



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:42 PM GMT

PDB ID : 3RIF
Title : C. elegans glutamate-gated chloride channel (GluCl) in complex with Fab, ivermectin and glutamate.
Authors : Hibbs, R.E.; Gouaux, E.
Deposited on : 2011-04-13
Resolution : 3.35 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

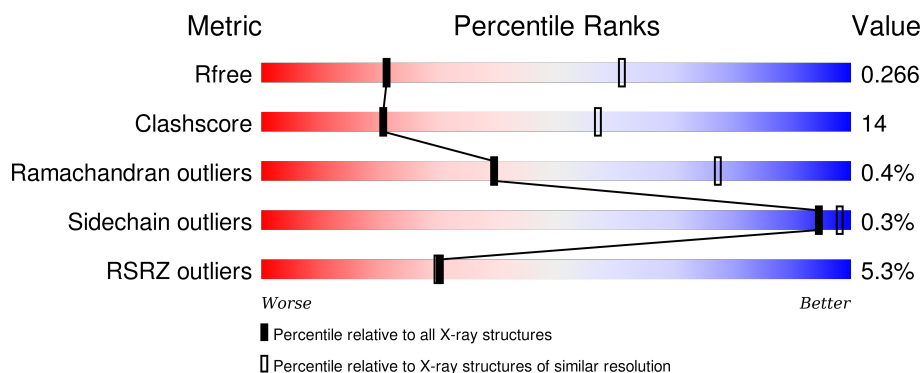
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1004 (3.40-3.28)
Clashscore	102246	1072 (3.40-3.28)
Ramachandran outliers	100387	1055 (3.40-3.28)
Sidechain outliers	100360	1054 (3.40-3.28)
RSRZ outliers	91569	1009 (3.40-3.28)

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	347	<div> <div>2%</div> <div>68%</div> <div>29%</div> <div>.</div> </div>
1	B	347	<div> <div>2%</div> <div>67%</div> <div>31%</div> <div>.</div> </div>
1	C	347	<div> <div>4%</div> <div>66%</div> <div>31%</div> <div>.</div> </div>
1	D	347	<div> <div>2%</div> <div>67%</div> <div>30%</div> <div>.</div> </div>
1	E	347	<div> <div>2%</div> <div>68%</div> <div>30%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	221	
2	G	221	
2	H	221	
2	I	221	
2	J	221	
3	K	210	
3	L	210	
3	M	210	
3	N	210	
3	O	210	

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
10	UND	B	406	-	-	-	X
4	GLU	A	401	-	-	-	X
4	GLU	D	401	-	-	-	X
6	IVM	B	403	-	-	-	X
6	IVM	E	402	-	-	-	X
7	LMT	A	405	-	-	-	X
8	OCT	B	405	-	-	-	X
8	OCT	D	403	-	-	-	X
9	NAG	B	400	-	-	-	X
9	NAG	C	400	-	-	-	X
9	NAG	E	400	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 29020 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 Avermectin-sensitive glutamate-gated chloride channel GluCl alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2720	1771	442	492	15			
1	B	340	Total	C	N	O	S	0	0	0
			2720	1771	442	492	15			
1	C	339	Total	C	N	O	S	0	0	0
			2710	1765	439	491	15			
1	D	340	Total	C	N	O	S	0	0	0
			2720	1771	442	492	15			
1	E	340	Total	C	N	O	S	0	0	0
			2720	1771	442	492	15			

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	303	ALA	-	LINKER	UNP O17793
A	304	GLY	-	LINKER	UNP O17793
A	305	THR	-	LINKER	UNP O17793
A	340	HIS	-	EXPRESSION TAG	UNP O17793
A	341	HIS	-	EXPRESSION TAG	UNP O17793
A	342	HIS	-	EXPRESSION TAG	UNP O17793
A	343	HIS	-	EXPRESSION TAG	UNP O17793
A	344	HIS	-	EXPRESSION TAG	UNP O17793
A	345	HIS	-	EXPRESSION TAG	UNP O17793
A	346	HIS	-	EXPRESSION TAG	UNP O17793
A	347	HIS	-	EXPRESSION TAG	UNP O17793
B	303	ALA	-	LINKER	UNP O17793
B	304	GLY	-	LINKER	UNP O17793
B	305	THR	-	LINKER	UNP O17793
B	340	HIS	-	EXPRESSION TAG	UNP O17793
B	341	HIS	-	EXPRESSION TAG	UNP O17793
B	342	HIS	-	EXPRESSION TAG	UNP O17793
B	343	HIS	-	EXPRESSION TAG	UNP O17793

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Chain	Residue	Modelled	Actual	Comment	Reference
B	344	HIS	-	EXPRESSION TAG	UNP O17793
B	345	HIS	-	EXPRESSION TAG	UNP O17793
B	346	HIS	-	EXPRESSION TAG	UNP O17793
B	347	HIS	-	EXPRESSION TAG	UNP O17793
C	303	ALA	-	LINKER	UNP O17793
C	304	GLY	-	LINKER	UNP O17793
C	305	THR	-	LINKER	UNP O17793
C	340	HIS	-	EXPRESSION TAG	UNP O17793
C	341	HIS	-	EXPRESSION TAG	UNP O17793
C	342	HIS	-	EXPRESSION TAG	UNP O17793
C	343	HIS	-	EXPRESSION TAG	UNP O17793
C	344	HIS	-	EXPRESSION TAG	UNP O17793
C	345	HIS	-	EXPRESSION TAG	UNP O17793
C	346	HIS	-	EXPRESSION TAG	UNP O17793
C	347	HIS	-	EXPRESSION TAG	UNP O17793
D	303	ALA	-	LINKER	UNP O17793
D	304	GLY	-	LINKER	UNP O17793
D	305	THR	-	LINKER	UNP O17793
D	340	HIS	-	EXPRESSION TAG	UNP O17793
D	341	HIS	-	EXPRESSION TAG	UNP O17793
D	342	HIS	-	EXPRESSION TAG	UNP O17793
D	343	HIS	-	EXPRESSION TAG	UNP O17793
D	344	HIS	-	EXPRESSION TAG	UNP O17793
D	345	HIS	-	EXPRESSION TAG	UNP O17793
D	346	HIS	-	EXPRESSION TAG	UNP O17793
D	347	HIS	-	EXPRESSION TAG	UNP O17793
E	303	ALA	-	LINKER	UNP O17793
E	304	GLY	-	LINKER	UNP O17793
E	305	THR	-	LINKER	UNP O17793
E	340	HIS	-	EXPRESSION TAG	UNP O17793
E	341	HIS	-	EXPRESSION TAG	UNP O17793
E	342	HIS	-	EXPRESSION TAG	UNP O17793
E	343	HIS	-	EXPRESSION TAG	UNP O17793
E	344	HIS	-	EXPRESSION TAG	UNP O17793
E	345	HIS	-	EXPRESSION TAG	UNP O17793
E	346	HIS	-	EXPRESSION TAG	UNP O17793
E	347	HIS	-	EXPRESSION TAG	UNP O17793

- Molecule 2 is a protein called Mouse monoclonal Fab fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	171	Total	C	N	O	S	0	0	0
			1324	846	213	259	6			

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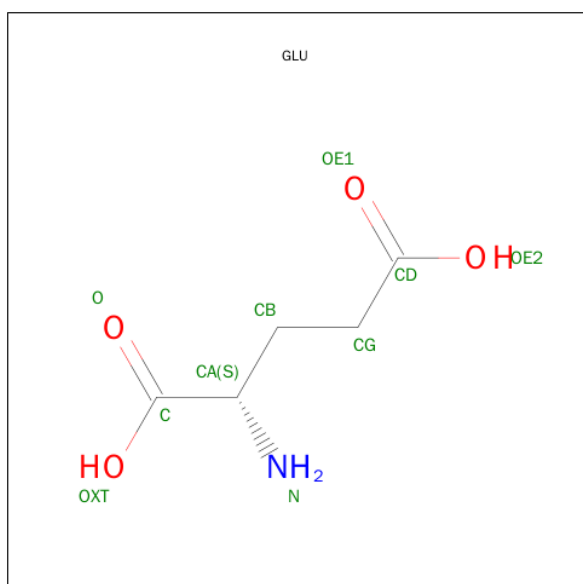
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	214	Total	C	N	O	S	0	0	0
			1631	1038	263	323	7			
2	H	221	Total	C	N	O	S	0	0	0
			1675	1061	271	335	8			
2	I	192	Total	C	N	O	S	0	0	0
			1466	932	238	288	8			
2	J	200	Total	C	N	O	S	0	0	0
			1526	971	247	301	7			

- Molecule 3 is a protein called Mouse monoclonal Fab fragment, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	210	Total	C	N	O	S	0	0	0
			1579	993	260	320	6			
3	L	210	Total	C	N	O	S	0	0	0
			1591	999	266	320	6			
3	M	210	Total	C	N	O	S	0	0	0
			1576	991	262	317	6			
3	N	148	Total	C	N	O	S	0	0	0
			1075	678	180	214	3			
3	O	195	Total	C	N	O	S	0	0	0
			1470	927	243	294	6			

- Molecule 4 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).

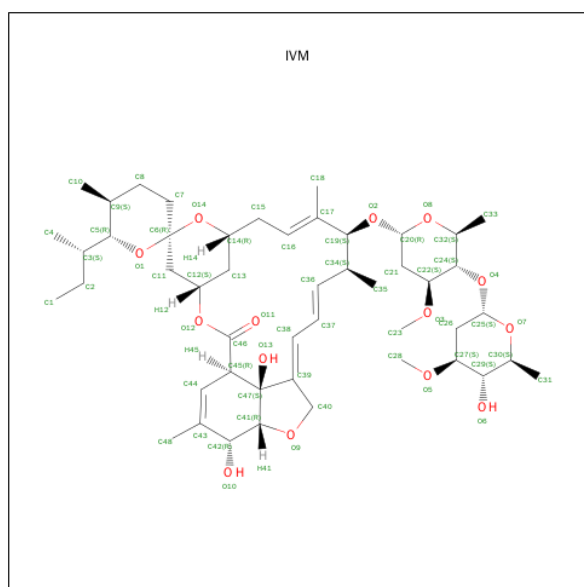


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	5	1	4		
4	B	1	Total	C	N	O	0	0
			10	5	1	4		
4	C	1	Total	C	N	O	0	0
			10	5	1	4		
4	D	1	Total	C	N	O	0	0
			10	5	1	4		
4	E	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is (2AE,4E,5'S,6S,6'R,7S,8E,11R,13R,15S,17AR,20R,20AR,20BS)-6'-[(2S)-BUTAN-2-YL]-20,20B-DIHYDROXY-5',6,8,19-TETRAMETHYL-17-OXO-3',4',5',6,6',10,11,14,15,17,17A,20,20A,20B-TETRADECAHYDRO-2H,7H-SPIRO[11,15-METHANOFURO[4,3,2-PQ][2,6]BENZODIOXACYCLOOCTADECINE-13,2'-PYRAN]-7-YL 2,6-DIDEOXY Y-4-O-(2,6-DIDEOXY-3-O-METHYL-ALPHA-L-ARABINO-HEXOPYRANOSYL)-3-O-METHYL-ALPHA-L-ARABINO-HEXOPYRANOSIDE (three-letter code: IVM) (formula: C₄₈H₇₄O₁₄).



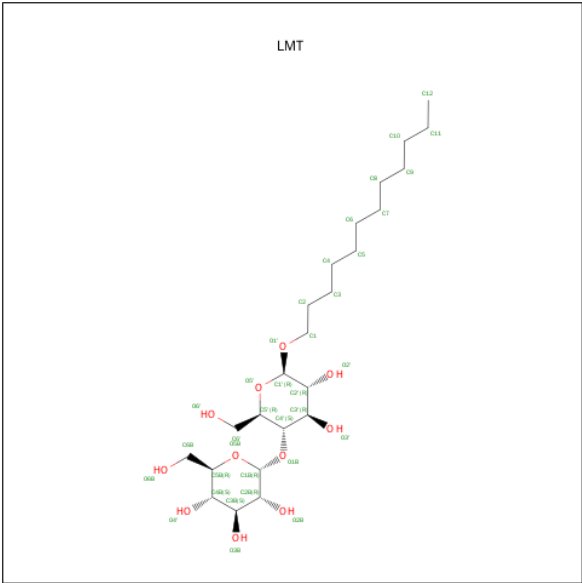
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			62	48	14		

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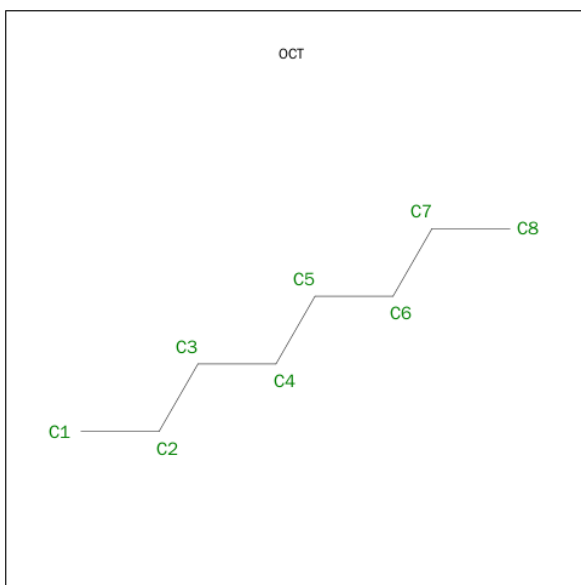
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			62	48	14		
6	D	1	Total	C	O	0	0
			62	48	14		
6	E	1	Total	C	O	0	0
			62	48	14		
6	A	1	Total	C	O	0	0
			62	48	14		

- Molecule 7 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



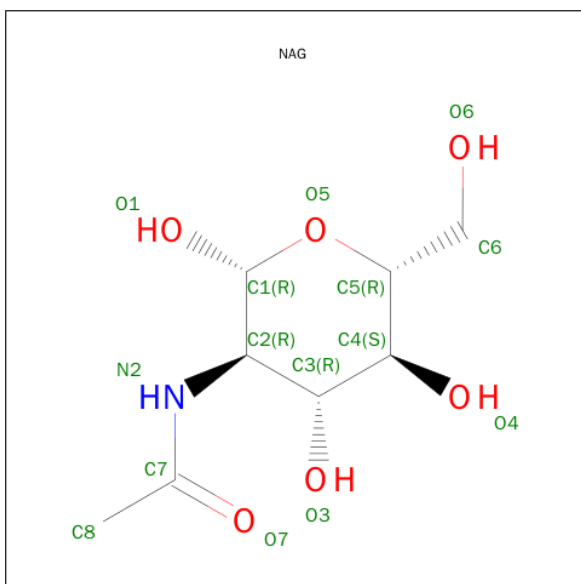
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			26	15	11		
7	B	1	Total	C	O	0	0
			26	15	11		
7	A	1	Total	C	O	0	0
			27	16	11		

- Molecule 8 is N-OCTANE (three-letter code: OCT) (formula: C₈H₁₈).



