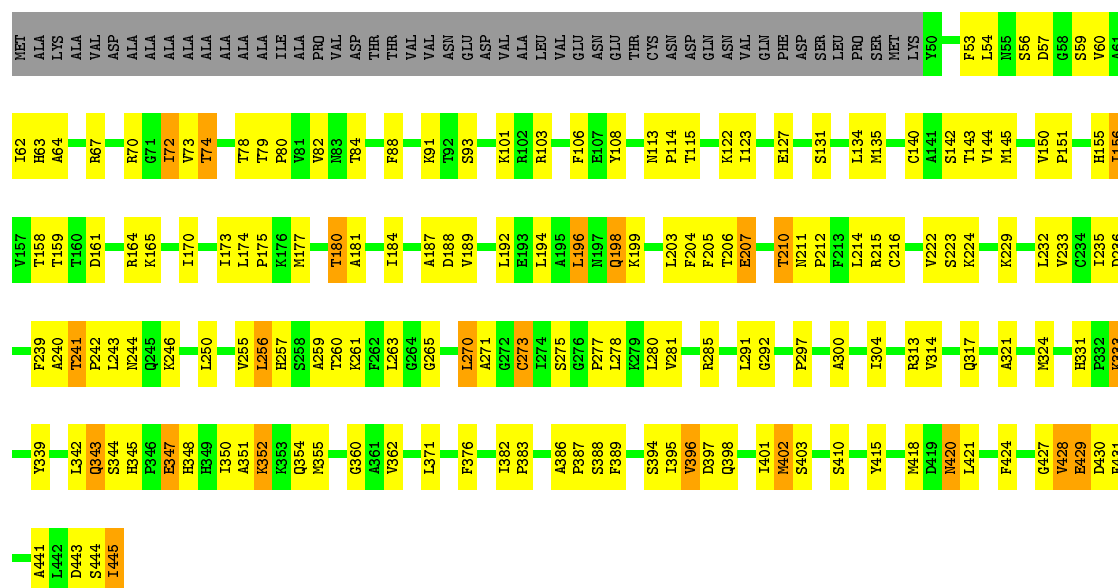
- Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE





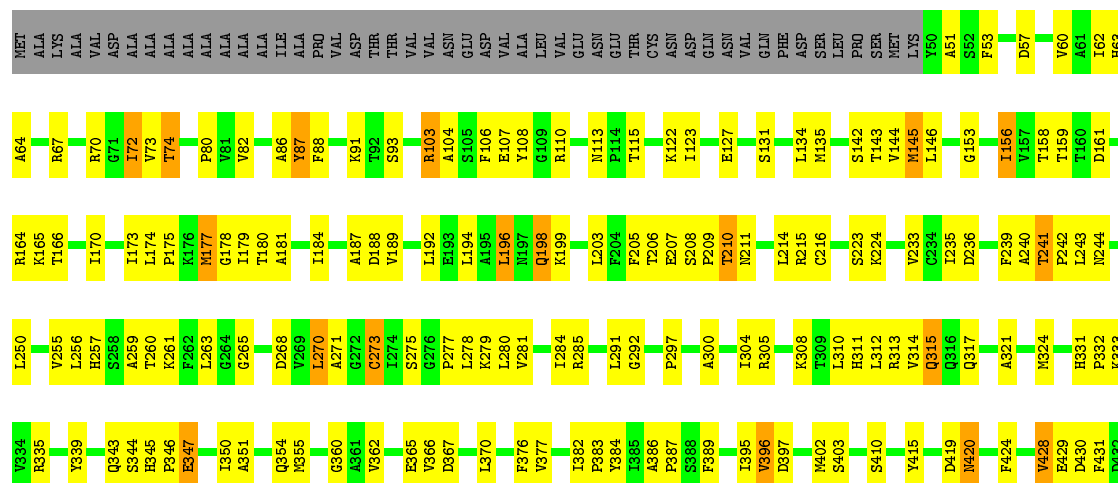
### • Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain K: 52% 32% 5% 11%



### • Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain L: 51% 34% 11%





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	309.60 Å   170.10 Å   162.10 Å 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 <sup>2</sup> )	22.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.30	0/3082	0.51	0/4179
1	B	0.30	0/3082	0.51	0/4179
1	C	0.30	0/3082	0.51	0/4179
1	D	0.30	0/3082	0.51	0/4179
1	E	0.30	0/3082	0.51	0/4179
1	F	0.29	0/3082	0.50	0/4179
1	G	0.30	0/3082	0.50	0/4179
1	H	0.30	0/3082	0.50	0/4179
1	I	0.30	0/3082	0.51	0/4179
1	J	0.30	0/3082	0.51	0/4179
1	K	0.30	0/3082	0.51	0/4179
1	L	0.30	0/3082	0.50	0/4179
All	All	0.30	0/36984	0.51	0/50148

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3023	0	3052	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3023	0	3052	114	0
1	C	3023	0	3052	106	0
1	D	3023	0	3052	102	0
1	E	3023	0	3052	127	0
1	F	3023	0	3052	108	0
1	G	3023	0	3052	111	0
1	H	3023	0	3052	119	0
1	I	3023	0	3052	120	0
1	J	3023	0	3052	109	0
1	K	3023	0	3052	115	0
1	L	3023	0	3052	120	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
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	1268	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 17.

