



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:22 PM GMT

PDB ID : 4I0U
Title : Improved structure of *Thermotoga maritima* CorA at 2.7 Å resolution
Authors : Nordin, N.; Guskov, A.; Phua, T.; Sahaf, N.; Xia, Y.; Lu, S.Y.; Eshaghi, H.;
Eshaghi, S.
Deposited on : 2012-11-19
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

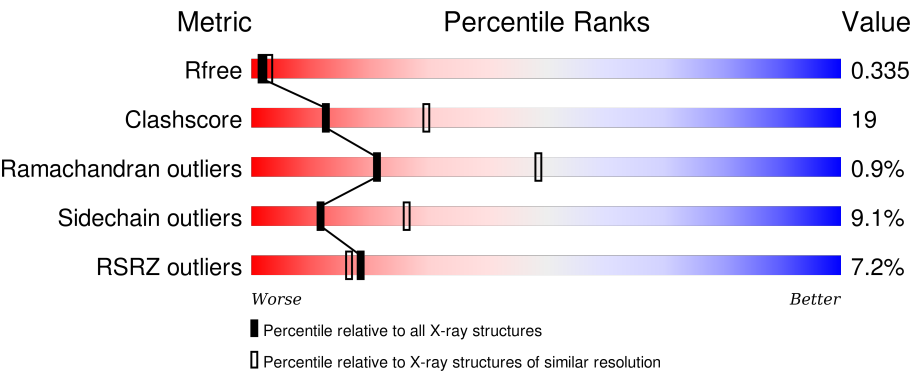
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	351	<div><div>7%</div><div>58%36%</div><div>..</div></div>
1	B	351	<div><div>4%</div><div>56%39%</div><div>..</div></div>
1	C	351	<div><div>8%</div><div>58%36%</div><div>..</div></div>
1	D	351	<div><div>9%</div><div>54%38%5%</div><div>.</div></div>
1	E	351	<div><div>7%</div><div>56%38%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	351	
1	G	351	
1	H	351	
1	I	351	
1	J	351	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	D	401	-	-	-	X
2	MG	D	403	-	-	-	X
2	MG	E	402	-	-	-	X
2	MG	J	401	-	-	-	X
3	CL	G	406	-	-	X	-
3	CL	J	404	-	-	-	X
4	LMT	A	403	-	-	X	X
4	LMT	B	406	-	-	X	-
5	PEG	C	406	-	-	X	-
5	PEG	J	405	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 29094 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 Magnesium transport protein CorA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2886	1880	471	525	10			
1	B	348	Total	C	N	O	S	0	0	0
			2895	1885	472	528	10			
1	C	347	Total	C	N	O	S	0	0	0
			2865	1862	469	525	9			
1	D	343	Total	C	N	O	S	0	0	0
			2849	1857	463	519	10			
1	E	345	Total	C	N	O	S	0	1	0
			2844	1850	465	519	10			
1	F	346	Total	C	N	O	S	0	0	0
			2856	1859	466	522	9			
1	G	346	Total	C	N	O	S	0	0	0
			2844	1850	465	519	10			
1	H	343	Total	C	N	O	S	0	0	0
			2826	1838	461	518	9			
1	I	345	Total	C	N	O	S	0	0	0
			2850	1857	462	521	10			
1	J	345	Total	C	N	O	S	0	0	0
			2844	1849	465	520	10			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	5	Total	Mg	0	0
			5	5		
2	J	3	Total	Mg	0	0
			3	3		
2	D	3	Total	Mg	0	0
			3	3		
2	E	2	Total	Mg	0	0
			2	2		

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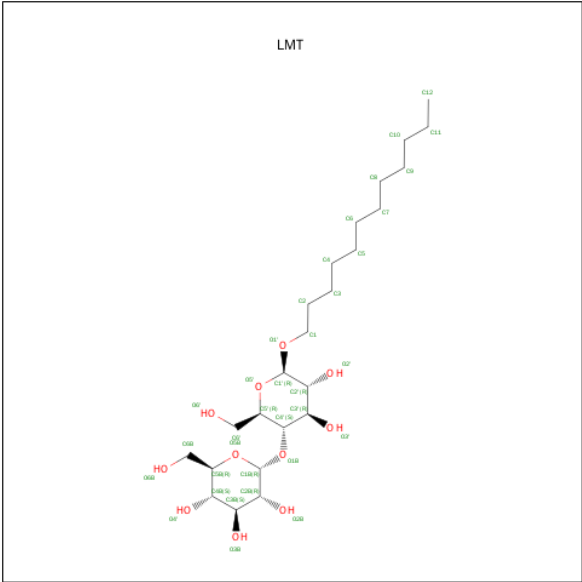
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total 3	Mg 3	0	0
2	I	3	Total 3	Mg 3	0	0
2	C	2	Total 2	Mg 2	0	0
2	A	1	Total 1	Mg 1	0	0
2	F	2	Total 2	Mg 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

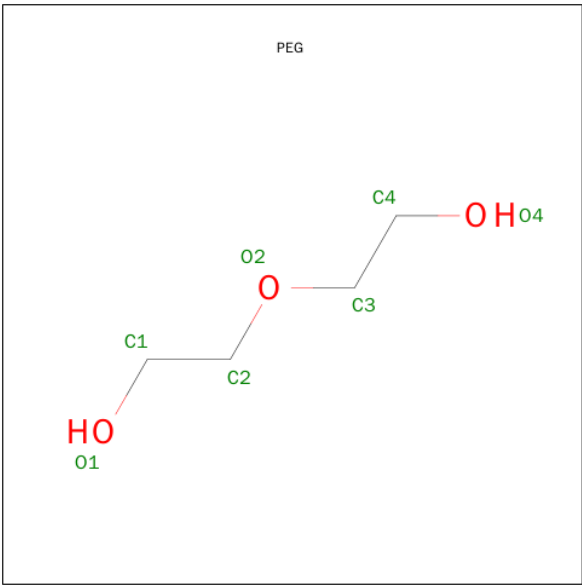
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total 2	Cl 2	0	0
3	J	1	Total 1	Cl 1	0	0
3	D	1	Total 1	Cl 1	0	0
3	E	2	Total 2	Cl 2	0	0
3	H	1	Total 1	Cl 1	0	0
3	B	2	Total 2	Cl 2	0	0
3	C	2	Total 2	Cl 2	0	0
3	A	1	Total 1	Cl 1	0	0
3	F	1	Total 1	Cl 1	0	0

- Molecule 4 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	24	11		
4	B	1	Total	C	O	0	0
			35	24	11		
4	B	1	Total	C	O	0	0
			32	21	11		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



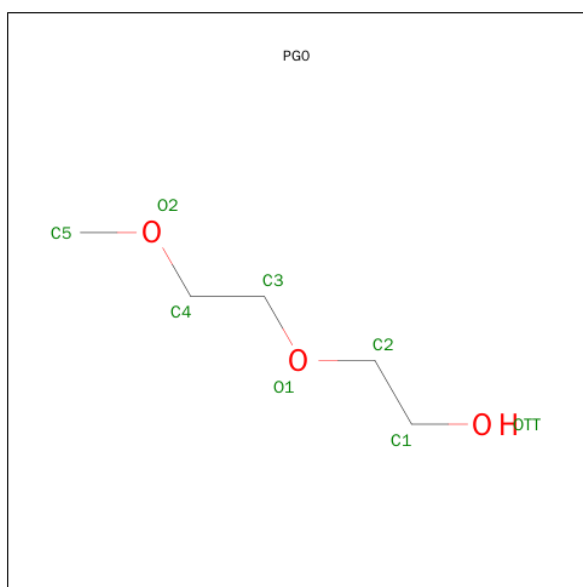
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		
5	F	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total	C	O	0	0
			7	4	3		
5	H	1	Total	C	O	0	0
			7	4	3		
5	I	1	Total	C	O	0	0
			7	4	3		
5	J	1	Total	C	O	0	0
			7	4	3		
5	J	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: C₅H₁₂O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			8	5	3		

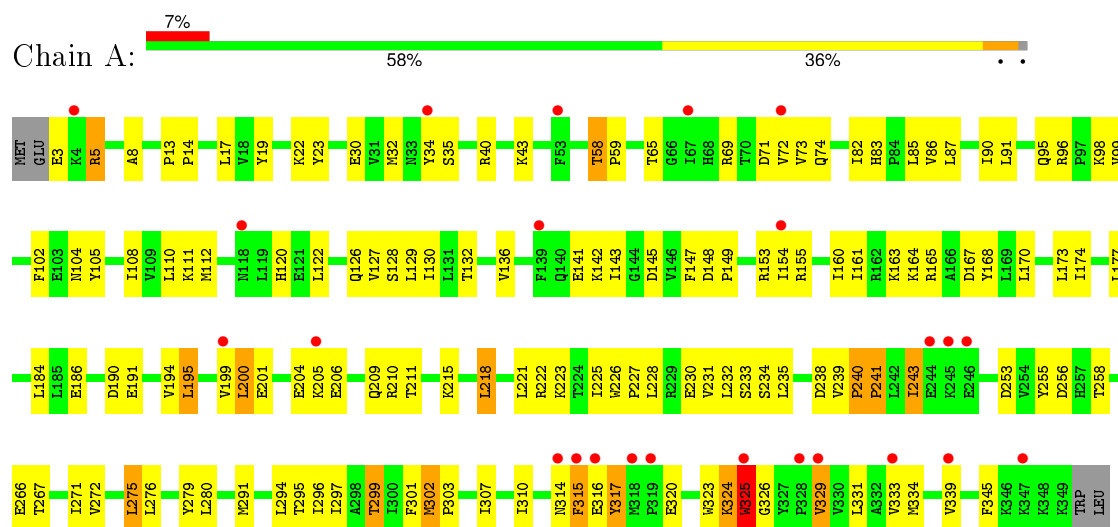
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	20	Total	O	0	0
			20	20		
7	B	28	Total	O	0	0
			28	28		
7	C	27	Total	O	0	0
			27	27		
7	D	25	Total	O	0	0
			25	25		
7	E	27	Total	O	0	0
			27	27		
7	F	20	Total	O	0	0
			20	20		
7	G	35	Total	O	0	0
			35	35		
7	H	15	Total	O	0	0
			15	15		
7	I	21	Total	O	0	0
			21	21		
7	J	23	Total	O	0	0
			23	23		

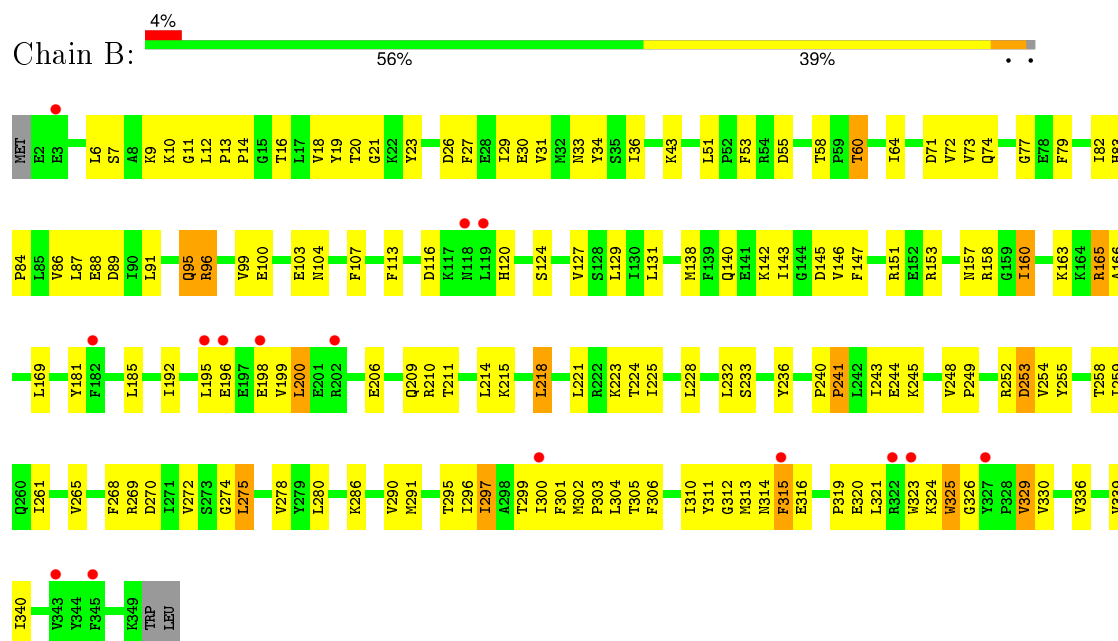
3 Residue-property plots

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.

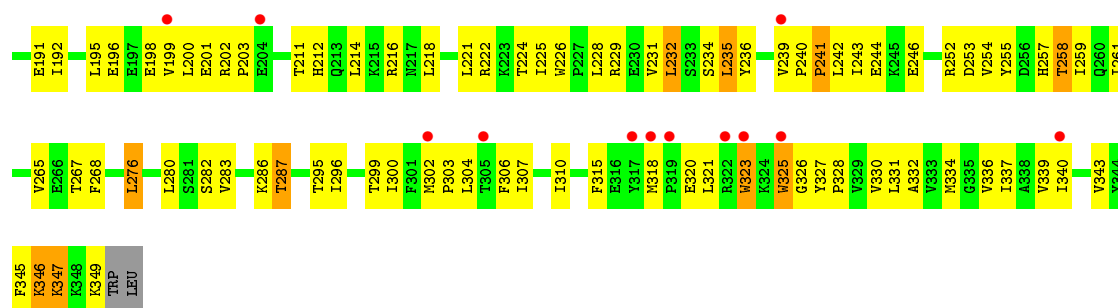
• Molecule 1: Magnesium transport protein CorA



• Molecule 1: Magnesium transport protein CorA

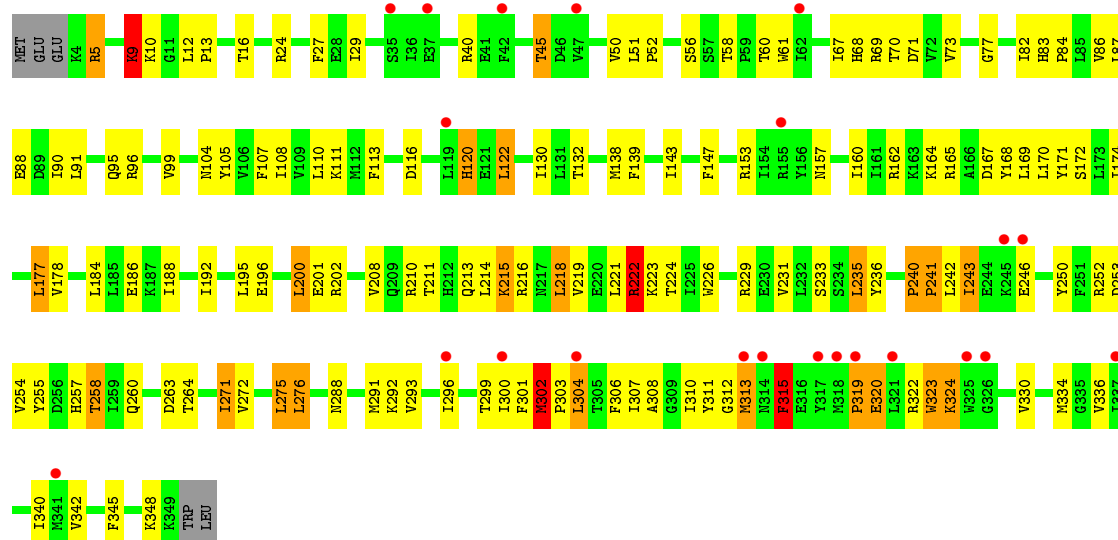


• Molecule 1: Magnesium transport protein CorA



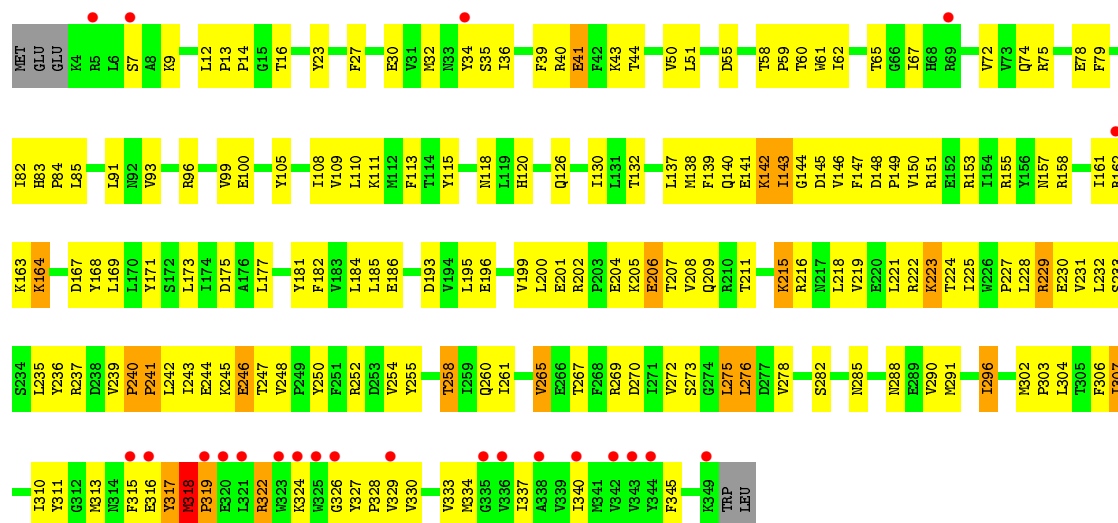
• Molecule 1: Magnesium transport protein CorA