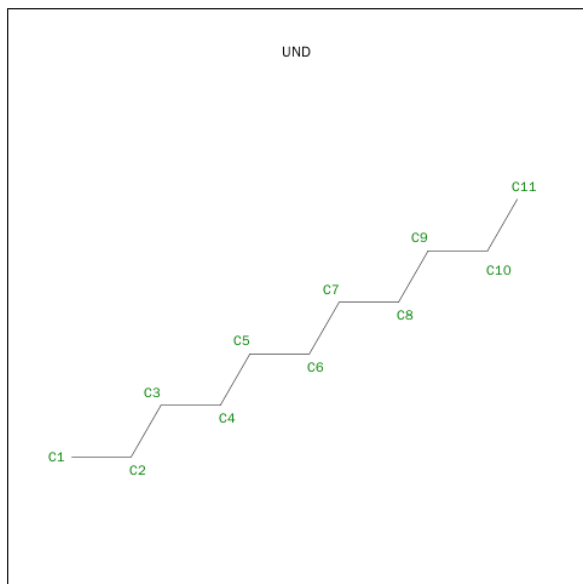
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total C 8 8	0	0
8	E	1	Total C 8 8	0	0
8	B	1	Total C 8 8	0	0

- Molecule 9 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

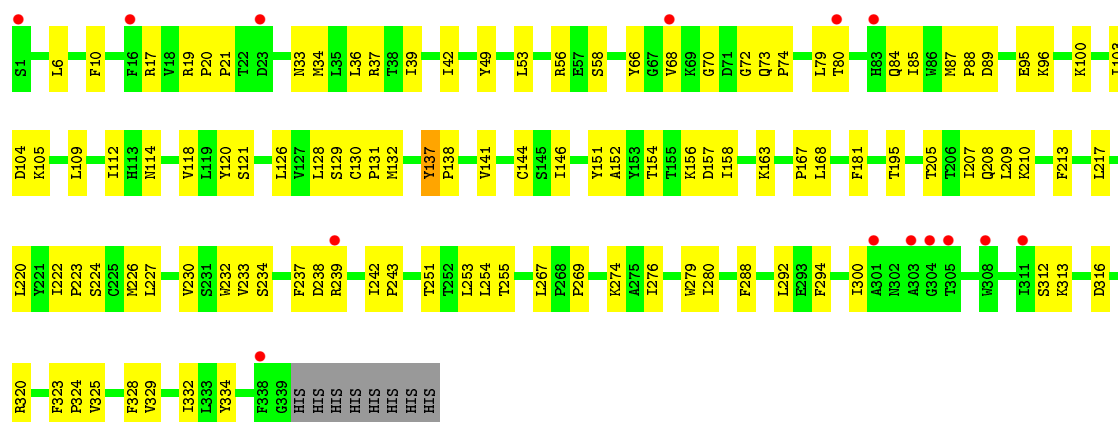


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	E	1	Total	C	N	O	0	0
			14	8	1	5		

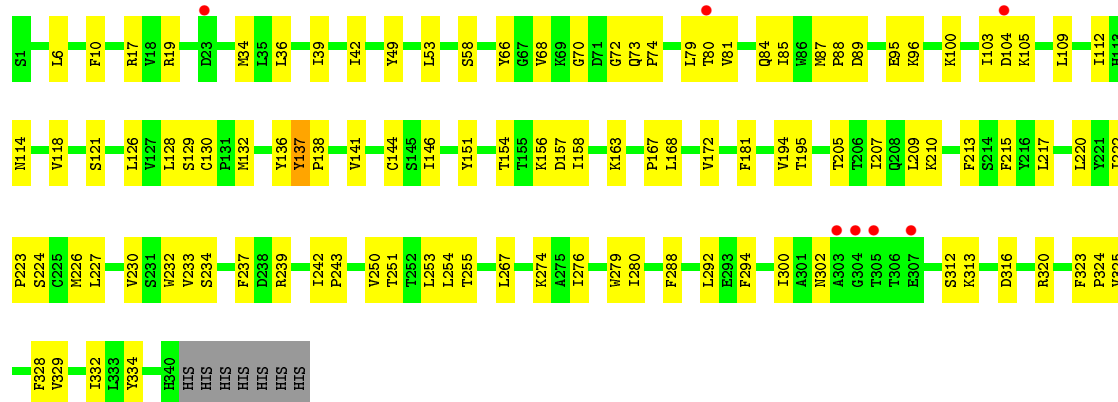
- Molecule 10 is UNDECANE (three-letter code: UND) (formula: C₁₁H₂₄).



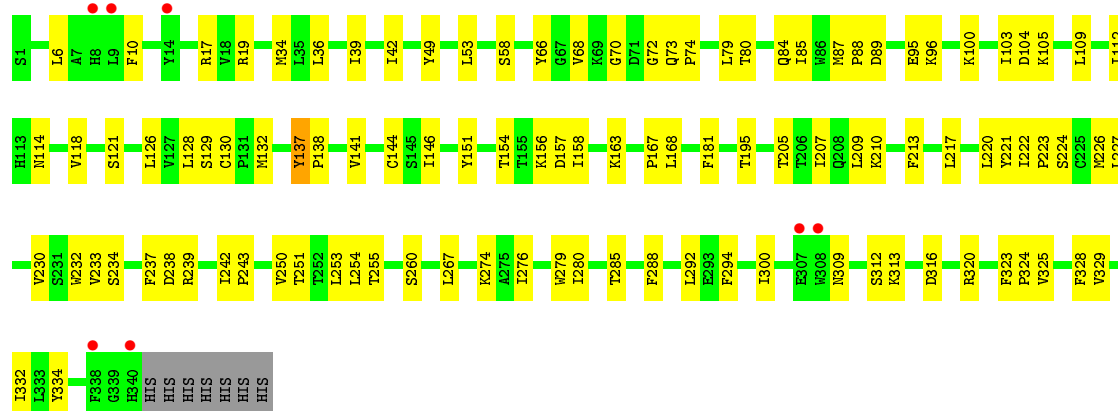
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	C	0	0
			11	11		



- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



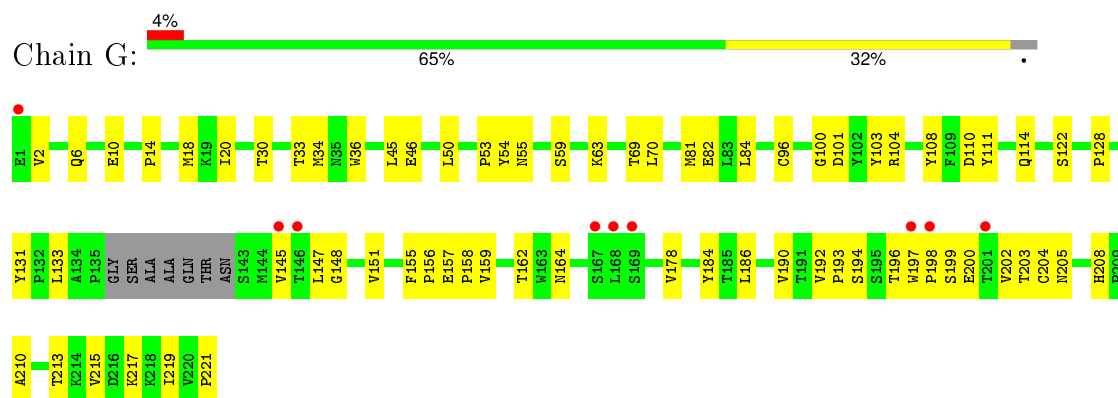
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



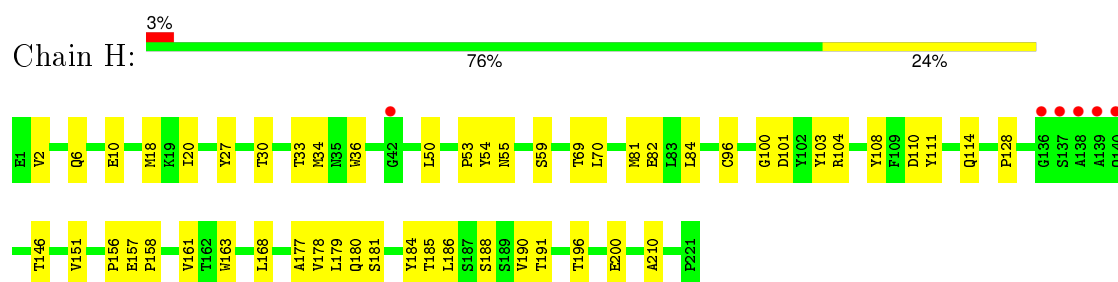
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



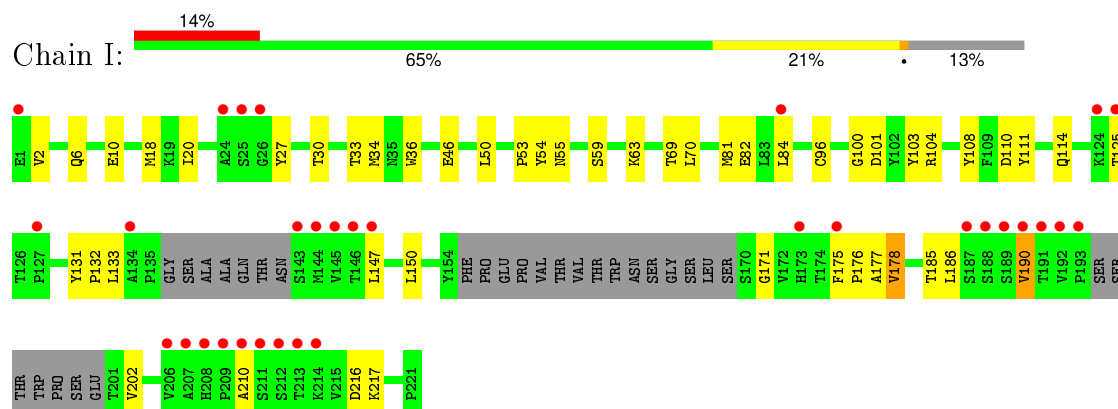
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

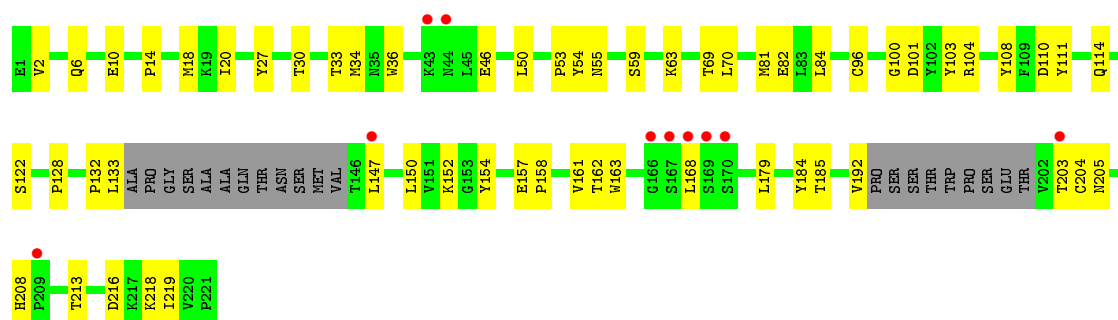


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

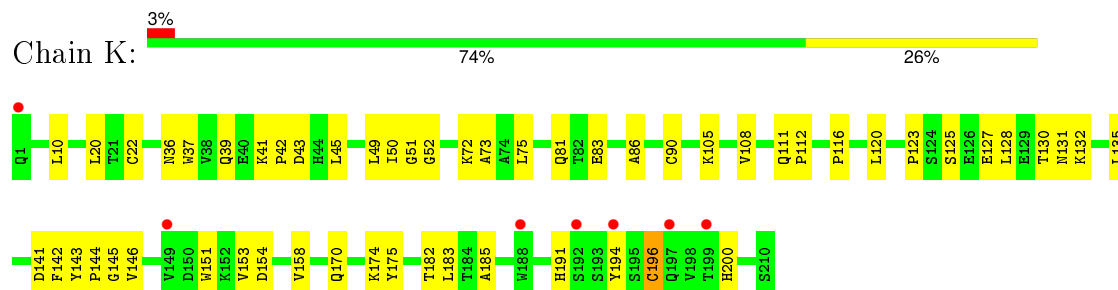


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

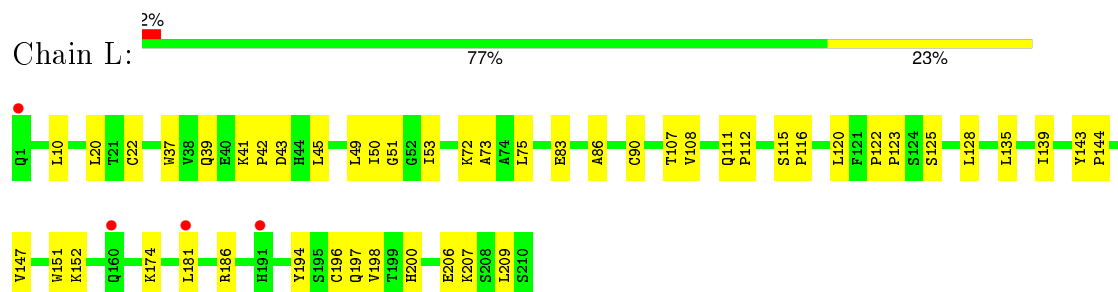




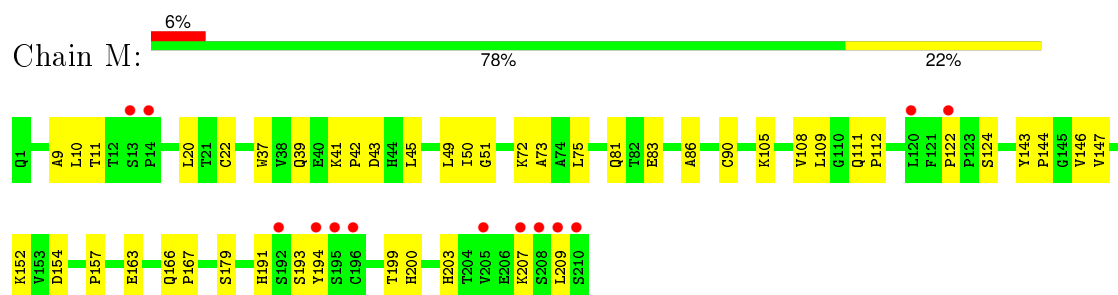
- Molecule 3: Mouse monoclonal Fab fragment, light chain



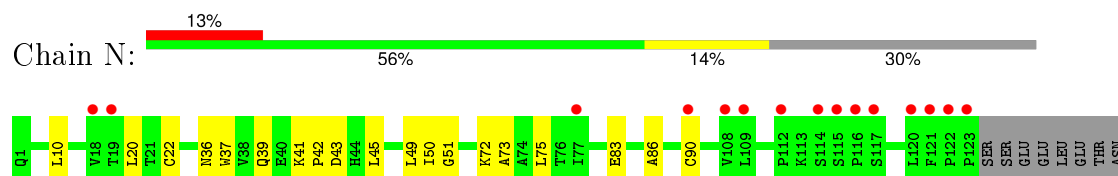
- Molecule 3: Mouse monoclonal Fab fragment, light chain