All (1268) 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
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:I:376:PHE:HB2	1:I:445:ILE:CD1	2.10	0.81
1:A:431:PHE:HE1	1:A:435:LYS:HB2	1.44	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:G:240:ALA:O	1:G:241:THR:HB	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:CYS:H	1:A:347:GLU:HG3	1.49	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:L:347:GLU:HB3	1:L:350:ILE:HD12	1.68	0.74
1:E:431:PHE:HE1	1:E:435:LYS:HB2	1.52	0.74
1:L:170:ILE:HG23	1:L:174:LEU:HD12	1.69	0.74
1:J:216:CYS:H	1:J:347:GLU:HG3	1.53	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
1:H:72:ILE:HD12	1:H:80:PRO:HG2	1.70	0.73
1:B:259:ALA:HA	1:B:263:LEU:HB2	1.71	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:O	1:C:72:ILE:HG23	1.89	0.72
1:L:259:ALA:HA	1:L:263:LEU:HB2	1.71	0.72
1:H:216:CYS:H	1:H:347:GLU:HG3	1.53	0.72
1:A:428:VAL:HG12	1:D:62:ILE:HD11	1.71	0.72
1:C:207:GLU:HB3	1:C:236:ASP:HB3	1.70	0.71
1:F:207:GLU:HB3	1:F:236:ASP:HB3	1.71	0.71
1:D:216:CYS:H	1:D:347:GLU:HG3	1.52	0.71
1:A:207:GLU:HB3	1:A:236:ASP:HB3	1.70	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:260:THR:HG23	1:K:270:LEU:HD22	1.72	0.71
1:K:259:ALA:HA	1:K:263:LEU:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:ALA:HA	1:D:263:LEU:HB2	1.73	0.71
1:B:313:ARG:O	1:B:317:GLN:HG3	1.91	0.70
1:E:431:PHE:CE1	1:E:435:LYS:HB2	2.26	0.70
1:L:259:ALA:HB3	1:L:271:ALA:HB3	1.73	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:F:72:ILE:HG23	1:F:72:ILE:O	1.91	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:J:313:ARG:O	1:J:317:GLN:HG3	1.91	0.70
1:G:383:PRO:HB2	1:G:396:VAL:HG22	1.72	0.70
1:G:313:ARG:O	1:G:317:GLN:HG3	1.91	0.70
1:K:72:ILE:HD12	1:K:80:PRO:HG2	1.72	0.69
1:C:259:ALA:HB3	1:C:271:ALA:HB3	1.73	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:L:174:LEU:N	1:L:175:PRO:HD2	2.07	0.69
1:H:72:ILE:O	1:H:72:ILE:HG23	1.93	0.69
1:E:72:ILE:O	1:E:72:ILE:HG23	1.91	0.69
1:G:72:ILE:HG23	1:G:72:ILE:O	1.91	0.69
1:H:115:THR:HG21	1:H:297:PRO:HB3	1.74	0.69
1:A:72:ILE:HG23	1:A:72:ILE:O	1.92	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: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:I:259:ALA:HB3	1:I:271:ALA:HB3	1.75	0.68
1:B:428:VAL:HG12	1:C:62:ILE:HD11	1.74	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:G:242:PRO:O	1:G:246:LYS:HE2	1.95	0.67
1:D:113:ASN:OD1	1:D:115:THR:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ILE:HD13	1:A:273:CYS:SG	2.34	0.67
1:E:216:CYS:H	1:E:347:GLU:HG3	1.59	0.67
1:K:72:ILE:HG23	1:K:72:ILE:O	1.92	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:L:72:ILE:HG23	1:L:72:ILE:O	1.94	0.66
1:I:63:HIS:HB3	1:I:67:ARG:HB2	1.77	0.66
1:K:347:GLU:HB3	1:K:350:ILE:HD12	1.76	0.66
1:E:431:PHE:C	1:E:431:PHE:HD1	1.98	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:F:216:CYS:H	1:F:347:GLU:HG3	1.60	0.66
1:C:250:LEU:HD11	1:C:354:GLN:HB2	1.76	0.66
1:C:174:LEU:N	1:C:175:PRO:HD2	2.11	0.66
1:J:174:LEU:N	1:J:175:PRO:HD2	2.11	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
1:D:313:ARG:O	1:D:317:GLN:HG3	1.96	0.66
1:B:54:LEU:HD22	1:B:59:SER:HB3	1.76	0.66
1:I:351:ALA:O	1:I:355:MET:HB2	1.96	0.66
1:F:259:ALA:HB3	1:F:271:ALA:HB3	1.77	0.66
1:C:210:THR:HG22	1:C:215:ARG:H	1.60	0.66
1:H:123:ILE:HD13	1:H:273:CYS:SG	2.36	0.66
1:I:260:THR:HG23	1:I:270:LEU:HD22	1.76	0.66
1:H:383:PRO:HB2	1:H:396:VAL:HG22	1.77	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:O	1:D:72:ILE:HG23	1.95	0.65
1:J:63:HIS:HB3	1:J:67:ARG:HB2	1.78	0.65
1:G:259:ALA:HA	1:G:263:LEU:HB2	1.78	0.65
1:L:216:CYS:H	1:L:347:GLU:HG3	1.62	0.65
1:J:159:THR:HA	1:J:184:ILE:O	1.97	0.65
1:L:383:PRO:HB2	1:L:396:VAL:HG22	1.78	0.65
1:D:174:LEU:N	1:D:175:PRO:HD2	2.11	0.65
1:D:156:ILE:HG22	1:D:181:ALA:CB	2.26	0.65
1:H:250:LEU:HD11	1:H:354:GLN:HB2	1.78	0.65
1:A:115:THR:HG21	1:A:297:PRO:HB3	1.79	0.65
1:E:431:PHE:O	1:E:431:PHE:HD1	1.79	0.65
1:L:123:ILE:HD13	1:L:273:CYS:SG	2.37	0.65
1:E:383:PRO:HB2	1:E:396:VAL:HG22	1.77	0.65
1:F:63:HIS:HB3	1:F:67:ARG:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:242:PRO:O	1:K:246:LYS:HE2	1.96	0.65
1:J:170:ILE:HG23	1:J:174:LEU:HD12	1.79	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:I:216:CYS:H	1:I:347:GLU:HG3	1.62	0.64
1:C:370:LEU:HD23	1:C:419:ASP:HB3	1.80	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:E:431:PHE:C	1:E:431:PHE:CD1	2.69	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
1:D:324:MET:HG2	1:D:431:PHE:HE1	1.63	0.63
1:H:60:VAL:HG13	1:H:64:ALA:HB2	1.81	0.63
1:C:210:THR:O	1:C:214:LEU:HA	1.98	0.63
1:H:156:ILE:HG22	1:H:181:ALA:CB	2.29	0.63
1:D:123:ILE:HD13	1:D:273:CYS:SG	2.38	0.63
1:L:115:THR:CG2	1:L:297:PRO:HB3	2.27	0.63
1:I:386:ALA:HB2	1:K:88:PHE:HA	1.80	0.63
1:H:174:LEU:N	1:H:175:PRO:HD2	2.13	0.63
1:H:159:THR:HA	1:H:184:ILE:O	1.98	0.63
1:H:144:VAL:HG22	1:H:291:LEU:HD12	1.80	0.63
1:F:88:PHE:HA	1:H:386:ALA:HB2	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:K:243:LEU:HD12	1:K:314:VAL:HG21	1.79	0.62
1:D:194:LEU:O	1:D:198:GLN:HG3	1.98	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:F:243:LEU:HD12	1:F:314:VAL:HG21	1.80	0.62
1:C:54:LEU:HD22	1:C:59:SER:HB3	1.82	0.62
1:A:259:ALA:HA	1:A:263:LEU:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:156:ILE:HG22	1:C:181:ALA:CB	2.29	0.62
1:E:60:VAL:HG13	1:E:64:ALA:HB2	1.80	0.62
1:A:431:PHE:C	1:A:431:PHE:HD1	2.02	0.62
1:A:431:PHE:C	1:A:431:PHE:CD1	2.73	0.62
1:H:211:ASN:HB2	1:H:239:PHE:HE2	1.65	0.62
1:E:260:THR:HG23	1:E:270:LEU:HD22	1.79	0.62
1:D:87:TYR:CE2	1:D:106:PHE:HB2	2.34	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:F:115:THR:HG21	1:F:297:PRO:HB3	1.82	0.62
1:A:211:ASN:HB2	1:A:239:PHE:HE2	1.65	0.62
1:I:431:PHE:CE1	1:I:435:LYS:HB2	2.35	0.62
1:K:113:ASN:OD1	1:K:115:THR:HG22	2.00	0.61
1:A:156:ILE:HG22	1:A:181:ALA:CB	2.29	0.61
1:C:313:ARG:O	1:C:317:GLN:HG3	2.00	0.61
1:F:442:LEU:HD23	1:F:445:ILE:HD12	1.82	0.61
1:I:209:PRO:HG3	1:I:355:MET:HE1	1.81	0.61
1:F:156:ILE:HG22	1:F:181:ALA:CB	2.31	0.61
1:L:115:THR:HG21	1:L:297:PRO:HB3	1.81	0.61
1:I:174:LEU:N	1:I:175:PRO:HD2	2.15	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:B:143:THR:HG21	1:D:291:LEU:HD22	1.82	0.61
1:I:431:PHE:HE1	1:I:435:LYS:HB2	1.66	0.61
1:G:60:VAL:HG13	1:G:64:ALA:HB2	1.82	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:L:72:ILE:HD12	1:L:80:PRO:HG2	1.83	0.60
1:E:170:ILE:HG23	1:E:174:LEU:HD12	1.82	0.60
1:E:88:PHE:HA	1:G:386:ALA:HB2	1.83	0.60
1:A:347:GLU:HB3	1:A:350:ILE:HD12	1.83	0.60
1:J:156:ILE:HG22	1:J:181:ALA:CB	2.31	0.60
1:B:386:ALA:HB2	1:D:88:PHE:HA	1.82	0.60
1:K:159:THR:HA	1:K:184:ILE:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:140:CYS:HB2	1:L:292:GLY:O	2.00	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:I:60:VAL:HG13	1:I:64:ALA:HB2	1.84	0.60
1:J:62:ILE:CD1	1:K:428:VAL:HG12	2.30	0.60
1:E:174:LEU:N	1:E:175:PRO:HD2	2.17	0.60
1:G:210:THR:HG22	1:G:215:ARG:H	1.66	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: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
1:D:158:THR:HG22	1:D:205:PHE:O	2.02	0.59
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: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:250:LEU:HD11	1:F:354:GLN:HB2	1.83	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:G:174:LEU:N	1:G:175:PRO:HD2	2.18	0.59
1:J:173:ILE:C	1:J:175:PRO:HD2	2.22	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: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:G:331:HIS:CE1	1:G:333:LYS:HB2	2.38	0.58
1:A:397:ASP:HB2	1:A:402:MET:HG3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:345:HIS:CE1	1:A:347:GLU:HG2	2.38	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:D:260:THR:HG23	1:D:270:LEU:HD22	1.85	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:A:158:THR:HG22	1:A:205:PHE:O	2.04	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:383:PRO:HB2	1:F:396:VAL:HG22	1.84	0.58
1:F:82:VAL:HG21	1:F:114:PRO:HG2	1.86	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:H:376:PHE:HB2	1:H:445:ILE:HD11	1.85	0.57
1:B:113:ASN:OD1	1:B:115:THR:HG22	2.04	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:F:60:VAL:HG13	1:F:64:ALA:HB2	1.86	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: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:E:313:ARG:O	1:E:317:GLN:HG3	2.03	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:D:64:ALA:O	1:D:122:LYS:HE2	2.04	0.57
1:I:115:THR:HG21	1:I:297:PRO:HB3	1.86	0.57
1:E:347:GLU:HB3	1:E:350:ILE:HD12	1.85	0.57
1:C:60:VAL:HG13	1:C:64:ALA:HB2	1.86	0.57
1:K:324:MET:HG2	1:K:431:PHE:HE1	1.70	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:G:256:LEU:HB2	1:G:273:CYS:O	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:242:PRO:HD3	1:F:257:HIS:CE1	2.40	0.57
1:D:397:ASP:HB2	1:D:402:MET:HG3	1.86	0.57
1:A:210:THR:HG23	1:A:211:ASN:N	2.19	0.57
1:H:210:THR:O	1:H:214:LEU:HA	2.05	0.57
1:B:60:VAL:HG13	1:B:64:ALA:HB2	1.87	0.57
1:A:323:ARG:CZ	1:A:431:PHE:HD2	2.17	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:F:73:VAL:O	1:F:74:THR:HG23	2.05	0.56
1:J:207:GLU:CB	1:J:236:ASP:HB3	2.33	0.56
1:A:207:GLU:CB	1:A:236:ASP:HB3	2.34	0.56
1:D:113:ASN:ND2	1:D:297:PRO:HG3	2.20	0.56
1:K:64:ALA:O	1:K:122:LYS:HE2	2.05	0.56
1:C:73:VAL:O	1:C:74:THR:HG23	2.05	0.56
1:J:428:VAL:HG13	1:J:428:VAL:O	2.04	0.56
1:F:386:ALA:HB2	1:H:88:PHE:HA	1.87	0.56
1:B:242:PRO:O	1:B:246:LYS:HE2	2.05	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:I:428:VAL:O	1:I:428:VAL:HG13	2.06	0.56
1:G:260:THR:HG23	1:G:270:LEU:HD22	1.87	0.56
1:B:194:LEU:O	1:B:198:GLN:HG3	2.06	0.56
1:I:210:THR:O	1:I:214:LEU:HA	2.04	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:E:250:LEU:HD11	1:E:354:GLN:HB2	1.86	0.56
1:E:194:LEU:O	1:E:198:GLN:HG3	2.05	0.56
1:E:82:VAL:HG21	1:E:114:PRO:HG2	1.86	0.56
1:K:300:ALA:O	1:K:304:ILE:HG13	2.06	0.56
1:B:291:LEU:HD22	1:D:143:THR:HG21	1.88	0.56
1:E:51:ALA:HB1	1:E:53:PHE:CE2	2.41	0.56
1:L:376:PHE:HB2	1:L:445:ILE:HD11	1.87	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:A:323:ARG:CZ	1:A:431:PHE:CD2	2.89	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:E:386:ALA:HB2	1:G:88:PHE:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:THR:HG21	1:C:291:LEU:HD22	1.88	0.56
1:C:242:PRO:O	1:C:246:LYS:HE2	2.05	0.55
1:A:115:THR:CG2	1:A:297:PRO:HB3	2.36	0.55
1:G:156:ILE:HG22	1:G:181:ALA:HB2	1.87	0.55
1:J:210:THR:O	1:J:214:LEU:HA	2.07	0.55
1:I:170:ILE:HG23	1:I:174:LEU:HD12	1.88	0.55
1:C:260:THR:CG2	1:C:270:LEU:HD22	2.36	0.55
1:D:347:GLU:HB3	1:D:350:ILE:HD12	1.89	0.55
1:C:383:PRO:HB2	1:C:396:VAL:CG2	2.35	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:L:194:LEU:O	1:L:198:GLN:HG3	2.07	0.55
1:K:351:ALA:O	1:K:355:MET:HB2	2.05	0.55
1:J:428:VAL:HG12	1:K:62:ILE:CD1	2.33	0.55
1:I:215:ARG:HD2	1:I:347:GLU:OE2	2.06	0.55
1:J:211:ASN:HB2	1:J:239:PHE:CE2	2.41	0.55
1:E:260:THR:CG2	1:E:270:LEU:HD22	2.37	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:L:260:THR:HG23	1:L:270:LEU:HD22	1.87	0.55
1:J:123:ILE:HD13	1:J:273:CYS:SG	2.47	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:A:310:LEU:O	1:A:314:VAL:HG23	2.07	0.55
1:A:156:ILE:HG22	1:A:181:ALA:HB2	1.89	0.55
1:G:339:TYR:CD1	1:G:362:VAL:HG22	2.41	0.55
1:D:115:THR:HG21	1:D:297:PRO:HB3	1.89	0.54
1:A:382:ILE:HG12	1:D:54:LEU:HD21	1.89	0.54
1:A:223:SER:HA	1:A:233:VAL:HG21	1.89	0.54
1:J:155:HIS:O	1:J:202:ASN:HB2	2.07	0.54