Chain F: 6% 57% 34% 6%

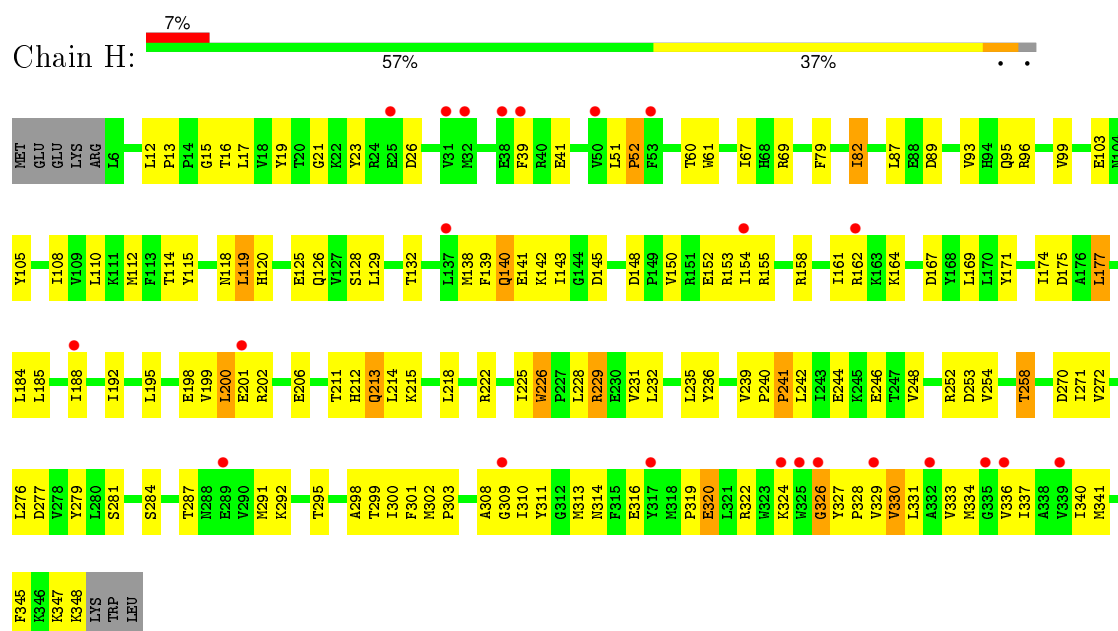


• Molecule 1: Magnesium transport protein CorA

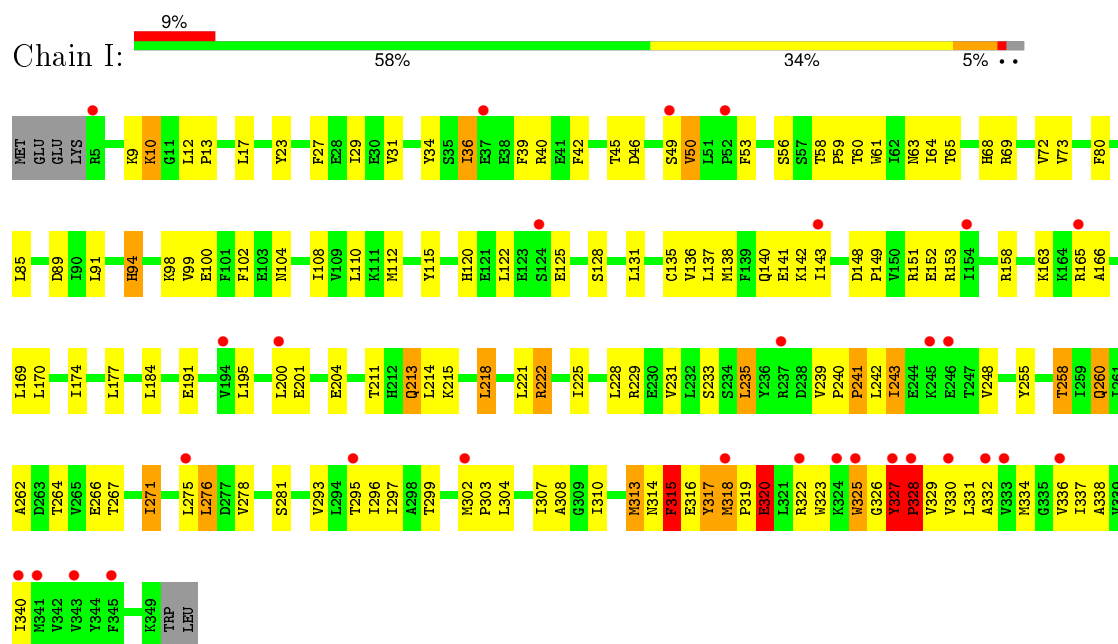
Chain G: 7% 48% 45% 6%



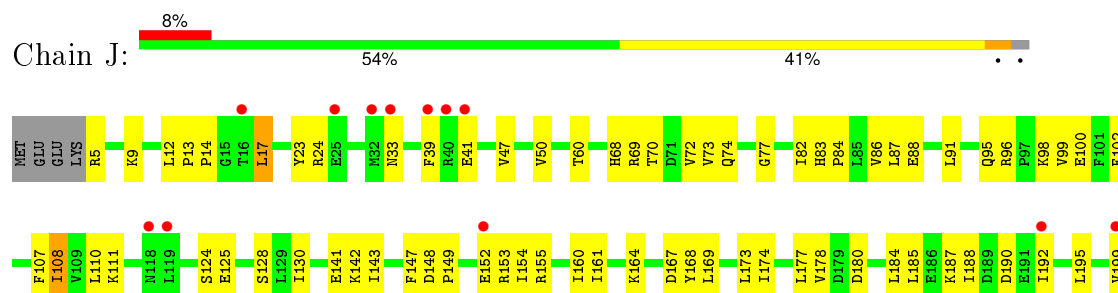
• Molecule 1: Magnesium transport protein CorA

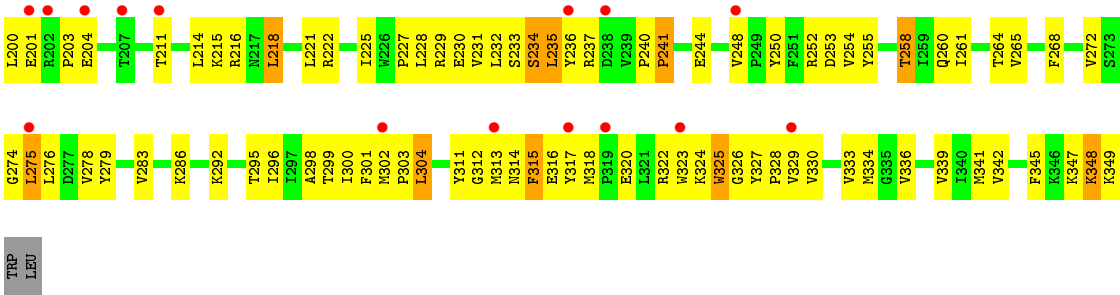


• Molecule 1: Magnesium transport protein CorA



• Molecule 1: Magnesium transport protein CorA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	116.25Å 151.50Å 143.36Å 90.00° 98.88° 90.00°	Depositor
Resolution (Å)	38.30 – 2.70 38.31 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.5 (38.30-2.70) 90.5 (38.31-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.228 , 0.289 0.279 , 0.335	Depositor DCC
R_{free} test set	6083 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 81.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	4 of 121642 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29094	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PEG, LMT, PG0, CL

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	0.51	0/2950	0.72	1/3997 (0.0%)
1	B	0.58	0/2959	0.78	1/4009 (0.0%)
1	C	0.53	0/2925	0.74	2/3962 (0.1%)
1	D	0.48	0/2913	0.70	1/3949 (0.0%)
1	E	0.50	0/2907	0.73	1/3941 (0.0%)
1	F	0.54	0/2918	0.76	5/3955 (0.1%)
1	G	0.57	0/2905	0.79	0/3938
1	H	0.51	0/2887	0.73	0/3915
1	I	0.54	1/2914 (0.0%)	0.75	4/3952 (0.1%)
1	J	0.55	0/2905	0.72	0/3939
All	All	0.53	1/29183 (0.0%)	0.74	15/39557 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
1	E	0	2
1	F	0	2
1	G	0	1
1	H	0	1
1	I	0	3
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	328	PRO	N-CD	5.23	1.55	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	122	LEU	CA-CB-CG	7.56	132.69	115.30
1	A	232	LEU	CA-CB-CG	-6.54	100.27	115.30
1	I	320	GLU	N-CA-C	6.53	128.64	111.00
1	I	315	PHE	N-CA-C	-6.49	93.49	111.00
1	I	327	TYR	C-N-CD	6.30	141.63	128.40
1	F	302	MET	C-N-CD	6.08	141.16	128.40
1	C	137	LEU	CA-CB-CG	-6.04	101.41	115.30
1	E	232	LEU	CA-CB-CG	-5.99	101.53	115.30
1	F	222	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	253	ASP	CB-CG-OD1	-5.76	113.12	118.30
1	D	232	LEU	CA-CB-CG	-5.68	102.23	115.30
1	F	323	TRP	N-CA-C	5.40	125.57	111.00
1	I	318	MET	C-N-CD	-5.29	108.96	120.60
1	F	9	LYS	N-CA-C	-5.09	97.24	111.00
1	C	89	ASP	CB-CG-OD1	-5.00	113.80	118.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	ALA	Peptide
1	C	326	GLY	Peptide
1	D	327	TYR	Peptide
1	E	323	TRP	Peptide
1	E	325	TRP	Peptide
1	F	315	PHE	Peptide
1	F	323	TRP	Peptide
1	G	317	TYR	Peptide
1	H	326	GLY	Peptide
1	I	320	GLU	Peptide
1	I	327	TYR	Peptide
1	I	94	HIS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2886	0	2938	105	0
1	B	2895	0	2944	126	0
1	C	2865	0	2915	112	0
1	D	2849	0	2895	116	0
1	E	2844	0	2890	118	0
1	F	2856	0	2897	134	0
1	G	2844	0	2882	143	0
1	H	2826	0	2862	104	0
1	I	2850	0	2879	138	0
1	J	2844	0	2882	118	0
2	A	1	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	5	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
3	A	1	0	0	1	0
3	B	2	0	0	1	0
3	C	2	0	0	1	0
3	D	1	0	0	0	0
3	E	2	0	0	2	0
3	F	1	0	0	1	0
3	G	2	0	0	2	0
3	H	1	0	0	1	0
3	J	1	0	0	1	0
4	A	35	0	46	27	0
4	B	67	0	83	35	0
5	B	28	0	40	5	0
5	C	14	0	20	4	0
5	D	7	0	10	0	0
5	E	28	0	40	1	0
5	F	7	0	10	0	0
5	G	35	0	50	8	0
5	H	7	0	10	0	0
5	I	7	0	10	0	0
5	J	14	0	20	2	0
6	E	8	0	12	0	0
7	A	20	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	28	0	0	8	0
7	C	27	0	0	4	0
7	D	25	0	0	8	0
7	E	27	0	0	4	0
7	F	20	0	0	2	0
7	G	35	0	0	12	0
7	H	15	0	0	3	0
7	I	21	0	0	4	0
7	J	23	0	0	6	0
All	All	29094	0	29335	1128	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 19.