- Molecule 3: Mouse monoclonal Fab fragment, light chain

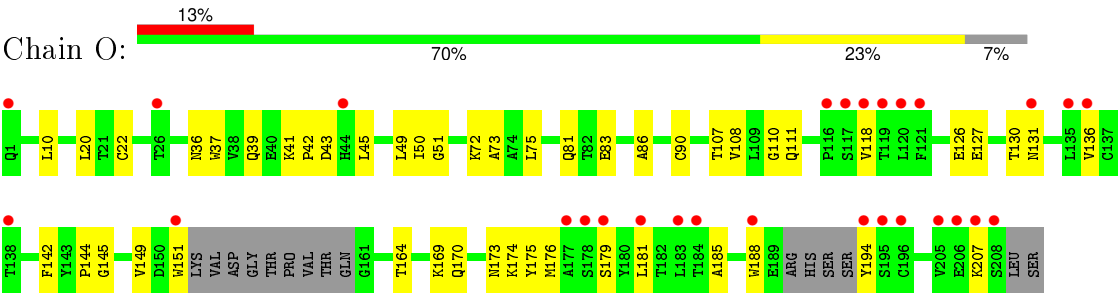


- Molecule 3: Mouse monoclonal Fab fragment, light chain





● Molecule 3: Mouse monoclonal Fab fragment, light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	155.44Å 155.44Å 575.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.73 – 3.35 39.73 – 3.34	Depositor EDS
% Data completeness (in resolution range)	93.0 (39.73-3.35) 99.4 (39.73-3.34)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.248 , 0.271 0.246 , 0.266	Depositor DCC
R_{free} test set	5138 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	87.8	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 43.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 102703 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	29020	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, IVM, LMT, UND, OCT

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	0.25	0/2793	0.39	0/3813
1	B	0.25	0/2793	0.39	0/3813
1	C	0.25	0/2782	0.39	0/3798
1	D	0.25	0/2793	0.39	0/3813
1	E	0.26	0/2793	0.39	0/3813
2	F	0.26	0/1359	0.41	0/1849
2	G	0.26	0/1676	0.44	0/2290
2	H	0.25	0/1721	0.42	0/2352
2	I	0.25	0/1501	0.41	0/2040
2	J	0.25	0/1565	0.41	0/2133
3	K	0.26	0/1617	0.43	0/2212
3	L	0.24	0/1629	0.43	0/2226
3	M	0.25	0/1614	0.42	0/2210
3	N	0.27	0/1098	0.42	0/1503
3	O	0.25	0/1504	0.42	0/2056
All	All	0.25	0/29238	0.41	0/39921

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

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	2720	0	2720	105	0
1	B	2720	0	2719	110	0
1	C	2710	0	2712	111	0
1	D	2720	0	2720	105	0
1	E	2720	0	2719	103	0
2	F	1324	0	1265	31	0
2	G	1631	0	1574	58	0
2	H	1675	0	1610	42	0
2	I	1466	0	1428	37	0
2	J	1526	0	1468	41	0
3	K	1579	0	1520	41	0
3	L	1591	0	1542	36	0
3	M	1576	0	1518	33	0
3	N	1075	0	1026	25	0
3	O	1470	0	1412	35	0
4	A	10	0	5	0	0
4	B	10	0	5	2	0
4	C	10	0	5	1	0
4	D	10	0	5	1	0
4	E	10	0	5	1	0
5	B	1	0	0	0	0
6	A	124	0	148	11	0
6	B	62	0	74	5	0
6	D	62	0	74	3	0
6	E	62	0	74	3	0
7	A	53	0	52	13	0
7	B	26	0	25	7	0
8	B	8	0	18	0	0
8	D	8	0	18	0	0
8	E	8	0	18	3	0
9	B	14	0	13	1	0
9	C	14	0	13	1	0
9	E	14	0	13	0	0
10	B	11	0	24	0	0
All	All	29020	0	28542	831	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 14.