1:D:96:ILE:O	1:D:100:GLU:HG3	2.07	0.54
1:A:428:VAL:O	1:A:428:VAL:HG13	2.07	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:G:115:THR:CG2	1:G:297:PRO:HB3	2.37	0.54
1:E:159:THR:HA	1:E:184:ILE:O	2.07	0.54
1:A:241:THR:HG22	1:A:243:LEU:N	2.14	0.54
1:L:256:LEU:HB2	1:L:273:CYS:O	2.07	0.54
1:L:87:TYR:N	1:L:87:TYR:CD2	2.76	0.54
1:I:242:PRO:HD3	1:I:257:HIS:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:THR:HG21	1:H:291:LEU:HD22	1.89	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:E:158:THR:HG22	1:E:205:PHE:O	2.07	0.54
1:C:262:PHE:CE1	1:C:390:GLY:HA2	2.43	0.54
1:E:166:THR:O	1:E:170:ILE:HG13	2.08	0.54
1:D:379:ALA:HB3	1:D:441:ALA:HB1	1.89	0.54
1:D:243:LEU:HD12	1:D:314:VAL:HG21	1.89	0.54
1:C:428:VAL:O	1:C:428:VAL:HG13	2.07	0.54
1:F:158:THR:HG22	1:F:205:PHE:O	2.07	0.54
1:E:428:VAL:HG12	1:H:62:ILE:CD1	2.36	0.54
1:B:156:ILE:HG22	1:B:181:ALA:HB2	1.90	0.54
1:K:170:ILE:HG23	1:K:174:LEU:HD12	1.89	0.54
1:H:166:THR:O	1:H:170:ILE:HG13	2.07	0.54
1:J:291:LEU:HD22	1:L:143:THR:HG21	1.90	0.54
1:L:144:VAL:HG22	1:L:291:LEU:HD12	1.89	0.54
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: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: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: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:B:260:THR:HG21	1:D:108:TYR:OH	2.08	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:D:215:ARG:NH1	1:D:347:GLU:OE2	2.41	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:I:345:HIS:CE1	1:I:347:GLU:HG2	2.43	0.53
1:F:313:ARG:O	1:F:317:GLN:HG3	2.08	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:D:428:VAL:HG13	1:D:428:VAL:O	2.07	0.53
1:B:210:THR:O	1:B:214:LEU:HA	2.08	0.53
1:D:242:PRO:O	1:D:246:LYS:HE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:78:THR:HG21	1:L:268:ASP:HB3	1.89	0.53
1:B:370:LEU:HD23	1:B:419:ASP:HB3	1.91	0.53
1:K:321:ALA:HB2	1:K:360:GLY:HA2	1.90	0.53
1:C:207:GLU:CB	1:C:236:ASP:HB3	2.39	0.53
1:B:428:VAL:O	1:B:428:VAL:HG13	2.09	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:B:155:HIS:HD1	1:B:180:THR:HG23	1.74	0.53
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:F:397:ASP:HB2	1:F:402:MET:HG3	1.91	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
1:K:250:LEU:HD11	1:K:354:GLN:HB2	1.92	0.52
1:G:310:LEU:O	1:G:314:VAL:HG23	2.10	0.52
1:A:62:ILE:CD1	1:D:428:VAL:HG12	2.40	0.52
1:C:211:ASN:HB2	1:C:239:PHE:CE2	2.45	0.52
1:I:431:PHE:C	1:I:431:PHE:CD1	2.82	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:K:80:PRO:HB3	1:L:82:VAL:HG22	1.91	0.52
1:B:242:PRO:HD3	1:B:257:HIS:CE1	2.43	0.52
1:G:207:GLU:CB	1:G:236:ASP:HB3	2.36	0.52
1:D:166:THR:O	1:D:170:ILE:HG13	2.10	0.52
1:A:60:VAL:HG13	1:A:64:ALA:HB2	1.92	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:L:210:THR:HG22	1:L:215:ARG:H	1.75	0.52
1:B:347:GLU:HB3	1:B:350:ILE:HD12	1.92	0.52
1:B:115:THR:HG21	1:B:297:PRO:HB3	1.91	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:H:345:HIS:HE1	1:H:347:GLU:HG2	1.75	0.52
1:E:63:HIS:CD2	1:E:67:ARG:HD3	2.45	0.52
1:B:386:ALA:HB1	1:B:387:PRO:CD	2.40	0.52
1:F:64:ALA:O	1:F:122:LYS:HE2	2.10	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: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:F:210:THR:O	1:F:214:LEU:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:144:VAL:HG22	1:J:291:LEU:HD12	1.92	0.51
1:I:313:ARG:O	1:I:317:GLN:HG3	2.10	0.51
1:G:351:ALA:O	1:G:355:MET:HB2	2.10	0.51
1:J:60:VAL:HG13	1:J:64:ALA:HB2	1.92	0.51
1:B:250:LEU:HD11	1:B:354:GLN:HB2	1.92	0.51
1:H:250:LEU:CD1	1:H:354:GLN:HB2	2.39	0.51
1:F:386:ALA:HB1	1:F:387:PRO:CD	2.41	0.51
1:A:131:SER:HB3	1:A:281:VAL:HG11	1.93	0.51
1:C:115:THR:CG2	1:C:297:PRO:HB3	2.39	0.51
1:A:260:THR:CG2	1:A:270:LEU:HD22	2.39	0.51
1:L:250:LEU:HD11	1:L:354:GLN:HB2	1.93	0.51
1:H:158:THR:HG22	1:H:205:PHE:O	2.10	0.51
1:F:241:THR:HG23	1:F:242:PRO:HD2	1.92	0.51
1:A:323:ARG:NH1	1:A:431:PHE:CD2	2.79	0.51
1:L:210:THR:O	1:L:214:LEU:HA	2.10	0.51
1:G:63:HIS:CD2	1:G:67:ARG:HD3	2.45	0.51
1:F:194:LEU:O	1:F:198:GLN:HG3	2.11	0.51
1:G:277:PRO:HG2	1:G:280:LEU:HB2	1.93	0.51
1:E:123:ILE:HD13	1:E:273:CYS:SG	2.51	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:365:GLU:HB3	1:I:420:ASN:HB3	1.93	0.51
1:I:250:LEU:HD11	1:I:354:GLN:HB2	1.91	0.51
1:L:310:LEU:O	1:L:314:VAL:HG23	2.11	0.51
1:I:96:ILE:O	1:I:100:GLU:HG3	2.11	0.51
1:C:339:TYR:CD1	1:C:362:VAL:HG22	2.46	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: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:G:260:THR:CG2	1:G:270:LEU:HD22	2.40	0.51
1:L:173:ILE:C	1:L:175:PRO:HD2	2.31	0.50
1:G:64:ALA:O	1:G:122:LYS:HE2	2.10	0.50
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:A:166:THR:O	1:A:170:ILE:HG13	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:397:ASP:HB2	1:B:402:MET:HG3	1.94	0.50
1:E:323:ARG:CZ	1:E:431:PHE:HD2	2.25	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:D:210:THR:O	1:D:214:LEU:HA	2.11	0.50
1:B:170:ILE:HA	1:B:174:LEU:HD12	1.94	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:A:88:PHE:HA	1:C:386:ALA:HB2	1.94	0.50
1:L:211:ASN:HB2	1:L:239:PHE:CE2	2.46	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:C:277:PRO:HG2	1:C:280:LEU:HB2	1.93	0.50
1:E:243:LEU:HD12	1:E:314:VAL:HG21	1.94	0.50
1:C:72:ILE:CG2	1:C:72:ILE:O	2.58	0.50
1:D:115:THR:CG2	1:D:297:PRO:HB3	2.41	0.50
1:H:256:LEU:HB2	1:H:273:CYS:O	2.12	0.50
1:B:173:ILE:C	1:B:175:PRO:HD2	2.32	0.50
1:F:123:ILE:HD13	1:F:273:CYS:SG	2.52	0.50
1:G:441:ALA:C	1:G:443:ASP:H	2.15	0.50
1:K:127:GLU:OE2	1:K:257:HIS:NE2	2.42	0.49
1:E:242:PRO:HD3	1:E:257:HIS:CE1	2.47	0.49
1:B:241:THR:CG2	1:B:243:LEU:H	2.18	0.49
1:F:138:GLY:N	2:F:500:PLP:O2P	2.46	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:I:311:HIS:HE2	1:L:428:VAL:HG13	1.77	0.49
1:F:428:VAL:HG13	1:F:428:VAL:O	2.12	0.49
1:B:379:ALA:HB3	1:B:441:ALA:HB1	1.92	0.49
1:G:397:ASP:HB2	1:G:402:MET:HG3	1.94	0.49
1:H:215:ARG:HD2	1:H:347:GLU:OE2	2.13	0.49
1:B:72:ILE:O	1:B:72:ILE:CG2	2.59	0.49
1:A:277:PRO:HG2	1:A:280:LEU:HB2	1.94	0.49
1:J:321:ALA:HB2	1:J:360:GLY:HA2	1.95	0.49
1:H:54:LEU:HD22	1:H:59:SER:CB	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:HIS:HE1	1:A:347:GLU:HG2	1.75	0.49
1:G:345:HIS:CE1	1:G:347:GLU:HG2	2.48	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:C:223:SER:HA	1:C:233:VAL:HG21	1.94	0.49
1:B:256:LEU:HB2	1:B:273:CYS:O	2.11	0.49
1:F:210:THR:HG23	1:F:211:ASN:N	2.27	0.49
1:B:115:THR:CG2	1:B:297:PRO:HB3	2.43	0.49
1:G:140:CYS:O	1:G:144:VAL:HG23	2.13	0.49
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:H:351:ALA:O	1:H:355:MET:HB2	2.13	0.49
1:L:60:VAL:HG13	1:L:64:ALA:HB2	1.94	0.49
1:B:82:VAL:HG21	1:B:114:PRO:HG2	1.95	0.49
1:K:210:THR:HG23	1:K:211:ASN:N	2.27	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:G:80:PRO:HB3	1:H:82:VAL:HG22	1.95	0.49
1:F:63:HIS:HE1	1:G:429:GLU:OE2	1.95	0.49
1:H:365:GLU:HB3	1:H:420:ASN:HB3	1.95	0.49
1:H:331:HIS:CE1	1:H:333:LYS:HB2	2.48	0.49
1:E:210:THR:HG23	1:E:211:ASN:N	2.27	0.49
1:D:386:ALA:HB1	1:D:387:PRO:CD	2.43	0.49
1:J:250:LEU:CD1	1:J:354:GLN:HB2	2.42	0.49
1:C:386:ALA:HB1	1:C:387:PRO:CD	2.41	0.49
1:J:223:SER:HA	1:J:233:VAL:HG21	1.95	0.49
1:K:174:LEU:N	1:K:175:PRO:CD	2.75	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:C:158:THR:HG22	1:C:205:PHE:O	2.13	0.49
1:G:194:LEU:O	1:G:198:GLN:HG3	2.13	0.49
1:H:255:VAL:HG13	1:H:255:VAL:O	2.13	0.49
1:G:131:SER:HB3	1:G:281:VAL:HG11	1.94	0.49
1:G:242:PRO:HD3	1:G:257:HIS:CE1	2.48	0.48
1:K:210:THR:O	1:K:214:LEU:HA	2.13	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:F:296:ASN:OD1	1:F:298:ASN:HB2	2.13	0.48
1:K:242:PRO:HD3	1:K:257:HIS:CE1	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:323:ARG:CZ	1:E:431:PHE:CD2	2.96	0.48
1:B:96:ILE:O	1:B:100:GLU:HG3	2.13	0.48
1:K:343:GLN:HA	1:K:348:HIS:CD2	2.48	0.48
1:F:300:ALA:O	1:F:304:ILE:HG13	2.13	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:G:113:ASN:ND2	1:G:297:PRO:HG3	2.29	0.48
1:D:87:TYR:CD2	1:D:106:PHE:HB2	2.47	0.48
1:J:73:VAL:O	1:J:74:THR:HG23	2.13	0.48
1:E:206:THR:O	1:E:235:ILE:HA	2.13	0.48
1:G:170:ILE:HA	1:G:174:LEU:HD12	1.96	0.48
1:I:215:ARG:NH1	1:I:347:GLU:OE2	2.44	0.48
1:K:156:ILE:HG22	1:K:181:ALA:HB2	1.94	0.48
1:K:387:PRO:HB3	3:K:610:PMC:HCA2	1.94	0.48
1:K:261:LYS:HD2	1:K:389:PHE:CZ	2.49	0.48
1:C:324:MET:HG2	1:C:431:PHE:HE1	1.78	0.48
1:A:321:ALA:HB2	1:A:360:GLY:HA2	1.95	0.48
1:I:156:ILE:HG22	1:I:181:ALA:CB	2.43	0.48
1:I:62:ILE:CD1	1:L:428:VAL:HG12	2.36	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: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:A:370:LEU:HD23	1:A:419:ASP:HB3	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:K:265:GLY:HA3	1:K:313:ARG:NH1	2.28	0.48
1:F:428:VAL:CG2	1:G:312:LEU:HD11	2.44	0.48
1:B:382:ILE:HB	1:B:383:PRO:HD3	1.96	0.48
1:A:140:CYS:O	1:A:144:VAL:HG23	2.14	0.48
1:E:173:ILE:O	1:E:176:LYS:HB2	2.14	0.48
1:I:140:CYS:HB2	1:K:292:GLY:O	2.14	0.48
1:K:70:ARG:HD3	1:K:79:THR:OG1	2.14	0.48
1:J:261:LYS:HD2	1:J:389:PHE:CZ	2.49	0.48
1:I:115:THR:CG2	1:I:297:PRO:HB3	2.42	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:D:159:THR:HA	1:D:184:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:346:PRO:HB2	1:L:347:GLU:OE2	2.14	0.48
1:D:54:LEU:HD22	1:D:59:SER:HB3	1.96	0.48
1:C:206:THR:O	1:C:235:ILE:HA	2.14	0.48
1:F:351:ALA:O	1:F:355:MET:HB2	2.13	0.48
1:I:143:THR:HG21	1:K:291:LEU:HD22	1.95	0.48
1:H:194:LEU:O	1:H:198:GLN:HG3	2.14	0.48
1:G:82:VAL:HG21	1:G:114:PRO:HG2	1.96	0.48
1:I:54:LEU:HD22	1:I:59:SER:HB3	1.95	0.48
1:A:113:ASN:ND2	1:A:297:PRO:HG3	2.28	0.47
1:I:156:ILE:HG22	1:I:181:ALA:HB2	1.96	0.47
1:B:159:THR:HA	1:B:184:ILE:O	2.14	0.47
1:L:365:GLU:HB3	1:L:420:ASN:HB3	1.96	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:K:204:PHE:HE2	1:K:222:VAL:HG11	1.78	0.47
1:I:56:SER:HB3	1:L:433:ASP:OD2	2.13	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:B:211:ASN:HB2	1:B:239:PHE:CE2	2.50	0.47
1:E:256:LEU:HB2	1:E:273:CYS:O	2.13	0.47
1:D:103:ARG:HG2	1:D:104:ALA:N	2.30	0.47
1:A:291:LEU:HD22	1:C:143:THR:HG21	1.96	0.47
1:C:296:ASN:OD1	1:C:298:ASN:HB2	2.15	0.47
1:A:242:PRO:O	1:A:246:LYS:HE2	2.14	0.47
1:F:72:ILE:CG2	1:F:72:ILE:O	2.62	0.47
1:J:382:ILE:HB	1:J:383:PRO:HD3	1.97	0.47
1:B:145:MET:HE2	1:B:146:LEU:HD23	1.96	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:F:57:ASP:HB3	1:F:243:LEU:CD2	2.44	0.47
1:E:127:GLU:OE2	1:E:257:HIS:NE2	2.45	0.47
1:B:166:THR:O	1:B:170:ILE:HG13	2.13	0.47
1:A:159:THR:HA	1:A:184:ILE:O	2.15	0.47
1:B:212:PRO:HG2	1:B:421:LEU:HD21	1.96	0.47
1:H:343:GLN:HA	1:H:348:HIS:CD2	2.49	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:K:428:VAL:HG13	1:K:428:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:THR:HG21	1:E:297:PRO:HB3	1.97	0.47
1:C:173:ILE:C	1:C:175:PRO:HD2	2.35	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:E:339:TYR:CD1	1:E:362:VAL:HG22	2.49	0.47
1:L:127:GLU:OE2	1:L:242:PRO:HB3	2.15	0.47
1:E:210:THR:O	1:E:214:LEU:HA	2.15	0.47
1:L:211:ASN:HB2	1:L:239:PHE:HE2	1.80	0.47
1:K:345:HIS:CE1	1:K:347:GLU:HG2	2.49	0.47
1:G:166:THR:O	1:G:170:ILE:HG13	2.14	0.47
1:B:428:VAL:CG2	1:C:312:LEU:HD11	2.45	0.47
1:L:386:ALA:HB1	1:L:387:PRO:CD	2.44	0.47
1:B:174:LEU:N	1:B:175:PRO:CD	2.77	0.47
1:K:115:THR:HG21	1:K:297:PRO:HB3	1.95	0.47
1:E:265:GLY:HA3	1:E:313:ARG:NH1	2.29	0.47
1:A:131:SER:CB	1:A:281:VAL:HG11	2.45	0.47
1:F:98:PHE:HE2	1:F:99:LYS:HE2	1.79	0.47