All (1128) 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:G:246:GLU:OE1	5:G:411:PEG:H22	1.24	1.32
4:A:403:LMT:H3B	4:B:406:LMT:C6'	1.59	1.32
4:A:403:LMT:C3B	4:B:406:LMT:H6E	1.83	1.08
4:A:403:LMT:H3B	4:B:406:LMT:H6E	1.07	1.06
1:G:246:GLU:OE1	5:G:411:PEG:C2	2.06	1.02
1:F:307:ILE:O	1:F:310:ILE:HG22	1.60	1.00
1:F:307:ILE:HD11	1:F:334:MET:CE	1.91	1.00
4:A:403:LMT:H3B	4:B:406:LMT:H6D	1.50	0.93
1:B:323:TRP:HB2	4:B:407:LMT:O4'	1.70	0.92
1:F:307:ILE:HD11	1:F:334:MET:CG	1.98	0.92
1:I:316:GLU:HB2	1:I:318:MET:HG2	1.49	0.92
1:I:326:GLY:HA3	1:I:328:PRO:HD3	1.50	0.92
1:I:330:VAL:O	1:I:334:MET:HG3	1.68	0.92
1:C:256:ASP:OD1	1:E:96[B]:ARG:NH2	2.03	0.91
4:A:403:LMT:C3B	4:B:406:LMT:C6'	2.47	0.91
1:F:301:PHE:HE2	1:I:303:PRO:HG3	1.32	0.91
1:C:316:GLU:HG2	1:E:321:LEU:HB3	1.53	0.90
1:B:43:LYS:HD2	5:B:410:PEG:H11	1.53	0.90
4:A:403:LMT:C3'	4:B:406:LMT:H4'	2.03	0.89
1:A:323:TRP:HB3	1:A:324:LYS:HA	1.54	0.88
1:D:203:PRO:HB2	7:D:521:HOH:O	1.73	0.88
1:G:61:TRP:HB2	1:G:169:LEU:HD21	1.56	0.87
1:G:196:GLU:OE1	1:H:212:HIS:NE2	2.06	0.86
1:F:110:LEU:HD13	1:F:177:LEU:HD22	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:PRO:CB	7:D:521:HOH:O	2.22	0.85
1:E:88:GLU:OE1	7:E:501:HOH:O	1.94	0.85
1:G:229:ARG:NH2	7:G:514:HOH:O	2.09	0.84
1:A:324:LYS:HD2	1:D:317:TYR:HB2	1.58	0.84
4:A:403:LMT:H3'	4:B:406:LMT:H4'	1.59	0.83
1:F:307:ILE:CD1	1:F:334:MET:CE	2.57	0.82
1:F:307:ILE:CD1	1:F:334:MET:HE3	2.09	0.82
1:A:13:PRO:HG3	1:D:153:ARG:HD3	1.62	0.81
1:D:229:ARG:HG2	1:D:258:THR:HG23	1.63	0.80
1:G:140:GLN:HE22	1:G:145:ASP:HB3	1.45	0.80
1:A:307:ILE:HD11	1:A:334:MET:HG2	1.64	0.80
1:I:235:LEU:HD12	1:I:242:LEU:HD11	1.63	0.80
1:I:89:ASP:OD2	7:I:505:HOH:O	1.99	0.79
1:B:74:GLN:NE2	7:B:526:HOH:O	2.15	0.79
1:C:126:GLN:NE2	7:C:522:HOH:O	2.14	0.79
1:F:13:PRO:HG3	1:I:153:ARG:HD3	1.63	0.79
4:A:403:LMT:H12	4:B:406:LMT:H51	1.62	0.79
7:F:513:HOH:O	1:G:223:LYS:NZ	2.16	0.79
1:F:306:PHE:CE1	1:G:304:LEU:HB3	2.18	0.79
1:J:88:GLU:OE2	7:J:507:HOH:O	2.01	0.78
1:B:252:ARG:NH2	5:C:406:PEG:O4	2.15	0.78
1:I:326:GLY:HA2	1:I:327:TYR:HB3	1.65	0.78
1:D:48:GLU:OE2	7:D:510:HOH:O	2.01	0.78
1:I:184:LEU:HD21	1:I:221:LEU:HD11	1.65	0.78
1:J:218:LEU:HD21	1:J:268:PHE:HB3	1.66	0.78
1:D:54:ARG:NH1	1:D:79:PHE:O	2.17	0.77
3:C:403:CL:CL	7:C:503:HOH:O	2.39	0.77
4:A:403:LMT:O2'	4:B:406:LMT:O3'	2.01	0.77
1:G:41:GLU:OE2	1:G:155:ARG:NE	2.16	0.77
1:D:199:VAL:HG13	1:D:279:TYR:HB2	1.66	0.77
1:G:168:TYR:OH	3:G:406:CL:CL	2.39	0.76
1:H:175:ASP:OD1	7:H:505:HOH:O	2.03	0.76
1:G:74:GLN:HE22	5:G:409:PEG:H31	1.48	0.76
1:I:327:TYR:CE1	1:J:318:MET:HE3	2.20	0.76
1:E:83:HIS:CD2	1:E:85:LEU:H	2.03	0.76
1:B:253:ASP:OD1	7:B:506:HOH:O	2.02	0.76
3:E:404:CL:CL	7:E:503:HOH:O	2.41	0.76
1:I:326:GLY:HA3	1:I:328:PRO:CD	2.14	0.76
1:C:192:ILE:HG12	1:C:214:LEU:HD21	1.68	0.76
1:I:325:TRP:HA	1:I:325:TRP:CE3	2.20	0.76
1:E:61:TRP:HB2	1:E:169:LEU:HD21	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:403:LMT:H12	4:B:406:LMT:C5	2.17	0.75
1:B:163:LYS:NZ	7:B:511:HOH:O	2.19	0.75
1:I:327:TYR:CE1	1:J:318:MET:CE	2.69	0.75
1:H:120:HIS:O	1:H:213:GLN:NE2	2.20	0.74
1:F:307:ILE:HG13	1:F:308:ALA:N	2.02	0.74
1:F:307:ILE:HD11	1:F:334:MET:HG2	1.69	0.74
1:H:195:LEU:HD21	1:H:211:THR:HA	1.68	0.74
1:D:73:VAL:HG21	1:D:91:LEU:HD21	1.68	0.74
1:G:232:LEU:HD13	1:G:254:VAL:HG12	1.68	0.74
4:A:403:LMT:C3'	4:B:406:LMT:O3'	2.36	0.73
1:I:63:ASN:HD22	1:I:151:ARG:HH22	1.32	0.73
1:D:140:GLN:HE22	1:D:145:ASP:HB3	1.52	0.73
1:F:311:TYR:HE2	1:F:330:VAL:HG21	1.53	0.73
1:I:327:TYR:HB2	1:J:315:PHE:HZ	1.53	0.73
1:I:331:LEU:O	1:I:334:MET:HB2	1.89	0.73
1:J:82:ILE:HG12	1:J:130:ILE:HD13	1.71	0.72
1:G:100:GLU:O	7:G:523:HOH:O	2.06	0.72
1:B:89:ASP:OD2	7:B:502:HOH:O	2.07	0.72
1:J:229:ARG:NH1	7:J:518:HOH:O	2.22	0.72
1:I:222:ARG:NE	1:I:266:GLU:OE1	2.23	0.72
1:I:211:THR:HG21	1:I:276:LEU:HD13	1.73	0.71
1:H:61:TRP:HB2	1:H:169:LEU:HD21	1.72	0.71
1:F:311:TYR:HB2	1:I:313:MET:HG2	1.72	0.71
1:E:200:LEU:HD12	1:E:201:GLU:HG3	1.73	0.71
1:E:327:TYR:HA	1:E:330:VAL:HB	1.72	0.71
1:H:125:GLU:HG3	1:H:141:GLU:HB2	1.72	0.71
1:D:61:TRP:HB2	1:D:169:LEU:HD21	1.73	0.71
1:B:198:GLU:OE1	1:B:210:ARG:NH1	2.24	0.71
1:D:184:LEU:HD21	1:D:221:LEU:HD11	1.72	0.70
3:H:401:CL:CL	1:J:14:PRO:HD2	2.28	0.70
1:C:8:ALA:O	7:C:511:HOH:O	2.09	0.70
1:A:184:LEU:HD21	1:A:221:LEU:HD11	1.72	0.70
1:C:263:ASP:OD2	1:E:96[A]:ARG:NH1	2.21	0.70
1:F:307:ILE:HD11	1:F:334:MET:HE2	1.73	0.70
1:C:200:LEU:HD12	1:C:201:GLU:HG3	1.72	0.70
1:A:314:ASN:ND2	1:B:314:ASN:OD1	2.25	0.70
1:E:83:HIS:HD2	1:E:85:LEU:H	1.40	0.69
1:I:307:ILE:HD11	1:I:334:MET:HG2	1.73	0.69
1:F:301:PHE:C	1:F:303:PRO:HD2	2.13	0.69
1:E:221:LEU:HG	1:E:225:ILE:HD12	1.74	0.69
1:C:83:HIS:ND1	1:C:84:PRO:HD2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:272:VAL:O	7:G:515:HOH:O	2.10	0.69
1:B:232:LEU:HD13	1:B:254:VAL:HG12	1.75	0.69
1:A:256:ASP:OD2	7:A:518:HOH:O	2.09	0.69
1:E:120:HIS:ND1	1:E:191:GLU:OE2	2.26	0.69
4:B:407:LMT:O2'	4:B:407:LMT:H31	1.93	0.69
1:A:99:VAL:HG22	1:A:231:VAL:HG13	1.74	0.69
1:F:301:PHE:CE2	1:I:303:PRO:HG3	2.23	0.68
4:B:407:LMT:O3'	4:B:407:LMT:H1B	1.91	0.68
1:E:195:LEU:HD21	1:E:211:THR:HA	1.76	0.68
1:H:200:LEU:HD12	1:H:201:GLU:HG3	1.76	0.68
1:B:153:ARG:HD3	1:C:13:PRO:HG3	1.74	0.68
1:A:302:MET:HE1	1:B:302:MET:HG3	1.75	0.67
1:D:222:ARG:HD2	1:D:266:GLU:OE1	1.93	0.67
1:J:253:ASP:OD1	7:J:512:HOH:O	2.11	0.67
1:J:228:LEU:HA	1:J:231:VAL:HB	1.76	0.67
1:H:105:TYR:HB3	1:H:132:THR:HB	1.76	0.66
1:C:316:GLU:HG2	1:E:321:LEU:CB	2.24	0.66
4:A:403:LMT:H3'	4:B:406:LMT:C4'	2.25	0.66
1:F:319:PRO:HB2	1:F:320:GLU:HA	1.77	0.66
1:G:318:MET:HG2	1:G:319:PRO:HD3	1.77	0.66
1:D:200:LEU:HD12	1:D:201:GLU:HG3	1.78	0.66
1:I:326:GLY:CA	1:I:328:PRO:HD3	2.24	0.66
1:I:328:PRO:CD	1:I:329:VAL:H	2.08	0.66
1:F:302:MET:HG3	1:I:302:MET:HE1	1.78	0.66
1:J:88:GLU:OE1	7:J:501:HOH:O	2.14	0.66
1:G:327:TYR:HB3	1:G:328:PRO:HD3	1.77	0.66
1:I:45:THR:O	7:I:509:HOH:O	2.14	0.66
1:F:264:THR:OG1	7:F:513:HOH:O	2.12	0.66
1:F:77:GLY:HA3	1:F:87:LEU:HD21	1.77	0.66
4:A:403:LMT:O3'	4:B:406:LMT:O3'	2.13	0.65
1:D:203:PRO:HB3	7:D:521:HOH:O	1.91	0.65
1:C:302:MET:HE1	1:E:302:MET:HG3	1.76	0.65
1:J:108:ILE:HD13	1:J:235:LEU:HD21	1.79	0.65
1:J:255:TYR:O	1:J:258:THR:HG22	1.96	0.65
1:G:193:ASP:OD2	7:G:513:HOH:O	2.14	0.65
1:E:90:ILE:HD11	1:E:130:ILE:HD11	1.77	0.65
1:F:165:ARG:HH12	1:F:243:ILE:HG21	1.61	0.65
1:H:308:ALA:N	1:H:309:GLY:HA3	2.11	0.65
1:A:153:ARG:HD3	1:B:13:PRO:HG3	1.78	0.65
1:B:27:PHE:CZ	1:B:72:VAL:HG21	2.32	0.65
1:F:61:TRP:HB2	1:F:169:LEU:HD21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:83:HIS:ND1	1:J:84:PRO:HD2	2.12	0.65
1:A:3:GLU:N	1:D:186:GLU:OE1	2.30	0.65
1:A:90:ILE:HD11	1:A:130:ILE:HD11	1.79	0.65
1:I:40:ARG:HH21	1:I:42:PHE:HE2	1.43	0.65
1:B:316:GLU:HB2	1:C:324:LYS:HG2	1.79	0.64
1:E:337:ILE:HA	1:E:340:ILE:HG12	1.79	0.64
1:F:302:MET:HG3	1:I:302:MET:CE	2.28	0.64
1:I:125:GLU:OE1	1:I:140:GLN:NE2	2.25	0.64
1:G:233:SER:OG	1:G:237:ARG:NH2	2.31	0.64
1:G:303:PRO:HG3	1:H:301:PHE:CE2	2.33	0.64
1:D:29:ILE:HG21	1:D:50:VAL:HG11	1.78	0.64
1:J:12:LEU:O	7:J:503:HOH:O	2.14	0.64
1:C:82:ILE:HG12	1:C:130:ILE:HD13	1.80	0.64
1:C:308:ALA:N	1:C:309:GLY:HA3	2.13	0.64
1:J:147:PHE:HZ	1:J:177:LEU:HD12	1.63	0.64
1:C:29:ILE:HG21	1:C:50:VAL:HG11	1.80	0.64
1:J:33:ASN:ND2	1:J:60:THR:OG1	2.31	0.63
1:G:221:LEU:HD23	1:G:265:VAL:HG21	1.80	0.63
1:G:184:LEU:HD21	1:G:221:LEU:HD11	1.80	0.63
1:G:306:PHE:CZ	5:G:408:PEG:H41	2.33	0.63
1:A:83:HIS:HE2	1:A:85:LEU:HD12	1.63	0.63
1:I:325:TRP:HA	1:I:325:TRP:HE3	1.63	0.63
1:A:253:ASP:OD1	7:A:504:HOH:O	2.15	0.63
1:E:82:ILE:HG13	1:E:105:TYR:CE2	2.33	0.63
1:E:231:VAL:HG12	1:E:232:LEU:HG	1.81	0.63
1:E:185:LEU:HD11	1:E:261:ILE:HG23	1.80	0.63
1:B:323:TRP:HB2	4:B:407:LMT:H4O1	1.64	0.62
1:A:95:GLN:HA	1:D:260:GLN:HE22	1.64	0.62
1:H:314:ASN:ND2	1:J:314:ASN:OD1	2.32	0.62
1:A:155:ARG:O	7:A:514:HOH:O	2.15	0.62
4:A:403:LMT:H3'	4:B:406:LMT:C3'	2.29	0.62
1:I:40:ARG:NH1	7:I:520:HOH:O	2.23	0.62
1:B:311:TYR:HE2	1:B:330:VAL:HG21	1.65	0.62
1:D:211:THR:HG21	1:D:276:LEU:HD13	1.80	0.62
1:B:324:LYS:HG2	1:B:325:TRP:H	1.63	0.62
1:F:192:ILE:HG12	1:F:214:LEU:HD21	1.81	0.62
1:E:236:TYR:CE1	1:E:252:ARG:HB2	2.34	0.62
1:F:200:LEU:HD13	1:G:209:GLN:HG2	1.81	0.62
1:I:327:TYR:HA	1:I:330:VAL:HB	1.81	0.62
1:H:115:TYR:HB2	1:H:184:LEU:HD11	1.82	0.62
1:G:315:PHE:HB3	1:H:327:TYR:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ILE:HD11	1:D:334:MET:HG2	1.82	0.62
1:G:30:GLU:HG3	1:G:43:LYS:HG2	1.80	0.62
1:F:9:LYS:HB2	1:F:12:LEU:HD12	1.80	0.62
1:A:168:TYR:OH	1:B:14:PRO:HG2	2.00	0.62
1:A:303:PRO:HG3	1:B:301:PHE:HE2	1.65	0.61
1:D:148:ASP:O	1:D:152:GLU:HG2	2.00	0.61
1:J:70:THR:HG22	1:J:91:LEU:HD13	1.81	0.61
1:D:348:LYS:HG2	1:D:349:LYS:H	1.66	0.61
1:B:55:ASP:HB3	5:B:411:PEG:H11	1.82	0.61
1:I:307:ILE:HD11	1:I:334:MET:CG	2.30	0.61
1:I:327:TYR:CE1	1:J:318:MET:HE2	2.34	0.61
1:D:209:GLN:HG2	1:E:200:LEU:HD22	1.81	0.61
1:G:175:ASP:OD2	7:G:510:HOH:O	2.16	0.61
1:J:200:LEU:HD12	1:J:201:GLU:HG3	1.83	0.61
1:C:243:ILE:HG13	1:C:246:GLU:HB2	1.83	0.61
1:G:150:VAL:HG11	1:G:173:LEU:HD23	1.83	0.60
1:G:153:ARG:HD3	1:H:13:PRO:HG3	1.83	0.60
1:D:14:PRO:HD2	3:E:403:CL:CL	2.38	0.60
1:E:12:LEU:HD13	1:E:16:THR:HG21	1.83	0.60
1:F:29:ILE:HG21	1:F:50:VAL:HG11	1.83	0.60
1:C:83:HIS:CD2	1:C:85:LEU:HB2	2.36	0.60
1:D:175:ASP:OD2	7:D:501:HOH:O	2.17	0.60
1:G:36:ILE:HD13	1:G:163:LYS:HG3	1.83	0.60
1:G:310:ILE:HG22	1:H:334:MET:HE1	1.83	0.60
1:G:272:VAL:HA	1:G:275:LEU:HD22	1.83	0.60
1:F:200:LEU:HD12	1:F:201:GLU:HG3	1.84	0.60
1:D:130:ILE:HB	1:D:137:LEU:HB2	1.84	0.60
1:H:152:GLU:HB2	1:H:158:ARG:HH21	1.66	0.60
1:F:165:ARG:NH1	1:F:243:ILE:HG21	2.17	0.60
1:A:199:VAL:HG13	1:A:279:TYR:HB2	1.83	0.60
1:C:98:LYS:NZ	1:C:100:GLU:OE1	2.21	0.59
1:A:19:TYR:OH	1:A:141:GLU:OE1	2.09	0.59
1:J:203:PRO:HG2	1:J:286:LYS:HE2	1.84	0.59
3:F:403:CL:CL	1:G:14:PRO:HD2	2.39	0.59
4:A:403:LMT:O3'	4:B:406:LMT:C4'	2.51	0.59
1:J:23:TYR:CE2	1:J:142:LYS:HD3	2.37	0.59
1:D:243:ILE:HG13	1:D:246:GLU:HB2	1.85	0.59
1:F:312:GLY:O	1:I:314:ASN:ND2	2.35	0.59
1:I:326:GLY:HA2	1:I:327:TYR:CB	2.31	0.59
1:H:112:MET:HG3	1:H:177:LEU:HD11	1.83	0.59
1:E:239:VAL:HA	1:E:242:LEU:HD12	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:165:ARG:NH2	1:I:243:ILE:HD12	2.18	0.59
1:C:34:TYR:O	1:C:59:PRO:HD2	2.02	0.59
1:G:195:LEU:HD21	1:G:211:THR:HA	1.84	0.59
1:H:99:VAL:HG22	1:H:108:ILE:HG12	1.85	0.59
1:F:5:ARG:O	1:F:5:ARG:NE	2.36	0.59
1:C:131:LEU:HD22	1:C:170:LEU:HD22	1.83	0.59
1:I:255:TYR:O	1:I:258:THR:HG22	2.03	0.59
1:C:174:ILE:O	1:C:178:VAL:HG23	2.02	0.59
1:I:27:PHE:CZ	1:I:72:VAL:HG21	2.38	0.59
1:G:143:ILE:HD13	1:G:144:GLY:H	1.68	0.58
1:B:33:ASN:HB2	1:B:60:THR:HG23	1.85	0.58
1:H:330:VAL:HA	1:H:333:VAL:HG12	1.84	0.58
1:F:195:LEU:HD11	1:F:210:ARG:HB3	1.83	0.58
4:A:403:LMT:O3'	4:B:406:LMT:H4'	2.03	0.58
1:B:324:LYS:O	1:B:326:GLY:N	2.36	0.58
1:J:225:ILE:HD12	1:J:228:LEU:HD23	1.84	0.58
1:B:306:PHE:CE1	1:C:304:LEU:HB3	2.38	0.58
1:B:140:GLN:HE22	1:B:145:ASP:HB3	1.67	0.58
1:A:323:TRP:CB	1:A:324:LYS:HA	2.28	0.58
1:D:120:HIS:H	1:D:120:HIS:CD2	2.19	0.58
1:F:288:ASN:HD21	1:F:292:LYS:HE3	1.69	0.58
1:F:178:VAL:HG21	1:F:254:VAL:HG13	1.85	0.58
1:H:326:GLY:O	1:H:329:VAL:HG12	2.03	0.58
1:E:229:ARG:NE	1:E:259:ILE:HG12	2.17	0.58
1:E:22:LYS:HE3	1:E:23:TYR:CZ	2.37	0.58
1:B:274:GLY:O	1:B:278:VAL:HG23	2.04	0.58
1:H:281:SER:HB3	1:J:279:TYR:HE2	1.68	0.58
1:D:117:LYS:HE3	1:D:187:LYS:HG2	1.85	0.58
1:D:320:GLU:HB3	1:E:315:PHE:CE1	2.39	0.58
1:F:83:HIS:ND1	1:F:84:PRO:HD2	2.19	0.58
1:I:326:GLY:CA	1:I:327:TYR:HB3	2.33	0.58
1:B:236:TYR:CZ	1:B:252:ARG:HG3	2.39	0.58
1:C:232:LEU:HD13	1:C:254:VAL:HG12	1.86	0.58
1:A:22:LYS:HE3	1:A:23:TYR:CE1	2.39	0.58
1:B:181:TYR:O	1:B:185:LEU:HG	2.04	0.58
1:D:195:LEU:HD23	1:D:275:LEU:HD23	1.86	0.58
1:F:229:ARG:HA	1:F:258:THR:HG21	1.86	0.57
1:B:34:TYR:OH	1:B:169:LEU:HD13	2.03	0.57
1:B:73:VAL:HG11	1:B:91:LEU:HD21	1.85	0.57
1:B:30:GLU:OE1	1:B:151:ARG:NH2	2.37	0.57
1:I:320:GLU:C	1:I:322:ARG:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:VAL:HA	1:G:126:GLN:OE1	2.04	0.57
1:E:346:LYS:HE3	1:E:346:LYS:H	1.69	0.57
1:J:311:TYR:HE2	1:J:330:VAL:HG21	1.69	0.57
5:E:405:PEG:H32	7:G:535:HOH:O	2.03	0.57
3:G:406:CL:CL	7:G:533:HOH:O	2.54	0.57
1:D:222:ARG:HD3	1:D:269:ARG:HD2	1.87	0.57
1:J:221:LEU:O	1:J:225:ILE:HG22	2.04	0.57
1:F:307:ILE:HD11	1:F:334:MET:HG3	1.86	0.57
1:G:255:TYR:O	1:G:258:THR:HG22	2.04	0.57
1:A:108:ILE:HD12	1:A:170:LEU:HD11	1.86	0.57
1:H:299:THR:HG1	1:H:345:PHE:HZ	1.50	0.57
1:D:328:PRO:HG2	1:D:329:VAL:HG13	1.86	0.57
1:J:47:VAL:HG21	1:J:72:VAL:HG13	1.86	0.57
1:E:253:ASP:OD1	7:E:507:HOH:O	2.18	0.57
1:E:323:TRP:O	1:E:326:GLY:N	2.38	0.57
1:C:100:GLU:HB3	1:C:102:PHE:CE1	2.40	0.56
1:D:327:TYR:CE1	1:E:318:MET:HG3	2.40	0.56
1:H:292:LYS:HD3	1:H:348:LYS:HB3	1.87	0.56
1:F:116:ASP:O	1:F:120:HIS:HA	2.04	0.56
1:F:312:GLY:HA2	1:I:314:ASN:HD22	1.68	0.56
1:I:328:PRO:CG	1:I:329:VAL:H	2.18	0.56
1:G:140:GLN:NE2	1:G:145:ASP:HB3	2.17	0.56
1:I:10:LYS:HD3	5:J:405:PEG:O4	2.05	0.56
1:B:153:ARG:HG2	1:B:158:ARG:HB2	1.87	0.56
1:B:336:VAL:O	1:B:340:ILE:HG23	2.06	0.56
1:E:17:LEU:HG	1:E:91:LEU:HD12	1.88	0.56
1:A:325:TRP:CE3	1:A:325:TRP:HA	2.39	0.56
1:H:300:ILE:O	1:H:303:PRO:HD2	2.05	0.56
1:C:316:GLU:CG	1:E:321:LEU:O	2.53	0.56
1:J:304:LEU:HD13	1:J:334:MET:HB3	1.86	0.56
1:H:120:HIS:HB2	1:H:213:GLN:HE22	1.70	0.56
1:D:327:TYR:HA	1:D:330:VAL:H	1.70	0.56
4:A:403:LMT:C3'	4:B:406:LMT:C4'	2.78	0.56
1:J:178:VAL:HG21	1:J:232:LEU:HD11	1.88	0.56
1:F:229:ARG:HA	1:F:258:THR:CG2	2.35	0.56
1:D:144:GLY:O	7:D:511:HOH:O	2.18	0.56
1:C:288:ASN:HD21	1:C:292:LYS:HE3	1.70	0.56
1:H:252:ARG:NH2	7:H:509:HOH:O	2.39	0.56
1:A:200:LEU:HD13	1:B:209:GLN:HG2	1.87	0.56
1:C:310:ILE:HD13	1:E:331:LEU:HD11	1.87	0.55
1:C:80:PHE:CD2	1:C:137:LEU:HD11	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:PHE:HA	1:E:321:LEU:HD22	1.87	0.55
1:H:313:MET:HA	1:J:312:GLY:HA2	1.89	0.55
1:B:129:LEU:CD2	1:B:138:MET:HG3	2.37	0.55
1:B:261:ILE:O	1:B:265:VAL:HG23	2.06	0.55
1:I:327:TYR:HE1	1:J:318:MET:HE3	1.68	0.55
1:C:225:ILE:HD12	1:C:228:LEU:HB3	1.89	0.55
1:J:77:GLY:HA3	1:J:87:LEU:HD11	1.87	0.55
1:G:109:VAL:O	1:G:110:LEU:HD23	2.06	0.55
1:F:243:ILE:HG13	1:F:246:GLU:HB2	1.87	0.55
1:F:315:PHE:HD2	1:G:318:MET:HE2	1.71	0.55
1:E:63:ASN:HA	1:E:138:MET:HB3	1.89	0.55
1:F:69:ARG:HB3	1:F:71:ASP:OD1	2.07	0.55
1:A:324:LYS:HE3	1:A:325:TRP:H	1.72	0.55
1:H:333:VAL:HA	1:H:336:VAL:HG12	1.88	0.55
1:B:86:VAL:HG13	1:B:107:PHE:CD2	2.42	0.55
1:E:157:ASN:CG	1:E:162:ARG:HG3	2.28	0.55
1:F:167:ASP:HB2	1:F:242:LEU:HD23	1.88	0.55
1:G:39:PHE:HE2	1:G:41:GLU:HG2	1.72	0.54
1:F:310:ILE:HG23	1:F:311:TYR:CD1	2.42	0.54
1:A:307:ILE:HA	1:A:310:ILE:HG12	1.87	0.54
1:B:252:ARG:NH2	1:C:100:GLU:HG2	2.21	0.54
1:D:208:VAL:HG13	1:D:276:LEU:HD11	1.88	0.54
1:I:63:ASN:ND2	1:I:151:ARG:HH22	2.02	0.54
1:J:174:ILE:HG21	1:J:232:LEU:HD21	1.89	0.54
1:H:222:ARG:HA	1:H:225:ILE:HG22	1.89	0.54
1:I:110:LEU:HD13	1:I:177:LEU:HD22	1.89	0.54
1:C:62:ILE:HD12	1:C:137:LEU:HD21	1.89	0.54
1:H:284:SER:HB3	1:J:283:VAL:HG11	1.87	0.54
1:H:270:ASP:OD2	1:J:215:LYS:HE2	2.07	0.54
1:E:111:LYS:O	1:E:181:TYR:OH	2.19	0.54
1:F:301:PHE:O	1:F:302:MET:HB2	2.08	0.54
1:D:325:TRP:O	1:D:328:PRO:HD3	2.07	0.54
1:I:61:TRP:HB2	1:I:169:LEU:HD21	1.90	0.54
1:B:310:ILE:HA	1:B:313:MET:HG3	1.89	0.54
1:E:327:TYR:O	1:E:331:LEU:N	2.36	0.54
1:B:195:LEU:HD21	1:B:211:THR:HA	1.88	0.54
1:J:188:ILE:HG23	1:J:214:LEU:HD11	1.90	0.54
4:A:403:LMT:H3'	4:B:406:LMT:H2'	1.89	0.54
1:G:61:TRP:HZ2	1:G:138:MET:HE1	1.73	0.54
1:E:82:ILE:HD11	1:E:130:ILE:HG21	1.89	0.54
1:C:63:ASN:OD1	1:C:138:MET:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LYS:NZ	1:A:126:GLN:OE1	2.41	0.54
1:G:222:ARG:HA	1:G:225:ILE:HG22	1.90	0.54
1:A:317:TYR:N	1:A:317:TYR:CD1	2.76	0.54
1:H:192:ILE:HG12	1:H:214:LEU:HD21	1.90	0.54
1:I:328:PRO:HD2	1:I:329:VAL:H	1.72	0.54
1:C:228:LEU:O	1:C:231:VAL:HB	2.07	0.54
1:G:200:LEU:HD12	1:G:201:GLU:HG3	1.90	0.54
1:D:82:ILE:HG13	1:D:105:TYR:CZ	2.42	0.53
1:I:302:MET:HG3	1:J:302:MET:HE1	1.90	0.53
1:E:318:MET:HB3	1:E:320:GLU:N	2.23	0.53
1:F:250:TYR:O	1:F:253:ASP:HB3	2.07	0.53
1:D:294:LEU:HD13	1:E:295:THR:HA	1.90	0.53
1:J:230:GLU:O	1:J:234:SER:OG	2.22	0.53
1:B:166:ALA:O	1:B:169:LEU:HB3	2.09	0.53
1:A:326:GLY:O	1:A:329:VAL:N	2.40	0.53
1:D:110:LEU:HD13	1:D:177:LEU:HD22	1.90	0.53
1:G:82:ILE:HG12	1:G:130:ILE:HD13	1.89	0.53
1:C:330:VAL:O	1:C:334:MET:HG2	2.08	0.53
1:F:90:ILE:HD11	1:F:130:ILE:HD11	1.89	0.53
1:H:281:SER:HB3	1:J:279:TYR:CE2	2.43	0.53
1:F:300:ILE:HG13	1:F:301:PHE:N	2.23	0.53
1:D:327:TYR:CG	1:D:327:TYR:O	2.61	0.53
1:E:346:LYS:NZ	1:E:347:LYS:HG3	2.23	0.53
1:D:110:LEU:HD11	1:D:174:ILE:HG12	1.91	0.53
1:A:149:PRO:HB3	1:B:11:GLY:HA2	1.91	0.53
1:F:313:MET:SD	1:G:311:TYR:HB2	2.48	0.53