All (831) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:HIS:CD2	7:A:404:LMT:H12	1.75	1.21
1:A:299:HIS:HD2	7:A:404:LMT:H12	1.25	0.97
1:B:100:LYS:HE2	1:C:104:ASP:H	1.27	0.96
1:D:89:ASP:HA	1:E:105:LYS:HG3	1.49	0.95
1:C:100:LYS:HE2	1:D:104:ASP:H	1.31	0.93
1:C:17:ARG:HB3	1:D:80:THR:HB	1.50	0.92
1:A:89:ASP:HA	1:B:105:LYS:HG3	1.57	0.87
1:A:104:ASP:H	1:E:100:LYS:HE2	1.39	0.87
3:L:107:THR:HG21	3:L:144:PRO:HB3	1.58	0.86
1:B:17:ARG:HB3	1:C:80:THR:HB	1.58	0.86
1:D:100:LYS:HE2	1:E:104:ASP:H	1.40	0.83
3:K:131:ASN:HA	3:K:185:ALA:HB2	1.61	0.83
1:B:195:THR:HA	2:F:55:ASN:HD21	1.43	0.82
1:A:80:THR:HB	1:E:17:ARG:HB3	1.63	0.81
1:A:105:LYS:HG3	1:E:89:ASP:HA	1.62	0.81
3:K:131:ASN:C	3:K:185:ALA:HB2	2.02	0.80
3:K:131:ASN:CA	3:K:185:ALA:HB2	2.11	0.79
1:B:195:THR:HA	2:F:55:ASN:ND2	1.98	0.78
7:A:404:LMT:H11	7:B:404:LMT:H2'	1.67	0.77
2:G:157:GLU:HB3	2:G:158:PRO:HA	1.67	0.76
1:A:100:LYS:HE2	1:B:104:ASP:H	1.50	0.76
3:L:125:SER:HA	3:L:128:LEU:HD12	1.67	0.76
1:B:100:LYS:HE2	1:C:104:ASP:N	2.00	0.76
2:F:208:HIS:HD2	2:F:211:SER:H	1.34	0.75
1:C:100:LYS:HE2	1:D:104:ASP:N	2.01	0.75
1:E:195:THR:HA	2:J:55:ASN:ND2	2.01	0.74
3:L:152:LYS:HD3	3:L:197:GLN:NE2	2.01	0.74
3:L:206:GLU:O	3:L:207:LYS:HD2	1.86	0.74
2:G:164:ASN:HD21	2:G:202:VAL:HG22	1.53	0.74
1:E:226:MET:HG3	6:E:402:IVM:H11A	1.70	0.74
3:L:139:ILE:HD12	3:L:198:VAL:HG21	1.70	0.74
2:J:128:PRO:HB3	2:J:154:TYR:HB3	1.69	0.73
1:D:226:MET:HG3	6:D:402:IVM:H11A	1.71	0.72
3:O:149:VAL:HB	3:O:164:THR:HG21	1.70	0.72
3:O:118:VAL:O	3:O:207:LYS:HE3	1.89	0.72
1:B:302:ASN:ND2	1:C:238:ASP:HB3	2.05	0.72
7:A:404:LMT:H1'	7:B:404:LMT:O3'	1.89	0.71
1:B:89:ASP:HA	1:C:105:LYS:HG3	1.71	0.71
1:E:195:THR:HA	2:J:55:ASN:HD21	1.54	0.71
2:G:164:ASN:OD1	2:G:202:VAL:HG13	1.89	0.70
3:N:169:LYS:NZ	3:N:169:LYS:HB3	2.07	0.70
3:L:122:PRO:HB3	3:L:209:LEU:HD11	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:ASP:HA	1:D:105:LYS:HG3	1.72	0.70
1:D:17:ARG:HB3	1:E:80:THR:HB	1.73	0.70
1:A:210:LYS:CE	7:A:405:LMT:O3B	2.40	0.69
1:A:195:THR:HA	2:H:55:ASN:ND2	2.08	0.68
1:A:195:THR:HA	2:H:55:ASN:HD21	1.58	0.68
1:D:195:THR:HA	2:I:55:ASN:ND2	2.08	0.68
1:D:195:THR:HA	2:I:55:ASN:HD21	1.58	0.68
1:D:224:SER:HB2	1:D:279:TRP:CH2	2.29	0.68
1:B:224:SER:HB2	1:B:279:TRP:CH2	2.29	0.67
1:B:250:VAL:CG1	1:C:251:THR:HG21	2.24	0.67
1:D:85:ILE:HD11	1:D:112:ILE:HD11	1.76	0.67
1:C:224:SER:HB2	1:C:279:TRP:CH2	2.29	0.67
3:L:120:LEU:HD12	3:L:196:CYS:HB3	1.77	0.67
1:B:151:TYR:O	4:B:401:GLU:HB2	1.93	0.67
1:D:151:TYR:O	4:D:401:GLU:HB2	1.95	0.67
3:O:39:GLN:HB2	3:O:49:LEU:HD21	1.76	0.67
1:E:224:SER:HB2	1:E:279:TRP:CH2	2.30	0.67
3:L:39:GLN:HB2	3:L:49:LEU:HD21	1.77	0.67
6:B:403:IVM:H11A	1:C:226:MET:HG3	1.75	0.66
3:K:39:GLN:HB2	3:K:49:LEU:HD21	1.77	0.66
3:K:132:LYS:NZ	3:K:182:THR:HG23	2.11	0.66
1:A:224:SER:HB2	1:A:279:TRP:CH2	2.30	0.66
3:M:39:GLN:HB2	3:M:49:LEU:HD21	1.76	0.66
1:C:100:LYS:CE	1:D:104:ASP:HA	2.26	0.66
3:N:39:GLN:HB2	3:N:49:LEU:HD21	1.76	0.66
1:A:42:ILE:HD13	1:A:209:LEU:HD13	1.76	0.66
1:D:79:LEU:HD22	1:D:85:ILE:HD12	1.78	0.66
1:D:42:ILE:HD13	1:D:209:LEU:HD13	1.77	0.66
1:D:288:PHE:CE2	1:D:292:LEU:HD11	2.31	0.65
3:N:139:ILE:HB	3:N:177:ALA:HB3	1.77	0.65
1:E:42:ILE:HD13	1:E:209:LEU:HD13	1.77	0.65
1:A:137:TYR:HB3	1:A:138:PRO:HD3	1.77	0.65
1:A:104:ASP:N	1:E:100:LYS:HE2	2.10	0.65
3:L:122:PRO:HB3	3:L:209:LEU:CD1	2.26	0.65
1:A:299:HIS:NE2	7:A:404:LMT:H12	2.09	0.65
1:E:288:PHE:CE2	1:E:292:LEU:HD11	2.32	0.65
3:O:170:GLN:OE1	3:O:176:MET:HB3	1.96	0.65
1:B:42:ILE:HD13	1:B:209:LEU:HD13	1.78	0.65
1:B:85:ILE:HD11	1:B:112:ILE:HD11	1.78	0.65
1:A:85:ILE:HD11	1:A:112:ILE:HD11	1.78	0.65
1:D:100:LYS:HE2	1:E:104:ASP:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ILE:HD13	1:C:209:LEU:HD13	1.77	0.65
1:A:288:PHE:CE2	1:A:292:LEU:HD11	2.31	0.65
1:E:85:ILE:HD11	1:E:112:ILE:HD11	1.78	0.65
1:C:85:ILE:HD11	1:C:112:ILE:HD11	1.79	0.64
1:A:210:LYS:NZ	7:A:405:LMT:O3B	2.31	0.64
1:C:288:PHE:CE2	1:C:292:LEU:HD11	2.33	0.64
6:B:403:IVM:H4B	1:C:226:MET:HB2	1.79	0.64
1:C:195:THR:HA	2:G:55:ASN:ND2	2.13	0.64
3:K:170:GLN:HG2	3:K:174:LYS:O	1.99	0.63
1:A:79:LEU:HD22	1:A:85:ILE:HD12	1.81	0.63
1:B:288:PHE:CE2	1:B:292:LEU:HD11	2.33	0.63
2:J:147:LEU:HD22	2:J:219:ILE:HG21	1.79	0.63
7:A:404:LMT:H6'2	7:B:404:LMT:O4'	1.98	0.63
1:E:79:LEU:HD22	1:E:85:ILE:HD12	1.81	0.63
1:C:79:LEU:HD22	1:C:85:ILE:HD12	1.81	0.63
2:H:6:GLN:H	2:H:114:GLN:HE22	1.47	0.63
3:L:135:LEU:HB2	3:L:181:LEU:HB3	1.80	0.62
1:A:226:MET:HB2	6:A:403:IVM:H4B	1.81	0.62
1:B:100:LYS:CE	1:C:104:ASP:HA	2.29	0.62
1:B:79:LEU:HD22	1:B:85:ILE:HD12	1.81	0.62
3:N:167:PRO:HA	3:N:176:MET:O	1.99	0.62
3:K:111:GLN:HG3	3:K:112:PRO:HD2	1.81	0.62
2:G:6:GLN:H	2:G:114:GLN:HE22	1.48	0.62
3:O:41:LYS:HE2	3:O:83:GLU:O	2.00	0.62
1:A:210:LYS:HE2	7:A:405:LMT:O3B	2.00	0.61
7:A:404:LMT:C6'	7:A:404:LMT:H1B	2.29	0.61
1:B:250:VAL:HG13	1:C:251:THR:HG21	1.83	0.61
3:M:41:LYS:HE2	3:M:83:GLU:O	2.01	0.61
1:E:137:TYR:HB3	1:E:138:PRO:HD3	1.83	0.61
3:N:41:LYS:HE2	3:N:83:GLU:O	2.00	0.61
1:D:137:TYR:HB3	1:D:138:PRO:HD3	1.82	0.61
1:A:17:ARG:HB3	1:B:80:THR:HB	1.83	0.60
2:J:6:GLN:H	2:J:114:GLN:HE22	1.48	0.60
1:A:19:ARG:HH11	1:A:157:ASP:HA	1.66	0.60
1:C:137:TYR:HB3	1:C:138:PRO:HD3	1.83	0.60
3:L:41:LYS:HE2	3:L:83:GLU:O	2.00	0.60
2:I:6:GLN:H	2:I:114:GLN:HE22	1.49	0.60
1:D:19:ARG:HH11	1:D:157:ASP:HA	1.66	0.60
2:F:208:HIS:CD2	2:F:211:SER:H	2.16	0.60
3:K:41:LYS:HE2	3:K:83:GLU:O	2.01	0.60
2:H:157:GLU:HG3	2:H:184:TYR:CD2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:ILE:HD11	1:D:294:PHE:HB3	1.82	0.60
1:A:104:ASP:HA	1:E:100:LYS:CE	2.31	0.60
1:E:19:ARG:HH11	1:E:157:ASP:HA	1.66	0.60
1:B:302:ASN:HD22	1:C:238:ASP:HB3	1.65	0.60
1:B:19:ARG:HH11	1:B:157:ASP:HA	1.67	0.60
1:E:242:ILE:HD11	1:E:294:PHE:HB3	1.83	0.60
2:G:162:THR:OG1	2:G:205:ASN:HB2	2.02	0.60
1:D:87:MET:O	1:E:105:LYS:NZ	2.35	0.59
1:B:137:TYR:HB3	1:B:138:PRO:HD3	1.82	0.59
1:A:242:ILE:HD11	1:A:294:PHE:HB3	1.84	0.59
1:B:88:PRO:HB3	1:B:158:ILE:HD11	1.85	0.59
1:B:17:ARG:HB3	1:C:80:THR:CB	2.31	0.59
1:C:19:ARG:HH11	1:C:157:ASP:HA	1.66	0.59
1:B:242:ILE:HD11	1:B:294:PHE:HB3	1.84	0.59
1:C:17:ARG:HB3	1:D:80:THR:CB	2.28	0.59
2:H:179:LEU:HD13	2:H:184:TYR:CE1	2.36	0.59
1:C:88:PRO:HB3	1:C:158:ILE:HD11	1.85	0.59
1:C:151:TYR:O	4:C:401:GLU:HB2	2.03	0.59
1:D:88:PRO:HB3	1:D:158:ILE:HD11	1.85	0.58
1:C:195:THR:HA	2:G:55:ASN:HD21	1.68	0.58
2:J:203:THR:HA	2:J:218:LYS:HA	1.85	0.58
2:H:156:PRO:HD2	2:H:210:ALA:CB	2.33	0.58
1:A:253:LEU:HD11	1:B:226:MET:CE	2.34	0.58
2:F:6:GLN:H	2:F:114:GLN:HE22	1.50	0.58
1:C:242:ILE:HD11	1:C:294:PHE:HB3	1.85	0.58
3:M:147:VAL:HG12	3:M:200:HIS:HB2	1.84	0.58
1:E:224:SER:HB2	1:E:279:TRP:HH2	1.69	0.58
1:E:234:SER:HA	1:E:237:PHE:HD2	1.69	0.58
1:D:234:SER:HA	1:D:237:PHE:HD2	1.68	0.58
1:B:234:SER:HA	1:B:237:PHE:HD2	1.69	0.58
1:D:36:LEU:HD23	1:D:39:ILE:HD11	1.86	0.58
2:G:131:TYR:CD1	3:K:127:GLU:HB3	2.39	0.58
1:D:224:SER:HB2	1:D:279:TRP:HH2	1.68	0.57
1:B:73:GLN:HB3	1:B:74:PRO:HD2	1.86	0.57
1:B:320:ARG:NH1	7:B:404:LMT:H6D	2.19	0.57
1:A:224:SER:HB2	1:A:279:TRP:HH2	1.69	0.57
1:C:234:SER:HA	1:C:237:PHE:HD2	1.70	0.57
3:K:131:ASN:HA	3:K:185:ALA:CB	2.34	0.57
3:O:169:LYS:HA	3:O:175:TYR:HA	1.86	0.57
1:A:234:SER:HA	1:A:237:PHE:HD2	1.69	0.57
1:A:88:PRO:HB3	1:A:158:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:50:ILE:HG22	3:K:51:GLY:H	1.69	0.57
1:E:88:PRO:HB3	1:E:158:ILE:HD11	1.85	0.57
1:B:224:SER:HB2	1:B:279:TRP:HH2	1.68	0.57
1:E:36:LEU:HD23	1:E:39:ILE:HD11	1.87	0.57
3:M:22:CYS:CB	3:M:90:CYS:SG	2.93	0.57
3:M:50:ILE:HG22	3:M:51:GLY:H	1.69	0.57
1:B:36:LEU:HD23	1:B:39:ILE:HD11	1.86	0.57
6:A:403:IVM:C18	8:E:403:OCT:H61	2.35	0.56
2:J:50:LEU:CD2	2:J:59:SER:HB3	2.35	0.56
3:O:50:ILE:HG22	3:O:51:GLY:H	1.70	0.56
3:N:50:ILE:HG22	3:N:51:GLY:H	1.70	0.56
7:A:404:LMT:H6E	7:A:404:LMT:H1B	1.87	0.56
2:I:50:LEU:CD2	2:I:59:SER:HB3	2.34	0.56
1:A:325:VAL:O	1:A:329:VAL:HG23	2.05	0.56
1:C:325:VAL:O	1:C:329:VAL:HG23	2.05	0.56
3:M:199:THR:HG23	3:M:203:HIS:O	2.06	0.56
1:C:73:GLN:HB3	1:C:74:PRO:HD2	1.85	0.56
3:K:132:LYS:HZ1	3:K:182:THR:HG23	1.69	0.56
1:A:36:LEU:HD23	1:A:39:ILE:HD11	1.87	0.56
1:C:36:LEU:HD23	1:C:39:ILE:HD11	1.87	0.56
2:H:50:LEU:CD2	2:H:59:SER:HB3	2.35	0.56
1:C:224:SER:HB2	1:C:279:TRP:HH2	1.68	0.56
2:G:50:LEU:CD2	2:G:59:SER:HB3	2.35	0.56
1:C:120:TYR:OH	1:D:104:ASP:OD1	2.19	0.56
2:G:203:THR:HG23	2:G:217:LYS:C	2.26	0.56
2:J:110:ASP:HB3	2:J:111:TYR:CD2	2.41	0.56
3:L:50:ILE:HG22	3:L:51:GLY:H	1.71	0.56
1:E:325:VAL:O	1:E:329:VAL:HG23	2.05	0.56
3:O:151:TRP:CE3	3:O:181:LEU:HD12	2.41	0.56
2:J:132:PRO:O	3:M:124:SER:HB3	2.06	0.56
2:G:197:TRP:HZ2	2:G:219:ILE:O	1.88	0.56
3:L:108:VAL:O	3:L:143:TYR:OH	2.24	0.56
2:F:50:LEU:CD2	2:F:59:SER:HB3	2.35	0.56
3:M:37:TRP:CE2	3:M:75:LEU:HB2	2.41	0.56
6:A:403:IVM:H18	8:E:403:OCT:H61	1.88	0.56
1:B:128:LEU:HD13	1:B:146:ILE:HG12	1.88	0.56
1:E:73:GLN:HB3	1:E:74:PRO:HD2	1.87	0.56
1:B:325:VAL:O	1:B:329:VAL:HG23	2.07	0.55
1:E:232:TRP:CH2	1:E:324:PRO:HA	2.41	0.55
1:B:232:TRP:CH2	1:B:324:PRO:HA	2.41	0.55
3:K:153:VAL:HG22	3:K:194:TYR:HD2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:37:TRP:CE2	3:L:75:LEU:HB2	2.41	0.55
1:D:325:VAL:O	1:D:329:VAL:HG23	2.06	0.55
3:N:37:TRP:CE2	3:N:75:LEU:HB2	2.41	0.55
1:A:73:GLN:HB3	1:A:74:PRO:HD2	1.86	0.55
1:C:230:VAL:O	1:C:233:VAL:HG22	2.07	0.55
3:L:107:THR:HG21	3:L:144:PRO:CB	2.34	0.55
1:C:232:TRP:CH2	1:C:324:PRO:HA	2.42	0.55
1:B:194:VAL:HG13	2:F:52:ASN:HD22	1.71	0.55
1:B:100:LYS:HZ1	1:C:104:ASP:HA	1.72	0.55
2:I:147:LEU:HD12	2:I:202:VAL:HG11	1.88	0.55
3:L:152:LYS:HD3	3:L:197:GLN:HE21	1.68	0.55
2:G:208:HIS:CE1	2:G:210:ALA:HB3	2.41	0.55
2:J:33:THR:HA	2:J:53:PRO:HD3	1.89	0.55
1:C:239:ARG:CZ	1:C:313:LYS:HG2	2.37	0.55
2:G:33:THR:HA	2:G:53:PRO:HD3	1.89	0.55
2:H:110:ASP:HB3	2:H:111:TYR:CD2	2.42	0.55
1:E:230:VAL:O	1:E:233:VAL:HG22	2.07	0.55
1:A:100:LYS:HE2	1:B:104:ASP:N	2.19	0.54
1:D:73:GLN:HB3	1:D:74:PRO:HD2	1.88	0.54
2:G:192:VAL:HG23	2:G:193:PRO:O	2.05	0.54
1:D:232:TRP:CH2	1:D:324:PRO:HA	2.42	0.54
2:G:110:ASP:HB3	2:G:111:TYR:CD2	2.42	0.54
7:A:404:LMT:H11	7:B:404:LMT:C2'	2.36	0.54
2:J:128:PRO:HD3	2:J:208:HIS:ND1	2.22	0.54
3:K:37:TRP:CE2	3:K:75:LEU:HB2	2.42	0.54
2:F:110:ASP:HB3	2:F:111:TYR:CD2	2.42	0.54
1:A:220:LEU:HD11	1:A:280:ILE:HD11	1.89	0.54
2:I:33:THR:HA	2:I:53:PRO:HD3	1.90	0.54
1:A:239:ARG:CZ	1:A:313:LYS:HG2	2.37	0.54
1:A:232:TRP:CH2	1:A:324:PRO:HA	2.41	0.54
2:J:133:LEU:HD21	2:J:150:LEU:HB2	1.90	0.54
2:H:33:THR:HA	2:H:53:PRO:HD3	1.90	0.54
1:C:79:LEU:HD13	1:C:112:ILE:HD11	1.90	0.54
2:H:50:LEU:HD21	2:H:59:SER:HB3	1.90	0.54
1:C:220:LEU:HD11	1:C:280:ILE:HD11	1.90	0.54
2:J:14:PRO:HD2	2:J:122:SER:HB3	1.90	0.54
3:O:107:THR:HG21	3:O:144:PRO:HB3	1.90	0.54
1:B:253:LEU:HD11	1:C:226:MET:CE	2.37	0.54
2:F:33:THR:HA	2:F:53:PRO:HD3	1.89	0.54
2:I:110:ASP:HB3	2:I:111:TYR:CD2	2.42	0.54
2:H:156:PRO:HD2	2:H:210:ALA:HB1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:50:LEU:HD21	2:I:59:SER:HB3	1.90	0.54
3:M:122:PRO:HG3	3:M:209:LEU:HD11	1.90	0.54
1:D:220:LEU:HD11	1:D:280:ILE:HD11	1.90	0.54
1:B:239:ARG:CZ	1:B:313:LYS:HG2	2.38	0.54
1:E:128:LEU:HD13	1:E:146:ILE:HG12	1.89	0.54
3:O:37:TRP:CE2	3:O:75:LEU:HB2	2.42	0.54
1:A:288:PHE:CD2	6:A:402:IVM:H8A	2.42	0.53
2:G:147:LEU:O	2:G:190:VAL:HG12	2.08	0.53
2:G:213:THR:HG22	2:G:215:VAL:HG23	1.89	0.53
2:F:175:PHE:CD1	3:N:178:SER:HB3	2.43	0.53
1:D:254:LEU:HD12	1:E:251:THR:HG23	1.90	0.53
1:A:230:VAL:O	1:A:233:VAL:HG22	2.08	0.53
1:B:320:ARG:HH11	7:B:404:LMT:H6D	1.73	0.53
1:D:128:LEU:HD13	1:D:146:ILE:HG12	1.89	0.53
1:B:100:LYS:NZ	1:C:104:ASP:HA	2.23	0.53
2:I:177:ALA:HB2	2:I:186:LEU:HD23	1.90	0.53
1:B:220:LEU:HD11	1:B:280:ILE:HD11	1.90	0.53
1:E:79:LEU:HD13	1:E:112:ILE:HD11	1.91	0.53
1:B:242:ILE:N	1:B:243:PRO:CD	2.72	0.53
1:E:220:LEU:HD11	1:E:280:ILE:HD11	1.90	0.53
2:J:69:THR:HB	2:J:82:GLU:HB2	1.90	0.53
1:A:128:LEU:HD13	1:A:146:ILE:HG12	1.89	0.53
2:J:162:THR:OG1	2:J:205:ASN:HB2	2.08	0.53
1:C:128:LEU:HD13	1:C:146:ILE:HG12	1.88	0.53
1:B:66:TYR:CE2	1:B:114:ASN:HA	2.44	0.53
2:I:69:THR:HB	2:I:82:GLU:HB2	1.91	0.53
1:B:254:LEU:HD12	1:C:251:THR:HG23	1.91	0.53
1:B:230:VAL:O	1:B:233:VAL:HG22	2.09	0.53
1:D:239:ARG:CZ	1:D:313:LYS:HG2	2.39	0.53
1:E:242:ILE:N	1:E:243:PRO:CD	2.72	0.53
2:F:50:LEU:HD21	2:F:59:SER:HB3	1.90	0.53
1:E:239:ARG:CZ	1:E:313:LYS:HG2	2.38	0.53
1:A:79:LEU:HD13	1:A:112:ILE:HD11	1.91	0.53
1:B:126:LEU:HD13	1:B:128:LEU:HD21	1.91	0.53