1:I:266:HIS:CD2	1:L:305:ARG:HG2	2.49	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:G:300:ALA:O	1:G:304:ILE:HG13	2.15	0.47
1:I:240:ALA:O	1:I:244:ASN:HB2	2.15	0.47
1:E:57:ASP:HB3	1:E:243:LEU:CD2	2.45	0.47
1:I:387:PRO:O	1:I:388:SER:HB3	2.14	0.47
1:H:373:THR:O	1:H:377:VAL:HG13	2.15	0.47
1:A:103:ARG:HG2	1:A:104:ALA:N	2.30	0.47
1:F:75:ASP:N	1:F:75:ASP:OD1	2.47	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:240:ALA:O	1:B:244:ASN:HB2	2.15	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:C:210:THR:HG23	1:C:211:ASN:N	2.29	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:H:428:VAL:HG13	1:H:428:VAL:O	2.14	0.46
1:F:418:MET:C	1:F:420:ASN:H	2.17	0.46
1:G:159:THR:HA	1:G:184:ILE:O	2.15	0.46
1:F:369:ASP:H	1:F:372:THR:HB	1.79	0.46
1:J:343:GLN:HA	1:J:348:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:310:LEU:O	1:F:314:VAL:HG23	2.15	0.46
1:I:207:GLU:CB	1:I:236:ASP:HB3	2.43	0.46
1:I:72:ILE:CG2	1:I:72:ILE:O	2.62	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: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:B:127:GLU:OE2	1:B:257:HIS:NE2	2.46	0.46
1:B:98:PHE:HE2	1:B:99:LYS:HE2	1.79	0.46
1:A:386:ALA:HB2	1:C:88:PHE:HA	1.97	0.46
1:C:153:GLY:HA2	1:C:178:GLY:O	2.15	0.46
1:E:255:VAL:O	1:E:255:VAL:HG13	2.15	0.46
1:I:291:LEU:HD22	1:K:143:THR:HG21	1.97	0.46
1:L:240:ALA:O	1:L:244:ASN:HB2	2.16	0.46
1:E:428:VAL:O	1:E:428:VAL:CG1	2.64	0.46
1:D:210:THR:HG22	1:D:215:ARG:H	1.80	0.46
1:G:383:PRO:HA	1:G:394:SER:O	2.16	0.46
1:L:72:ILE:O	1:L:72:ILE:CG2	2.64	0.46
1:K:63:HIS:HB3	1:K:67:ARG:CB	2.45	0.46
1:E:96:ILE:O	1:E:100:GLU:HG3	2.16	0.46
1:A:215:ARG:HD2	1:A:347:GLU:OE2	2.16	0.46
1:L:174:LEU:N	1:L:175:PRO:CD	2.75	0.46
1:F:211:ASN:HB2	1:F:239:PHE:HE2	1.80	0.46
1:C:174:LEU:N	1:C:175:PRO:CD	2.77	0.46
1:H:210:THR:HG23	1:H:211:ASN:N	2.30	0.46
1:E:156:ILE:HG22	1:E:181:ALA:HB2	1.96	0.46
1:C:103:ARG:HG2	1:C:104:ALA:N	2.30	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: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:K:72:ILE:O	1:K:72:ILE:CG2	2.63	0.46
1:I:166:THR:O	1:I:170:ILE:HG13	2.16	0.46
1:E:370:LEU:HD23	1:E:419:ASP:HB3	1.98	0.46
1:G:72:ILE:CG2	1:G:72:ILE:O	2.61	0.46
1:J:63:HIS:HE1	1:K:429:GLU:OE2	1.99	0.46
1:B:396:VAL:HG13	1:B:424:PHE:CD2	2.50	0.46
1:L:277:PRO:HG2	1:L:280:LEU:HB2	1.98	0.46
1:I:321:ALA:HB2	1:I:360:GLY:HA2	1.98	0.46
1:G:261:LYS:HD2	1:G:389:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:255:VAL:HG13	1:J:255:VAL:O	2.15	0.46
1:E:240:ALA:O	1:E:244:ASN:HB2	2.16	0.46
1:A:431:PHE:O	1:A:431:PHE:HD1	1.99	0.46
1:H:53:PHE:HD1	1:H:54:LEU:HG	1.80	0.46
1:L:166:THR:O	1:L:170:ILE:HG13	2.15	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:H:386:ALA:HB1	1:H:387:PRO:CD	2.46	0.46
1:K:250:LEU:CD1	1:K:354:GLN:HB2	2.46	0.46
1:B:418:MET:C	1:B:420:ASN:H	2.18	0.46
1:F:370:LEU:HD23	1:F:419:ASP:HB3	1.97	0.46
1:J:331:HIS:ND1	1:J:332:PRO:HD2	2.31	0.46
1:C:345:HIS:CE1	1:C:347:GLU:HG2	2.51	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:K:386:ALA:HB1	1:K:387:PRO:CD	2.46	0.46
1:D:131:SER:OG	1:D:281:VAL:HG11	2.16	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:53:PHE:CD1	1:K:54:LEU:HG	2.51	0.45
1:G:250:LEU:CD1	1:G:354:GLN:HB2	2.45	0.45
1:F:383:PRO:HB3	1:F:394:SER:HB3	1.97	0.45
1:J:64:ALA:O	1:J:122:LYS:HE2	2.16	0.45
1:G:212:PRO:HG2	1:G:421:LEU:HD21	1.98	0.45
1:A:337:VAL:HG22	1:A:364:PHE:HB3	1.98	0.45
1:G:206:THR:O	1:G:235:ILE:HA	2.16	0.45
1:L:57:ASP:HB3	1:L:243:LEU:CD2	2.46	0.45
1:E:312:LEU:HD11	1:H:428:VAL:CG2	2.46	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:G:53:PHE:CE1	1:G:54:LEU:HG	2.51	0.45
1:F:82:VAL:HG21	1:F:114:PRO:CG	2.46	0.45
1:F:321:ALA:HB2	1:F:360:GLY:HA2	1.97	0.45
1:F:206:THR:O	1:F:235:ILE:HA	2.16	0.45
1:K:215:ARG:HD2	1:K:347:GLU:OE2	2.16	0.45
1:B:207:GLU:CB	1:B:236:ASP:HB3	2.45	0.45
1:L:192:LEU:HG	1:L:196:LEU:HD23	1.97	0.45
1:K:241:THR:HG22	1:K:243:LEU:N	2.14	0.45
1:C:241:THR:CG2	1:C:243:LEU:H	2.16	0.45
1:L:428:VAL:O	1:L:428:VAL:CG1	2.63	0.45
1:J:346:PRO:HB2	1:J:347:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:72:ILE:HD11	1:J:72:ILE:HD11	1.97	0.45
1:J:386:ALA:HB1	1:J:387:PRO:CD	2.46	0.45
1:I:131:SER:CB	1:I:281:VAL:HG11	2.46	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:L:351:ALA:O	1:L:355:MET:HB2	2.16	0.45
1:H:206:THR:O	1:H:235:ILE:HA	2.16	0.45
1:F:335:ARG:HH21	1:F:367:ASP:HA	1.81	0.45
1:H:212:PRO:HG2	1:H:421:LEU:HD21	1.99	0.45
1:C:98:PHE:HE2	1:C:99:LYS:HE2	1.81	0.45
1:K:206:THR:O	1:K:235:ILE:HA	2.15	0.45
1:I:243:LEU:HD12	1:I:314:VAL:HG21	1.98	0.45
1:E:241:THR:HG23	1:E:242:PRO:HD2	1.98	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:I:63:HIS:HE1	1:L:429:GLU:OE2	1.99	0.45
1:I:343:GLN:HA	1:I:348:HIS:CD2	2.51	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:A:215:ARG:NH1	1:A:347:GLU:OE2	2.50	0.45
1:F:210:THR:HG22	1:F:215:ARG:H	1.81	0.45
1:D:256:LEU:HB2	1:D:273:CYS:O	2.17	0.45
1:I:323:ARG:CZ	1:I:431:PHE:HD2	2.30	0.45
1:B:163:TYR:CE2	1:B:165:LYS:HB2	2.52	0.45
1:D:365:GLU:HB3	1:D:420:ASN:HB3	1.97	0.45
1:H:310:LEU:O	1:H:314:VAL:HG23	2.16	0.45
1:J:240:ALA:O	1:J:244:ASN:HB2	2.16	0.45
1:C:428:VAL:O	1:C:428:VAL:CG1	2.64	0.45
1:G:259:ALA:HB3	1:G:271:ALA:HB3	1.98	0.45
1:E:250:LEU:CD1	1:E:354:GLN:HB2	2.46	0.45
1:D:192:LEU:HG	1:D:196:LEU:HD23	1.99	0.45
1:E:261:LYS:HD2	1:E:389:PHE:CZ	2.52	0.45
1:J:98:PHE:HE2	1:J:99:LYS:HE2	1.81	0.45
1:B:62:ILE:CD1	1:C:428:VAL:HG12	2.45	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:K:396:VAL:HG13	1:K:424:PHE:CD2	2.51	0.45
1:F:256:LEU:HB2	1:F:273:CYS:O	2.17	0.45
1:A:386:ALA:HB1	1:A:387:PRO:CD	2.46	0.45
1:C:397:ASP:HB2	1:C:402:MET:HG3	1.99	0.45
1:B:106:PHE:O	1:B:108:TYR:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:379:ALA:HB3	1:I:441:ALA:HB1	1.99	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: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:A:127:GLU:OE2	1:A:257:HIS:NE2	2.49	0.44
1:H:242:PRO:HD3	1:H:257:HIS:CE1	2.51	0.44
1:H:144:VAL:HG12	1:H:284:ILE:HG23	2.00	0.44
1:D:144:VAL:HG22	1:D:291:LEU:HD12	1.99	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:H:174:LEU:N	1:H:175:PRO:CD	2.81	0.44
1:C:258:SER:O	1:C:260:THR:N	2.51	0.44
1:I:192:LEU:HD22	1:I:222:VAL:HG22	1.98	0.44
1:H:196:LEU:HD12	1:H:229:LYS:HB2	1.97	0.44
1:H:192:LEU:HG	1:H:196:LEU:HD23	1.99	0.44
1:K:106:PHE:O	1:K:108:TYR:N	2.50	0.44
1:L:106:PHE:O	1:L:108:TYR:N	2.50	0.44
1:H:369:ASP:H	1:H:372:THR:HB	1.82	0.44
1:I:382:ILE:HB	1:I:383:PRO:HD3	1.99	0.44
1:C:122:LYS:NZ	1:C:308:LYS:HE2	2.32	0.44
1:I:255:VAL:O	1:I:255:VAL:HG13	2.18	0.44
1:J:420:ASN:HA	1:J:420:ASN:HD22	1.58	0.44
1:L:64:ALA:O	1:L:122:LYS:HE2	2.17	0.44
1:H:331:HIS:ND1	1:H:332:PRO:HD2	2.32	0.44
1:K:418:MET:C	1:K:420:ASN:H	2.20	0.44
1:L:207:GLU:CB	1:L:236:ASP:HB3	2.46	0.44
1:L:345:HIS:CE1	1:L:347:GLU:HG2	2.53	0.44
1:H:212:PRO:HD2	1:H:213:PHE:CD2	2.53	0.44
1:L:324:MET:HG2	1:L:431:PHE:HE1	1.83	0.44
1:I:428:VAL:HG22	1:L:312:LEU:HD11	2.00	0.44
1:E:242:PRO:O	1:E:246:LYS:HE2	2.18	0.44
1:A:428:VAL:O	1:A:428:VAL:CG1	2.65	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:C:170:ILE:HG23	1:C:174:LEU:HD12	2.00	0.44
1:F:82:VAL:CG2	1:F:114:PRO:HG2	2.48	0.44
1:E:208:SER:HA	1:E:209:PRO:C	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LEU:HA	1:C:196:LEU:HD13	1.87	0.44
1:C:376:PHE:CB	1:C:445:ILE:HD11	2.29	0.44
1:A:127:GLU:CD	1:A:242:PRO:HB3	2.37	0.44
1:F:428:VAL:HG12	1:G:62:ILE:CD1	2.40	0.44
1:A:420:ASN:HD22	1:A:420:ASN:HA	1.56	0.44
1:I:143:THR:HG22	1:I:144:VAL:N	2.33	0.44
1:K:155:HIS:ND1	1:K:180:THR:HG23	2.33	0.44
1:G:217:VAL:O	1:G:219:ILE:N	2.51	0.44
1:E:277:PRO:HG2	1:E:280:LEU:HB2	1.99	0.44
1:I:331:HIS:CE1	1:I:333:LYS:HB2	2.52	0.44
1:D:348:HIS:O	1:D:352:LYS:HB2	2.18	0.44
1:G:241:THR:HG23	1:G:242:PRO:HD2	2.00	0.44
1:D:383:PRO:HB2	1:D:396:VAL:CG2	2.48	0.44
1:J:383:PRO:HB3	1:J:394:SER:HB3	1.99	0.44
1:J:210:THR:HG22	1:J:215:ARG:H	1.82	0.44
1:D:82:VAL:HG21	1:D:114:PRO:HG2	2.00	0.44
1:A:376:PHE:HB2	1:A:445:ILE:HD11	2.00	0.44
1:J:129:ALA:HB2	1:J:248:LEU:CD1	2.48	0.44
1:K:131:SER:OG	1:K:281:VAL:HG11	2.17	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:G:382:ILE:HB	1:G:383:PRO:HD3	1.99	0.44
1:E:346:PRO:HB2	1:E:347:GLU:OE2	2.18	0.44
1:J:212:PRO:HG2	1:J:421:LEU:HD21	1.99	0.44
1:H:192:LEU:O	1:H:196:LEU:HB2	2.17	0.44
1:B:262:PHE:CE1	1:B:390:GLY:HA2	2.52	0.44
1:I:261:LYS:HD2	1:I:389:PHE:CZ	2.53	0.44
1:E:207:GLU:HG3	1:E:210:THR:HA	1.99	0.43
1:L:347:GLU:CB	1:L:350:ILE:HD12	2.41	0.43
1:G:174:LEU:N	1:G:175:PRO:CD	2.81	0.43
1:D:396:VAL:HG13	1:D:424:PHE:CD2	2.53	0.43
1:K:115:THR:CG2	1:K:297:PRO:HB3	2.48	0.43
1:C:138:GLY:O	1:C:141:ALA:HB3	2.18	0.43
1:J:268:ASP:HB3	1:K:78:THR:HG21	1.99	0.43
1:D:255:VAL:O	1:D:255:VAL:HG13	2.18	0.43
1:L:321:ALA:HB2	1:L:360:GLY:HA2	1.99	0.43
1:L:86:ALA:C	1:L:87:TYR:CD2	2.92	0.43
1:L:144:VAL:HG12	1:L:284:ILE:HG23	1.99	0.43
1:E:65:GLY:O	1:E:118:VAL:HG13	2.18	0.43
1:C:255:VAL:HG13	1:C:255:VAL:O	2.17	0.43
1:I:134:LEU:HD22	1:I:295:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:ASP:H	1:C:372:THR:HB	1.82	0.43
1:K:63:HIS:CD2	1:K:67:ARG:HD3	2.54	0.43
1:J:82:VAL:HG21	1:J:114:PRO:HG2	1.99	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:I:428:VAL:CG2	1:L:312:LEU:HD11	2.47	0.43
1:L:127:GLU:CD	1:L:242:PRO:HB3	2.39	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:L:383:PRO:HB2	1:L:396:VAL:CG2	2.48	0.43
1:D:383:PRO:HA	1:D:394:SER:O	2.18	0.43
1:E:339:TYR:HB3	1:E:342:LEU:HG	2.00	0.43
1:B:323:ARG:NH1	1:B:431:PHE:CD2	2.86	0.43
1:B:223:SER:HA	1:B:233:VAL:HG21	2.00	0.43
1:E:331:HIS:CE1	1:E:333:LYS:HB2	2.54	0.43
1:J:339:TYR:CZ	1:J:358:PHE:HB2	2.53	0.43
1:K:232:LEU:HA	1:K:232:LEU:HD23	1.89	0.43
1:E:431:PHE:CE1	1:E:435:LYS:HD3	2.53	0.43
1:A:428:VAL:HG21	1:D:312:LEU:HD11	2.00	0.43
1:G:210:THR:HG23	1:G:211:ASN:N	2.33	0.43
1:E:396:VAL:O	1:E:397:ASP:HB3	2.19	0.43
1:A:143:THR:HG22	1:A:144:VAL:N	2.33	0.43
1:J:206:THR:O	1:J:235:ILE:HA	2.19	0.43
1:K:150:VAL:HA	1:K:151:PRO:HD3	1.87	0.43
1:G:383:PRO:HB3	1:G:394:SER:HB3	1.99	0.43
1:G:215:ARG:NH1	1:G:347:GLU:OE2	2.52	0.43
1:H:382:ILE:HB	1:H:383:PRO:HD3	1.99	0.43
1:B:63:HIS:CD2	1:B:67:ARG:HD3	2.54	0.43
1:E:196:LEU:HA	1:E:196:LEU:HD13	1.86	0.43
1:H:370:LEU:HD23	1:H:419:ASP:HB3	2.01	0.43
1:K:441:ALA:C	1:K:443:ASP:H	2.22	0.43
1:K:57:ASP:HB3	1:K:243:LEU:CD2	2.48	0.43
1:B:243:LEU:HD12	1:B:314:VAL:HG21	1.99	0.43
1:L:242:PRO:HD3	1:L:257:HIS:CE1	2.54	0.43
1:C:70:ARG:C	1:C:72:ILE:H	2.21	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:A:86:ALA:HB1	1:C:387:PRO:HD2	1.99	0.43
1:K:187:ALA:O	1:K:189:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:145:MET:HE2	1:I:146:LEU:HA	2.01	0.43
1:L:208:SER:HA	1:L:209:PRO:C	2.39	0.43
1:E:343:GLN:HA	1:E:348:HIS:CD2	2.53	0.43
1:F:240:ALA:O	1:F:244:ASN:HB2	2.18	0.43
1:J:127:GLU:OE2	1:J:242:PRO:HB3	2.18	0.43
1:D:428:VAL:CG1	1:D:428:VAL:O	2.67	0.43
1:F:345:HIS:CE1	1:F:347:GLU:HG2	2.54	0.43
1:A:174:LEU:N	1:A:175:PRO:CD	2.80	0.43
1:J:122:LYS:NZ	1:J:308:LYS:HE2	2.33	0.43
1:A:212:PRO:HG2	1:A:421:LEU:HD21	2.01	0.43
1:C:310:LEU:HA	1:C:313:ARG:NH2	2.34	0.43
1:J:339:TYR:OH	1:J:358:PHE:HB2	2.19	0.43
1:A:438:ILE:O	1:A:442:LEU:HD12	2.18	0.43
1:I:129:ALA:HB2	1:I:248:LEU:CD1	2.49	0.43
1:H:150:VAL:HA	1:H:151:PRO:HD3	1.89	0.43
1:B:296:ASN:OD1	1:B:298:ASN:HB2	2.18	0.43
1:F:232:LEU:HA	1:F:232:LEU:HD23	1.92	0.43
1:D:258:SER:O	1:D:260:THR:N	2.52	0.43
1:B:418:MET:C	1:B:420:ASN:N	2.71	0.43
1:L:73:VAL:O	1:L:74:THR:HG23	2.19	0.43