1:D:206:GLU:HG3	1:D:207:THR:N	2.24	0.53
1:D:212:HIS:NE2	1:E:196:GLU:OE1	2.39	0.53
1:A:195:LEU:HD21	1:A:211:THR:HA	1.91	0.53
1:D:239:VAL:HA	1:D:242:LEU:HD12	1.91	0.53
1:J:99:VAL:HG23	1:J:231:VAL:HG22	1.90	0.53
1:J:108:ILE:HD12	1:J:174:ILE:HD11	1.91	0.53
1:F:168:TYR:OH	1:G:14:PRO:HG2	2.09	0.53
1:H:99:VAL:HG23	1:H:231:VAL:HG22	1.91	0.53
1:A:297:ILE:HG22	1:D:302:MET:HE3	1.89	0.53
1:H:82:ILE:HG13	1:H:105:TYR:CE2	2.43	0.53
1:H:327:TYR:CZ	1:H:331:LEU:HD11	2.43	0.53
1:F:186:GLU:OE2	1:G:7:SER:HB3	2.09	0.53
1:B:19:TYR:CZ	1:B:21:GLY:HA3	2.44	0.53
1:C:110:LEU:HD21	1:C:228:LEU:HD13	1.91	0.52
1:G:225:ILE:HD12	1:G:228:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:100:GLU:OE2	7:J:515:HOH:O	2.19	0.52
1:F:293:VAL:HA	1:F:296:ILE:HG12	1.91	0.52
1:I:13:PRO:HG3	1:J:153:ARG:HD3	1.91	0.52
1:F:307:ILE:CD1	1:F:334:MET:HE2	2.35	0.52
1:I:29:ILE:HG21	1:I:50:VAL:HG11	1.91	0.52
1:D:145:ASP:OD2	1:D:151:ARG:NH2	2.33	0.52
1:F:195:LEU:HD21	1:F:211:THR:HA	1.89	0.52
1:I:328:PRO:HG2	1:I:329:VAL:H	1.74	0.52
1:I:63:ASN:HD22	1:I:151:ARG:NH2	2.03	0.52
1:D:125:GLU:HG3	1:D:141:GLU:HB2	1.90	0.52
1:I:148:ASP:O	1:I:152:GLU:HG2	2.08	0.52
1:E:165:ARG:NH2	1:E:243:ILE:HG21	2.24	0.52
1:F:307:ILE:HD11	1:F:334:MET:SD	2.49	0.52
1:J:147:PHE:CZ	1:J:177:LEU:HD12	2.42	0.52
1:B:311:TYR:CE2	1:B:330:VAL:HG21	2.43	0.52
1:B:312:GLY:H	1:B:313:MET:HB2	1.74	0.52
1:B:296:ILE:HA	1:B:299:THR:HG22	1.90	0.52
1:B:301:PHE:O	1:B:305:THR:N	2.39	0.52
1:J:316:GLU:HG2	1:J:317:TYR:H	1.74	0.52
1:F:307:ILE:CG1	1:F:334:MET:HE2	2.39	0.52
1:J:73:VAL:HG21	1:J:91:LEU:HD21	1.92	0.52
1:H:310:ILE:HD11	1:J:334:MET:HE1	1.92	0.52
1:I:99:VAL:CG2	1:I:231:VAL:HG13	2.40	0.52
1:B:221:LEU:HG	1:B:225:ILE:HD12	1.91	0.52
1:E:164:LYS:NZ	1:E:246:GLU:HB3	2.24	0.52
1:I:304:LEU:HD11	1:I:338:ALA:HB2	1.92	0.52
1:E:44:THR:HG1	1:E:46:ASP:H	1.58	0.52
1:G:83:HIS:ND1	1:G:84:PRO:HD2	2.25	0.52
1:I:326:GLY:CA	1:I:327:TYR:CB	2.87	0.52
1:I:240:PRO:HB2	1:I:241:PRO:HD3	1.91	0.52
1:E:89:ASP:OD2	7:E:516:HOH:O	2.19	0.52
1:C:218:LEU:HD21	1:C:268:PHE:HB3	1.90	0.52
1:B:27:PHE:HZ	1:B:72:VAL:HG21	1.74	0.51
1:F:105:TYR:HB3	1:F:132:THR:HB	1.91	0.51
1:A:82:ILE:HG12	1:A:130:ILE:HD13	1.93	0.51
1:A:23:TYR:CE2	1:A:142:LYS:HD3	2.45	0.51
1:F:301:PHE:HE2	1:I:303:PRO:CG	2.14	0.51
5:G:408:PEG:H32	5:G:408:PEG:O1	2.10	0.51
1:A:195:LEU:HD11	1:A:210:ARG:HB3	1.92	0.51
1:A:240:PRO:HB2	1:A:241:PRO:HD3	1.92	0.51
1:I:328:PRO:CG	1:I:329:VAL:N	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:ILE:HG12	1:E:299:THR:OG1	2.10	0.51
1:G:319:PRO:HG2	1:G:322:ARG:O	2.10	0.51
1:G:307:ILE:HD11	1:G:334:MET:SD	2.50	0.51
1:I:120:HIS:ND1	1:I:191:GLU:OE2	2.38	0.51
1:G:12:LEU:HD13	1:G:16:THR:HG21	1.92	0.51
1:I:165:ARG:CZ	1:I:243:ILE:HD12	2.41	0.51
1:F:157:ASN:CG	1:F:162:ARG:HG3	2.31	0.51
1:A:65:THR:OG1	7:A:516:HOH:O	2.19	0.51
1:D:198:GLU:O	1:D:202:ARG:N	2.43	0.51
1:A:209:GLN:HG2	1:D:200:LEU:HD13	1.91	0.51
1:D:323:TRP:O	1:D:325:TRP:N	2.44	0.51
1:H:295:THR:O	1:H:299:THR:HG23	2.11	0.51
5:B:408:PEG:H41	7:B:526:HOH:O	2.11	0.51
1:H:336:VAL:O	1:H:340:ILE:HG23	2.11	0.51
1:G:215:LYS:O	1:G:219:VAL:HG23	2.10	0.51
1:B:303:PRO:HG3	1:C:301:PHE:CE2	2.45	0.51
1:H:239:VAL:HG11	1:H:248:VAL:HG22	1.91	0.51
1:F:153:ARG:HD3	1:G:13:PRO:HG3	1.93	0.51
1:J:295:THR:O	1:J:299:THR:HG23	2.11	0.51
1:H:171:TYR:HE1	1:H:254:VAL:HG23	1.76	0.51
1:A:334:MET:HE1	1:D:310:ILE:HD11	1.93	0.51
1:D:109:VAL:O	1:D:110:LEU:HD23	2.11	0.51
1:H:244:GLU:HA	1:H:248:VAL:HG23	1.93	0.51
1:H:41:GLU:OE1	1:H:155:ARG:NH2	2.44	0.51
1:A:320:GLU:OE2	4:A:403:LMT:H1B	2.09	0.51
1:G:61:TRP:CZ2	1:G:138:MET:HE1	2.46	0.51
1:E:83:HIS:CE1	1:E:84:PRO:HD2	2.45	0.51
1:G:330:VAL:O	1:G:334:MET:HG2	2.10	0.51
1:G:113:PHE:HD2	1:G:181:TYR:HE1	1.59	0.51
1:I:326:GLY:CA	1:I:328:PRO:CD	2.85	0.50
1:C:110:LEU:HD13	1:C:177:LEU:HD22	1.93	0.50
1:C:233:SER:OG	1:C:237:ARG:NH2	2.43	0.50
1:G:34:TYR:O	1:G:59:PRO:HD2	2.11	0.50
1:G:316:GLU:HG3	1:H:324:LYS:HB3	1.93	0.50
1:F:307:ILE:CD1	1:F:334:MET:CG	2.83	0.50
1:D:327:TYR:HE1	1:E:318:MET:HG3	1.76	0.50
1:G:146:VAL:HG21	1:G:177:LEU:HA	1.93	0.50
1:C:86:VAL:HG13	1:C:107:PHE:CE2	2.46	0.50
1:I:195:LEU:HD21	1:I:211:THR:HA	1.94	0.50
1:I:125:GLU:HG3	1:I:141:GLU:HB2	1.94	0.50
1:A:317:TYR:HD1	1:A:317:TYR:N	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ILE:HG12	1:B:64:ILE:HG12	1.93	0.50
1:B:232:LEU:CD1	1:B:254:VAL:HG12	2.39	0.50
1:E:44:THR:OG1	1:E:45:THR:N	2.45	0.50
1:A:14:PRO:HG3	1:D:171:TYR:OH	2.11	0.50
1:H:277:ASP:HB3	1:J:276:LEU:HD23	1.93	0.50
1:F:208:VAL:HG12	1:I:278:VAL:HG13	1.93	0.50
1:D:167:ASP:OD2	1:D:243:ILE:N	2.31	0.50
1:E:73:VAL:HG21	1:E:91:LEU:HD21	1.93	0.50
1:B:129:LEU:HD23	1:B:138:MET:HG3	1.94	0.50
1:E:93:VAL:HA	1:E:126:GLN:NE2	2.25	0.50
1:J:233:SER:OG	1:J:237:ARG:NH2	2.44	0.50
1:D:239:VAL:HG11	1:D:248:VAL:HG22	1.94	0.50
1:E:115:TYR:OH	1:E:120:HIS:HB3	2.12	0.50
1:A:227:PRO:O	1:A:230:GLU:N	2.44	0.50
1:D:96:ARG:NH1	1:D:227:PRO:HB3	2.27	0.50
1:F:222:ARG:HH11	1:F:222:ARG:CG	2.24	0.50
1:C:228:LEU:HA	1:C:231:VAL:HB	1.93	0.50
1:E:29:ILE:HG21	1:E:50:VAL:HG11	1.94	0.50
1:B:244:GLU:HA	1:B:248:VAL:HG23	1.94	0.50
1:G:270:ASP:O	1:G:273:SER:OG	2.22	0.50
1:E:51:LEU:N	1:E:52:PRO:HD2	2.26	0.50
1:F:99:VAL:HG22	1:F:108:ILE:HG12	1.94	0.50
1:A:110:LEU:HD11	1:A:174:ILE:HG12	1.92	0.50
1:I:153:ARG:HG2	1:I:158:ARG:HB2	1.94	0.50
1:B:302:MET:HE1	1:C:302:MET:HG3	1.94	0.50
1:I:46:ASP:O	1:I:49:SER:OG	2.26	0.50
1:E:296:ILE:HG22	1:E:345:PHE:CE2	2.47	0.50
1:B:255:TYR:CE2	1:B:259:ILE:HD11	2.46	0.50
1:J:187:LYS:O	1:J:190:ASP:HB2	2.12	0.50
1:A:136:VAL:HG11	1:A:173:LEU:HD12	1.94	0.50
1:A:73:VAL:HG21	1:A:91:LEU:HD21	1.93	0.50
1:I:307:ILE:HG13	1:I:334:MET:HE2	1.94	0.50
1:G:229:ARG:HA	1:G:258:THR:HG21	1.94	0.50
1:F:315:PHE:HE1	1:G:327:TYR:HD2	1.59	0.50
1:H:188:ILE:O	1:H:192:ILE:HG13	2.11	0.50
1:E:255:TYR:O	1:E:258:THR:HG22	2.12	0.49
1:B:255:TYR:CZ	1:B:259:ILE:HD11	2.47	0.49
1:G:326:GLY:HA2	1:G:329:VAL:HG22	1.93	0.49
1:I:73:VAL:HG21	1:I:91:LEU:HD21	1.94	0.49
1:D:253:ASP:O	1:D:256:ASP:N	2.44	0.49
1:G:99:VAL:HG23	1:G:231:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:306:PHE:HE1	1:G:304:LEU:HB3	1.71	0.49
1:G:74:GLN:NE2	5:G:409:PEG:H31	2.24	0.49
1:E:336:VAL:O	1:E:340:ILE:HG23	2.12	0.49
1:C:167:ASP:OD2	1:C:243:ILE:N	2.43	0.49
1:B:34:TYR:O	1:B:58:THR:HB	2.12	0.49
1:D:167:ASP:OD1	1:D:168:TYR:N	2.44	0.49
1:I:228:LEU:O	1:I:231:VAL:HB	2.12	0.49
1:B:83:HIS:ND1	1:B:84:PRO:HD2	2.28	0.49
1:G:167:ASP:OD2	1:G:243:ILE:HG12	2.12	0.49
1:I:328:PRO:CD	1:I:329:VAL:N	2.72	0.49
1:F:211:THR:HG21	1:F:276:LEU:HD13	1.94	0.49
1:G:239:VAL:HB	1:G:242:LEU:HB2	1.93	0.49
1:I:34:TYR:CE1	1:I:59:PRO:HB2	2.47	0.49
1:B:323:TRP:NE1	4:B:407:LMT:O6'	2.44	0.49
1:G:315:PHE:CD2	1:H:327:TYR:HA	2.47	0.49
1:C:88:GLU:HB3	7:C:504:HOH:O	2.11	0.49
1:C:272:VAL:HA	1:C:275:LEU:HD22	1.93	0.49
1:G:246:GLU:OE1	5:G:411:PEG:C1	2.60	0.49
1:I:328:PRO:O	1:I:331:LEU:N	2.45	0.49
1:A:303:PRO:HG3	1:B:301:PHE:CE2	2.45	0.49
1:I:60:THR:HB	1:I:135:CYS:SG	2.52	0.49
1:E:192:ILE:HG12	1:E:214:LEU:HD21	1.92	0.49
1:J:333:VAL:O	1:J:336:VAL:HG12	2.12	0.49
1:J:195:LEU:O	1:J:199:VAL:HG23	2.12	0.49
7:B:506:HOH:O	1:C:89:ASP:OD2	2.20	0.49
1:C:165:ARG:NH2	1:C:243:ILE:HG21	2.28	0.49
1:J:230:GLU:HA	1:J:233:SER:HB3	1.95	0.49
1:F:257:HIS:O	1:F:260:GLN:N	2.45	0.49
1:B:315:PHE:HD2	1:C:327:TYR:HD1	1.59	0.49
1:G:35:SER:HB3	1:G:58:THR:HG21	1.95	0.49
1:A:222:ARG:HG3	1:A:226:TRP:CD1	2.47	0.49
1:E:83:HIS:ND1	1:E:84:PRO:HD2	2.28	0.49
1:H:239:VAL:HG21	1:H:244:GLU:HG3	1.93	0.49
1:H:51:LEU:N	1:H:52:PRO:HD2	2.28	0.49
1:J:47:VAL:O	1:J:50:VAL:HG22	2.12	0.49
1:H:120:HIS:HB2	1:H:213:GLN:NE2	2.28	0.49
1:J:303:PRO:HG2	1:J:304:LEU:HD23	1.95	0.49
1:J:192:ILE:HG12	1:J:214:LEU:HD21	1.95	0.49
1:G:239:VAL:HG12	1:G:242:LEU:HD12	1.94	0.49
1:C:116:ASP:O	1:C:120:HIS:HA	2.13	0.49
1:J:167:ASP:OD1	1:J:168:TYR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:295:THR:O	1:I:299:THR:HG22	2.13	0.49
1:B:300:ILE:O	1:B:304:LEU:HG	2.13	0.49
1:A:320:GLU:OE2	4:A:403:LMT:C1B	2.60	0.48
1:E:83:HIS:CG	1:E:84:PRO:HD2	2.47	0.48
1:B:138:MET:HE1	1:B:147:PHE:CD2	2.47	0.48
1:A:204:GLU:HG2	1:A:205:LYS:H	1.77	0.48
1:F:138:MET:HE1	1:F:147:PHE:CD2	2.48	0.48
1:F:307:ILE:HD12	1:F:334:MET:HE3	1.91	0.48
1:C:101:PHE:H	5:C:406:PEG:C4	2.26	0.48
1:G:93:VAL:O	1:G:111:LYS:NZ	2.46	0.48
1:H:302:MET:HE2	1:J:301:PHE:HB2	1.95	0.48
1:I:85:LEU:HD11	1:J:250:TYR:CD1	2.47	0.48
1:E:328:PRO:O	1:E:332:ALA:N	2.45	0.48
1:G:113:PHE:HE2	1:G:224:THR:HG21	1.78	0.48
1:A:190:ASP:O	1:A:194:VAL:HG23	2.14	0.48
1:C:260:GLN:O	1:C:264:THR:OG1	2.16	0.48
1:B:31:VAL:HG11	1:B:53:PHE:CE2	2.48	0.48
1:D:51:LEU:N	1:D:52:PRO:HD2	2.28	0.48
1:G:171:TYR:HE1	1:G:254:VAL:HG23	1.78	0.48
1:D:299:THR:HG21	1:D:345:PHE:CZ	2.47	0.48
1:H:236:TYR:CD1	1:H:252:ARG:HB2	2.49	0.48
1:D:160:ILE:HG22	1:D:164:LYS:HG2	1.96	0.48
4:A:403:LMT:C3'	4:B:406:LMT:C3'	2.92	0.48
1:F:301:PHE:O	1:F:303:PRO:HD2	2.13	0.48
1:F:303:PRO:HG2	1:F:304:LEU:H	1.79	0.48
1:J:95:GLN:HE22	1:J:98:LYS:NZ	2.12	0.48
1:C:277:ASP:HB3	1:E:276:LEU:HD23	1.94	0.48
1:C:24:ARG:HA	1:C:68:HIS:CD2	2.49	0.48
1:D:288:ASN:HD21	1:D:292:LYS:HE3	1.79	0.48
1:J:330:VAL:O	1:J:334:MET:HG3	2.14	0.48
1:A:186:GLU:OE2	1:B:7:SER:HB3	2.12	0.48
1:F:27:PHE:CD2	1:F:45:THR:HG22	2.48	0.48
1:I:36:ILE:HD13	1:I:163:LYS:HD2	1.95	0.48
1:J:324:LYS:O	1:J:326:GLY:N	2.47	0.48
1:B:192:ILE:HG12	1:B:214:LEU:HD21	1.95	0.48
4:A:403:LMT:C3B	4:B:406:LMT:H6D	2.28	0.48
1:B:324:LYS:C	1:B:326:GLY:H	2.17	0.48
1:D:51:LEU:HD13	1:D:79:PHE:CD2	2.49	0.48
1:E:323:TRP:O	1:E:325:TRP:N	2.47	0.48
1:A:291:MET:SD	1:D:291:MET:HE1	2.54	0.48
1:A:129:LEU:HD13	1:A:170:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:319:PRO:HA	1:H:320:GLU:C	2.31	0.47
1:D:128:SER:HB2	1:D:139:PHE:HB2	1.95	0.47
1:I:23:TYR:CD2	1:I:142:LYS:HD3	2.49	0.47
1:D:299:THR:HG21	1:D:345:PHE:CE2	2.49	0.47
1:F:336:VAL:O	1:F:340:ILE:HG23	2.15	0.47
1:D:317:TYR:CG	1:D:318:MET:N	2.83	0.47
1:C:12:LEU:HD22	1:C:16:THR:HG21	1.96	0.47
1:I:320:GLU:C	1:I:322:ARG:N	2.68	0.47
1:G:227:PRO:HA	7:G:521:HOH:O	2.13	0.47
1:H:51:LEU:HD22	1:H:79:PHE:CD2	2.50	0.47
1:J:292:LYS:HE2	1:J:348:LYS:O	2.14	0.47
1:B:51:LEU:HB3	1:B:79:PHE:CE2	2.49	0.47
1:G:302:MET:HE1	1:H:302:MET:HG3	1.96	0.47
1:E:218:LEU:HD21	1:E:268:PHE:HB3	1.96	0.47
1:A:5:ARG:O	1:A:5:ARG:NE	2.46	0.47
1:C:31:VAL:HG11	1:C:53:PHE:CE2	2.50	0.47
1:I:314:ASN:O	1:I:316:GLU:N	2.45	0.47
1:G:147:PHE:O	1:G:150:VAL:HB	2.15	0.47
1:D:327:TYR:HB2	1:D:330:VAL:HB	1.97	0.47
1:A:112:MET:HG3	1:A:177:LEU:HD11	1.97	0.47
1:I:68:HIS:CE1	1:I:69:ARG:HG2	2.50	0.47
1:I:80:PHE:CD2	1:I:137:LEU:HD11	2.50	0.47
1:I:239:VAL:HG11	1:I:248:VAL:HG22	1.97	0.47
1:H:271:ILE:HD13	1:J:216:ARG:NH1	2.30	0.47
1:G:258:THR:HA	1:G:261:ILE:HD12	1.97	0.47
1:C:167:ASP:HB2	1:C:242:LEU:HD23	1.97	0.47
1:F:160:ILE:HG13	1:F:164:LYS:HG3	1.97	0.47
1:C:319:PRO:CB	1:C:322:ARG:HB3	2.44	0.47
1:E:77:GLY:HA3	1:E:87:LEU:HD21	1.96	0.47
1:F:311:TYR:CE2	1:F:330:VAL:HG21	2.40	0.47
1:B:323:TRP:CE2	4:B:407:LMT:H6E	2.50	0.47
1:I:330:VAL:HG12	1:I:331:LEU:N	2.29	0.47
1:I:170:LEU:O	1:I:174:ILE:HG13	2.14	0.47
1:J:95:GLN:HE22	1:J:98:LYS:HZ3	1.63	0.47
1:H:316:GLU:O	1:H:319:PRO:HD2	2.13	0.47
1:B:95:GLN:HG2	1:B:96:ARG:N	2.29	0.47
1:B:240:PRO:HB2	1:B:241:PRO:HD3	1.97	0.47
1:C:196:GLU:OE1	1:E:212:HIS:NE2	2.46	0.47
1:H:154:ILE:HG12	1:H:161:ILE:HD13	1.97	0.47
1:C:236:TYR:CE1	1:C:252:ARG:HB2	2.50	0.47
1:C:17:LEU:HG	1:C:91:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:PHE:H	5:C:406:PEG:H42	1.78	0.47
1:E:229:ARG:HA	1:E:258:THR:CG2	2.44	0.47
1:H:302:MET:HE1	1:J:298:ALA:HA	1.96	0.47
1:A:210:ARG:NH2	7:A:513:HOH:O	2.46	0.47
1:G:285:ASN:O	1:G:288:ASN:HB3	2.15	0.47
1:C:51:LEU:HD22	1:C:79:PHE:CG	2.50	0.47
1:F:13:PRO:HG3	1:I:153:ARG:CD	2.41	0.47
1:B:272:VAL:HA	1:B:275:LEU:HD22	1.97	0.47
1:J:39:PHE:HE2	1:J:41:GLU:HG2	1.80	0.47
1:D:19:TYR:CZ	1:D:21:GLY:HA3	2.50	0.47
1:B:323:TRP:HE1	4:B:407:LMT:H6'	1.62	0.47
1:E:232:LEU:HD22	1:E:254:VAL:CG1	2.44	0.47
1:C:288:ASN:ND2	1:C:292:LYS:HE3	2.30	0.47
1:G:182:PHE:O	1:G:186:GLU:HG3	2.15	0.47
1:C:62:ILE:HB	1:C:137:LEU:HD23	1.96	0.46
1:H:310:ILE:HA	1:H:313:MET:SD	2.55	0.46
1:A:111:LYS:O	1:A:177:LEU:HD21	2.15	0.46
1:I:99:VAL:HG13	1:I:108:ILE:HG12	1.97	0.46
1:G:230:GLU:HB2	7:G:521:HOH:O	2.14	0.46
1:H:12:LEU:HD13	1:H:16:THR:HG21	1.97	0.46
1:E:140:GLN:HB3	1:E:140:GLN:HE21	1.55	0.46
1:J:154:ILE:HG12	1:J:161:ILE:HD13	1.97	0.46
1:C:316:GLU:HG2	1:E:321:LEU:O	2.14	0.46
1:B:225:ILE:HD13	1:B:265:VAL:HG21	1.97	0.46
1:E:345:PHE:O	1:E:349:LYS:HA	2.15	0.46
1:E:30:GLU:HG3	1:E:43:LYS:HG2	1.96	0.46
1:A:34:TYR:O	1:A:59:PRO:HD2	2.15	0.46
1:H:110:LEU:HD22	1:H:228:LEU:HD13	1.98	0.46
1:G:62:ILE:HB	1:G:137:LEU:HD23	1.97	0.46
1:F:307:ILE:HD11	1:F:334:MET:HE3	1.72	0.46
1:J:227:PRO:O	1:J:231:VAL:N	2.41	0.46
1:F:188:ILE:HG21	1:F:218:LEU:HD11	1.96	0.46
1:E:235:LEU:HD12	1:E:242:LEU:HD11	1.97	0.46
1:A:120:HIS:ND1	1:A:191:GLU:OE2	2.47	0.46
1:B:286:LYS:O	1:B:290:VAL:N	2.48	0.46
1:I:328:PRO:HG2	1:I:329:VAL:N	2.30	0.46
1:G:32:MET:HG2	1:G:41:GLU:HB2	1.96	0.46
1:A:297:ILE:HG21	1:D:299:THR:HA	1.96	0.46
1:D:303:PRO:O	1:D:306:PHE:HB3	2.16	0.46
1:F:215:LYS:O	1:F:219:VAL:HG23	2.16	0.46
1:I:307:ILE:HA	1:I:310:ILE:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:TRP:HD1	1:A:324:LYS:O	1.98	0.46
1:D:209:GLN:HE21	1:E:200:LEU:HD13	1.79	0.46
1:D:116:ASP:O	1:D:120:HIS:HA	2.15	0.46
1:J:86:VAL:HG13	1:J:107:PHE:CE2	2.51	0.46
1:E:110:LEU:HD13	1:E:177:LEU:HD22	1.98	0.46
1:F:82:ILE:HD11	1:F:130:ILE:HG21	1.97	0.46
1:C:225:ILE:HG12	1:C:261:ILE:HG22	1.97	0.46
1:D:304:LEU:HB3	1:E:306:PHE:CE1	2.51	0.46
1:G:65:THR:HG21	1:G:143:ILE:HA	1.98	0.46
1:D:320:GLU:H	1:D:322:ARG:N	2.13	0.46
1:I:115:TYR:OH	1:I:120:HIS:HB3	2.16	0.46
1:F:271:ILE:HD11	1:G:216:ARG:HG2	1.97	0.46
1:A:69:ARG:HB3	1:A:71:ASP:OD1	2.16	0.46
1:I:89:ASP:OD2	1:I:98:LYS:NZ	2.32	0.46
1:H:82:ILE:HG22	1:H:87:LEU:HG	1.98	0.46
1:B:199:VAL:HG11	1:B:278:VAL:HB	1.98	0.46
1:C:232:LEU:HD13	1:C:254:VAL:CG1	2.46	0.46
1:D:300:ILE:O	1:D:303:PRO:HD2	2.15	0.46
1:E:113:PHE:HE2	1:E:224:THR:HG21	1.81	0.46
1:F:67:ILE:HG21	1:F:139:PHE:HB3	1.98	0.46
1:I:314:ASN:HD21	1:J:314:ASN:ND2	2.14	0.46
1:F:276:LEU:HA	1:F:276:LEU:HD12	1.56	0.46
1:E:164:LYS:HZ1	1:E:246:GLU:HB3	1.81	0.46
1:I:65:THR:HG21	1:I:143:ILE:HA	1.98	0.46
1:A:145:ASP:HB2	1:A:147:PHE:HD2	1.81	0.46
1:E:131:LEU:HD22	1:E:170:LEU:HD22	1.98	0.46
1:J:185:LEU:HD11	1:J:261:ILE:HG23	1.98	0.46
1:B:324:LYS:CG	1:B:325:TRP:H	2.29	0.46
1:G:138:MET:SD	1:G:147:PHE:CE2	3.09	0.46
1:C:100:GLU:HB3	1:C:102:PHE:HE1	1.79	0.46
1:D:327:TYR:HB3	1:E:315:PHE:CD2	2.51	0.46
1:A:165:ARG:NH2	1:A:243:ILE:HG21	2.31	0.46
1:J:160:ILE:HG12	3:J:404:CL:CL	2.53	0.46
1:B:325:TRP:O	1:B:329:VAL:HB	2.15	0.45
5:G:408:PEG:H22	1:H:331:LEU:HD22	1.98	0.45
1:E:174:ILE:HG21	1:E:232:LEU:HD21	1.99	0.45
1:H:148:ASP:O	1:H:152:GLU:HG2	2.17	0.45
1:E:22:LYS:HE3	1:E:23:TYR:OH	2.17	0.45
1:G:110:LEU:HD12	1:G:177:LEU:HD13	1.97	0.45
1:E:93:VAL:O	1:E:111:LYS:NZ	2.48	0.45
1:G:23:TYR:CE2	1:G:142:LYS:HD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:PHE:CD2	1:D:45:THR:HG22	2.51	0.45
4:A:403:LMT:H3'	4:B:406:LMT:C2'	2.46	0.45
1:B:30:GLU:HG3	1:B:43:LYS:HG2	1.98	0.45
1:F:200:LEU:HD13	1:G:209:GLN:HE21	1.81	0.45
1:C:239:VAL:HA	1:C:242:LEU:HD12	1.98	0.45
1:C:231:VAL:HG12	1:C:232:LEU:HG	1.97	0.45
1:G:337:ILE:HA	1:G:340:ILE:HG12	1.99	0.45
1:A:280:LEU:HD23	1:B:280:LEU:HD21	1.97	0.45
1:F:240:PRO:HB2	1:F:241:PRO:CD	2.46	0.45
1:I:225:ILE:HG13	1:I:262:ALA:HB2	1.98	0.45
1:D:102:PHE:CD2	1:D:105:TYR:CE2	3.05	0.45
1:H:153:ARG:HH11	1:H:153:ARG:HG3	1.80	0.45
1:J:274:GLY:O	1:J:278:VAL:HG23	2.17	0.45
1:F:73:VAL:HG21	1:F:91:LEU:HD21	1.97	0.45
1:D:296:ILE:HA	1:D:299:THR:HG22	1.98	0.45
1:D:276:LEU:HA	1:D:276:LEU:HD12	1.74	0.45
1:H:99:VAL:CG2	1:H:231:VAL:HG13	2.47	0.45
1:E:22:LYS:NZ	1:E:123:GLU:OE2	2.38	0.45
1:C:120:HIS:H	1:C:120:HIS:CD2	2.34	0.45
1:C:36:ILE:HD13	1:C:163:LYS:HG3	1.98	0.45
1:J:221:LEU:HA	1:J:221:LEU:HD12	1.61	0.45
1:E:228:LEU:O	1:E:231:VAL:HB	2.17	0.45
1:I:23:TYR:CE2	1:I:142:LYS:HD3	2.51	0.45
1:E:232:LEU:HD22	1:E:254:VAL:HG12	1.98	0.45
1:B:299:THR:OG1	1:C:297:ILE:HG12	2.16	0.45
1:A:240:PRO:HB2	1:A:241:PRO:CD	2.47	0.45
1:E:131:LEU:HD12	1:E:136:VAL:HG22	1.99	0.45
1:G:9:LYS:HG3	1:G:9:LYS:O	2.16	0.45
1:B:87:LEU:HA	1:B:87:LEU:HD23	1.73	0.45
1:D:275:LEU:HA	1:D:275:LEU:HD12	1.70	0.45
1:J:195:LEU:HD21	1:J:211:THR:HA	1.99	0.45
1:B:51:LEU:HD13	1:B:79:PHE:CG	2.51	0.45
1:H:153:ARG:HD3	1:J:13:PRO:HG3	1.98	0.45
1:F:113:PHE:HB2	1:F:184:LEU:HD22	1.97	0.45
1:A:276:LEU:HA	1:A:276:LEU:HD12	1.85	0.45
1:D:296:ILE:HG13	1:D:297:ILE:HD12	1.98	0.45
1:C:235:LEU:HA	1:C:235:LEU:HD12	1.86	0.45
1:G:171:TYR:CZ	1:G:250:TYR:HB3	2.52	0.45