2:J:179:LEU:HD13	2:J:184:TYR:CE1	2.44	0.53
1:D:100:LYS:CE	1:E:104:ASP:HA	2.38	0.53
1:D:230:VAL:O	1:D:233:VAL:HG22	2.09	0.53
2:H:186:LEU:C	2:H:186:LEU:HD12	2.29	0.53
1:C:87:MET:O	1:D:105:LYS:NZ	2.42	0.52
2:G:50:LEU:HD21	2:G:59:SER:HB3	1.91	0.52
2:G:69:THR:HB	2:G:82:GLU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:22:CYS:O	3:M:72:LYS:HB2	2.09	0.52
1:A:100:LYS:CE	1:B:104:ASP:HA	2.39	0.52
1:B:79:LEU:HD13	1:B:112:ILE:HD11	1.91	0.52
1:A:242:ILE:N	1:A:243:PRO:CD	2.72	0.52
1:C:163:LYS:O	1:C:167:PRO:HG3	2.09	0.52
1:D:79:LEU:HD13	1:D:112:ILE:HD11	1.92	0.52
2:I:131:TYR:CD2	3:O:127:GLU:HG2	2.45	0.52
1:A:163:LYS:O	1:A:167:PRO:HG3	2.10	0.52
3:L:123:PRO:HD3	3:L:135:LEU:HD13	1.90	0.52
2:F:2:VAL:HG21	2:F:111:TYR:CD2	2.45	0.52
1:D:250:VAL:CG1	1:E:251:THR:HG21	2.40	0.52
1:E:163:LYS:O	1:E:167:PRO:HG3	2.09	0.52
1:D:242:ILE:N	1:D:243:PRO:CD	2.73	0.52
2:J:2:VAL:HG21	2:J:111:TYR:CD2	2.45	0.52
1:A:80:THR:CB	1:E:17:ARG:HB3	2.38	0.52
2:J:50:LEU:HD21	2:J:59:SER:HB3	1.91	0.52
1:C:66:TYR:CE2	1:C:114:ASN:HA	2.45	0.52
3:N:172:ASN:O	3:N:173:ASN:HB2	2.10	0.52
2:H:2:VAL:HG21	2:H:111:TYR:CD2	2.45	0.52
1:D:126:LEU:HD13	1:D:128:LEU:HD21	1.92	0.52
1:D:234:SER:HA	1:D:237:PHE:CD2	2.45	0.52
1:C:126:LEU:HD13	1:C:128:LEU:HD21	1.92	0.52
1:A:105:LYS:NZ	1:E:87:MET:O	2.43	0.51
1:A:234:SER:HA	1:A:237:PHE:CD2	2.45	0.51
1:B:234:SER:HA	1:B:237:PHE:CD2	2.45	0.51
3:K:50:ILE:HG22	3:K:51:GLY:N	2.25	0.51
1:D:163:LYS:O	1:D:167:PRO:HG3	2.10	0.51
3:O:42:PRO:O	3:O:43:ASP:HB2	2.10	0.51
3:L:22:CYS:O	3:L:72:LYS:HB2	2.10	0.51
1:A:66:TYR:CE2	1:A:114:ASN:HA	2.45	0.51
2:I:2:VAL:HG21	2:I:111:TYR:CD2	2.45	0.51
3:O:142:PHE:HE1	3:O:145:GLY:HA2	1.74	0.51
2:F:69:THR:HB	2:F:82:GLU:HB2	1.90	0.51
2:F:133:LEU:HD11	2:F:150:LEU:HB2	1.93	0.51
3:L:111:GLN:HB2	3:L:112:PRO:HD2	1.93	0.51
3:O:22:CYS:O	3:O:72:LYS:HB2	2.11	0.51
2:H:69:THR:HB	2:H:82:GLU:HB2	1.92	0.51
1:C:242:ILE:N	1:C:243:PRO:CD	2.73	0.51
1:E:66:TYR:CE2	1:E:114:ASN:HA	2.45	0.51
2:J:168:LEU:HD21	2:J:192:VAL:HG12	1.91	0.51
3:K:22:CYS:O	3:K:72:LYS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:169:LYS:HZ3	3:N:169:LYS:HB3	1.74	0.51
3:M:50:ILE:HG22	3:M:51:GLY:N	2.25	0.51
2:G:203:THR:HG23	2:G:217:LYS:O	2.11	0.51
1:C:100:LYS:HZ1	1:D:104:ASP:HA	1.75	0.51
1:E:234:SER:HA	1:E:237:PHE:CD2	2.46	0.51
1:B:163:LYS:O	1:B:167:PRO:HG3	2.11	0.51
1:E:226:MET:HB2	6:E:402:IVM:H4B	1.93	0.50
1:D:66:TYR:CE2	1:D:114:ASN:HA	2.45	0.50
1:E:126:LEU:HD13	1:E:128:LEU:HD21	1.92	0.50
3:M:111:GLN:HB2	3:M:112:PRO:HD2	1.92	0.50
1:A:104:ASP:HA	1:E:100:LYS:HZ1	1.77	0.50
1:E:96:LYS:HD2	1:E:129:SER:HB3	1.94	0.50
1:B:96:LYS:HD2	1:B:129:SER:HB3	1.94	0.50
3:M:22:CYS:HB2	3:M:90:CYS:SG	2.52	0.50
6:A:403:IVM:H48B	1:E:260:SER:HB3	1.91	0.50
1:C:234:SER:HA	1:C:237:PHE:CD2	2.46	0.50
2:I:30:THR:HA	2:I:53:PRO:HB2	1.94	0.50
1:C:96:LYS:HD2	1:C:129:SER:HB3	1.93	0.50
2:G:196:THR:O	2:G:200:GLU:HB3	2.10	0.50
3:M:42:PRO:O	3:M:43:ASP:HB2	2.12	0.50
1:A:39:ILE:HD13	1:A:207:ILE:CD1	2.42	0.50
1:A:126:LEU:HD13	1:A:128:LEU:HD21	1.92	0.50
3:L:42:PRO:O	3:L:43:ASP:HB2	2.11	0.50
3:K:42:PRO:O	3:K:43:ASP:HB2	2.11	0.50
3:O:50:ILE:HG22	3:O:51:GLY:N	2.27	0.50
2:G:197:TRP:CZ2	2:G:219:ILE:O	2.64	0.50
3:M:105:LYS:HD2	3:M:146:VAL:HG22	1.93	0.50
1:D:224:SER:HB2	1:D:279:TRP:CZ3	2.47	0.50
2:G:178:VAL:O	2:G:184:TYR:HA	2.12	0.49
2:G:203:THR:HG22	2:G:204:CYS:N	2.26	0.49
2:G:186:LEU:HD12	2:G:186:LEU:C	2.32	0.49
1:D:96:LYS:HD2	1:D:129:SER:HB3	1.94	0.49
1:E:39:ILE:HD13	1:E:207:ILE:CD1	2.42	0.49
1:B:39:ILE:HD13	1:B:207:ILE:CD1	2.42	0.49
1:B:128:LEU:CD1	1:B:146:ILE:HG12	2.42	0.49
3:N:22:CYS:O	3:N:72:LYS:HB2	2.11	0.49
3:N:50:ILE:HG22	3:N:51:GLY:N	2.26	0.49
3:L:50:ILE:HG22	3:L:51:GLY:N	2.27	0.49
2:G:2:VAL:HG21	2:G:111:TYR:CD2	2.47	0.49
3:K:125:SER:HA	3:K:128:LEU:HD12	1.94	0.49
1:C:17:ARG:HD2	1:D:81:VAL:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:LEU:CD1	1:C:146:ILE:HG12	2.43	0.49
2:H:177:ALA:HA	2:H:186:LEU:HB3	1.93	0.49
1:D:253:LEU:HD11	1:E:226:MET:CE	2.43	0.49
1:E:224:SER:HB2	1:E:279:TRP:CZ3	2.48	0.49
3:N:42:PRO:O	3:N:43:ASP:HB2	2.12	0.49
1:C:39:ILE:HD13	1:C:207:ILE:CD1	2.43	0.49
2:J:30:THR:HA	2:J:53:PRO:HB2	1.94	0.49
1:A:130:CYS:O	1:A:132:MET:HG3	2.13	0.49
1:A:84:GLN:HE21	1:A:84:GLN:HA	1.78	0.49
1:D:39:ILE:HD13	1:D:207:ILE:CD1	2.43	0.49
3:O:169:LYS:CG	3:O:173:ASN:HA	2.42	0.49
2:J:161:VAL:HA	2:J:205:ASN:O	2.13	0.49
1:A:250:VAL:CG1	1:B:251:THR:HG21	2.42	0.49
2:H:178:VAL:HG22	2:H:185:THR:O	2.12	0.49
2:J:157:GLU:HB3	2:J:158:PRO:HA	1.95	0.49
3:O:131:ASN:OD1	3:O:185:ALA:HB3	2.12	0.49
1:B:224:SER:HB2	1:B:279:TRP:CZ3	2.48	0.49
1:A:224:SER:HB2	1:A:279:TRP:CZ3	2.48	0.49
1:A:137:TYR:CE1	1:A:267:LEU:HD21	2.48	0.49
1:A:234:SER:HG	1:A:294:PHE:HZ	1.60	0.49
2:F:30:THR:HA	2:F:53:PRO:HB2	1.94	0.49
2:G:157:GLU:HB3	2:G:158:PRO:CA	2.41	0.49
2:G:30:THR:HA	2:G:53:PRO:HB2	1.95	0.49
3:K:120:LEU:HD12	3:K:196:CYS:H	1.77	0.49
2:H:36:TRP:CD1	2:H:70:LEU:HD22	2.48	0.49
1:A:103:ILE:HG23	1:A:103:ILE:O	2.13	0.48
2:I:46:GLU:OE1	2:I:63:LYS:HE2	2.12	0.48
1:C:100:LYS:NZ	1:D:104:ASP:HA	2.27	0.48
1:A:253:LEU:HD11	1:B:226:MET:HE1	1.94	0.48
2:F:46:GLU:OE1	2:F:63:LYS:HE2	2.13	0.48
1:A:96:LYS:HD2	1:A:129:SER:HB3	1.95	0.48
1:B:87:MET:O	1:C:105:LYS:NZ	2.47	0.48
1:C:224:SER:HB2	1:C:279:TRP:CZ3	2.48	0.48
1:C:208:GLN:HB2	9:C:400:NAG:H82	1.95	0.48
3:L:120:LEU:HD23	3:L:120:LEU:C	2.34	0.48
3:M:152:LYS:HG2	3:M:157:PRO:HA	1.95	0.48
2:I:36:TRP:CD1	2:I:70:LEU:HD22	2.49	0.48
1:E:130:CYS:O	1:E:132:MET:HG3	2.13	0.48
2:H:168:LEU:HD23	2:H:190:VAL:HG21	1.94	0.48
3:N:10:LEU:HD12	3:N:20:LEU:CD2	2.44	0.48
2:G:156:PRO:HD2	2:G:210:ALA:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LEU:CD1	1:A:146:ILE:HG12	2.44	0.48
1:B:130:CYS:O	1:B:132:MET:HG3	2.13	0.48
1:E:70:GLY:C	1:E:72:GLY:H	2.17	0.48
1:D:84:GLN:HE21	1:D:84:GLN:HA	1.79	0.48
1:E:288:PHE:HE2	1:E:292:LEU:HD11	1.77	0.48
3:O:151:TRP:CD2	3:O:181:LEU:HD12	2.48	0.48
1:D:172:VAL:HA	2:G:54:TYR:OH	2.13	0.48
1:D:128:LEU:CD1	1:D:146:ILE:HG12	2.44	0.48
1:B:187:SER:HB3	9:B:400:NAG:O7	2.13	0.48
1:B:253:LEU:HD11	1:C:226:MET:HE1	1.95	0.48
1:D:137:TYR:CE1	1:D:267:LEU:HD21	2.49	0.48
1:D:130:CYS:O	1:D:132:MET:HG3	2.13	0.48
2:H:157:GLU:HB3	2:H:158:PRO:HA	1.96	0.48
3:K:10:LEU:HD12	3:K:20:LEU:CD2	2.44	0.48
3:L:10:LEU:HD12	3:L:20:LEU:CD2	2.44	0.48
2:J:208:HIS:HB3	2:J:213:THR:HB	1.96	0.47
2:G:46:GLU:OE1	2:G:63:LYS:HE2	2.14	0.47
2:G:133:LEU:HB2	2:G:148:GLY:O	2.14	0.47
1:A:104:ASP:HA	1:E:100:LYS:NZ	2.29	0.47
3:L:151:TRP:CZ3	3:L:196:CYS:HB2	2.49	0.47
2:G:145:VAL:HG13	2:G:192:VAL:HG22	1.96	0.47
2:J:163:TRP:CZ3	2:J:204:CYS:HB3	2.49	0.47
2:F:84:LEU:N	2:F:84:LEU:HD12	2.30	0.47
2:I:100:GLY:HA3	2:I:108:TYR:CZ	2.49	0.47
2:J:46:GLU:OE1	2:J:63:LYS:HE2	2.14	0.47
1:A:70:GLY:C	1:A:72:GLY:H	2.17	0.47
1:A:226:MET:CE	1:E:253:LEU:HD11	2.44	0.47
2:J:203:THR:CG2	2:J:216:ASP:HB3	2.44	0.47
1:C:137:TYR:CE1	1:C:267:LEU:HD21	2.50	0.47
2:I:6:GLN:N	2:I:114:GLN:HE22	2.12	0.47
2:F:36:TRP:CD1	2:F:70:LEU:HD22	2.48	0.47
2:J:36:TRP:CD1	2:J:70:LEU:HD22	2.50	0.47
3:M:143:TYR:HA	3:M:144:PRO:C	2.35	0.47
2:H:30:THR:HA	2:H:53:PRO:HB2	1.94	0.47
1:E:128:LEU:CD1	1:E:146:ILE:HG12	2.44	0.47
1:A:254:LEU:HD12	1:B:251:THR:HG23	1.95	0.47
2:H:100:GLY:HA3	2:H:108:TYR:CZ	2.50	0.47
2:H:84:LEU:HD12	2:H:84:LEU:N	2.30	0.47
1:B:84:GLN:HA	1:B:84:GLN:HE21	1.80	0.47
1:B:70:GLY:C	1:B:72:GLY:H	2.17	0.47
2:H:6:GLN:N	2:H:114:GLN:HE22	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:6:GLN:N	2:G:114:GLN:HE22	2.11	0.47
1:E:84:GLN:HA	1:E:84:GLN:HE21	1.79	0.47
3:K:130:THR:HG22	3:K:130:THR:O	2.14	0.47
1:C:253:LEU:HD11	1:D:226:MET:CE	2.45	0.47
2:H:110:ASP:HB3	2:H:111:TYR:HD2	1.80	0.47
2:J:101:ASP:HB3	2:J:104:ARG:HG3	1.96	0.47
2:G:36:TRP:CD1	2:G:70:LEU:HD22	2.49	0.47
2:J:84:LEU:HD12	2:J:84:LEU:N	2.30	0.47
2:I:101:ASP:HB3	2:I:104:ARG:HG3	1.97	0.47
2:J:100:GLY:HA3	2:J:108:TYR:CZ	2.50	0.47
1:C:154:THR:HG23	1:C:156:LYS:H	1.80	0.47
1:A:288:PHE:HE2	1:A:292:LEU:HD11	1.78	0.47
1:E:137:TYR:CE1	1:E:267:LEU:HD21	2.50	0.47
1:B:137:TYR:CE1	1:B:267:LEU:HD21	2.50	0.47
1:B:34:MET:SD	1:B:205:THR:HG21	2.55	0.47
1:C:242:ILE:HG22	1:C:243:PRO:HD3	1.95	0.47
2:G:147:LEU:HD22	2:G:219:ILE:HG21	1.97	0.47
1:C:34:MET:SD	1:C:205:THR:HG21	2.55	0.47
3:M:10:LEU:HD12	3:M:20:LEU:CD2	2.45	0.47
2:F:6:GLN:N	2:F:114:GLN:HE22	2.13	0.47
1:C:234:SER:HG	1:C:294:PHE:HZ	1.62	0.47
1:C:130:CYS:O	1:C:132:MET:HG3	2.15	0.47
3:K:116:PRO:HA	3:K:142:PHE:HB3	1.96	0.47
1:E:103:ILE:HG23	1:E:103:ILE:O	2.15	0.46
1:D:288:PHE:HE2	1:D:292:LEU:HD11	1.77	0.46
1:E:154:THR:HG23	1:E:156:LYS:H	1.80	0.46
1:D:103:ILE:HG23	1:D:103:ILE:O	2.15	0.46
1:C:288:PHE:HE2	1:C:292:LEU:HD11	1.79	0.46
1:B:242:ILE:HG22	1:B:243:PRO:HD3	1.98	0.46
1:C:70:GLY:C	1:C:72:GLY:H	2.17	0.46
2:F:100:GLY:HA3	2:F:108:TYR:CZ	2.49	0.46
2:H:146:THR:HG22	2:H:191:THR:HB	1.97	0.46
2:G:84:LEU:N	2:G:84:LEU:HD12	2.30	0.46
1:B:236:TRP:CH2	7:B:404:LMT:H12	2.50	0.46
1:E:242:ILE:HG22	1:E:243:PRO:HD3	1.97	0.46
1:D:70:GLY:C	1:D:72:GLY:H	2.18	0.46
1:C:84:GLN:HE21	1:C:84:GLN:HA	1.80	0.46
1:A:87:MET:O	1:B:105:LYS:NZ	2.49	0.46
1:C:103:ILE:HG23	1:C:103:ILE:O	2.15	0.46
1:D:242:ILE:HG22	1:D:243:PRO:HD3	1.97	0.46
3:M:11:THR:HG23	3:M:109:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:VAL:HG12	1:D:210:LYS:HA	1.96	0.46
1:E:141:VAL:HG12	1:E:210:LYS:HA	1.97	0.46
1:A:242:ILE:HG22	1:A:243:PRO:HD3	1.98	0.46
1:A:84:GLN:NE2	1:A:84:GLN:HA	2.31	0.46
2:I:216:ASP:O	2:I:217:LYS:HD2	2.15	0.46
2:H:101:ASP:HB3	2:H:104:ARG:HG3	1.97	0.46
3:K:37:TRP:CZ3	3:K:90:CYS:HB3	2.50	0.46
2:F:110:ASP:HB3	2:F:111:TYR:HD2	1.80	0.46
3:O:37:TRP:CZ3	3:O:90:CYS:HB3	2.51	0.46
1:C:222:ILE:N	1:C:223:PRO:HD2	2.31	0.46
3:N:41:LYS:HB2	3:N:45:LEU:HB2	1.98	0.46
2:G:110:ASP:HB3	2:G:111:TYR:HD2	1.80	0.46
2:J:179:LEU:HD13	2:J:184:TYR:CZ	2.50	0.46
1:A:251:THR:HG21	1:E:250:VAL:CG1	2.45	0.46
2:G:100:GLY:HA3	2:G:108:TYR:CZ	2.50	0.46
2:I:84:LEU:N	2:I:84:LEU:HD12	2.31	0.46
3:M:22:CYS:HG	3:M:90:CYS:HG	0.46	0.46
1:E:34:MET:SD	1:E:205:THR:HG21	2.56	0.46
3:K:41:LYS:HD3	3:K:86:ALA:HB2	1.98	0.46
2:J:30:THR:HG23	2:J:103:TYR:OH	2.16	0.46
2:F:30:THR:HG23	2:F:103:TYR:OH	2.16	0.46
1:C:141:VAL:HG12	1:C:210:LYS:HA	1.97	0.46
2:F:101:ASP:HB3	2:F:104:ARG:HG3	1.97	0.46
3:O:164:THR:HG22	3:O:179:SER:OG	2.15	0.46
2:H:30:THR:HG23	2:H:103:TYR:OH	2.16	0.46
2:I:132:PRO:HD3	2:I:217:LYS:HE2	1.98	0.46
1:D:328:PHE:CE2	1:D:332:ILE:HD11	2.51	0.46
3:L:37:TRP:CZ3	3:L:90:CYS:HB3	2.51	0.45
2:J:30:THR:O	2:J:54:TYR:HB2	2.17	0.45
1:B:141:VAL:HG12	1:B:210:LYS:HA	1.97	0.45
3:O:10:LEU:HD12	3:O:20:LEU:CD2	2.45	0.45
2:G:101:ASP:HB3	2:G:104:ARG:HG3	1.97	0.45
3:O:41:LYS:HB2	3:O:45:LEU:HB2	1.98	0.45
2:J:6:GLN:N	2:J:114:GLN:HE22	2.12	0.45
1:E:323:PHE:HB2	1:E:324:PRO:HD3	1.99	0.45
1:D:84:GLN:NE2	1:D:84:GLN:HA	2.32	0.45
1:A:222:ILE:N	1:A:223:PRO:HD2	2.32	0.45
3:M:41:LYS:HB3	3:M:42:PRO:HD2	1.98	0.45
1:A:103:ILE:C	1:A:105:LYS:H	2.20	0.45
2:G:196:THR:HB	2:G:200:GLU:OE2	2.16	0.45
3:O:131:ASN:HA	3:O:185:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:THR:HG23	1:B:156:LYS:H	1.81	0.45
1:D:154:THR:HG23	1:D:156:LYS:H	1.81	0.45
1:B:288:PHE:CD2	6:B:403:IVM:H8A	2.52	0.45
3:O:41:LYS:HD3	3:O:86:ALA:HB2	1.98	0.45
1:E:36:LEU:HD13	1:E:168:LEU:HD11	1.98	0.45
1:C:323:PHE:HB2	1:C:324:PRO:HD3	1.99	0.45
2:I:110:ASP:HB3	2:I:111:TYR:HD2	1.80	0.45
1:B:36:LEU:HD13	1:B:168:LEU:HD11	1.99	0.45
3:N:37:TRP:CZ3	3:N:90:CYS:HB3	2.51	0.45
2:H:20:ILE:HD11	2:H:81:MET:HE1	1.98	0.45
3:K:145:GLY:HA3	3:K:175:TYR:CG	2.51	0.45
1:B:224:SER:CB	1:B:279:TRP:CZ3	3.00	0.45
3:K:41:LYS:HB2	3:K:45:LEU:HB2	1.99	0.45
1:B:234:SER:HG	1:B:294:PHE:HZ	1.64	0.45
1:B:323:PHE:HB2	1:B:324:PRO:HD3	1.99	0.45
3:M:154:ASP:OD2	3:M:191:HIS:ND1	2.44	0.45
1:B:103:ILE:HG23	1:B:103:ILE:O	2.15	0.45
2:G:30:THR:HG23	2:G:103:TYR:OH	2.16	0.45
2:G:159:VAL:CG2	2:G:186:LEU:HD21	2.47	0.45
1:D:222:ILE:N	1:D:223:PRO:HD2	2.32	0.45
1:E:316:ASP:O	1:E:320:ARG:HG3	2.17	0.45
1:C:254:LEU:HD12	1:D:251:THR:HG23	1.99	0.45
1:A:141:VAL:HG12	1:A:210:LYS:HA	1.98	0.45
1:E:279:TRP:HB2	1:E:334:TYR:CE1	2.52	0.45
2:J:110:ASP:HB3	2:J:111:TYR:HD2	1.79	0.45
3:O:142:PHE:CE1	3:O:145:GLY:HA2	2.51	0.45
1:D:302:ASN:ND2	1:E:238:ASP:HB3	2.32	0.45
2:H:128:PRO:HB3	2:H:151:VAL:HG12	1.99	0.45
1:C:279:TRP:HB2	1:C:334:TYR:CE1	2.52	0.45
3:K:182:THR:O	3:K:183:LEU:HD23	2.17	0.45
3:N:41:LYS:HB3	3:N:42:PRO:HD2	1.99	0.45
2:G:14:PRO:HD2	2:G:122:SER:HB3	1.99	0.45
1:A:154:THR:HG23	1:A:156:LYS:H	1.80	0.45