1:H:79:THR:HA	1:H:80:PRO:HD3	1.88	0.42
1:B:215:ARG:NH1	1:B:347:GLU:OE2	2.52	0.42
1:B:428:VAL:HG22	1:C:312:LEU:HD11	2.01	0.42
1:B:380:LEU:HD13	1:B:396:VAL:HG21	2.00	0.42
1:L:265:GLY:HA3	1:L:313:ARG:NH1	2.34	0.42
1:C:144:VAL:HG22	1:C:291:LEU:HD12	2.00	0.42
1:J:155:HIS:HA	1:J:180:THR:O	2.19	0.42
1:E:331:HIS:CG	1:E:332:PRO:HD2	2.54	0.42
1:F:164:ARG:HD2	1:F:404:TYR:CE2	2.53	0.42
1:J:103:ARG:HG2	1:J:104:ALA:N	2.34	0.42
1:H:73:VAL:O	1:H:74:THR:HG23	2.18	0.42
1:A:240:ALA:O	1:A:244:ASN:HB2	2.19	0.42
1:I:113:ASN:ND2	1:I:297:PRO:HG3	2.34	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:E:79:THR:HA	1:E:80:PRO:HD3	1.90	0.42
1:C:215:ARG:NH1	1:C:347:GLU:OE2	2.49	0.42
1:D:250:LEU:CD1	1:D:354:GLN:HB2	2.45	0.42
1:J:383:PRO:HA	1:J:394:SER:O	2.19	0.42
1:B:123:ILE:HD13	1:B:273:CYS:SG	2.59	0.42
1:I:106:PHE:O	1:I:108:TYR:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:SER:HB3	1:C:281:VAL:HG11	2.00	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:J:428:VAL:O	1:J:428:VAL:CG1	2.68	0.42
1:A:428:VAL:HG22	1:D:312:LEU:HD11	2.01	0.42
1:E:215:ARG:HD2	1:E:347:GLU:OE2	2.20	0.42
1:K:173:ILE:C	1:K:175:PRO:HD2	2.40	0.42
1:E:82:VAL:CG2	1:E:114:PRO:HG2	2.50	0.42
1:A:64:ALA:O	1:A:122:LYS:HE2	2.18	0.42
1:L:206:THR:O	1:L:235:ILE:HA	2.19	0.42
1:A:339:TYR:CZ	1:A:358:PHE:HB2	2.54	0.42
1:B:339:TYR:CD1	1:B:362:VAL:HG22	2.54	0.42
1:E:57:ASP:HB3	1:E:243:LEU:HD22	2.01	0.42
1:J:209:PRO:HD3	1:J:240:ALA:HB2	2.01	0.42
1:G:366:VAL:HG11	1:G:445:ILE:HD13	2.02	0.42
1:D:173:ILE:C	1:D:175:PRO:HD2	2.39	0.42
1:C:258:SER:C	1:C:260:THR:N	2.71	0.42
1:L:63:HIS:CD2	1:L:67:ARG:HD3	2.54	0.42
1:E:339:TYR:OH	1:E:358:PHE:HB2	2.20	0.42
1:L:384:TYR:O	1:L:395:ILE:HG23	2.19	0.42
1:A:374:ALA:O	1:A:377:VAL:HG22	2.19	0.42
1:H:232:LEU:HA	1:H:232:LEU:HD23	1.92	0.42
1:G:255:VAL:O	1:G:255:VAL:HG13	2.19	0.42
1:L:331:HIS:CG	1:L:332:PRO:HD2	2.54	0.42
1:L:57:ASP:HB3	1:L:243:LEU:HD22	2.01	0.42
1:I:58:GLY:O	1:I:62:ILE:HG13	2.19	0.42
1:L:210:THR:HG23	1:L:211:ASN:N	2.34	0.42
1:K:72:ILE:HD11	1:L:72:ILE:HD11	2.01	0.42
1:G:173:ILE:C	1:G:175:PRO:HD2	2.39	0.42
1:G:72:ILE:HD12	1:G:80:PRO:HG2	2.00	0.42
1:J:256:LEU:HB2	1:J:273:CYS:O	2.18	0.42
1:C:420:ASN:HA	1:C:420:ASN:HD22	1.56	0.42
1:F:261:LYS:HD2	1:F:389:PHE:CZ	2.55	0.42
1:A:292:GLY:O	1:C:140:CYS:HB2	2.18	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:J:57:ASP:HB3	1:J:243:LEU:CD2	2.50	0.42
1:H:113:ASN:ND2	1:H:297:PRO:HG3	2.33	0.42
1:E:80:PRO:O	1:E:115:THR:HB	2.20	0.42
1:I:396:VAL:HG13	1:I:424:PHE:CD2	2.53	0.42
1:A:210:THR:O	1:A:214:LEU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:196:LEU:HD13	1:K:196:LEU:HA	1.93	0.42
1:J:265:GLY:O	1:J:391:GLY:HA2	2.20	0.42
1:H:339:TYR:CD1	1:H:362:VAL:HG22	2.54	0.42
1:J:312:LEU:HD11	1:K:428:VAL:CG2	2.49	0.42
1:G:366:VAL:HG12	1:G:367:ASP:N	2.34	0.42
1:D:211:ASN:HA	1:D:212:PRO:HA	1.86	0.42
1:J:331:HIS:CE1	1:J:333:LYS:HB2	2.55	0.42
1:I:280:LEU:O	1:I:283:GLU:HB2	2.20	0.42
1:D:82:VAL:HG12	1:D:84:THR:HG22	2.02	0.42
1:E:155:HIS:HA	1:E:180:THR:O	2.20	0.42
1:A:323:ARG:NH1	1:A:431:PHE:CE2	2.88	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:E:374:ALA:HB1	1:G:92:THR:HG21	2.02	0.42
1:D:398:GLN:O	1:D:401:ILE:N	2.53	0.42
1:F:223:SER:HA	1:F:233:VAL:HG21	2.01	0.42
1:I:429:GLU:OE2	1:L:63:HIS:CE1	2.72	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: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: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:I:206:THR:O	1:I:235:ILE:HA	2.20	0.42
1:E:291:LEU:HD22	1:G:143:THR:HG21	2.01	0.42
1:C:321:ALA:HB2	1:C:360:GLY:HA2	2.01	0.42
1:C:159:THR:HA	1:C:184:ILE:O	2.20	0.42
1:H:296:ASN:HA	1:H:297:PRO:HD3	1.94	0.41
1:C:383:PRO:CB	1:C:396:VAL:HG22	2.46	0.41
1:K:395:ILE:HG22	1:K:396:VAL:N	2.34	0.41
1:F:265:GLY:HA3	1:F:313:ARG:NH1	2.35	0.41
1:B:145:MET:CE	1:B:146:LEU:HD23	2.50	0.41
1:J:331:HIS:CG	1:J:332:PRO:HD2	2.54	0.41
1:A:339:TYR:CD1	1:A:362:VAL:HG22	2.55	0.41
1:L:331:HIS:ND1	1:L:332:PRO:HD2	2.35	0.41
1:K:398:GLN:O	1:K:401:ILE:N	2.53	0.41
1:A:194:LEU:O	1:A:198:GLN:HG3	2.19	0.41
1:L:255:VAL:O	1:L:255:VAL:HG13	2.20	0.41
1:B:310:LEU:O	1:B:314:VAL:HG23	2.20	0.41
1:G:211:ASN:HB2	1:G:239:PHE:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:THR:CG2	1:E:297:PRO:HB3	2.50	0.41
1:J:211:ASN:HA	1:J:212:PRO:HA	1.91	0.41
1:B:419:ASP:OD1	1:B:419:ASP:N	2.52	0.41
1:F:366:VAL:HG12	1:F:367:ASP:N	2.34	0.41
1:D:418:MET:C	1:D:420:ASN:H	2.22	0.41
1:K:418:MET:C	1:K:420:ASN:N	2.73	0.41
1:B:138:GLY:N	2:B:500:PLP:O2P	2.53	0.41
1:H:127:GLU:OE2	1:H:257:HIS:NE2	2.52	0.41
1:I:312:LEU:HD11	1:L:428:VAL:CG2	2.51	0.41
1:H:394:SER:OG	1:H:427:GLY:N	2.43	0.41
1:E:270:LEU:HD23	1:E:270:LEU:N	2.36	0.41
1:I:173:ILE:C	1:I:175:PRO:HD2	2.39	0.41
1:E:82:VAL:HG21	1:E:114:PRO:CG	2.50	0.41
1:E:280:LEU:O	1:E:283:GLU:HB2	2.20	0.41
1:I:404:TYR:O	1:I:412:ARG:HD3	2.20	0.41
1:B:373:THR:O	1:B:377:VAL:HG13	2.20	0.41
1:H:126:LEU:HA	1:H:126:LEU:HD23	1.86	0.41
1:G:127:GLU:OE2	1:G:257:HIS:NE2	2.53	0.41
1:G:57:ASP:HB3	1:G:243:LEU:CD2	2.51	0.41
1:K:270:LEU:N	1:K:270:LEU:HD23	2.35	0.41
1:G:79:THR:HA	1:G:80:PRO:HD3	1.90	0.41
1:A:256:LEU:HB2	1:A:273:CYS:O	2.20	0.41
1:L:382:ILE:HB	1:L:383:PRO:HD3	2.03	0.41
1:G:386:ALA:HB1	1:G:387:PRO:CD	2.50	0.41
1:L:87:TYR:N	1:L:87:TYR:HD2	2.16	0.41
1:I:418:MET:C	1:I:420:ASN:H	2.23	0.41
1:H:131:SER:CB	1:H:281:VAL:HG11	2.51	0.41
1:C:418:MET:C	1:C:420:ASN:H	2.23	0.41
1:L:370:LEU:HD23	1:L:419:ASP:HB3	2.01	0.41
1:E:187:ALA:O	1:E:189:VAL:HG23	2.20	0.41
1:G:337:VAL:HG22	1:G:364:PHE:HB3	2.02	0.41
1:L:339:TYR:CD1	1:L:362:VAL:HG22	2.55	0.41
1:B:160:THR:HG23	1:B:183:VAL:HG12	2.03	0.41
1:A:250:LEU:HD11	1:A:354:GLN:HB2	2.03	0.41
1:I:241:THR:HG22	1:I:243:LEU:N	2.15	0.41
1:H:240:ALA:O	1:H:241:THR:CB	2.57	0.41
1:G:207:GLU:H	1:G:207:GLU:HG2	1.75	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:L:260:THR:CG2	1:L:270:LEU:HD22	2.49	0.41
1:B:331:HIS:CE1	1:B:333:LYS:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:VAL:HA	1:C:151:PRO:HD3	1.90	0.41
1:H:280:LEU:O	1:H:283:GLU:HB2	2.20	0.41
1:H:241:THR:HG23	1:H:242:PRO:HD2	2.01	0.41
1:K:339:TYR:HB3	1:K:342:LEU:HG	2.02	0.41
1:H:324:MET:HG3	1:H:426:PHE:CE1	2.56	0.41
1:H:262:PHE:CE1	1:H:390:GLY:HA2	2.56	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:J:217:VAL:O	1:J:219:ILE:N	2.54	0.41
1:E:129:ALA:HB2	1:E:248:LEU:CD1	2.50	0.41
1:G:196:LEU:HA	1:G:196:LEU:HD13	1.85	0.41
1:K:240:ALA:O	1:K:241:THR:CB	2.59	0.41
1:J:347:GLU:CB	1:J:350:ILE:HD12	2.46	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:F:215:ARG:NH1	1:F:347:GLU:OE2	2.54	0.41
1:J:210:THR:HG23	1:J:211:ASN:N	2.35	0.41
1:J:156:ILE:CG1	1:J:203:LEU:HD23	2.51	0.41
1:D:258:SER:C	1:D:260:THR:N	2.74	0.41
1:B:64:ALA:O	1:B:122:LYS:HE2	2.20	0.41
1:I:265:GLY:HA3	1:I:313:ARG:NH1	2.36	0.41
1:A:278:LEU:HA	1:A:281:VAL:HG12	2.02	0.41
1:C:377:VAL:HA	1:C:380:LEU:HD12	2.02	0.41
1:F:419:ASP:N	1:F:419:ASP:OD1	2.54	0.41
1:C:398:GLN:O	1:C:399:PRO:C	2.58	0.41
1:L:187:ALA:O	1:L:189:VAL:HG23	2.21	0.41
1:E:420:ASN:HA	1:E:420:ASN:HD22	1.58	0.41
1:L:311:HIS:O	1:L:315:GLN:HB2	2.20	0.41
1:G:265:GLY:HA3	1:G:313:ARG:NH1	2.36	0.41
1:A:72:ILE:CG2	1:A:72:ILE:O	2.63	0.41
1:A:220:GLU:HA	1:A:250:LEU:O	2.20	0.41
1:F:140:CYS:O	1:F:144:VAL:HG23	2.20	0.41
1:D:135:MET:SD	1:D:141:ALA:HA	2.61	0.41
1:G:96:ILE:O	1:G:100:GLU:HG3	2.21	0.41
1:B:192:LEU:HG	1:B:196:LEU:HD23	2.02	0.41
1:J:426:PHE:HE1	1:J:438:ILE:HD11	1.86	0.41
1:E:212:PRO:HG2	1:E:421:LEU:HD21	2.03	0.41
1:A:243:LEU:HD12	1:A:314:VAL:HG21	2.03	0.41
1:I:241:THR:HG23	1:I:242:PRO:HD2	2.03	0.41
1:L:243:LEU:CD1	1:L:311:HIS:HA	2.51	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:D:207:GLU:HG2	1:D:207:GLU:H	1.77	0.41
1:D:234:CYS:SG	1:D:256:LEU:HD23	2.61	0.41
1:C:56:SER:O	1:C:60:VAL:HG23	2.20	0.41
1:H:420:ASN:HD22	1:H:420:ASN:HA	1.55	0.41
1:A:387:PRO:HD2	1:C:86:ALA:HB1	2.02	0.41
1:E:196:LEU:HD12	1:E:229:LYS:HB2	2.03	0.41
1:I:248:LEU:HA	1:I:248:LEU:HD23	1.87	0.41
1:B:196:LEU:HD13	1:B:196:LEU:HA	1.85	0.41
1:D:232:LEU:HA	1:D:232:LEU:HD23	1.94	0.41
1:B:119:LEU:HG	1:B:134:LEU:HD11	2.03	0.41
1:A:331:HIS:CE1	1:A:333:LYS:HB2	2.55	0.41
1:J:65:GLY:O	1:J:118:VAL:HG13	2.21	0.41
1:E:75:ASP:O	1:F:87:TYR:HA	2.20	0.41
1:K:255:VAL:O	1:K:255:VAL:HG13	2.21	0.41
1:L:127:GLU:OE2	1:L:257:HIS:NE2	2.53	0.41
1:F:418:MET:C	1:F:420:ASN:N	2.75	0.41
1:I:54:LEU:HD22	1:I:59:SER:CB	2.51	0.41
1:C:123:ILE:HD13	1:C:273:CYS:SG	2.60	0.41
1:L:335:ARG:HH21	1:L:367:ASP:HA	1.85	0.41
1:E:192:LEU:HG	1:E:196:LEU:HD23	2.03	0.41
1:C:117:VAL:HA	1:C:120:GLU:HB2	2.03	0.41
1:G:163:TYR:CE2	1:G:165:LYS:HB2	2.56	0.41
1:G:155:HIS:O	1:G:202:ASN:HB2	2.20	0.41
1:E:164:ARG:O	1:E:167:ARG:HB3	2.20	0.41
1:K:241:THR:HG23	1:K:242:PRO:HD2	2.04	0.40
1:J:270:LEU:HD23	1:J:270:LEU:N	2.36	0.40
1:A:131:SER:OG	1:A:281:VAL:HG11	2.21	0.40
1:H:355:MET:HB3	1:H:357:GLY:O	2.21	0.40
1:B:145:MET:HE2	1:B:146:LEU:HA	2.03	0.40
1:K:155:HIS:HA	1:K:180:THR:O	2.21	0.40
1:D:296:ASN:OD1	1:D:298:ASN:HB2	2.22	0.40
1:H:94:GLU:O	1:H:97:ASP:HB2	2.21	0.40
1:B:321:ALA:HB2	1:B:360:GLY:HA2	2.03	0.40
1:F:196:LEU:HA	1:F:196:LEU:HD13	1.87	0.40
1:J:366:VAL:HG12	1:J:367:ASP:N	2.35	0.40
1:I:51:ALA:HB1	1:I:53:PHE:CE2	2.56	0.40
1:F:336:HIS:ND1	1:F:337:VAL:N	2.70	0.40
1:D:212:PRO:HG2	1:D:421:LEU:HD21	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:242:PRO:O	1:H:246:LYS:HE2	2.21	0.40
1:C:50:TYR:CE2	1:C:64:ALA:HA	2.56	0.40
1:A:140:CYS:HA	1:C:291:LEU:O	2.21	0.40
1:K:348:HIS:O	1:K:352:LYS:HB2	2.22	0.40
1:H:138:GLY:N	2:H:500:PLP:O2P	2.54	0.40
1:B:164:ARG:O	1:B:167:ARG:HB3	2.22	0.40
1:L:103:ARG:HG2	1:L:104:ALA:N	2.36	0.40
1:F:204:PHE:CE2	1:F:222:VAL:HG11	2.57	0.40
1:B:208:SER:HA	1:B:209:PRO:C	2.41	0.40
1:I:428:VAL:O	1:I:428:VAL:CG1	2.67	0.40
1:H:60:VAL:O	1:H:62:ILE:N	2.54	0.40
1:L:396:VAL:HG13	1:L:424:PHE:CD2	2.57	0.40
1:H:143:THR:HG22	1:H:144:VAL:N	2.37	0.40
1:K:387:PRO:HD3	1:K:402:MET:HE1	2.03	0.40
1:B:334:VAL:HG11	1:B:337:VAL:HG23	2.04	0.40
1:E:339:TYR:CZ	1:E:358:PHE:HB2	2.57	0.40
1:L:108:TYR:CD2	1:L:110:ARG:HB2	2.55	0.40
1:A:324:MET:HE2	1:A:438:ILE:HD12	2.02	0.40
1:I:164:ARG:HD2	1:I:404:TYR:CE2	2.56	0.40
1:F:192:LEU:HG	1:F:196:LEU:HD23	2.04	0.40
1:C:204:PHE:CE2	1:C:222:VAL:HG11	2.57	0.40
1:L:145:MET:HE2	1:L:146:LEU:HD23	2.04	0.40
1:B:153:GLY:HA2	1:B:178:GLY:O	2.22	0.40
1:J:153:GLY:HA2	1:J:178:GLY:O	2.21	0.40
1:J:280:LEU:HA	1:J:280:LEU:HD23	1.92	0.40
1:D:155:HIS:HA	1:D:180:THR:O	2.21	0.40
1:E:62:ILE:CD1	1:H:428:VAL:HG12	2.45	0.40
1:H:170:ILE:HG23	1:H:174:LEU:HD12	2.03	0.40
1:E:194:LEU:HG	1:E:198:GLN:CD	2.42	0.40
1:B:420:ASN:HA	1:B:420:ASN:HD22	1.53	0.40
1:B:204:PHE:CE2	1:B:222:VAL:HG11	2.56	0.40
1:F:268:ASP:HB3	1:G:78:THR:HG21	2.04	0.40
1:I:98:PHE:HE2	1:I:99:LYS:HE2	1.86	0.40
1:D:366:VAL:HG12	1:D:367:ASP:N	2.36	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%)	34	72
1	B	394/445 (88%)	364 (92%)	25 (6%)	5 (1%)	15	50
1	C	394/445 (88%)	353 (90%)	37 (9%)	4 (1%)	19	58
1	D	394/445 (88%)	363 (92%)	27 (7%)	4 (1%)	19	58
1	E	394/445 (88%)	354 (90%)	35 (9%)	5 (1%)	15	50
1	F	394/445 (88%)	356 (90%)	35 (9%)	3 (1%)	24	63
1	G	394/445 (88%)	357 (91%)	33 (8%)	4 (1%)	19	58
1	H	394/445 (88%)	363 (92%)	28 (7%)	3 (1%)	24	63
1	I	394/445 (88%)	354 (90%)	37 (9%)	3 (1%)	24	63
1	J	394/445 (88%)	354 (90%)	37 (9%)	3 (1%)	24	63
1	K	394/445 (88%)	359 (91%)	30 (8%)	5 (1%)	15	50
1	L	394/445 (88%)	356 (90%)	34 (9%)	4 (1%)	19	58
All	All	4728/5340 (88%)	4288 (91%)	395 (8%)	45 (1%)	19	58