1:E:51:LEU:HB3	1:E:79:PHE:CE2	2.52	0.45
1:H:128:SER:HB2	1:H:139:PHE:HB2	1.99	0.45
1:B:16:THR:HG22	1:B:18:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LEU:HA	1:A:87:LEU:HD23	1.76	0.45
1:J:218:LEU:HD12	1:J:218:LEU:HA	1.74	0.45
1:H:185:LEU:HD23	1:H:185:LEU:HA	1.70	0.45
1:B:295:THR:O	1:B:299:THR:HG22	2.17	0.45
1:B:160:ILE:HG12	3:B:404:CL:CL	2.54	0.45
1:H:140:GLN:HE22	1:H:145:ASP:HB3	1.82	0.45
1:C:337:ILE:HA	1:C:340:ILE:HG12	1.99	0.45
1:F:216:ARG:HG2	1:I:271:ILE:HG12	1.97	0.45
1:I:327:TYR:CD2	1:I:327:TYR:O	2.70	0.44
1:B:43:LYS:NZ	5:B:410:PEG:H22	2.32	0.44
1:D:295:THR:O	1:D:299:THR:HG22	2.16	0.44
1:E:48:GLU:HA	1:E:51:LEU:HD12	1.99	0.44
1:H:23:TYR:CE2	1:H:142:LYS:HD3	2.51	0.44
1:D:225:ILE:HD13	1:D:265:VAL:HG21	1.97	0.44
1:D:23:TYR:CE2	1:D:142:LYS:HD3	2.52	0.44
1:J:339:VAL:O	1:J:342:VAL:HB	2.17	0.44
1:F:307:ILE:CD1	1:F:334:MET:HG3	2.47	0.44
1:I:307:ILE:HD11	1:I:334:MET:CE	2.47	0.44
1:C:34:TYR:CE2	1:C:154:ILE:HD13	2.53	0.44
1:B:312:GLY:H	1:B:313:MET:CB	2.30	0.44
1:F:99:VAL:HG23	1:F:231:VAL:HG22	1.99	0.44
1:H:240:PRO:HB2	1:H:241:PRO:HD3	1.99	0.44
1:D:241:PRO:HA	7:D:522:HOH:O	2.17	0.44
1:B:228:LEU:O	1:B:228:LEU:HD12	2.16	0.44
1:B:252:ARG:CZ	1:C:100:GLU:HG2	2.48	0.44
1:G:39:PHE:CZ	1:G:155:ARG:HG2	2.52	0.44
1:B:16:THR:O	1:B:88:GLU:HG3	2.16	0.44
1:I:337:ILE:HA	1:I:340:ILE:HG12	2.00	0.44
1:B:71:ASP:N	1:B:71:ASP:OD1	2.47	0.44
4:A:403:LMT:H1'	4:B:406:LMT:H32	1.99	0.44
4:A:403:LMT:C2'	4:B:406:LMT:O3'	2.65	0.44
1:E:218:LEU:HD12	1:E:218:LEU:HA	1.74	0.44
1:J:261:ILE:O	1:J:265:VAL:HG23	2.18	0.44
1:B:103:GLU:HG2	7:B:508:HOH:O	2.16	0.44
1:A:17:LEU:HD23	1:A:74:GLN:HB2	1.99	0.44
1:H:167:ASP:HB2	1:H:242:LEU:HD23	1.99	0.44
1:H:199:VAL:HG13	1:H:279:TYR:HB2	1.99	0.44
1:E:16:THR:O	1:E:88:GLU:HG3	2.17	0.44
1:G:236:TYR:CE1	1:G:252:ARG:HB2	2.53	0.44
1:A:22:LYS:HG3	1:A:23:TYR:CD1	2.53	0.44
1:D:288:ASN:ND2	1:D:292:LYS:HE3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:PHE:CE2	1:D:303:PRO:HG3	2.52	0.44
1:G:157:ASN:ND2	1:G:162:ARG:HG3	2.32	0.44
1:I:308:ALA:HA	1:J:313:MET:HE2	2.00	0.44
1:G:296:ILE:HB	1:G:345:PHE:CE2	2.53	0.44
1:G:55:ASP:HA	7:G:527:HOH:O	2.18	0.44
1:I:331:LEU:HA	1:I:331:LEU:HD23	1.74	0.44
1:I:222:ARG:HA	1:I:225:ILE:HG22	1.99	0.44
1:D:307:ILE:HG13	1:D:334:MET:HE3	2.00	0.44
1:G:307:ILE:HA	1:G:310:ILE:HG12	1.99	0.44
1:H:185:LEU:HD23	1:H:188:ILE:HD12	1.99	0.44
1:B:248:VAL:N	1:B:249:PRO:HD2	2.33	0.44
1:B:77:GLY:HA3	1:B:87:LEU:HD11	1.99	0.44
1:F:170:LEU:O	1:F:174:ILE:HG13	2.17	0.44
1:A:272:VAL:HA	1:A:275:LEU:HD22	2.00	0.44
1:A:32:MET:HE2	1:A:154:ILE:HG21	1.98	0.44
1:A:221:LEU:HA	1:A:221:LEU:HD12	1.70	0.44
1:D:298:ALA:O	1:D:302:MET:HB2	2.17	0.44
1:B:10:LYS:C	1:B:12:LEU:H	2.20	0.44
1:E:185:LEU:HD23	1:E:185:LEU:HA	1.72	0.44
1:D:322:ARG:O	1:D:323:TRP:HB2	2.16	0.44
1:C:292:LYS:O	1:C:296:ILE:HG23	2.18	0.44
1:I:99:VAL:HG23	1:I:231:VAL:HG22	1.99	0.44
1:J:272:VAL:HA	1:J:275:LEU:HD22	2.00	0.44
1:C:306:PHE:CE1	1:E:304:LEU:HD23	2.53	0.44
1:J:148:ASP:N	1:J:149:PRO:HD2	2.33	0.44
1:D:337:ILE:O	1:D:341:MET:HG2	2.17	0.44
1:E:240:PRO:HB2	1:E:241:PRO:HD3	1.99	0.44
1:D:33:ASN:ND2	1:D:60:THR:OG1	2.50	0.44
1:C:307:ILE:C	1:C:309:GLY:HA3	2.38	0.44
1:C:34:TYR:O	1:C:58:THR:HB	2.17	0.44
1:H:311:TYR:CD2	1:H:330:VAL:HG21	2.53	0.44
1:F:222:ARG:HD2	1:F:226:TRP:HE1	1.83	0.44
1:E:47:VAL:O	1:E:51:LEU:HG	2.18	0.44
1:J:345:PHE:O	1:J:348:LYS:HD3	2.18	0.44
1:C:240:PRO:HB2	1:C:241:PRO:HD3	2.00	0.44
1:D:301:PHE:CE2	1:E:303:PRO:HG3	2.53	0.44
1:J:169:LEU:O	1:J:173:LEU:HG	2.17	0.44
1:H:119:LEU:H	1:H:119:LEU:HG	1.56	0.44
1:B:323:TRP:CZ3	1:B:325:TRP:HB2	2.53	0.44
1:B:55:ASP:HB3	5:B:411:PEG:H31	2.00	0.44
1:H:214:LEU:HD23	1:H:272:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:PRO:HA	1:B:320:GLU:C	2.38	0.44
1:G:291:MET:HE1	1:H:291:MET:HG2	2.00	0.44
1:G:206:GLU:HG3	1:G:207:THR:N	2.33	0.44
1:A:225:ILE:O	1:A:228:LEU:HB3	2.17	0.44
1:C:125:GLU:HG3	1:C:141:GLU:HB2	2.00	0.43
1:B:302:MET:HE1	1:C:298:ALA:HA	2.00	0.43
1:H:82:ILE:HA	1:H:105:TYR:CE2	2.53	0.43
1:G:318:MET:SD	1:G:318:MET:N	2.92	0.43
1:E:339:VAL:O	1:E:343:VAL:N	2.41	0.43
1:J:301:PHE:HA	1:J:304:LEU:HB2	1.99	0.43
1:A:148:ASP:N	1:A:149:PRO:HD2	2.33	0.43
1:J:100:GLU:HB3	1:J:102:PHE:HE1	1.84	0.43
1:H:15:GLY:O	1:H:17:LEU:HD13	2.18	0.43
1:J:244:GLU:HA	1:J:248:VAL:HG23	1.99	0.43
1:G:105:TYR:HB3	1:G:132:THR:HB	2.00	0.43
1:I:56:SER:OG	1:I:58:THR:O	2.34	0.43
1:F:307:ILE:CG1	1:F:334:MET:CE	2.97	0.43
1:I:317:TYR:O	1:I:317:TYR:HD1	2.02	0.43
1:E:257:HIS:O	1:E:261:ILE:HG13	2.19	0.43
1:C:296:ILE:HG22	1:C:345:PHE:CE2	2.53	0.43
1:B:86:VAL:HG13	1:B:107:PHE:CG	2.53	0.43
1:G:222:ARG:HD3	1:G:269:ARG:CD	2.48	0.43
1:C:252:ARG:O	1:C:252:ARG:HG2	2.18	0.43
1:B:113:PHE:CE1	1:B:124:SER:HB3	2.53	0.43
1:F:56:SER:HG	1:F:58:THR:H	1.66	0.43
1:B:6:LEU:HD13	1:B:20:THR:O	2.18	0.43
1:B:245:LYS:HD3	1:B:245:LYS:HA	1.63	0.43
5:C:406:PEG:H32	5:C:406:PEG:H12	1.57	0.43
1:G:239:VAL:HG11	1:G:248:VAL:HG22	2.00	0.43
1:J:148:ASP:O	1:J:152:GLU:HG2	2.18	0.43
1:A:160:ILE:HG22	1:A:164:LYS:HG2	2.00	0.43
1:A:102:PHE:HD2	1:A:105:TYR:CZ	2.36	0.43
1:I:112:MET:HE2	1:I:112:MET:HB2	1.82	0.43
1:A:314:ASN:O	1:B:321:LEU:HD22	2.19	0.43
1:J:110:LEU:CD2	1:J:228:LEU:HD13	2.48	0.43
3:A:402:CL:CL	1:B:14:PRO:HD2	2.56	0.43
1:H:226:TRP:CE2	1:H:229:ARG:NH2	2.87	0.43
1:C:347:LYS:HE3	1:C:348:LYS:HB3	1.99	0.43
1:J:180:ASP:HB2	5:J:405:PEG:H41	2.00	0.43
1:I:108:ILE:HD12	1:I:174:ILE:HD11	2.01	0.43
1:J:225:ILE:O	1:J:228:LEU:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLN:HE22	1:A:98:LYS:CE	2.32	0.43
1:F:178:VAL:HG21	1:F:254:VAL:CG1	2.48	0.43
1:I:61:TRP:HE1	1:I:138:MET:HE2	1.83	0.43
1:G:260:GLN:OE1	1:H:95:GLN:HA	2.19	0.43
1:G:51:LEU:HB3	1:G:79:PHE:CE2	2.54	0.43
1:I:31:VAL:HG11	1:I:53:PHE:CE2	2.54	0.43
1:B:12:LEU:HA	1:B:13:PRO:HD3	1.91	0.43
1:G:208:VAL:HG13	1:G:276:LEU:HD11	2.00	0.43
1:H:337:ILE:HA	1:H:340:ILE:HG12	2.01	0.43
1:E:346:LYS:HZ2	1:E:347:LYS:HG3	1.82	0.43
1:F:184:LEU:HD21	1:F:221:LEU:HD11	2.00	0.43
1:I:200:LEU:HD12	1:I:201:GLU:HG3	2.01	0.43
1:B:23:TYR:CZ	1:B:142:LYS:HD3	2.54	0.43
1:D:249:PRO:O	1:D:252:ARG:HB3	2.18	0.43
1:I:293:VAL:HA	1:I:296:ILE:HG12	2.00	0.43
1:I:218:LEU:HD12	1:I:218:LEU:HA	1.75	0.43
1:B:297:ILE:HA	1:B:297:ILE:HD12	1.85	0.43
1:I:276:LEU:HA	1:I:276:LEU:HD12	1.59	0.43
1:A:99:VAL:HG13	1:A:108:ILE:HG12	2.01	0.43
1:F:82:ILE:HG12	1:F:130:ILE:HD13	2.00	0.43
1:J:185:LEU:HD13	1:J:264:THR:CG2	2.48	0.43
1:A:233:SER:HB2	1:A:255:TYR:CE1	2.54	0.43
1:J:111:LYS:O	1:J:177:LEU:HD21	2.19	0.43
1:A:316:GLU:HA	1:A:317:TYR:HA	1.71	0.43
1:G:83:HIS:HD2	1:G:85:LEU:HB2	1.84	0.43
1:D:337:ILE:HA	1:D:340:ILE:HG12	2.01	0.43
1:F:233:SER:HB2	1:F:255:TYR:CE1	2.54	0.43
1:C:39:PHE:CZ	1:C:155:ARG:HA	2.54	0.43
1:H:19:TYR:CE1	1:H:21:GLY:HA3	2.53	0.43
1:I:9:LYS:HB2	1:I:12:LEU:HD12	2.00	0.43
4:A:403:LMT:H12	4:B:406:LMT:H52	1.98	0.42
1:A:324:LYS:CE	1:A:325:TRP:H	2.30	0.42
1:D:202:ARG:HA	1:D:203:PRO:HD3	1.82	0.42
1:B:299:THR:HA	1:C:297:ILE:HG21	2.01	0.42
1:E:51:LEU:O	1:E:79:PHE:HE2	2.02	0.42
1:J:41:GLU:OE2	1:J:155:ARG:NE	2.47	0.42
1:H:89:ASP:OD1	7:H:502:HOH:O	2.21	0.42
1:E:202:ARG:HA	1:E:203:PRO:HD3	1.82	0.42
1:J:325:TRP:C	1:J:328:PRO:HD2	2.39	0.42
1:F:291:MET:HE2	1:G:290:VAL:HG12	1.99	0.42
1:I:100:GLU:HB3	1:I:102:PHE:CE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:307:ILE:HG13	1:F:334:MET:HE2	2.01	0.42
1:F:303:PRO:HG2	1:F:304:LEU:N	2.34	0.42
1:H:105:TYR:CB	1:H:132:THR:HB	2.46	0.42
1:G:221:LEU:HD23	1:G:265:VAL:CG2	2.49	0.42
1:D:143:ILE:HD12	1:D:144:GLY:H	1.84	0.42
1:E:243:ILE:HG13	1:E:246:GLU:HB2	2.00	0.42
1:B:233:SER:HB2	1:B:255:TYR:CE1	2.54	0.42
1:C:41:GLU:OE2	1:C:155:ARG:NE	2.52	0.42
1:G:148:ASP:N	1:G:149:PRO:HD2	2.34	0.42
1:A:35:SER:HB3	1:A:58:THR:HG21	2.02	0.42
1:A:163:LYS:HD2	1:A:163:LYS:N	2.34	0.42
1:F:9:LYS:HE3	1:F:9:LYS:HB2	1.83	0.42
1:C:304:LEU:HD11	1:C:338:ALA:HB2	2.01	0.42
1:B:129:LEU:HD21	1:B:138:MET:HG3	2.01	0.42
1:D:115:TYR:HE2	1:D:191:GLU:HG3	1.83	0.42
1:I:94:HIS:O	1:J:260:GLN:NE2	2.53	0.42
1:B:218:LEU:HD21	1:B:268:PHE:HB3	2.01	0.42
1:G:91:LEU:HA	1:G:91:LEU:HD23	1.71	0.42
1:H:115:TYR:OH	1:H:120:HIS:HB3	2.19	0.42
1:H:298:ALA:O	1:H:302:MET:HB2	2.19	0.42
1:C:339:VAL:O	1:C:343:VAL:HG23	2.19	0.42
1:H:198:GLU:O	1:H:202:ARG:N	2.52	0.42
1:J:347:LYS:HD3	1:J:349:LYS:HG3	2.01	0.42
1:H:103:GLU:H	1:H:103:GLU:HG2	1.59	0.42
1:I:328:PRO:O	1:I:332:ALA:N	2.53	0.42
1:C:12:LEU:HA	1:C:13:PRO:HD3	1.89	0.42
1:E:340:ILE:HA	1:E:343:VAL:HB	2.01	0.42
1:C:221:LEU:O	1:C:225:ILE:HG22	2.20	0.42
1:F:153:ARG:CD	1:G:13:PRO:HG3	2.49	0.42
1:H:232:LEU:HD13	1:H:254:VAL:HG12	2.02	0.42
1:I:80:PHE:CE2	1:I:137:LEU:HD21	2.55	0.42
1:E:198:GLU:O	1:E:202:ARG:N	2.52	0.42
1:G:199:VAL:HG12	1:G:278:VAL:HG12	2.02	0.42
1:F:51:LEU:N	1:F:52:PRO:HD2	2.34	0.42
1:F:111:LYS:HB2	1:F:224:THR:HG21	2.02	0.42
4:B:407:LMT:H31	4:B:407:LMT:H61	1.68	0.42
1:A:315:PHE:HD2	1:B:321:LEU:HA	1.85	0.42
1:I:34:TYR:O	1:I:59:PRO:HD2	2.19	0.42
1:C:41:GLU:CD	1:C:155:ARG:HE	2.23	0.42
1:D:83:HIS:HA	1:D:84:PRO:HD3	1.96	0.42
1:C:61:TRP:CZ3	1:C:151:ARG:HG2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:THR:O	1:A:299:THR:N	2.42	0.42
1:F:235:LEU:HD12	1:F:235:LEU:HA	1.96	0.42
1:B:269:ARG:NH2	1:B:269:ARG:HB3	2.35	0.42
1:F:86:VAL:O	1:F:90:ILE:HG13	2.20	0.42
1:J:300:ILE:HG13	1:J:301:PHE:CD1	2.55	0.42
1:E:212:HIS:O	1:E:216:ARG:HG3	2.18	0.42
1:E:67:ILE:HG23	1:E:140:GLN:O	2.19	0.42
1:J:240:PRO:HB2	1:J:241:PRO:HD3	2.00	0.42
1:J:17:LEU:HD23	1:J:74:GLN:HB2	2.01	0.42
1:G:78:GLU:OE1	7:G:525:HOH:O	2.21	0.42
1:C:276:LEU:HA	1:C:276:LEU:HD12	1.88	0.42
1:J:232:LEU:HD13	1:J:254:VAL:O	2.20	0.42
1:G:153:ARG:HA	1:G:158:ARG:HB2	2.00	0.42
1:C:225:ILE:O	1:C:228:LEU:HB3	2.19	0.42
1:D:272:VAL:O	1:D:275:LEU:HB2	2.20	0.42
1:E:306:PHE:O	1:E:310:ILE:HG12	2.19	0.42
1:I:296:ILE:HG13	1:I:297:ILE:HD12	2.01	0.42
1:A:167:ASP:OD1	1:A:167:ASP:N	2.52	0.42
1:C:181:TYR:CD1	1:C:181:TYR:N	2.88	0.42
1:H:300:ILE:HG13	1:H:301:PHE:CD1	2.54	0.42
1:J:185:LEU:HD13	1:J:264:THR:HG21	2.01	0.42
1:J:125:GLU:OE1	1:J:141:GLU:N	2.52	0.42
1:F:312:GLY:CA	1:I:314:ASN:HD22	2.33	0.42
1:G:145:ASP:HB2	1:G:147:PHE:CD2	2.55	0.42
1:B:55:ASP:OD1	7:B:519:HOH:O	2.21	0.42
1:G:276:LEU:HA	1:G:276:LEU:HD12	1.72	0.42
1:I:319:PRO:C	1:I:320:GLU:HG3	2.41	0.42
1:I:166:ALA:O	1:I:169:LEU:HB3	2.20	0.42
1:C:275:LEU:HD12	1:C:275:LEU:HA	1.75	0.42
1:I:213:GLN:HA	1:I:213:GLN:NE2	2.35	0.42
1:I:316:GLU:HA	1:I:317:TYR:HB3	2.02	0.41
1:G:252:ARG:O	1:G:255:TYR:HB3	2.20	0.41
1:G:310:ILE:O	1:G:313:MET:HB3	2.20	0.41
1:G:12:LEU:HD13	1:G:16:THR:CG2	2.50	0.41
1:J:195:LEU:HD23	1:J:275:LEU:HD23	2.02	0.41
1:G:27:PHE:CZ	1:G:72:VAL:HG21	2.56	0.41
1:A:30:GLU:HG2	1:A:43:LYS:HG2	2.02	0.41
1:B:165:ARG:N	1:B:165:ARG:HD2	2.35	0.41
1:F:61:TRP:HB2	1:F:169:LEU:CD2	2.47	0.41
1:G:211:THR:HG21	1:G:276:LEU:HD13	2.02	0.41
1:H:311:TYR:HD2	1:H:330:VAL:HG21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:47:VAL:CG2	1:J:72:VAL:HG13	2.50	0.41
1:A:204:GLU:HG2	1:A:205:LYS:N	2.35	0.41
1:D:300:ILE:O	1:D:304:LEU:HG	2.21	0.41
1:H:229:ARG:HA	1:H:258:THR:CG2	2.50	0.41
1:F:236:TYR:CE1	1:F:252:ARG:HB2	2.55	0.41
4:A:403:LMT:C4B	4:B:406:LMT:H6D	2.50	0.41
1:I:307:ILE:CG1	1:I:334:MET:HE2	2.50	0.41
1:D:165:ARG:CZ	1:D:243:ILE:HG21	2.50	0.41
1:C:86:VAL:HG13	1:C:107:PHE:CZ	2.55	0.41
1:C:337:ILE:O	1:C:341:MET:HG2	2.20	0.41
1:C:19:TYR:OH	1:C:141:GLU:OE1	2.32	0.41
1:J:327:TYR:HB3	1:J:328:PRO:HD3	2.02	0.41
1:F:24:ARG:HA	1:F:68:HIS:CD2	2.55	0.41
1:A:296:ILE:HG22	1:A:345:PHE:CZ	2.55	0.41
1:G:115:TYR:OH	1:G:120:HIS:HB3	2.20	0.41
4:B:407:LMT:O2'	4:B:407:LMT:H61	2.20	0.41
1:D:302:MET:HG3	1:E:302:MET:HE1	2.02	0.41
1:C:130:ILE:HB	1:C:137:LEU:HB2	2.02	0.41
1:F:288:ASN:ND2	1:F:292:LYS:HE3	2.33	0.41
1:F:292:LYS:HG2	1:F:348:LYS:HD3	2.02	0.41
1:C:147:PHE:CZ	1:C:177:LEU:HD12	2.55	0.41
1:H:347:LYS:HG3	1:H:348:LYS:HD2	2.02	0.41
1:F:222:ARG:HD2	1:F:226:TRP:NE1	2.35	0.41
1:A:105:TYR:HB3	1:A:132:THR:HB	2.03	0.41
1:G:139:PHE:N	1:G:139:PHE:CD1	2.87	0.41
1:J:254:VAL:O	1:J:258:THR:HB	2.20	0.41
1:A:83:HIS:O	1:A:86:VAL:HB	2.21	0.41
1:F:188:ILE:O	1:F:192:ILE:HG13	2.20	0.41
1:A:149:PRO:CB	1:B:11:GLY:HA2	2.51	0.41
1:I:131:LEU:HD22	1:I:170:LEU:HB2	2.02	0.41
1:G:240:PRO:HB2	1:G:241:PRO:CD	2.50	0.41
1:F:16:THR:O	1:F:88:GLU:HG3	2.21	0.41
1:B:9:LYS:O	1:B:9:LYS:HG3	2.20	0.41
1:F:302:MET:HG3	1:I:302:MET:HE3	2.00	0.41
1:A:315:PHE:N	1:A:315:PHE:CD1	2.88	0.41
1:G:143:ILE:HD13	1:G:144:GLY:N	2.35	0.41
1:I:136:VAL:CG2	1:I:169:LEU:HD23	2.50	0.41
1:G:224:THR:O	1:G:227:PRO:HG2	2.20	0.41
1:G:75:ARG:HA	7:G:525:HOH:O	2.20	0.41
1:G:244:GLU:HB3	1:G:245:LYS:HE2	2.03	0.41
1:E:283:VAL:O	1:E:287:THR:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:GLY:HA3	1:D:87:LEU:HD21	2.02	0.41
1:E:280:LEU:HD12	1:E:280:LEU:HA	1.83	0.41
1:C:87:LEU:HA	1:C:87:LEU:HD23	1.90	0.41
1:A:294:LEU:O	1:A:294:LEU:HD12	2.20	0.41
1:F:304:LEU:HD12	1:F:304:LEU:HA	1.85	0.41
1:G:32:MET:O	1:G:60:THR:HA	2.20	0.41
1:I:211:THR:O	1:I:214:LEU:N	2.54	0.41
1:G:324:LYS:HA	1:G:324:LYS:HD3	1.87	0.41
1:G:322:ARG:O	1:G:324:LYS:N	2.53	0.41
1:F:86:VAL:HG13	1:F:107:PHE:CD2	2.55	0.41
1:H:328:PRO:HA	1:H:331:LEU:HB2	2.03	0.41
1:J:23:TYR:CD2	1:J:142:LYS:HD3	2.55	0.41
1:F:160:ILE:HD12	1:F:164:LYS:HE3	2.02	0.41
1:C:347:LYS:CD	1:C:348:LYS:H	2.34	0.41
1:E:307:ILE:HD11	1:E:334:MET:HG2	2.02	0.41
1:E:334:MET:HB2	1:E:334:MET:HE2	1.77	0.41
4:B:406:LMT:H6'2	4:B:406:LMT:H1B	1.87	0.41
1:I:148:ASP:N	1:I:149:PRO:HD2	2.36	0.41
1:F:257:HIS:O	1:F:260:GLN:HB3	2.21	0.41
1:A:255:TYR:O	1:A:258:THR:HG22	2.21	0.41
1:H:93:VAL:HA	1:H:126:GLN:OE1	2.21	0.41
1:H:164:LYS:NZ	1:H:246:GLU:HB3	2.36	0.41
1:C:244:GLU:HA	1:C:248:VAL:HG23	2.03	0.41
1:A:218:LEU:HD12	1:A:218:LEU:HA	1.85	0.41
1:G:164:LYS:HA	1:G:164:LYS:HD2	2.00	0.41
1:B:116:ASP:O	1:B:120:HIS:HA	2.20	0.41
1:F:311:TYR:O	1:I:314:ASN:N	2.49	0.41
1:F:82:ILE:HG22	1:F:87:LEU:HG	2.01	0.41
1:C:54:ARG:HD3	1:C:80:PHE:HA	2.03	0.41
1:C:164:LYS:HE2	1:C:246:GLU:HB3	2.03	0.41
1:F:171:TYR:OH	1:G:14:PRO:HG3	2.21	0.41
1:D:321:LEU:HB3	1:D:322:ARG:H	1.60	0.41
1:G:93:VAL:HG21	1:G:141:GLU:OE1	2.21	0.41
1:E:165:ARG:CZ	1:E:243:ILE:HG21	2.51	0.41
1:F:138:MET:SD	1:F:147:PHE:CE2	3.14	0.41
1:A:71:ASP:OD1	1:A:72:VAL:HG23	2.21	0.41
1:J:185:LEU:HD23	1:J:185:LEU:HA	1.65	0.41
1:G:333:VAL:O	1:G:337:ILE:HG22	2.21	0.41
1:D:60:THR:HB	1:D:135:CYS:SG	2.61	0.41
1:B:218:LEU:HD12	1:B:218:LEU:HA	1.75	0.41
1:F:272:VAL:O	1:F:275:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:ARG:HA	1:E:258:THR:HG23	2.03	0.41
1:J:300:ILE:HG22	1:J:341:MET:CB	2.51	0.41
1:E:113:PHE:CE2	1:E:224:THR:HG21	2.56	0.41
1:B:99:VAL:HG12	1:B:100:GLU:N	2.35	0.41
1:D:185:LEU:HD11	1:D:261:ILE:HG23	2.03	0.41
1:D:229:ARG:HA	1:D:258:THR:HG23	2.03	0.40
1:H:23:TYR:CD2	1:H:142:LYS:HD3	2.56	0.40
1:J:68:HIS:CE1	1:J:69:ARG:HG2	2.56	0.40
1:I:264:THR:O	1:I:267:THR:HB	2.21	0.40
1:G:204:GLU:HG2	1:G:205:LYS:H	1.87	0.40
1:A:239:VAL:O	1:A:239:VAL:HG23	2.22	0.40
1:B:199:VAL:HG21	1:B:275:LEU:HG	2.02	0.40
1:C:110:LEU:HB3	1:C:177:LEU:HD22	2.03	0.40
1:F:120:HIS:H	1:F:120:HIS:CD2	2.38	0.40
1:G:99:VAL:HG13	1:G:108:ILE:HG12	2.04	0.40
1:H:153:ARG:NH1	1:H:153:ARG:HG3	2.36	0.40
1:B:196:GLU:O	1:B:200:LEU:HG	2.22	0.40
1:D:257:HIS:HE1	7:D:503:HOH:O	2.03	0.40
1:J:184:LEU:HD21	1:J:221:LEU:HD11	2.04	0.40
1:G:30:GLU:OE1	1:G:151:ARG:NH2	2.54	0.40
1:I:29:ILE:HG12	1:I:64:ILE:HG12	2.03	0.40
1:G:278:VAL:HA	1:H:276:LEU:HD21	2.03	0.40
1:I:315:PHE:O	7:I:521:HOH:O	2.22	0.40
1:F:196:GLU:HB3	1:F:275:LEU:HD11	2.04	0.40
1:A:267:THR:O	1:A:271:ILE:HG13	2.22	0.40
1:F:95:GLN:HA	1:I:260:GLN:HE22	1.85	0.40
1:H:129:LEU:HD21	1:H:138:MET:SD	2.61	0.40
1:I:328:PRO:C	1:I:330:VAL:N	2.73	0.40
1:B:236:TYR:CE1	1:B:252:ARG:HG3	2.57	0.40
1:J:177:LEU:O	1:J:177:LEU:HD23	2.22	0.40
1:A:200:LEU:HD12	1:A:201:GLU:HG3	2.04	0.40
1:E:276:LEU:HA	1:E:276:LEU:HD12	1.63	0.40
1:J:325:TRP:O	1:J:329:VAL:HG22	2.21	0.40
1:F:236:TYR:CD1	1:F:252:ARG:HB2	2.56	0.40
1:F:342:VAL:O	1:F:345:PHE:N	2.55	0.40
1:F:322:ARG:O	1:F:324:LYS:HA	2.21	0.40
1:J:236:TYR:OH	1:J:252:ARG:HD2	2.21	0.40
1:D:103:GLU:HG2	1:D:103:GLU:H	1.53	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	345/351 (98%)	323 (94%)	19 (6%)	3 (1%)	21	49
1	B	346/351 (99%)	320 (92%)	24 (7%)	2 (1%)	30	59
1	C	345/351 (98%)	321 (93%)	22 (6%)	2 (1%)	30	59
1	D	341/351 (97%)	316 (93%)	22 (6%)	3 (1%)	21	49
1	E	344/351 (98%)	321 (93%)	22 (6%)	1 (0%)	46	75
1	F	344/351 (98%)	318 (92%)	22 (6%)	4 (1%)	16	39
1	G	344/351 (98%)	317 (92%)	21 (6%)	6 (2%)	11	29
1	H	341/351 (97%)	322 (94%)	17 (5%)	2 (1%)	30	59
1	I	343/351 (98%)	315 (92%)	25 (7%)	3 (1%)	21	49
1	J	343/351 (98%)	322 (94%)	17 (5%)	4 (1%)	16	39
All	All	3436/3510 (98%)	3195 (93%)	211 (6%)	30 (1%)	21	49