1:C:152:ALA:HB1	1:D:109:LEU:HD13	1.99	0.45
1:E:222:ILE:N	1:E:223:PRO:HD2	2.32	0.45
3:O:41:LYS:HB3	3:O:42:PRO:HD2	1.99	0.44
3:N:41:LYS:HD3	3:N:86:ALA:HB2	1.98	0.44
1:D:224:SER:CB	1:D:279:TRP:CZ3	3.00	0.44
1:D:36:LEU:HD13	1:D:168:LEU:HD11	1.99	0.44
2:G:30:THR:O	2:G:54:TYR:HB2	2.16	0.44
1:A:34:MET:CG	1:A:53:LEU:HD12	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:MET:HG3	1:C:53:LEU:HD12	1.99	0.44
3:M:166:GLN:HG3	3:M:167:PRO:HD2	1.99	0.44
2:I:20:ILE:HD11	2:I:81:MET:HE1	1.99	0.44
1:E:109:LEU:HB3	1:E:121:SER:HB3	1.99	0.44
1:C:100:LYS:CE	1:D:104:ASP:CA	2.95	0.44
1:C:17:ARG:CD	1:D:81:VAL:O	2.66	0.44
1:B:288:PHE:HE2	1:B:292:LEU:HD11	1.79	0.44
3:M:41:LYS:HD3	3:M:86:ALA:HB2	1.99	0.44
1:D:323:PHE:HB2	1:D:324:PRO:HD3	1.99	0.44
1:D:34:MET:SD	1:D:205:THR:HG21	2.57	0.44
2:J:20:ILE:HD11	2:J:81:MET:HE1	1.99	0.44
1:E:213:PHE:CE2	1:E:217:LEU:HB2	2.52	0.44
3:L:41:LYS:HB3	3:L:42:PRO:HD2	1.99	0.44
1:C:36:LEU:HD13	1:C:168:LEU:HD11	1.98	0.44
2:I:30:THR:HG23	2:I:103:TYR:OH	2.16	0.44
1:B:84:GLN:NE2	1:B:84:GLN:HA	2.33	0.44
1:C:84:GLN:NE2	1:C:84:GLN:HA	2.33	0.44
1:C:213:PHE:CE2	1:C:217:LEU:HB2	2.52	0.44
3:K:41:LYS:HB3	3:K:42:PRO:HD2	1.99	0.44
2:I:125:THR:HG21	2:I:210:ALA:O	2.17	0.44
2:H:34:MET:CE	2:H:96:CYS:HB2	2.48	0.44
1:A:213:PHE:CE2	1:A:217:LEU:HB2	2.53	0.44
1:C:328:PHE:CE2	1:C:332:ILE:HD11	2.53	0.44
1:C:224:SER:CB	1:C:279:TRP:CZ3	3.00	0.44
2:I:30:THR:O	2:I:54:TYR:HB2	2.17	0.44
1:A:34:MET:SD	1:A:205:THR:HG21	2.57	0.44
3:L:111:GLN:HE22	3:L:174:LYS:HG3	1.83	0.44
1:A:58:SER:HA	1:A:118:VAL:O	2.17	0.44
2:F:128:PRO:HB3	2:F:154:TYR:HB3	2.00	0.44
1:C:100:LYS:HE2	1:D:104:ASP:CA	2.48	0.44
1:A:224:SER:CB	1:A:279:TRP:CZ3	3.01	0.44
1:D:267:LEU:HD13	1:D:274:LYS:HE3	1.99	0.44
1:D:58:SER:HA	1:D:118:VAL:O	2.18	0.44
3:L:115:SER:HB3	3:L:116:PRO:HD2	1.99	0.44
1:B:279:TRP:HB2	1:B:334:TYR:CE1	2.53	0.44
1:B:39:ILE:HD13	1:B:207:ILE:HD13	2.00	0.44
1:E:84:GLN:HA	1:E:84:GLN:NE2	2.32	0.44
1:B:222:ILE:N	1:B:223:PRO:HD2	2.33	0.44
1:C:58:SER:HA	1:C:118:VAL:O	2.18	0.44
1:B:213:PHE:CE2	1:B:217:LEU:HB2	2.53	0.44
3:M:37:TRP:CZ3	3:M:90:CYS:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ILE:C	1:C:105:LYS:H	2.21	0.44
3:K:143:TYR:HA	3:K:144:PRO:C	2.38	0.44
1:E:151:TYR:O	4:E:401:GLU:HB2	2.17	0.44
1:B:109:LEU:HB3	1:B:121:SER:HB3	2.00	0.44
1:E:267:LEU:HD13	1:E:274:LYS:HE3	1.99	0.43
1:B:34:MET:HG3	1:B:53:LEU:HD12	2.00	0.43
1:C:34:MET:CG	1:C:53:LEU:HD12	2.47	0.43
3:N:22:CYS:HB3	3:N:73:ALA:HB3	2.00	0.43
1:A:227:LEU:HD21	1:A:255:THR:CG2	2.48	0.43
1:A:103:ILE:O	1:A:103:ILE:CG2	2.65	0.43
1:D:279:TRP:HB2	1:D:334:TYR:CE1	2.53	0.43
1:A:279:TRP:HB2	1:A:334:TYR:CE1	2.52	0.43
1:A:323:PHE:HB2	1:A:324:PRO:HD3	1.99	0.43
1:C:109:LEU:HB3	1:C:121:SER:HB3	2.00	0.43
1:A:109:LEU:HB3	1:A:121:SER:HB3	2.00	0.43
1:E:224:SER:CB	1:E:279:TRP:CZ3	3.01	0.43
2:F:30:THR:O	2:F:54:TYR:HB2	2.17	0.43
1:A:34:MET:HG3	1:A:53:LEU:HD12	2.00	0.43
3:N:10:LEU:HD12	3:N:20:LEU:HD23	2.01	0.43
1:A:251:THR:HG23	1:E:254:LEU:HD12	2.00	0.43
1:E:58:SER:HA	1:E:118:VAL:O	2.18	0.43
6:B:403:IVM:H14	6:B:403:IVM:H1B	2.00	0.43
6:A:402:IVM:H14	6:A:402:IVM:H1B	2.00	0.43
3:M:41:LYS:HB2	3:M:45:LEU:HB2	2.00	0.43
3:L:41:LYS:HD3	3:L:86:ALA:HB2	1.99	0.43
1:A:328:PHE:CE2	1:A:332:ILE:HD11	2.53	0.43
2:F:20:ILE:HD11	2:F:81:MET:HE1	2.01	0.43
6:E:402:IVM:H14	6:E:402:IVM:H1B	2.00	0.43
1:C:267:LEU:HD13	1:C:274:LYS:HE3	1.99	0.43
2:F:10:GLU:HG3	2:F:18:MET:CE	2.49	0.43
1:D:213:PHE:CE2	1:D:217:LEU:HB2	2.53	0.43
1:B:58:SER:HA	1:B:118:VAL:O	2.18	0.43
2:G:198:PRO:HG3	2:G:221:PRO:HG3	2.00	0.43
3:M:22:CYS:HB3	3:M:73:ALA:HB3	2.01	0.43
2:I:34:MET:CE	2:I:96:CYS:HB2	2.49	0.43
2:I:10:GLU:HG3	2:I:18:MET:CE	2.49	0.43
1:A:6:LEU:O	1:A:10:PHE:HD2	2.01	0.43
1:A:222:ILE:HG23	6:A:403:IVM:H2A	2.00	0.43
1:E:39:ILE:HD13	1:E:207:ILE:HD13	2.00	0.43
1:A:36:LEU:HD13	1:A:168:LEU:HD11	1.99	0.43
3:K:153:VAL:HG22	3:K:194:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:30:THR:O	2:H:54:TYR:HB2	2.18	0.43
1:E:34:MET:CG	1:E:53:LEU:HD12	2.48	0.43
3:K:142:PHE:HB2	3:K:200:HIS:CE1	2.54	0.43
1:E:6:LEU:O	1:E:10:PHE:HD2	2.02	0.43
2:G:157:GLU:CB	2:G:158:PRO:HA	2.35	0.43
1:B:267:LEU:HD13	1:B:274:LYS:HE3	2.01	0.43
2:J:2:VAL:HG21	2:J:111:TYR:CE2	2.54	0.43
1:D:34:MET:CG	1:D:53:LEU:HD12	2.48	0.43
2:H:180:GLN:O	2:H:181:SER:HB2	2.17	0.43
1:D:103:ILE:C	1:D:105:LYS:H	2.21	0.43
3:L:41:LYS:HB2	3:L:45:LEU:HB2	2.00	0.43
1:A:39:ILE:HD13	1:A:207:ILE:HD13	2.00	0.43
1:B:34:MET:CG	1:B:53:LEU:HD12	2.48	0.43
2:I:131:TYR:CD1	3:O:126:GLU:HB3	2.54	0.43
1:B:6:LEU:O	1:B:10:PHE:HD2	2.02	0.43
1:D:300:ILE:HG13	1:D:312:SER:HB2	2.01	0.43
1:D:6:LEU:O	1:D:10:PHE:HD2	2.02	0.43
1:B:103:ILE:C	1:B:105:LYS:H	2.22	0.43
1:C:42:ILE:HD12	1:C:181:PHE:CD2	2.54	0.43
3:L:22:CYS:HB3	3:L:73:ALA:HB3	2.01	0.43
1:B:227:LEU:HD21	1:B:255:THR:CG2	2.49	0.43
1:D:109:LEU:HB3	1:D:121:SER:HB3	2.00	0.42
1:A:20:PRO:HA	1:A:21:PRO:HD3	1.86	0.42
3:O:188:TRP:HA	3:O:194:TYR:OH	2.19	0.42
6:A:402:IVM:H11A	1:B:226:MET:HG3	2.00	0.42
3:N:36:ASN:O	3:N:90:CYS:HA	2.19	0.42
1:D:276:ILE:O	1:D:280:ILE:HG12	2.19	0.42
2:I:171:GLY:O	2:I:190:VAL:HA	2.19	0.42
3:K:154:ASP:OD2	3:K:191:HIS:ND1	2.50	0.42
3:O:130:THR:O	3:O:130:THR:HG22	2.19	0.42
1:A:267:LEU:HD13	1:A:274:LYS:HE3	2.01	0.42
3:N:166:GLN:HA	3:N:167:PRO:HD3	1.95	0.42
2:G:203:THR:CG2	2:G:204:CYS:N	2.82	0.42
3:K:22:CYS:HB3	3:K:73:ALA:HB3	2.00	0.42
2:J:34:MET:CE	2:J:96:CYS:HB2	2.48	0.42
1:C:227:LEU:HD21	1:C:255:THR:CG2	2.49	0.42
1:B:100:LYS:HE2	1:C:104:ASP:CA	2.49	0.42
1:E:103:ILE:CG2	1:E:103:ILE:O	2.67	0.42
1:C:39:ILE:HD13	1:C:207:ILE:HD13	2.00	0.42
1:E:227:LEU:HD21	1:E:255:THR:CG2	2.50	0.42
3:O:22:CYS:HB3	3:O:73:ALA:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:34:MET:CE	2:F:96:CYS:HB2	2.49	0.42
1:C:316:ASP:O	1:C:320:ARG:HG3	2.19	0.42
2:H:10:GLU:HG3	2:H:18:MET:CE	2.50	0.42
6:D:402:IVM:H1B	6:D:402:IVM:H14	2.00	0.42
3:O:151:TRP:CE2	3:O:181:LEU:HB2	2.54	0.42
2:G:155:PHE:CD2	2:G:156:PRO:HA	2.55	0.42
2:G:156:PRO:HD2	2:G:210:ALA:HB1	2.01	0.42
1:A:276:ILE:O	1:A:280:ILE:HG12	2.19	0.42
1:D:34:MET:HG3	1:D:53:LEU:HD12	2.01	0.42
2:G:20:ILE:HD11	2:G:81:MET:HE1	2.00	0.42
3:K:123:PRO:HD3	3:K:135:LEU:HG	2.02	0.42
1:E:328:PHE:CE2	1:E:332:ILE:HD11	2.55	0.42
2:G:157:GLU:HG3	2:G:184:TYR:CD2	2.55	0.42
1:D:194:VAL:HG11	2:I:33:THR:HG21	2.00	0.42
1:C:146:ILE:HB	1:C:205:THR:CG2	2.50	0.42
3:N:137:CYS:HB3	3:N:179:SER:HB3	2.00	0.42
2:H:163:TRP:HZ2	2:H:188:SER:O	2.01	0.42
1:D:253:LEU:HD11	1:E:226:MET:HE1	2.02	0.42
2:G:155:PHE:CG	2:G:156:PRO:HA	2.55	0.42
2:H:2:VAL:HG21	2:H:111:TYR:CE2	2.55	0.42
1:E:146:ILE:HB	1:E:205:THR:CG2	2.50	0.42
2:H:161:VAL:HG11	2:H:188:SER:HB3	2.02	0.42
1:D:227:LEU:HD21	1:D:255:THR:CG2	2.50	0.42
1:D:89:ASP:HA	1:E:105:LYS:CG	2.35	0.42
1:A:42:ILE:CD1	1:A:209:LEU:HD13	2.49	0.42
2:I:2:VAL:HG12	2:I:27:TYR:HB3	2.02	0.42
2:I:2:VAL:HG21	2:I:111:TYR:CE2	2.55	0.42
1:A:227:LEU:HD21	1:A:255:THR:HG22	2.02	0.42
2:J:10:GLU:HG3	2:J:18:MET:CE	2.50	0.42
1:B:316:ASP:O	1:B:320:ARG:HG3	2.20	0.42
3:L:194:TYR:HB2	3:L:209:LEU:HD21	2.02	0.42
1:D:103:ILE:CG2	1:D:103:ILE:O	2.68	0.42
6:A:402:IVM:H4B	1:B:226:MET:HB2	2.01	0.42
1:A:146:ILE:HB	1:A:205:THR:CG2	2.49	0.42
2:F:10:GLU:HG3	2:F:18:MET:HE1	2.02	0.42
2:H:10:GLU:HG3	2:H:18:MET:HE1	2.01	0.42
2:G:128:PRO:HB2	2:G:151:VAL:HG13	2.01	0.42
3:M:193:SER:O	3:M:194:TYR:CG	2.73	0.42
1:C:20:PRO:HA	1:C:21:PRO:HD3	1.85	0.42
3:K:146:VAL:O	3:K:146:VAL:HG23	2.20	0.42
1:D:234:SER:HG	1:D:294:PHE:HZ	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ILE:HD13	1:D:207:ILE:HD13	2.01	0.41
2:F:2:VAL:HG21	2:F:111:TYR:CE2	2.55	0.41
3:M:10:LEU:HD12	3:M:20:LEU:HD23	2.02	0.41
3:K:105:LYS:HD2	3:K:146:VAL:HG13	2.02	0.41
1:C:49:TYR:CE2	1:C:144:CYS:HB3	2.55	0.41
1:C:6:LEU:O	1:C:10:PHE:HD2	2.02	0.41
1:B:273:ILE:HD11	6:B:403:IVM:H30	2.02	0.41
2:H:157:GLU:HG3	2:H:184:TYR:CE2	2.54	0.41
1:C:276:ILE:O	1:C:280:ILE:HG12	2.20	0.41
3:L:10:LEU:HD12	3:L:20:LEU:HD23	2.02	0.41
2:I:150:LEU:HD13	3:O:136:VAL:HG21	2.02	0.41
1:C:269:PRO:HB3	1:D:215:PHE:CG	2.55	0.41
2:G:34:MET:CE	2:G:96:CYS:HB2	2.50	0.41
3:K:151:TRP:HB2	3:K:158:VAL:HB	2.02	0.41
1:A:303:ALA:CB	7:A:404:LMT:H6D	2.50	0.41
1:E:103:ILE:C	1:E:105:LYS:H	2.23	0.41
1:A:81:VAL:O	1:E:17:ARG:HD2	2.20	0.41
1:D:42:ILE:HD12	1:D:181:PHE:CD2	2.55	0.41
1:B:42:ILE:CD1	1:B:209:LEU:HD13	2.50	0.41
1:B:146:ILE:HB	1:B:205:THR:CG2	2.50	0.41
1:D:146:ILE:HB	1:D:205:THR:CG2	2.50	0.41
1:B:328:PHE:CE2	1:B:332:ILE:HD11	2.55	0.41
3:M:81:GLN:O	3:M:108:VAL:HG21	2.20	0.41
1:E:103:ILE:HD12	1:E:103:ILE:HA	1.98	0.41
1:D:226:MET:HB2	6:D:402:IVM:H4B	2.01	0.41
1:A:137:TYR:CB	1:A:138:PRO:HD3	2.46	0.41
6:A:403:IVM:H1B	6:A:403:IVM:H14	2.01	0.41
2:J:2:VAL:HG12	2:J:27:TYR:HB3	2.02	0.41
3:O:81:GLN:O	3:O:108:VAL:HG21	2.21	0.41
1:B:49:TYR:CE2	1:B:144:CYS:HB3	2.55	0.41
1:C:33:ASN:OD1	1:C:56:ARG:HD2	2.21	0.41
1:E:234:SER:HG	1:E:294:PHE:HZ	1.63	0.41
1:D:316:ASP:O	1:D:320:ARG:HG3	2.20	0.41
2:J:152:LYS:HA	2:J:185:THR:HG23	2.01	0.41
3:M:207:LYS:HA	3:M:207:LYS:HD3	1.94	0.41
1:A:300:ILE:HG13	1:A:312:SER:HB2	2.01	0.41
1:C:103:ILE:CG2	1:C:103:ILE:O	2.68	0.41
1:A:42:ILE:HD12	1:A:181:PHE:CD2	2.56	0.41
1:E:34:MET:HG3	1:E:53:LEU:HD12	2.01	0.41
1:B:276:ILE:O	1:B:280:ILE:HG12	2.19	0.41
3:N:170:GLN:CB	3:N:172:ASN:OD1	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:10:LEU:HD12	3:K:20:LEU:HD23	2.01	0.41
1:E:227:LEU:HD12	1:E:227:LEU:HA	1.91	0.41
1:E:309:ASN:O	1:E:312:SER:HB3	2.21	0.41
2:I:175:PHE:HB3	2:I:176:PRO:HD2	2.03	0.41
2:G:147:LEU:HD22	2:G:219:ILE:CG2	2.50	0.41
3:K:36:ASN:O	3:K:90:CYS:HA	2.21	0.41
3:L:186:ARG:H	3:L:186:ARG:HG2	1.74	0.41
1:A:49:TYR:CE2	1:A:144:CYS:HB3	2.56	0.41
1:B:103:ILE:CG2	1:B:103:ILE:O	2.68	0.41
3:N:169:LYS:NZ	3:N:169:LYS:CB	2.80	0.41
2:F:2:VAL:HG12	2:F:27:TYR:HB3	2.02	0.41
3:M:9:ALA:HB2	3:M:146:VAL:HG21	2.03	0.41
1:D:302:ASN:HD22	1:E:238:ASP:HB3	1.86	0.41
2:H:128:PRO:HB3	2:H:151:VAL:CG1	2.50	0.41
1:A:302:ASN:HD22	1:B:238:ASP:HB3	1.85	0.41
3:L:53:ILE:HD13	3:L:53:ILE:HA	1.93	0.41
2:H:157:GLU:CB	2:H:158:PRO:HA	2.50	0.41
2:I:133:LEU:HD11	2:I:150:LEU:HB2	2.03	0.41
1:A:302:ASN:ND2	1:B:238:ASP:HB3	2.36	0.41
2:G:10:GLU:HG3	2:G:18:MET:CE	2.50	0.41
3:M:163:GLU:O	3:M:179:SER:HA	2.20	0.41
1:E:49:TYR:CE2	1:E:144:CYS:HB3	2.55	0.41
1:B:100:LYS:CE	1:C:104:ASP:CA	2.96	0.41
3:O:111:GLN:HE22	3:O:174:LYS:HE3	1.86	0.41
1:B:220:LEU:HD23	1:B:221:TYR:CE2	2.56	0.40
1:E:220:LEU:HD23	1:E:221:TYR:CE2	2.56	0.40
1:C:130:CYS:HA	1:C:131:PRO:HD2	1.95	0.40
1:B:227:LEU:HD21	1:B:255:THR:HG22	2.03	0.40
1:B:300:ILE:HG13	1:B:312:SER:HB2	2.02	0.40
1:B:42:ILE:HD12	1:B:181:PHE:CD2	2.56	0.40
1:B:137:TYR:CB	1:B:138:PRO:HD3	2.51	0.40
3:O:36:ASN:O	3:O:90:CYS:HA	2.21	0.40
1:C:300:ILE:HG13	1:C:312:SER:HB2	2.02	0.40
3:L:147:VAL:HG12	3:L:200:HIS:HB2	2.03	0.40
4:B:401:GLU:OXT	1:C:37:ARG:NH2	2.54	0.40
1:E:42:ILE:HD12	1:E:181:PHE:CD2	2.56	0.40
1:E:285:THR:HG21	8:E:403:OCT:H21	2.01	0.40
1:C:73:GLN:CB	1:C:74:PRO:HD2	2.51	0.40
1:E:73:GLN:CB	1:E:74:PRO:HD2	2.52	0.40
1:E:300:ILE:HG13	1:E:312:SER:HB2	2.02	0.40
3:K:81:GLN:O	3:K:108:VAL:HG21	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:178:VAL:HG22	2:I:185:THR:O	2.22	0.40
1:D:49:TYR:CE2	1:D:144:CYS:HB3	2.56	0.40
1:D:42:ILE:CD1	1:D:209:LEU:HD13	2.49	0.40
1:A:226:MET:HG3	6:A:403:IVM:H11A	2.04	0.40
1:D:250:VAL:HG13	1:E:251:THR:HG21	2.02	0.40
1:D:136:TYR:O	1:D:137:TYR:C	2.59	0.40
2:H:2:VAL:HG12	2:H:27:TYR:HB3	2.02	0.40
1:E:276:ILE:O	1:E:280:ILE:HG12	2.20	0.40
2:G:108:TYR:HB3	3:K:52:GLY:N	2.37	0.40
2:H:196:THR:O	2:H:200:GLU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	338/347 (97%)	317 (94%)	19 (6%)	2 (1%)	30	69
1	B	338/347 (97%)	317 (94%)	19 (6%)	2 (1%)	30	69
1	C	337/347 (97%)	316 (94%)	19 (6%)	2 (1%)	30	69
1	D	338/347 (97%)	317 (94%)	19 (6%)	2 (1%)	30	69
1	E	338/347 (97%)	317 (94%)	19 (6%)	2 (1%)	30	69
2	F	163/221 (74%)	150 (92%)	12 (7%)	1 (1%)	30	69
2	G	210/221 (95%)	196 (93%)	13 (6%)	1 (0%)	34	73
2	H	219/221 (99%)	206 (94%)	13 (6%)	0	100	100
2	I	184/221 (83%)	172 (94%)	10 (5%)	2 (1%)	17	57
2	J	194/221 (88%)	180 (93%)	14 (7%)	0	100	100
3	K	208/210 (99%)	189 (91%)	19 (9%)	0	100	100
3	L	208/210 (99%)	195 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	208/210 (99%)	194 (93%)	14 (7%)	0	100	100
3	N	140/210 (67%)	128 (91%)	11 (8%)	1 (1%)	26	67
3	O	189/210 (90%)	168 (89%)	20 (11%)	1 (0%)	34	73
All	All	3612/3890 (93%)	3362 (93%)	234 (6%)	16 (0%)	39	77