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

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Mol	Chain	Res	Type
1	D	198	GLN
1	D	259	ALA
1	H	198	GLN
1	I	198	GLN
1	K	198	GLN
1	L	198	GLN
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%)	278 (85%)	49 (15%)	3	15
1	B	327/364 (90%)	278 (85%)	49 (15%)	3	15
1	C	327/364 (90%)	284 (87%)	43 (13%)	5	21
1	D	327/364 (90%)	282 (86%)	45 (14%)	4	19
1	E	327/364 (90%)	281 (86%)	46 (14%)	4	18
1	F	327/364 (90%)	279 (85%)	48 (15%)	4	16
1	G	327/364 (90%)	281 (86%)	46 (14%)	4	18
1	H	327/364 (90%)	279 (85%)	48 (15%)	4	16
1	I	327/364 (90%)	281 (86%)	46 (14%)	4	18
1	J	327/364 (90%)	284 (87%)	43 (13%)	5	21
1	K	327/364 (90%)	281 (86%)	46 (14%)	4	18
1	L	327/364 (90%)	283 (86%)	44 (14%)	5	20
All	All	3924/4368 (90%)	3371 (86%)	553 (14%)	4	18

All (553) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	72	ILE
1	A	74	THR
1	A	91	LYS
1	A	93	SER
1	A	101	LYS
1	A	134	LEU
1	A	135	MET
1	A	142	SER
1	A	143	THR
1	A	145	MET
1	A	151	PRO
1	A	156	ILE
1	A	161	ASP
1	A	164	ARG
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	210	THR

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Mol	Chain	Res	Type
1	A	224	LYS
1	A	229	LYS
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	279	LYS
1	A	285	ARG
1	A	333	LYS
1	A	343	GLN
1	A	344	SER
1	A	347	GLU
1	A	352	LYS
1	A	371	LEU
1	A	396	VAL
1	A	397	ASP
1	A	402	MET
1	A	403	SER
1	A	410	SER
1	A	415	TYR
1	A	420	ASN
1	A	428	VAL
1	A	430	ASP
1	A	431	PHE
1	A	444	SER
1	B	52	SER
1	B	70	ARG
1	B	72	ILE
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	164	ARG

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Mol	Chain	Res	Type
1	B	165	LYS
1	B	177	MET
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	224	LYS
1	B	229	LYS
1	B	241	THR
1	B	273	CYS
1	B	275	SER
1	B	278	LEU
1	B	279	LYS
1	B	285	ARG
1	B	315	GLN
1	B	343	GLN
1	B	344	SER
1	B	347	GLU
1	B	352	LYS
1	B	371	LEU
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	420	ASN
1	B	423	ARG
1	B	428	VAL
1	B	430	ASP
1	B	444	SER
1	C	70	ARG
1	C	72	ILE
1	C	74	THR
1	C	91	LYS
1	C	93	SER
1	C	103	ARG
1	C	134	LEU
1	C	135	MET

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Mol	Chain	Res	Type
1	C	142	SER
1	C	145	MET
1	C	156	ILE
1	C	161	ASP
1	C	164	ARG
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	224	LYS
1	C	229	LYS
1	C	241	THR
1	C	273	CYS
1	C	278	LEU
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	377	VAL
1	C	396	VAL
1	C	397	ASP
1	C	402	MET
1	C	403	SER
1	C	410	SER
1	C	415	TYR
1	C	420	ASN
1	C	428	VAL
1	C	430	ASP
1	C	443	ASP
1	D	70	ARG
1	D	72	ILE
1	D	74	THR
1	D	91	LYS
1	D	93	SER
1	D	101	LYS
1	D	103	ARG

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Mol	Chain	Res	Type
1	D	131	SER
1	D	134	LEU
1	D	135	MET
1	D	142	SER
1	D	145	MET
1	D	156	ILE
1	D	161	ASP
1	D	164	ARG
1	D	165	LYS
1	D	177	MET
1	D	180	THR
1	D	196	LEU
1	D	199	LYS
1	D	203	LEU
1	D	207	GLU
1	D	210	THR
1	D	224	LYS
1	D	229	LYS
1	D	273	CYS
1	D	275	SER
1	D	278	LEU
1	D	285	ARG
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	377	VAL
1	D	396	VAL
1	D	397	ASP
1	D	402	MET
1	D	403	SER
1	D	410	SER
1	D	415	TYR
1	D	420	ASN
1	D	428	VAL
1	D	430	ASP
1	E	70	ARG
1	E	72	ILE
1	E	74	THR
1	E	91	LYS

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Mol	Chain	Res	Type
1	E	93	SER
1	E	103	ARG
1	E	124	SER
1	E	134	LEU
1	E	135	MET
1	E	142	SER
1	E	145	MET
1	E	161	ASP
1	E	164	ARG
1	E	165	LYS
1	E	177	MET
1	E	180	THR
1	E	196	LEU
1	E	199	LYS
1	E	203	LEU
1	E	210	THR
1	E	224	LYS
1	E	229	LYS
1	E	245	GLN
1	E	270	LEU
1	E	273	CYS
1	E	275	SER
1	E	278	LEU
1	E	279	LYS
1	E	285	ARG
1	E	315	GLN
1	E	343	GLN
1	E	344	SER
1	E	347	GLU
1	E	377	VAL
1	E	396	VAL
1	E	397	ASP
1	E	402	MET
1	E	403	SER
1	E	410	SER
1	E	415	TYR
1	E	420	ASN
1	E	428	VAL
1	E	430	ASP
1	E	431	PHE
1	E	442	LEU
1	E	444	SER

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Mol	Chain	Res	Type
1	F	70	ARG
1	F	72	ILE
1	F	74	THR
1	F	91	LYS
1	F	93	SER
1	F	101	LYS
1	F	103	ARG
1	F	115	THR
1	F	134	LEU
1	F	135	MET
1	F	142	SER
1	F	145	MET
1	F	156	ILE
1	F	161	ASP
1	F	164	ARG
1	F	165	LYS
1	F	177	MET
1	F	180	THR
1	F	196	LEU
1	F	203	LEU
1	F	207	GLU
1	F	210	THR
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	285	ARG
1	F	333	LYS
1	F	343	GLN
1	F	344	SER
1	F	347	GLU
1	F	371	LEU
1	F	377	VAL
1	F	396	VAL
1	F	397	ASP
1	F	402	MET
1	F	403	SER

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Mol	Chain	Res	Type
1	F	410	SER
1	F	415	TYR
1	F	420	ASN
1	F	428	VAL
1	F	430	ASP
1	F	444	SER
1	G	72	ILE
1	G	91	LYS
1	G	93	SER
1	G	103	ARG
1	G	115	THR
1	G	124	SER
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	164	ARG
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	224	LYS
1	G	229	LYS
1	G	270	LEU
1	G	273	CYS
1	G	275	SER
1	G	278	LEU
1	G	279	LYS
1	G	285	ARG
1	G	333	LYS
1	G	343	GLN
1	G	347	GLU
1	G	352	LYS
1	G	371	LEU
1	G	377	VAL