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	302	MET
1	I	327	TYR
1	B	325	TRP
1	D	324	LYS
1	H	67	ILE
1	I	328	PRO
1	A	241	PRO
1	B	241	PRO
1	C	241	PRO
1	G	317	TYR
1	H	241	PRO
1	I	241	PRO
1	J	322	ARG
1	J	323	TRP

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Mol	Chain	Res	Type
1	J	325	TRP
1	F	241	PRO
1	G	322	ARG
1	J	241	PRO
1	F	240	PRO
1	G	241	PRO
1	G	318	MET
1	A	325	TRP
1	D	240	PRO
1	D	241	PRO
1	F	319	PRO
1	A	240	PRO
1	E	241	PRO
1	C	240	PRO
1	G	319	PRO
1	G	240	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	326/330 (99%)	294 (90%)	32 (10%)	10	23
1	B	327/330 (99%)	298 (91%)	29 (9%)	12	27
1	C	323/330 (98%)	299 (93%)	24 (7%)	17	39
1	D	322/330 (98%)	292 (91%)	30 (9%)	11	25
1	E	320/330 (97%)	291 (91%)	29 (9%)	12	26
1	F	321/330 (97%)	287 (89%)	34 (11%)	8	19
1	G	319/330 (97%)	289 (91%)	30 (9%)	11	25
1	H	318/330 (96%)	287 (90%)	31 (10%)	10	23
1	I	320/330 (97%)	290 (91%)	30 (9%)	11	25
1	J	320/330 (97%)	298 (93%)	22 (7%)	19	43
All	All	3216/3300 (98%)	2925 (91%)	291 (9%)	12	27