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	TYR
1	B	137	TYR
1	C	137	TYR
1	D	137	TYR
1	E	137	TYR
2	I	190	VAL
1	A	68	VAL
1	B	68	VAL
1	C	68	VAL
1	D	68	VAL
1	E	68	VAL
2	G	199	SER
3	N	173	ASN
2	I	178	VAL
3	O	110	GLY
2	F	178	VAL

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	308/316 (98%)	307 (100%)	1 (0%)	94	98
1	B	308/316 (98%)	307 (100%)	1 (0%)	94	98
1	C	307/316 (97%)	306 (100%)	1 (0%)	94	98
1	D	308/316 (98%)	307 (100%)	1 (0%)	94	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	308/316 (98%)	307 (100%)	1 (0%)	94	98
2	F	145/190 (76%)	145 (100%)	0	100	100
2	G	184/190 (97%)	182 (99%)	2 (1%)	80	91
2	H	188/190 (99%)	188 (100%)	0	100	100
2	I	164/190 (86%)	164 (100%)	0	100	100
2	J	170/190 (90%)	170 (100%)	0	100	100
3	K	176/178 (99%)	174 (99%)	2 (1%)	80	91
3	L	178/178 (100%)	178 (100%)	0	100	100
3	M	175/178 (98%)	175 (100%)	0	100	100
3	N	115/178 (65%)	115 (100%)	0	100	100
3	O	162/178 (91%)	162 (100%)	0	100	100
All	All	3196/3420 (94%)	3187 (100%)	9 (0%)	94	98