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Mol	Chain	Res	Type
1	G	396	VAL
1	G	397	ASP
1	G	402	MET
1	G	403	SER
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	H	70	ARG
1	H	72	ILE
1	H	74	THR
1	H	91	LYS
1	H	93	SER
1	H	103	ARG
1	H	134	LEU
1	H	135	MET
1	H	142	SER
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	222	VAL
1	H	224	LYS
1	H	229	LYS
1	H	256	LEU
1	H	273	CYS
1	H	275	SER
1	H	278	LEU
1	H	279	LYS
1	H	285	ARG
1	H	333	LYS
1	H	343	GLN

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Mol	Chain	Res	Type
1	H	344	SER
1	H	347	GLU
1	H	352	LYS
1	H	371	LEU
1	H	377	VAL
1	H	396	VAL
1	H	397	ASP
1	H	402	MET
1	H	403	SER
1	H	410	SER
1	H	414	LYS
1	H	415	TYR
1	H	420	ASN
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	134	LEU
1	I	135	MET
1	I	142	SER
1	I	145	MET
1	I	156	ILE
1	I	161	ASP
1	I	162	CYS
1	I	164	ARG
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
1	I	224	LYS
1	I	229	LYS
1	I	256	LEU
1	I	273	CYS

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Mol	Chain	Res	Type
1	I	275	SER
1	I	278	LEU
1	I	279	LYS
1	I	285	ARG
1	I	333	LYS
1	I	343	GLN
1	I	347	GLU
1	I	353	LYS
1	I	371	LEU
1	I	377	VAL
1	I	396	VAL
1	I	397	ASP
1	I	402	MET
1	I	403	SER
1	I	410	SER
1	I	415	TYR
1	I	420	ASN
1	I	428	VAL
1	I	430	ASP
1	I	431	PHE
1	J	70	ARG
1	J	72	ILE
1	J	74	THR
1	J	91	LYS
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
1	J	180	THR
1	J	196	LEU
1	J	199	LYS
1	J	203	LEU
1	J	210	THR
1	J	224	LYS
1	J	229	LYS

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Mol	Chain	Res	Type
1	J	256	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	343	GLN
1	J	344	SER
1	J	347	GLU
1	J	352	LYS
1	J	371	LEU
1	J	377	VAL
1	J	396	VAL
1	J	402	MET
1	J	403	SER
1	J	410	SER
1	J	415	TYR
1	J	420	ASN
1	J	428	VAL
1	J	430	ASP
1	K	72	ILE
1	K	74	THR
1	K	91	LYS
1	K	93	SER
1	K	101	LYS
1	K	103	ARG
1	K	134	LEU
1	K	135	MET
1	K	142	SER
1	K	145	MET
1	K	156	ILE
1	K	161	ASP
1	K	164	ARG
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

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Mol	Chain	Res	Type
1	K	224	LYS
1	K	229	LYS
1	K	256	LEU
1	K	270	LEU
1	K	273	CYS
1	K	275	SER
1	K	278	LEU
1	K	285	ARG
1	K	333	LYS
1	K	343	GLN
1	K	344	SER
1	K	347	GLU
1	K	352	LYS
1	K	371	LEU
1	K	396	VAL
1	K	397	ASP
1	K	402	MET
1	K	403	SER
1	K	410	SER
1	K	415	TYR
1	K	420	ASN
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	74	THR
1	L	87	TYR
1	L	91	LYS
1	L	93	SER
1	L	103	ARG
1	L	134	LEU
1	L	135	MET
1	L	142	SER
1	L	145	MET
1	L	156	ILE
1	L	161	ASP
1	L	164	ARG
1	L	165	LYS
1	L	177	MET
1	L	180	THR

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Mol	Chain	Res	Type
1	L	196	LEU
1	L	199	LYS
1	L	203	LEU
1	L	210	THR
1	L	224	LYS
1	L	270	LEU
1	L	273	CYS
1	L	275	SER
1	L	278	LEU
1	L	279	LYS
1	L	285	ARG
1	L	315	GLN
1	L	333	LYS
1	L	343	GLN
1	L	344	SER
1	L	347	GLU
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	428	VAL
1	L	430	ASP
1	L	444	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	288	HIS
1	A	343	GLN
1	A	420	ASN
1	B	63	HIS
1	B	343	GLN
1	B	420	ASN
1	C	63	HIS
1	C	288	HIS
1	C	343	GLN
1	C	420	ASN

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Mol	Chain	Res	Type
1	D	63	HIS
1	D	343	GLN
1	D	420	ASN
1	E	63	HIS
1	E	83	ASN
1	E	288	HIS
1	E	298	ASN
1	E	343	GLN
1	E	420	ASN
1	F	63	HIS
1	F	343	GLN
1	F	420	ASN
1	G	63	HIS
1	G	288	HIS
1	G	343	GLN
1	G	420	ASN
1	H	63	HIS
1	H	343	GLN
1	H	420	ASN
1	I	63	HIS
1	I	288	HIS
1	I	343	GLN
1	I	420	ASN
1	J	63	HIS
1	J	83	ASN
1	J	288	HIS
1	J	298	ASN
1	J	343	GLN
1	J	420	ASN
1	K	63	HIS
1	K	343	GLN
1	K	420	ASN
1	L	63	HIS
1	L	343	GLN
1	L	420	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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$
2	PLP	A	500	1	15,15,16	4.25	5 (33%)	21,22,23	2.46	10 (47%)
3	PMC	A	600	-	11,14,14	2.29	5 (45%)	13,20,20	1.61	2 (15%)
2	PLP	B	500	1	15,15,16	4.70	5 (33%)	21,22,23	2.50	11 (52%)
3	PMC	B	601	-	11,14,14	2.16	6 (54%)	13,20,20	1.57	2 (15%)
2	PLP	C	500	1	15,15,16	3.86	5 (33%)	21,22,23	2.42	11 (52%)
3	PMC	C	602	-	11,14,14	2.28	4 (36%)	13,20,20	1.63	2 (15%)
2	PLP	D	500	1	15,15,16	5.07	5 (33%)	21,22,23	2.61	10 (47%)
3	PMC	D	603	-	11,14,14	2.01	5 (45%)	13,20,20	1.47	2 (15%)
2	PLP	E	500	1	15,15,16	3.95	5 (33%)	21,22,23	2.37	9 (42%)
3	PMC	E	604	-	11,14,14	2.25	4 (36%)	13,20,20	1.67	2 (15%)
2	PLP	F	500	1	15,15,16	4.59	5 (33%)	21,22,23	2.38	11 (52%)
3	PMC	F	605	-	11,14,14	2.18	4 (36%)	13,20,20	1.61	2 (15%)
2	PLP	G	500	1	15,15,16	3.96	5 (33%)	21,22,23	2.38	9 (42%)
3	PMC	G	606	-	11,14,14	1.99	3 (27%)	13,20,20	1.50	2 (15%)
2	PLP	H	500	1	15,15,16	4.72	6 (40%)	21,22,23	2.51	11 (52%)
3	PMC	H	607	-	11,14,14	2.11	5 (45%)	13,20,20	1.60	2 (15%)
2	PLP	I	500	1	15,15,16	4.10	5 (33%)	21,22,23	2.34	10 (47%)
3	PMC	I	608	-	11,14,14	2.08	5 (45%)	13,20,20	1.54	2 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PLP	J	500	1	15,15,16	3.85	5 (33%)	21,22,23	2.32	8 (38%)
3	PMC	J	609	-	11,14,14	2.03	5 (45%)	13,20,20	1.48	2 (15%)
2	PLP	K	500	1	15,15,16	4.84	5 (33%)	21,22,23	2.60	10 (47%)
3	PMC	K	610	-	11,14,14	2.19	5 (45%)	13,20,20	1.62	2 (15%)
2	PLP	L	500	1	15,15,16	3.42	5 (33%)	21,22,23	2.38	8 (38%)
3	PMC	L	611	-	11,14,14	2.03	4 (36%)	13,20,20	1.51	2 (15%)

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
2	PLP	A	500	1	-	0/6/6/8	0/1/1/1
3	PMC	A	600	-	-	0/5/9/9	0/1/1/1
2	PLP	B	500	1	-	0/6/6/8	0/1/1/1
3	PMC	B	601	-	-	0/5/9/9	0/1/1/1
2	PLP	C	500	1	-	0/6/6/8	0/1/1/1
3	PMC	C	602	-	-	0/5/9/9	0/1/1/1
2	PLP	D	500	1	-	0/6/6/8	0/1/1/1
3	PMC	D	603	-	-	0/5/9/9	0/1/1/1
2	PLP	E	500	1	-	0/6/6/8	0/1/1/1
3	PMC	E	604	-	-	0/5/9/9	0/1/1/1
2	PLP	F	500	1	-	0/6/6/8	0/1/1/1
3	PMC	F	605	-	-	0/5/9/9	0/1/1/1
2	PLP	G	500	1	-	0/6/6/8	0/1/1/1
3	PMC	G	606	-	-	0/5/9/9	0/1/1/1
2	PLP	H	500	1	-	0/6/6/8	0/1/1/1
3	PMC	H	607	-	-	0/5/9/9	0/1/1/1
2	PLP	I	500	1	-	0/6/6/8	0/1/1/1
3	PMC	I	608	-	-	0/5/9/9	0/1/1/1
2	PLP	J	500	1	-	0/6/6/8	0/1/1/1
3	PMC	J	609	-	-	0/5/9/9	0/1/1/1
2	PLP	K	500	1	-	0/6/6/8	0/1/1/1
3	PMC	K	610	-	-	0/5/9/9	0/1/1/1
2	PLP	L	500	1	-	0/6/6/8	0/1/1/1
3	PMC	L	611	-	-	0/5/9/9	0/1/1/1

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	PLP	P-O2P	-2.74	1.44	1.54
2	F	500	PLP	P-O2P	-2.73	1.44	1.54
2	H	500	PLP	P-O2P	-2.71	1.45	1.54
2	B	500	PLP	P-O2P	-2.68	1.45	1.54
2	G	500	PLP	P-O2P	-2.68	1.45	1.54
2	J	500	PLP	P-O2P	-2.60	1.45	1.54
2	C	500	PLP	P-O2P	-2.59	1.45	1.54
2	I	500	PLP	P-O2P	-2.54	1.45	1.54
2	L	500	PLP	P-O2P	-2.49	1.45	1.54
2	A	500	PLP	P-O2P	-2.42	1.46	1.54
2	K	500	PLP	P-O2P	-2.41	1.46	1.54
2	L	500	PLP	P-O3P	-2.37	1.46	1.54
3	L	611	PMC	P1-O3	-2.36	1.49	1.54
2	D	500	PLP	P-O2P	-2.34	1.46	1.54
2	F	500	PLP	P-O3P	-2.28	1.46	1.54
2	E	500	PLP	P-O3P	-2.24	1.46	1.54
2	I	500	PLP	P-O3P	-2.23	1.46	1.54
3	D	603	PMC	P1-O3	-2.22	1.49	1.54
3	A	600	PMC	P1-O3	-2.19	1.49	1.54
3	C	602	PMC	P1-O3	-2.17	1.49	1.54
2	A	500	PLP	P-O3P	-2.17	1.46	1.54
2	J	500	PLP	P-O3P	-2.14	1.47	1.54
3	J	609	PMC	P1-O3	-2.14	1.49	1.54
2	G	500	PLP	P-O3P	-2.13	1.47	1.54
2	H	500	PLP	P-O3P	-2.13	1.47	1.54
3	B	601	PMC	P1-O3	-2.10	1.49	1.54
2	C	500	PLP	P-O3P	-2.10	1.47	1.54
3	I	608	PMC	P1-O3	-2.09	1.49	1.54
3	E	604	PMC	P1-O3	-2.09	1.49	1.54
3	H	607	PMC	P1-O3	-2.09	1.49	1.54
3	A	600	PMC	P1-O2	-2.09	1.49	1.54
3	F	605	PMC	P1-O3	-2.08	1.49	1.54
2	K	500	PLP	P-O3P	-2.08	1.47	1.54
3	D	603	PMC	P1-O2	-2.06	1.49	1.54
2	D	500	PLP	P-O3P	-2.05	1.47	1.54
2	B	500	PLP	P-O3P	-2.05	1.47	1.54
3	K	610	PMC	P1-O3	-2.04	1.49	1.54
3	K	610	PMC	P1-O2	-2.02	1.50	1.54
3	B	601	PMC	P1-O2	-2.00	1.50	1.54
3	J	609	PMC	C4-C3	2.01	1.43	1.39
3	I	608	PMC	C4-C3	2.02	1.43	1.39
3	H	607	PMC	C4-C3	2.02	1.43	1.39
3	B	601	PMC	C4-C3	2.07	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	500	PLP	C5A-C5	2.26	1.57	1.50
3	I	608	PMC	C2-C3	2.27	1.45	1.41
3	F	605	PMC	C2-C3	2.34	1.45	1.41
3	D	603	PMC	C2-C3	2.42	1.45	1.41
3	G	606	PMC	C2-C3	2.42	1.45	1.41
3	J	609	PMC	C2-C3	2.45	1.45	1.41
3	K	610	PMC	C2-C3	2.48	1.45	1.41
3	B	601	PMC	C2-C3	2.50	1.45	1.41
3	H	607	PMC	C2-C3	2.53	1.45	1.41
2	L	500	PLP	C2-N1	2.55	1.39	1.34
2	E	500	PLP	C2-N1	2.56	1.39	1.34
2	G	500	PLP	C2-N1	2.63	1.39	1.34
3	J	609	PMC	CA-C3	2.66	1.55	1.51
3	A	600	PMC	C2-C3	2.67	1.45	1.41
2	K	500	PLP	C2-N1	2.68	1.39	1.34
3	G	606	PMC	CA-C3	2.75	1.55	1.51
2	A	500	PLP	C2-N1	2.80	1.40	1.34
3	I	608	PMC	CA-C3	2.85	1.55	1.51
3	L	611	PMC	C2-C3	2.86	1.46	1.41
2	D	500	PLP	C2-N1	2.89	1.40	1.34
3	L	611	PMC	CA-C3	2.89	1.55	1.51
3	D	603	PMC	CA-C3	2.96	1.55	1.51
2	J	500	PLP	C2-N1	2.97	1.40	1.34
2	C	500	PLP	C2-N1	2.97	1.40	1.34
3	H	607	PMC	CA-C3	3.02	1.55	1.51
3	C	602	PMC	C2-C3	3.05	1.46	1.41
3	B	601	PMC	CA-C3	3.10	1.55	1.51
2	B	500	PLP	C2-N1	3.10	1.40	1.34
3	E	604	PMC	C2-C3	3.12	1.46	1.41
3	L	611	PMC	P1-CA	3.22	1.84	1.79
3	F	605	PMC	CA-C3	3.31	1.56	1.51
2	F	500	PLP	C2-N1	3.33	1.41	1.34
3	A	600	PMC	CA-C3	3.33	1.56	1.51
2	I	500	PLP	C2-N1	3.34	1.41	1.34
3	K	610	PMC	CA-C3	3.37	1.56	1.51
2	H	500	PLP	C2-N1	3.43	1.41	1.34
3	G	606	PMC	P1-CA	3.47	1.84	1.79
3	E	604	PMC	CA-C3	3.48	1.56	1.51
3	D	603	PMC	P1-CA	3.49	1.84	1.79
3	C	602	PMC	CA-C3	3.54	1.56	1.51
3	J	609	PMC	P1-CA	3.64	1.84	1.79
3	H	607	PMC	P1-CA	3.75	1.84	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	608	PMC	P1-CA	3.90	1.85	1.79
3	B	601	PMC	P1-CA	3.95	1.85	1.79
3	E	604	PMC	P1-CA	4.01	1.85	1.79
3	K	610	PMC	P1-CA	4.03	1.85	1.79
3	C	602	PMC	P1-CA	4.07	1.85	1.79
3	F	605	PMC	P1-CA	4.15	1.85	1.79
3	A	600	PMC	P1-CA	4.30	1.85	1.79
2	L	500	PLP	C3-C2	5.95	1.44	1.40
2	I	500	PLP	C3-C2	7.62	1.46	1.40
2	C	500	PLP	C3-C2	7.74	1.46	1.40
2	J	500	PLP	C3-C2	7.87	1.46	1.40
2	G	500	PLP	C3-C2	8.86	1.46	1.40
2	E	500	PLP	C3-C2	9.51	1.47	1.40
2	A	500	PLP	C3-C2	9.74	1.47	1.40
2	L	500	PLP	C5-C4	10.60	1.52	1.40
2	E	500	PLP	C5-C4	10.82	1.53	1.40
2	F	500	PLP	C3-C2	10.92	1.48	1.40
2	B	500	PLP	C3-C2	11.13	1.48	1.40
2	G	500	PLP	C5-C4	11.41	1.53	1.40
2	J	500	PLP	C5-C4	11.51	1.53	1.40
2	H	500	PLP	C3-C2	11.63	1.48	1.40
2	C	500	PLP	C5-C4	11.65	1.54	1.40
2	K	500	PLP	C5-C4	11.84	1.54	1.40
2	A	500	PLP	C5-C4	12.21	1.54	1.40
2	H	500	PLP	C5-C4	12.68	1.55	1.40
2	I	500	PLP	C5-C4	12.81	1.55	1.40
2	F	500	PLP	C5-C4	12.86	1.55	1.40
2	D	500	PLP	C5-C4	12.95	1.55	1.40
2	B	500	PLP	C5-C4	13.31	1.55	1.40
2	K	500	PLP	C3-C2	13.64	1.50	1.40
2	D	500	PLP	C3-C2	13.71	1.50	1.40