All (291) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	40	ARG
1	A	58	THR
1	A	96	ARG
1	A	104	ASN
1	A	122	LEU
1	A	127	VAL
1	A	128	SER
1	A	143	ILE
1	A	161	ILE
1	A	195	LEU
1	A	200	LEU
1	A	206	GLU
1	A	215	LYS
1	A	218	LEU
1	A	223	LYS
1	A	234	SER
1	A	235	LEU
1	A	238	ASP
1	A	243	ILE
1	A	266	GLU
1	A	275	LEU
1	A	299	THR
1	A	302	MET
1	A	315	PHE
1	A	317	TYR
1	A	324	LYS
1	A	325	TRP
1	A	329	VAL
1	A	331	LEU
1	A	333	VAL
1	A	339	VAL
1	B	26	ASP
1	B	36	ILE
1	B	60	THR
1	B	82	ILE
1	B	95	GLN
1	B	96	ARG
1	B	104	ASN
1	B	127	VAL
1	B	131	LEU
1	B	143	ILE

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Mol	Chain	Res	Type
1	B	146	VAL
1	B	157	ASN
1	B	160	ILE
1	B	165	ARG
1	B	200	LEU
1	B	206	GLU
1	B	215	LYS
1	B	218	LEU
1	B	223	LYS
1	B	224	THR
1	B	243	ILE
1	B	258	THR
1	B	270	ASP
1	B	275	LEU
1	B	291	MET
1	B	297	ILE
1	B	315	PHE
1	B	329	VAL
1	B	339	VAL
1	C	6	LEU
1	C	26	ASP
1	C	50	VAL
1	C	60	THR
1	C	104	ASN
1	C	118	ASN
1	C	120	HIS
1	C	123	GLU
1	C	128	SER
1	C	143	ILE
1	C	177	LEU
1	C	218	LEU
1	C	222	ARG
1	C	235	LEU
1	C	258	THR
1	C	265	VAL
1	C	273	SER
1	C	275	LEU
1	C	297	ILE
1	C	299	THR
1	C	307	ILE
1	C	321	LEU
1	C	322	ARG

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Mol	Chain	Res	Type
1	C	347	LYS
1	D	39	PHE
1	D	44	THR
1	D	45	THR
1	D	50	VAL
1	D	96	ARG
1	D	99	VAL
1	D	103	GLU
1	D	106	VAL
1	D	120	HIS
1	D	122	LEU
1	D	162	ARG
1	D	206	GLU
1	D	215	LYS
1	D	218	LEU
1	D	221	LEU
1	D	229	ARG
1	D	232	LEU
1	D	235	LEU
1	D	253	ASP
1	D	258	THR
1	D	260	GLN
1	D	267	THR
1	D	275	LEU
1	D	282	SER
1	D	315	PHE
1	D	322	ARG
1	D	323	TRP
1	D	325	TRP
1	D	327	TYR
1	D	349	LYS
1	E	17	LEU
1	E	24	ARG
1	E	39	PHE
1	E	44	THR
1	E	60	THR
1	E	82	ILE
1	E	109	VAL
1	E	114	THR
1	E	120	HIS
1	E	127	VAL
1	E	128	SER

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Mol	Chain	Res	Type
1	E	135	CYS
1	E	143	ILE
1	E	199	VAL
1	E	222	ARG
1	E	226	TRP
1	E	234	SER
1	E	235	LEU
1	E	244	GLU
1	E	258	THR
1	E	265	VAL
1	E	267	THR
1	E	276	LEU
1	E	282	SER
1	E	286	LYS
1	E	287	THR
1	E	300	ILE
1	E	346	LYS
1	E	347	LYS
1	F	5	ARG
1	F	9	LYS
1	F	10	LYS
1	F	40	ARG
1	F	45	THR
1	F	60	THR
1	F	70	THR
1	F	96	ARG
1	F	104	ASN
1	F	120	HIS
1	F	122	LEU
1	F	143	ILE
1	F	172	SER
1	F	177	LEU
1	F	200	LEU
1	F	202	ARG
1	F	213	GLN
1	F	215	LYS
1	F	218	LEU
1	F	222	ARG
1	F	223	LYS
1	F	235	LEU
1	F	243	ILE
1	F	258	THR

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Mol	Chain	Res	Type
1	F	263	ASP
1	F	271	ILE
1	F	275	LEU
1	F	276	LEU
1	F	299	THR
1	F	304	LEU
1	F	313	MET
1	F	315	PHE
1	F	320	GLU
1	F	324	LYS
1	G	40	ARG
1	G	41	GLU
1	G	44	THR
1	G	50	VAL
1	G	67	ILE
1	G	96	ARG
1	G	118	ASN
1	G	142	LYS
1	G	143	ILE
1	G	161	ILE
1	G	164	LYS
1	G	185	LEU
1	G	202	ARG
1	G	206	GLU
1	G	215	LYS
1	G	218	LEU
1	G	223	LYS
1	G	229	ARG
1	G	235	LEU
1	G	246	GLU
1	G	247	THR
1	G	258	THR
1	G	265	VAL
1	G	267	THR
1	G	275	LEU
1	G	276	LEU
1	G	282	SER
1	G	296	ILE
1	G	307	ILE
1	G	318	MET
1	H	26	ASP
1	H	39	PHE

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Mol	Chain	Res	Type
1	H	52	PRO
1	H	60	THR
1	H	69	ARG
1	H	82	ILE
1	H	96	ARG
1	H	114	THR
1	H	118	ASN
1	H	119	LEU
1	H	140	GLN
1	H	143	ILE
1	H	150	VAL
1	H	162	ARG
1	H	174	ILE
1	H	177	LEU
1	H	200	LEU
1	H	206	GLU
1	H	213	GLN
1	H	215	LYS
1	H	218	LEU
1	H	226	TRP
1	H	229	ARG
1	H	235	LEU
1	H	253	ASP
1	H	258	THR
1	H	287	THR
1	H	320	GLU
1	H	322	ARG
1	H	330	VAL
1	H	341	MET
1	I	10	LYS
1	I	17	LEU
1	I	36	ILE
1	I	39	PHE
1	I	50	VAL
1	I	104	ASN
1	I	122	LEU
1	I	128	SER
1	I	204	GLU
1	I	213	GLN
1	I	215	LYS
1	I	218	LEU
1	I	222	ARG

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Mol	Chain	Res	Type
1	I	229	ARG
1	I	233	SER
1	I	235	LEU
1	I	243	ILE
1	I	258	THR
1	I	260	GLN
1	I	271	ILE
1	I	275	LEU
1	I	276	LEU
1	I	281	SER
1	I	313	MET
1	I	315	PHE
1	I	317	TYR
1	I	320	GLU
1	I	323	TRP
1	I	325	TRP
1	I	336	VAL
1	J	5	ARG
1	J	9	LYS
1	J	17	LEU
1	J	24	ARG
1	J	96	ARG
1	J	108	ILE
1	J	124	SER
1	J	128	SER
1	J	143	ILE
1	J	164	LYS
1	J	204	GLU
1	J	218	LEU
1	J	222	ARG
1	J	234	SER
1	J	235	LEU
1	J	258	THR
1	J	275	LEU
1	J	296	ILE
1	J	304	LEU
1	J	315	PHE
1	J	320	GLU
1	J	348	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	157	ASN
1	B	74	GLN
1	B	209	GLN
1	C	33	ASN
1	C	94	HIS
1	C	126	GLN
1	C	288	ASN
1	D	33	ASN
1	D	95	GLN
1	D	140	GLN
1	D	288	ASN
1	D	314	ASN
1	E	83	HIS
1	E	118	ASN
1	E	126	GLN
1	E	209	GLN
1	E	260	GLN
1	F	118	ASN
1	F	288	ASN
1	G	63	ASN
1	G	74	GLN
1	G	95	GLN
1	G	118	ASN
1	G	140	GLN
1	G	157	ASN
1	G	209	GLN
1	H	95	GLN
1	H	213	GLN
1	H	288	ASN
1	H	314	ASN
1	I	63	ASN
1	I	95	GLN
1	I	213	GLN
1	I	260	GLN
1	I	314	ASN
1	J	33	ASN
1	J	95	GLN
1	J	260	GLN
1	J	314	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 ⓘ

Of 62 ligands modelled in this entry, 37 are monoatomic - leaving 25 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	LMT	A	403	-	36,36,36	0.39	0	47,47,47	0.70	1 (2%)
4	LMT	B	406	-	36,36,36	0.41	0	47,47,47	0.83	2 (4%)
4	LMT	B	407	-	33,33,36	0.43	0	44,44,47	0.86	2 (4%)
5	PEG	B	408	-	6,6,6	0.54	0	5,5,5	0.72	0
5	PEG	B	409	-	6,6,6	0.35	0	5,5,5	0.45	0
5	PEG	B	410	-	6,6,6	0.37	0	5,5,5	0.39	0
5	PEG	B	411	-	6,6,6	0.55	0	5,5,5	1.31	1 (20%)
5	PEG	C	405	-	6,6,6	0.29	0	5,5,5	0.44	0
5	PEG	C	406	-	6,6,6	0.65	0	5,5,5	0.95	0
5	PEG	D	405	-	6,6,6	0.38	0	5,5,5	0.99	0
5	PEG	E	405	-	6,6,6	0.60	0	5,5,5	0.60	0
5	PEG	E	406	-	6,6,6	0.55	0	5,5,5	1.31	1 (20%)
5	PEG	E	407	-	6,6,6	0.59	0	5,5,5	0.49	0
5	PEG	E	408	-	6,6,6	0.44	0	5,5,5	1.33	1 (20%)
6	PG0	E	409	-	7,7,7	0.39	0	6,6,6	1.07	1 (16%)
5	PEG	F	404	-	6,6,6	0.56	0	5,5,5	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEG	G	408	-	6,6,6	0.55	0	5,5,5	0.69	0
5	PEG	G	409	-	6,6,6	0.53	0	5,5,5	0.87	0
5	PEG	G	410	-	6,6,6	0.34	0	5,5,5	0.46	0
5	PEG	G	411	-	6,6,6	0.36	0	5,5,5	0.31	0
5	PEG	G	412	-	6,6,6	0.58	0	5,5,5	1.07	0
5	PEG	H	402	-	6,6,6	0.33	0	5,5,5	0.27	0
5	PEG	I	404	-	6,6,6	0.57	0	5,5,5	0.71	0
5	PEG	J	405	-	6,6,6	0.50	0	5,5,5	0.79	0
5	PEG	J	406	-	6,6,6	0.58	0	5,5,5	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LMT	A	403	-	-	0/21/61/61	0/2/2/2
4	LMT	B	406	-	-	0/21/61/61	0/2/2/2
4	LMT	B	407	-	-	0/18/58/61	0/2/2/2
5	PEG	B	408	-	-	0/4/4/4	0/0/0/0
5	PEG	B	409	-	-	0/4/4/4	0/0/0/0
5	PEG	B	410	-	-	0/4/4/4	0/0/0/0
5	PEG	B	411	-	-	0/4/4/4	0/0/0/0
5	PEG	C	405	-	-	0/4/4/4	0/0/0/0
5	PEG	C	406	-	-	0/4/4/4	0/0/0/0
5	PEG	D	405	-	-	0/4/4/4	0/0/0/0
5	PEG	E	405	-	-	0/4/4/4	0/0/0/0
5	PEG	E	406	-	-	0/4/4/4	0/0/0/0
5	PEG	E	407	-	-	0/4/4/4	0/0/0/0
5	PEG	E	408	-	-	0/4/4/4	0/0/0/0
6	PG0	E	409	-	-	0/5/5/5	0/0/0/0
5	PEG	F	404	-	-	0/4/4/4	0/0/0/0
5	PEG	G	408	-	-	0/4/4/4	0/0/0/0
5	PEG	G	409	-	-	0/4/4/4	0/0/0/0
5	PEG	G	410	-	-	0/4/4/4	0/0/0/0
5	PEG	G	411	-	-	0/4/4/4	0/0/0/0
5	PEG	G	412	-	-	0/4/4/4	0/0/0/0
5	PEG	H	402	-	-	0/4/4/4	0/0/0/0
5	PEG	I	404	-	-	0/4/4/4	0/0/0/0
5	PEG	J	405	-	-	0/4/4/4	0/0/0/0
5	PEG	J	406	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	LMT	C1B-O1B-C4'	-2.38	111.79	118.01
4	B	407	LMT	C1B-O1B-C4'	-2.37	111.82	118.01
4	B	406	LMT	C1B-O1B-C4'	-2.17	112.35	118.01
4	B	406	LMT	C3B-C4B-C5B	2.08	113.83	110.20
4	B	407	LMT	C3B-C4B-C5B	2.14	113.93	110.20
6	E	409	PG0	C2-O1-C3	2.23	122.89	113.31
5	B	411	PEG	C3-O2-C2	2.27	123.07	113.31
5	E	406	PEG	C3-O2-C2	2.81	125.37	113.31
5	E	408	PEG	C3-O2-C2	2.93	125.89	113.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	LMT	27	0
4	B	406	LMT	26	0
4	B	407	LMT	9	0
5	B	408	PEG	1	0
5	B	410	PEG	2	0
5	B	411	PEG	2	0
5	C	406	PEG	4	0
5	E	405	PEG	1	0
5	G	408	PEG	3	0
5	G	409	PEG	2	0
5	G	411	PEG	3	0
5	J	405	PEG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	347/351 (98%)	0.49	24 (6%) 20 18	33, 72, 122, 180	0
1	B	348/351 (99%)	0.27	15 (4%) 39 38	27, 58, 126, 158	0
1	C	347/351 (98%)	0.53	29 (8%) 14 11	25, 75, 145, 230	0
1	D	343/351 (97%)	0.41	30 (8%) 13 10	40, 77, 133, 197	0
1	E	345/351 (98%)	0.39	25 (7%) 18 16	35, 71, 149, 187	0
1	F	346/351 (98%)	0.35	22 (6%) 23 21	32, 70, 135, 202	0
1	G	346/351 (98%)	0.38	23 (6%) 22 20	30, 57, 141, 234	0
1	H	343/351 (97%)	0.39	23 (6%) 21 19	30, 71, 127, 191	0
1	I	345/351 (98%)	0.54	30 (8%) 13 10	38, 71, 143, 246	0
1	J	345/351 (98%)	0.49	27 (7%) 16 14	32, 71, 151, 192	0
All	All	3455/3510 (98%)	0.43	248 (7%) 18 16	25, 70, 140, 246	0

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	322	ARG	11.3
1	G	325	TRP	9.7
1	G	319	PRO	8.8
1	G	326	GLY	8.5
1	F	317	TYR	8.0
1	F	325	TRP	7.4
1	G	323	TRP	7.3
1	J	317	TYR	7.2
1	A	245	LYS	7.2
1	G	343	VAL	6.8
1	I	245	LYS	6.5
1	C	317	TYR	5.9
1	I	200	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	H	39	PHE	5.4
1	D	317	TYR	5.2
1	E	323	TRP	5.2
1	D	325	TRP	5.1
1	F	318	MET	5.1
1	C	316	GLU	5.0
1	H	339	VAL	4.9
1	C	325	TRP	4.9
1	J	236	TYR	4.8
1	J	201	GLU	4.7
1	C	245	LYS	4.6
1	G	340	ILE	4.6
1	C	38	GLU	4.6
1	C	315	PHE	4.6
1	F	319	PRO	4.6
1	C	343	VAL	4.5
1	C	319	PRO	4.5
1	J	319	PRO	4.5
1	C	321	LEU	4.4
1	G	329	VAL	4.3
1	D	37	GLU	4.3
1	H	332	ALA	4.1
1	J	39	PHE	4.1
1	H	326	GLY	4.1
1	C	104	ASN	4.0
1	H	325	TRP	4.0
1	B	343	VAL	3.9
1	H	336	VAL	3.9
1	E	319	PRO	3.9
1	J	202	ARG	3.8
1	J	152	GLU	3.8
1	A	316	GLU	3.7
1	I	318	MET	3.7
1	B	119	LEU	3.7
1	A	328	PRO	3.7
1	A	329	VAL	3.7
1	H	154	ILE	3.7
1	I	330	VAL	3.7
1	D	50	VAL	3.7
1	C	339	VAL	3.7
1	H	317	TYR	3.6
1	G	315	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	53	PHE	3.6
1	D	318	MET	3.6
1	H	324	LYS	3.5
1	J	33	ASN	3.5
1	J	199	VAL	3.5
1	D	203	PRO	3.5
1	D	339	VAL	3.5
1	A	205	LYS	3.5
1	A	319	PRO	3.4
1	H	201	GLU	3.4
1	C	342	VAL	3.4
1	F	35	SER	3.4
1	G	349	LYS	3.4
1	I	343	VAL	3.4
1	D	346	LYS	3.4
1	A	244	GLU	3.4
1	J	323	TRP	3.4
1	I	345	PHE	3.4
1	A	325	TRP	3.4
1	H	335	GLY	3.4
1	B	315	PHE	3.3
1	A	339	VAL	3.3
1	F	326	GLY	3.3
1	D	154	ILE	3.3
1	I	340	ILE	3.3
1	E	24	ARG	3.2
1	G	321	LEU	3.2
1	H	32	MET	3.2
1	A	347	LYS	3.2
1	B	198	GLU	3.2
1	J	211	THR	3.1
1	A	118	ASN	3.1
1	A	67	ILE	3.1
1	D	343	VAL	3.1
1	E	133	LYS	3.0
1	I	246	GLU	3.0
1	F	47	VAL	3.0
1	C	314	ASN	3.0
1	C	324	LYS	3.0
1	G	316	GLU	3.0
1	E	42	PHE	3.0
1	I	325	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	35	SER	3.0
1	C	336	VAL	3.0
1	F	314	ASN	2.9
1	F	37	GLU	2.9
1	F	304	LEU	2.9
1	C	278	VAL	2.9
1	H	50	VAL	2.9
1	H	329	VAL	2.9
1	F	313	MET	2.9
1	J	32	MET	2.9
1	C	332	ALA	2.9
1	A	199	VAL	2.9
1	F	119	LEU	2.9
1	H	38	GLU	2.9
1	E	305	THR	2.9
1	C	47	VAL	2.8
1	A	53	PHE	2.8
1	D	42	PHE	2.8
1	E	325	TRP	2.8
1	J	40	ARG	2.8
1	A	314	ASN	2.8
1	B	322	ARG	2.8
1	G	320	GLU	2.8
1	J	329	VAL	2.8
1	I	5	ARG	2.8
1	J	118	ASN	2.7
1	B	3	GLU	2.7
1	J	207	THR	2.7
1	C	205	LYS	2.7
1	E	154	ILE	2.7
1	D	30	GLU	2.7
1	G	7	SER	2.7
1	E	204	GLU	2.7
1	I	327	TYR	2.7
1	F	62	ILE	2.7
1	D	323	TRP	2.6
1	I	322	ARG	2.6
1	J	313	MET	2.6
1	C	39	PHE	2.6
1	H	289	GLU	2.6
1	C	236	TYR	2.6
1	E	158	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	4	LYS	2.6
1	F	337	ILE	2.6
1	E	34	TYR	2.6
1	C	335	GLY	2.6
1	I	165	ARG	2.6
1	B	182	PHE	2.6
1	D	32	MET	2.6
1	J	238	ASP	2.5
1	F	246	GLU	2.5
1	A	154	ILE	2.5
1	A	4	LYS	2.5
1	G	336	VAL	2.5
1	B	202	ARG	2.5
1	E	163	LYS	2.5
1	I	52	PRO	2.5
1	B	118	ASN	2.5
1	G	344	TYR	2.5
1	F	245	LYS	2.5
1	G	324	LYS	2.5
1	A	34	TYR	2.5
1	E	155	ARG	2.5
1	J	204	GLU	2.5
1	D	328	PRO	2.5
1	G	342	VAL	2.4
1	C	151	ARG	2.4
1	D	345	PHE	2.4
1	D	119	LEU	2.4
1	D	143	ILE	2.4
1	J	119	LEU	2.4
1	F	42	PHE	2.4
1	I	194	VAL	2.4
1	A	318	MET	2.4
1	C	241	PRO	2.4
1	D	283	VAL	2.4
1	E	37	GLU	2.4
1	B	345	PHE	2.4
1	H	53	PHE	2.4
1	E	239	VAL	2.4
1	I	37	GLU	2.4
1	G	34	TYR	2.4
1	D	340	ILE	2.4
1	E	340	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	195	LEU	2.3
1	E	318	MET	2.3
1	J	275	LEU	2.3
1	B	323	TRP	2.3
1	F	300	ILE	2.3
1	C	103	GLU	2.3
1	I	275	LEU	2.3
1	I	302	MET	2.3
1	D	326	GLY	2.3
1	J	302	MET	2.3
1	E	39	PHE	2.3
1	D	336	VAL	2.3
1	A	246	GLU	2.2
1	A	139	PHE	2.2
1	G	69	ARG	2.2
1	I	237	ARG	2.2
1	E	32	MET	2.2
1	I	324	LYS	2.2
1	B	196	GLU	2.2
1	E	31	VAL	2.2
1	G	162	ARG	2.2
1	I	341	MET	2.2
1	D	29	ILE	2.2
1	H	162	ARG	2.2
1	A	315	PHE	2.2
1	J	41	GLU	2.2
1	G	338	ALA	2.2
1	D	322	ARG	2.2
1	F	296	ILE	2.2
1	D	115	TYR	2.2
1	E	317	TYR	2.1
1	D	62	ILE	2.1
1	F	155	ARG	2.1
1	I	332	ALA	2.1
1	A	333	VAL	2.1
1	B	195	LEU	2.1
1	I	49	SER	2.1
1	I	124	SER	2.1
1	I	143	ILE	2.1
1	B	327	TYR	2.1
1	J	16	THR	2.1
1	I	154	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	306	PHE	2.1
1	A	72	VAL	2.1
1	D	276	LEU	2.1
1	E	199	VAL	2.1
1	H	25	GLU	2.1
1	H	309	GLY	2.1
1	I	295	THR	2.1
1	J	192	ILE	2.1
1	C	105	TYR	2.1
1	I	336	VAL	2.1
1	E	302	MET	2.1
1	F	341	MET	2.1
1	H	188	ILE	2.1
1	I	333	VAL	2.0
1	B	300	ILE	2.0
1	D	142	LYS	2.0
1	I	328	PRO	2.0
1	G	5	ARG	2.0
1	H	137	LEU	2.0
1	H	31	VAL	2.0
1	E	25	GLU	2.0
1	J	25	GLU	2.0
1	G	335	GLY	2.0
1	F	321	LEU	2.0
1	J	248	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	D	401	1/1	0.88	1.61	21.53	86,86,86,86	0
5	PEG	J	405	7/7	0.81	0.28	9.35	49,53,59,63	0
2	MG	J	401	1/1	0.89	0.58	8.75	107,107,107,107	0
2	MG	E	402	1/1	0.93	0.27	3.60	56,56,56,56	0
4	LMT	A	403	35/35	0.79	0.47	3.00	72,129,136,142	35
2	MG	D	403	1/1	0.77	0.23	2.64	57,57,57,57	0
3	CL	J	404	1/1	0.85	0.28	2.02	46,46,46,46	0
2	MG	F	401	1/1	0.97	0.25	1.73	42,42,42,42	0
2	MG	J	403	1/1	0.88	0.22	1.13	50,50,50,50	0
5	PEG	C	406	7/7	0.91	0.26	0.90	49,60,63,75	0
5	PEG	H	402	7/7	0.89	0.23	0.61	73,84,92,97	0
2	MG	B	401	1/1	0.92	0.24	0.58	45,45,45,45	0
2	MG	I	403	1/1	0.97	0.22	0.15	45,45,45,45	0
2	MG	I	401	1/1	0.91	0.19	-0.01	56,56,56,56	0
5	PEG	G	408	7/7	0.72	0.22	-0.03	91,103,105,109	0
3	CL	B	404	1/1	0.80	0.16	-0.08	57,57,57,57	0
3	CL	F	403	1/1	0.69	0.18	-0.12	60,60,60,60	0
2	MG	G	405	1/1	0.98	0.17	-0.22	39,39,39,39	0
2	MG	C	402	1/1	0.99	0.18	-0.34	45,45,45,45	0
3	CL	E	403	1/1	0.86	0.20	-0.36	62,62,62,62	0
2	MG	C	401	1/1	0.94	0.13	-0.82	53,53,53,53	0
2	MG	E	401	1/1	0.95	0.14	-0.85	34,34,34,34	0
2	MG	A	401	1/1	0.81	0.13	-0.96	65,65,65,65	0
2	MG	G	404	1/1	0.97	0.14	-0.98	45,45,45,45	0
2	MG	D	402	1/1	0.96	0.13	-1.02	35,35,35,35	0
3	CL	H	401	1/1	0.90	0.11	-1.45	52,52,52,52	0
2	MG	J	402	1/1	0.92	0.12	-1.52	43,43,43,43	0
2	MG	G	403	1/1	0.95	0.11	-1.62	54,54,54,54	0
3	CL	A	402	1/1	0.90	0.10	-1.88	52,52,52,52	0
3	CL	C	404	1/1	0.96	0.07	-2.45	44,44,44,44	0
3	CL	G	406	1/1	0.91	0.08	-2.89	46,46,46,46	0
2	MG	I	402	1/1	0.92	0.10	-3.30	58,58,58,58	0
5	PEG	F	404	7/7	0.44	0.33	-	92,113,123,126	0
2	MG	G	401	1/1	0.91	0.94	-	61,61,61,61	0
5	PEG	D	405	7/7	0.78	0.17	-	62,80,92,108	0
5	PEG	B	410	7/7	0.81	0.29	-	57,74,82,87	0
2	MG	F	402	1/1	0.92	0.17	-	57,57,57,57	0
5	PEG	G	412	7/7	0.81	0.23	-	72,74,87,90	0
5	PEG	G	409	7/7	0.29	0.25	-	75,92,99,102	0
5	PEG	G	411	7/7	0.54	0.18	-	203,214,221,223	0
3	CL	D	404	1/1	0.80	0.44	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CL	C	403	1/1	0.95	0.24	-	41,41,41,41	0
4	LMT	B	406	35/35	0.78	0.30	-	89,123,133,135	0
5	PEG	J	406	7/7	0.55	0.49	-	78,88,95,100	0
2	MG	B	403	1/1	0.94	0.12	-	45,45,45,45	0
3	CL	E	404	1/1	0.93	0.16	-	52,52,52,52	0
5	PEG	B	409	7/7	0.82	0.37	-	67,87,95,95	0
3	CL	B	405	1/1	0.93	0.82	-	50,50,50,50	0
5	PEG	G	410	7/7	0.76	0.20	-	98,101,110,114	0
5	PEG	B	408	7/7	0.87	0.15	-	64,77,83,85	0
5	PEG	B	411	7/7	0.88	0.17	-	61,68,72,78	0
5	PEG	I	404	7/7	0.83	0.15	-	77,82,84,89	0
5	PEG	E	408	7/7	0.85	0.21	-	67,71,77,82	0
5	PEG	C	405	7/7	0.85	0.27	-	79,82,95,100	0
6	PG0	E	409	8/8	0.90	0.10	-	72,83,97,98	0
5	PEG	E	405	7/7	0.90	0.11	-	82,84,92,95	0
3	CL	G	407	1/1	0.77	0.16	-	65,65,65,65	0
5	PEG	E	406	7/7	0.93	0.34	-	65,75,91,107	0
2	MG	G	402	1/1	0.87	0.44	-	69,69,69,69	0
2	MG	B	402	1/1	0.97	0.17	-	39,39,39,39	0
4	LMT	B	407	32/35	0.78	0.36	-	114,176,197,203	0
5	PEG	E	407	7/7	0.79	0.40	-	77,83,87,96	0

6.5 Other polymers

There are no such residues in this entry.