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	500	PLP	O3-C3-C2	-3.78	111.09	117.66
2	D	500	PLP	C3-C4-C5	-3.68	114.77	118.78
2	K	500	PLP	O3-C3-C2	-3.53	111.51	117.66
2	B	500	PLP	O3-C3-C2	-3.49	111.59	117.66
2	G	500	PLP	O3-C3-C2	-3.42	111.72	117.66
2	D	500	PLP	O3-C3-C2	-3.41	111.73	117.66
2	C	500	PLP	O3-C3-C2	-3.38	111.78	117.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	500	PLP	O3-C3-C2	-3.38	111.79	117.66
2	K	500	PLP	C3-C4-C5	-3.34	115.13	118.78
2	J	500	PLP	O3-C3-C2	-3.21	112.07	117.66
2	E	500	PLP	O3-C3-C2	-3.08	112.31	117.66
2	A	500	PLP	O3-C3-C2	-3.08	112.31	117.66
2	H	500	PLP	O4P-P-O1P	-3.05	99.38	107.14
2	L	500	PLP	C5-C6-N1	-2.95	118.74	123.86
2	I	500	PLP	O3-C3-C2	-2.93	112.57	117.66
2	I	500	PLP	C5-C6-N1	-2.92	118.79	123.86
2	B	500	PLP	C3-C4-C5	-2.78	115.74	118.78
2	F	500	PLP	C3-C2-N1	-2.75	116.81	120.61
2	C	500	PLP	C5-C6-N1	-2.75	119.09	123.86
2	L	500	PLP	O3-C3-C2	-2.73	112.92	117.66
2	B	500	PLP	C3-C2-N1	-2.65	116.95	120.61
2	J	500	PLP	C5-C6-N1	-2.58	119.38	123.86
2	L	500	PLP	C3-C2-N1	-2.57	117.06	120.61
2	H	500	PLP	C3-C2-N1	-2.55	117.09	120.61
2	I	500	PLP	C3-C2-N1	-2.54	117.10	120.61
2	A	500	PLP	C3-C2-N1	-2.53	117.11	120.61
2	C	500	PLP	C3-C2-N1	-2.50	117.15	120.61
2	E	500	PLP	C5-C6-N1	-2.49	119.54	123.86
2	F	500	PLP	C5-C6-N1	-2.48	119.55	123.86
2	G	500	PLP	C5-C6-N1	-2.47	119.57	123.86
2	I	500	PLP	O4P-P-O1P	-2.43	100.96	107.14
2	E	500	PLP	C3-C2-N1	-2.42	117.27	120.61
2	K	500	PLP	C3-C2-N1	-2.40	117.29	120.61
2	J	500	PLP	C3-C2-N1	-2.39	117.31	120.61
2	J	500	PLP	O4P-P-O1P	-2.39	101.06	107.14
2	B	500	PLP	C5-C6-N1	-2.38	119.72	123.86
2	H	500	PLP	C5-C6-N1	-2.36	119.76	123.86
2	H	500	PLP	C3-C4-C5	-2.36	116.21	118.78
2	G	500	PLP	C3-C2-N1	-2.36	117.35	120.61
2	A	500	PLP	C5-C6-N1	-2.32	119.83	123.86
2	F	500	PLP	C3-C4-C5	-2.31	116.26	118.78
2	D	500	PLP	C3-C2-N1	-2.22	117.55	120.61
2	D	500	PLP	C5-C6-N1	-2.19	120.07	123.86
2	C	500	PLP	O3P-P-O4P	-2.15	100.38	106.56
2	K	500	PLP	C5-C6-N1	-2.08	120.25	123.86
2	B	500	PLP	O3P-P-O2P	2.04	115.13	107.38
2	I	500	PLP	O2P-P-O1P	2.07	117.23	110.58
2	A	500	PLP	O2P-P-O4P	2.11	112.63	106.56
2	A	500	PLP	O3P-P-O2P	2.20	115.75	107.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	PLP	C4A-C4-C5	2.22	123.20	120.88
2	G	500	PLP	C6-C5-C4	2.24	120.05	118.15
2	E	500	PLP	O3P-P-O2P	2.25	115.94	107.38
2	A	500	PLP	C4A-C4-C5	2.25	123.22	120.88
2	L	500	PLP	O3P-P-O2P	2.26	115.97	107.38
2	E	500	PLP	C6-C5-C4	2.28	120.08	118.15
3	G	606	PMC	P1-CA-C3	2.33	118.62	114.10
2	F	500	PLP	O3P-P-O2P	2.37	116.39	107.38
2	C	500	PLP	C6-C5-C4	2.39	120.18	118.15
3	J	609	PMC	P1-CA-C3	2.46	118.86	114.10
3	D	603	PMC	P1-CA-C3	2.49	118.92	114.10
2	H	500	PLP	C6-C5-C4	2.51	120.27	118.15
2	I	500	PLP	C4A-C4-C5	2.52	123.51	120.88
3	I	608	PMC	P1-CA-C3	2.60	119.14	114.10
2	F	500	PLP	C4A-C4-C5	2.62	123.61	120.88
2	H	500	PLP	C4A-C4-C5	2.66	123.66	120.88
3	B	601	PMC	P1-CA-C3	2.73	119.38	114.10
2	F	500	PLP	C6-C5-C4	2.73	120.47	118.15
2	B	500	PLP	C6-C5-C4	2.76	120.49	118.15
2	D	500	PLP	C6-N1-C2	2.77	124.92	119.28
2	F	500	PLP	O4P-C5A-C5	2.86	113.72	108.99
2	C	500	PLP	O3P-P-O2P	2.87	118.29	107.38
3	L	611	PMC	P1-CA-C3	2.87	119.66	114.10
2	K	500	PLP	C6-N1-C2	2.89	125.17	119.28
2	G	500	PLP	C4A-C4-C5	2.91	123.91	120.88
3	H	607	PMC	P1-CA-C3	2.94	119.80	114.10
3	F	605	PMC	P1-CA-C3	3.00	119.91	114.10
2	H	500	PLP	C6-N1-C2	3.07	125.54	119.28
2	D	500	PLP	O3-C3-C4	3.09	126.80	118.12
2	I	500	PLP	O3-C3-C4	3.10	126.83	118.12
3	A	600	PMC	P1-CA-C3	3.13	120.16	114.10
3	K	610	PMC	P1-CA-C3	3.14	120.18	114.10
2	B	500	PLP	O3-C3-C4	3.16	127.01	118.12
2	G	500	PLP	C6-N1-C2	3.20	125.81	119.28
3	L	611	PMC	C6-N1-C2	3.23	122.88	116.64
2	E	500	PLP	C6-N1-C2	3.24	125.89	119.28
2	F	500	PLP	O3-C3-C4	3.24	127.24	118.12
2	B	500	PLP	C6-N1-C2	3.24	125.90	119.28
2	A	500	PLP	O3-C3-C4	3.25	127.25	118.12
2	J	500	PLP	C6-N1-C2	3.25	125.91	119.28
2	F	500	PLP	C6-N1-C2	3.29	126.00	119.28
2	K	500	PLP	O4P-C5A-C5	3.29	114.44	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	500	PLP	O3-C3-C4	3.30	127.40	118.12
3	I	608	PMC	C6-N1-C2	3.30	123.01	116.64
2	A	500	PLP	C6-N1-C2	3.31	126.02	119.28
3	D	603	PMC	C6-N1-C2	3.31	123.03	116.64
3	J	609	PMC	C6-N1-C2	3.31	123.03	116.64
3	B	601	PMC	C6-N1-C2	3.32	123.04	116.64
3	C	602	PMC	C6-N1-C2	3.33	123.06	116.64
3	A	600	PMC	C6-N1-C2	3.33	123.06	116.64
3	E	604	PMC	C6-N1-C2	3.33	123.06	116.64
3	G	606	PMC	C6-N1-C2	3.33	123.07	116.64
2	J	500	PLP	O3-C3-C4	3.34	127.50	118.12
3	H	607	PMC	C6-N1-C2	3.35	123.10	116.64
3	C	602	PMC	P1-CA-C3	3.36	120.61	114.10
3	K	610	PMC	C6-N1-C2	3.37	123.14	116.64
2	L	500	PLP	O3-C3-C4	3.37	127.61	118.12
2	E	500	PLP	O3-C3-C4	3.41	127.71	118.12
2	G	500	PLP	O3-C3-C4	3.41	127.72	118.12
3	F	605	PMC	C6-N1-C2	3.42	123.24	116.64
2	H	500	PLP	O3-C3-C4	3.44	127.80	118.12
2	C	500	PLP	C6-N1-C2	3.45	126.32	119.28
2	I	500	PLP	C6-N1-C2	3.45	126.33	119.28
2	C	500	PLP	O3-C3-C4	3.48	127.90	118.12
2	K	500	PLP	C6-C5-C4	3.48	121.10	118.15
2	G	500	PLP	O4P-C5A-C5	3.49	114.76	108.99
2	I	500	PLP	O4P-C5A-C5	3.56	114.88	108.99
2	B	500	PLP	C4A-C4-C5	3.58	124.62	120.88
3	E	604	PMC	P1-CA-C3	3.58	121.04	114.10
2	D	500	PLP	C6-C5-C4	3.66	121.25	118.15
2	L	500	PLP	C6-N1-C2	3.69	126.80	119.28
2	B	500	PLP	O4P-C5A-C5	3.76	115.21	108.99
2	D	500	PLP	O4P-C5A-C5	3.77	115.22	108.99
2	C	500	PLP	O4P-C5A-C5	3.84	115.34	108.99
2	K	500	PLP	C4A-C4-C5	3.92	124.97	120.88
2	H	500	PLP	O4P-C5A-C5	4.17	115.88	108.99
2	D	500	PLP	C4A-C4-C5	4.26	125.32	120.88
2	E	500	PLP	O4P-C5A-C5	4.33	116.16	108.99
2	L	500	PLP	O4P-C5A-C5	4.51	116.45	108.99
2	J	500	PLP	O4P-C5A-C5	4.59	116.58	108.99
2	A	500	PLP	O4P-C5A-C5	4.86	117.03	108.99
2	J	500	PLP	C2A-C2-C3	5.14	127.24	121.04
2	G	500	PLP	C2A-C2-C3	5.39	127.54	121.04
2	I	500	PLP	C2A-C2-C3	5.48	127.65	121.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	500	PLP	C2A-C2-C3	5.49	127.66	121.04
2	C	500	PLP	C2A-C2-C3	5.51	127.68	121.04
2	D	500	PLP	C2A-C2-C3	5.57	127.75	121.04
2	B	500	PLP	C2A-C2-C3	5.64	127.84	121.04
2	A	500	PLP	C2A-C2-C3	5.83	128.06	121.04
2	F	500	PLP	C2A-C2-C3	5.83	128.07	121.04
2	E	500	PLP	C2A-C2-C3	5.84	128.08	121.04
2	L	500	PLP	C2A-C2-C3	5.86	128.10	121.04
2	K	500	PLP	C2A-C2-C3	5.95	128.22	121.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

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

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.