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	GLU
1	B	95	GLU
1	C	95	GLU
1	D	95	GLU
1	E	95	GLU
2	G	45	LEU
2	G	194	SER
3	K	141	ASP
3	K	196	CYS

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	46	ASN
1	A	84	GLN
1	A	101	HIS
1	A	169	GLN
1	A	264	ASN
1	B	46	ASN
1	B	84	GLN
1	B	101	HIS

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Mol	Chain	Res	Type
1	B	169	GLN
1	B	264	ASN
1	C	46	ASN
1	C	84	GLN
1	C	101	HIS
1	C	169	GLN
1	C	264	ASN
1	D	46	ASN
1	D	84	GLN
1	D	101	HIS
1	D	169	GLN
1	D	264	ASN
1	E	46	ASN
1	E	84	GLN
1	E	101	HIS
1	E	169	GLN
1	E	264	ASN
2	F	5	GLN
2	F	55	ASN
2	F	62	GLN
2	F	180	GLN
2	F	208	HIS
2	G	5	GLN
2	G	62	GLN
2	H	5	GLN
2	H	62	GLN
2	H	180	GLN
2	I	5	GLN
2	I	55	ASN
2	I	62	GLN
2	I	180	GLN
2	J	5	GLN
2	J	62	GLN
3	L	111	GLN
3	L	197	GLN
3	M	160	GLN
3	N	166	GLN
3	O	166	GLN

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 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	GLU	A	401	-	3,9,9	0.33	0	2,11,11	0.10	0
6	IVM	A	402	-	63,68,68	0.78	1 (1%)	72,102,102	1.62	15 (20%)
6	IVM	A	403	-	63,68,68	0.78	1 (1%)	72,102,102	1.62	14 (19%)
7	LMT	A	404	-	27,27,36	1.44	4 (14%)	38,38,47	1.85	13 (34%)
7	LMT	A	405	-	28,28,36	1.39	5 (17%)	39,39,47	1.39	5 (12%)
9	NAG	B	400	1	14,14,15	0.56	0	15,19,21	0.63	0
4	GLU	B	401	-	3,9,9	0.34	0	2,11,11	0.06	0
6	IVM	B	403	-	63,68,68	0.78	1 (1%)	72,102,102	1.61	14 (19%)
7	LMT	B	404	-	27,27,36	1.41	4 (14%)	38,38,47	1.55	9 (23%)
8	OCT	B	405	-	7,7,7	0.25	0	6,6,6	0.42	0
10	UND	B	406	-	10,10,10	0.26	0	9,9,9	0.47	0
9	NAG	C	400	1	14,14,15	0.46	0	15,19,21	1.69	1 (6%)
4	GLU	C	401	-	3,9,9	0.37	0	2,11,11	0.10	0
4	GLU	D	401	-	3,9,9	0.35	0	2,11,11	0.03	0
6	IVM	D	402	-	63,68,68	0.78	1 (1%)	72,102,102	1.61	14 (19%)
8	OCT	D	403	-	7,7,7	0.25	0	6,6,6	0.43	0
9	NAG	E	400	1	14,14,15	0.44	0	15,19,21	1.15	2 (13%)
4	GLU	E	401	-	3,9,9	0.35	0	2,11,11	0.11	0
6	IVM	E	402	-	63,68,68	0.78	1 (1%)	72,102,102	1.62	14 (19%)
8	OCT	E	403	-	7,7,7	0.25	0	6,6,6	0.47	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	GLU	A	401	-	-	0/3/9/9	0/0/0/0
6	IVM	A	402	-	-	0/43/141/141	0/5/7/7
6	IVM	A	403	-	-	0/43/141/141	0/5/7/7
7	LMT	A	404	-	-	0/12/52/61	0/2/2/2
7	LMT	A	405	-	-	0/13/53/61	0/2/2/2
9	NAG	B	400	1	-	0/6/23/26	0/1/1/1
4	GLU	B	401	-	-	0/3/9/9	0/0/0/0
6	IVM	B	403	-	-	0/43/141/141	0/5/7/7
7	LMT	B	404	-	-	0/12/52/61	0/2/2/2
8	OCT	B	405	-	-	0/5/5/5	0/0/0/0
10	UND	B	406	-	-	0/8/8/8	0/0/0/0
9	NAG	C	400	1	-	0/6/23/26	0/1/1/1
4	GLU	C	401	-	-	0/3/9/9	0/0/0/0
4	GLU	D	401	-	-	0/3/9/9	0/0/0/0
6	IVM	D	402	-	-	0/43/141/141	0/5/7/7
8	OCT	D	403	-	-	0/5/5/5	0/0/0/0
9	NAG	E	400	1	-	0/6/23/26	0/1/1/1
4	GLU	E	401	-	-	0/3/9/9	0/0/0/0
6	IVM	E	402	-	-	0/43/141/141	0/5/7/7
8	OCT	E	403	-	-	0/5/5/5	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	404	LMT	C3'-C4'	-3.76	1.41	1.52
7	A	404	LMT	C3'-C4'	-3.73	1.41	1.52
7	A	405	LMT	C3'-C4'	-3.52	1.42	1.52
7	A	405	LMT	C4B-C3B	-3.41	1.43	1.52
7	B	404	LMT	C4B-C3B	-3.41	1.43	1.52
7	A	404	LMT	C4B-C3B	-3.36	1.43	1.52
7	A	405	LMT	C3B-C2B	-2.72	1.45	1.52
7	A	404	LMT	C3B-C2B	-2.47	1.45	1.52
7	B	404	LMT	C3B-C2B	-2.40	1.46	1.52
7	A	404	LMT	O2'-C2'	-2.28	1.37	1.43
7	B	404	LMT	O2'-C2'	-2.06	1.38	1.43
7	A	405	LMT	O2'-C2'	-2.03	1.38	1.43
7	A	405	LMT	O5'-C5'	2.04	1.49	1.44
6	D	402	IVM	O12-C46	4.70	1.45	1.34
6	A	403	IVM	O12-C46	4.73	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	402	IVM	O12-C46	4.75	1.45	1.34
6	B	403	IVM	O12-C46	4.75	1.45	1.34
6	E	402	IVM	O12-C46	4.76	1.45	1.34

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	402	IVM	C13-C14-C15	-4.79	106.68	113.57
6	A	402	IVM	C13-C14-C15	-4.74	106.74	113.57
6	D	402	IVM	C13-C14-C15	-4.73	106.76	113.57
6	B	403	IVM	C13-C14-C15	-4.64	106.89	113.57
6	A	403	IVM	C13-C14-C15	-4.47	107.14	113.57
7	A	404	LMT	C1B-O5B-C5B	-4.07	105.85	113.75
6	A	402	IVM	C15-C16-C17	-3.84	120.58	127.15
6	B	403	IVM	C15-C16-C17	-3.78	120.67	127.15
6	E	402	IVM	C15-C16-C17	-3.77	120.68	127.15
6	A	403	IVM	C15-C16-C17	-3.77	120.69	127.15
6	D	402	IVM	C15-C16-C17	-3.74	120.73	127.15
6	D	402	IVM	O9-C40-C39	-3.56	102.24	105.72
6	B	403	IVM	O9-C40-C39	-3.47	102.32	105.72
6	A	403	IVM	O9-C40-C39	-3.45	102.34	105.72
6	A	403	IVM	C12-O12-C46	-3.45	112.50	117.67
6	A	402	IVM	O9-C40-C39	-3.44	102.35	105.72
6	E	402	IVM	C12-O12-C46	-3.38	112.60	117.67
6	E	402	IVM	O9-C40-C39	-3.37	102.42	105.72
6	B	403	IVM	C12-O12-C46	-3.32	112.70	117.67
6	A	402	IVM	C12-O12-C46	-3.27	112.77	117.67
6	D	402	IVM	C12-O12-C46	-3.21	112.86	117.67
7	A	405	LMT	O3'-C3'-C2'	-2.98	103.62	110.34
7	B	404	LMT	O3'-C3'-C2'	-2.91	103.79	110.34
7	A	404	LMT	O1B-C1B-O5B	-2.77	103.66	110.68
7	A	404	LMT	O3'-C3'-C2'	-2.67	104.33	110.34
6	A	403	IVM	C3-C5-C9	-2.62	111.64	116.37
6	E	402	IVM	C3-C5-C9	-2.60	111.69	116.37
6	E	402	IVM	O12-C46-O11	-2.53	118.68	123.89
6	D	402	IVM	C3-C5-C9	-2.51	111.84	116.37
6	D	402	IVM	C38-C37-C36	-2.51	117.81	124.18
6	B	403	IVM	C3-C5-C9	-2.51	111.85	116.37
6	A	403	IVM	C37-C38-C39	-2.49	122.77	130.32
6	A	402	IVM	C3-C5-C9	-2.49	111.89	116.37
6	E	402	IVM	C37-C38-C39	-2.48	122.78	130.32
6	D	402	IVM	C37-C38-C39	-2.48	122.81	130.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	402	IVM	O12-C46-O11	-2.47	118.80	123.89
6	A	403	IVM	O12-C46-O11	-2.46	118.81	123.89
6	B	403	IVM	O12-C46-O11	-2.46	118.82	123.89
6	D	402	IVM	O12-C46-O11	-2.44	118.86	123.89
6	B	403	IVM	C37-C38-C39	-2.44	122.93	130.32
6	A	403	IVM	C38-C37-C36	-2.44	118.00	124.18
6	A	402	IVM	C38-C37-C36	-2.40	118.10	124.18
6	E	402	IVM	C38-C37-C36	-2.40	118.11	124.18
6	A	402	IVM	C37-C38-C39	-2.40	123.05	130.32
7	B	404	LMT	C1B-O1B-C4'	-2.34	111.90	118.01
7	A	404	LMT	O3B-C3B-C4B	-2.33	105.08	110.34
6	B	403	IVM	C38-C37-C36	-2.32	118.30	124.18
6	A	403	IVM	O11-C46-C45	-2.31	120.33	124.80
7	B	404	LMT	O3B-C3B-C4B	-2.25	105.27	110.34
7	A	405	LMT	C1B-O1B-C4'	-2.22	112.20	118.01
6	A	402	IVM	O11-C46-C45	-2.21	120.52	124.80
6	E	402	IVM	O11-C46-C45	-2.21	120.53	124.80
6	D	402	IVM	O11-C46-C45	-2.21	120.54	124.80
6	B	403	IVM	O11-C46-C45	-2.18	120.58	124.80
7	A	404	LMT	O1B-C4'-C3'	-2.07	101.82	107.17
7	A	404	LMT	O2'-C2'-C3'	-2.05	105.72	110.34
6	A	402	IVM	O1-C6-C11	2.01	109.12	106.16
7	A	404	LMT	C1'-C2'-C3'	2.02	113.94	109.97
6	B	403	IVM	O14-C14-C13	2.06	113.01	108.85
6	A	402	IVM	O1-C5-C3	2.07	109.55	106.27
6	A	403	IVM	O14-C14-C13	2.09	113.07	108.85
6	E	402	IVM	O14-C14-C13	2.09	113.07	108.85
9	E	400	NAG	C2-N2-C7	2.11	125.75	123.04
7	A	404	LMT	O5B-C5B-C6B	2.11	111.69	106.36
6	A	402	IVM	O14-C14-C13	2.12	113.13	108.85
6	E	402	IVM	O1-C5-C3	2.12	109.62	106.27
6	D	402	IVM	O1-C5-C3	2.12	109.62	106.27
7	B	404	LMT	O6'-C6'-C5'	2.13	118.36	111.33
6	D	402	IVM	O14-C14-C13	2.18	113.25	108.85
7	B	404	LMT	O6B-C6B-C5B	2.18	118.53	111.33
6	E	402	IVM	C18-C17-C19	2.18	119.39	115.58
6	D	402	IVM	C18-C17-C19	2.20	119.44	115.58
6	A	403	IVM	O1-C5-C3	2.21	109.77	106.27
6	B	403	IVM	C18-C17-C19	2.22	119.46	115.58
6	A	403	IVM	C18-C17-C19	2.25	119.51	115.58
7	A	405	LMT	O6'-C6'-C5'	2.25	118.78	111.33
6	B	403	IVM	O1-C5-C3	2.26	109.84	106.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	405	LMT	O1'-C1-C2	2.27	118.92	109.88
7	B	404	LMT	O1'-C1'-C2'	2.30	110.94	108.04
6	A	402	IVM	C18-C17-C19	2.35	119.70	115.58
6	A	403	IVM	O14-C14-C15	2.38	108.23	106.00
6	D	402	IVM	O14-C14-C15	2.38	108.23	106.00
6	E	402	IVM	O14-C14-C15	2.46	108.30	106.00
6	A	402	IVM	O14-C14-C15	2.50	108.34	106.00
7	A	404	LMT	C3B-C4B-C5B	2.56	114.67	110.20
6	B	403	IVM	O14-C14-C15	2.60	108.44	106.00
7	B	404	LMT	O1B-C1B-C2B	2.71	114.69	108.10
7	A	404	LMT	C1-O1'-C1'	2.92	119.05	113.94
9	E	400	NAG	C1-O5-C5	2.94	115.97	112.25
7	A	404	LMT	O1'-C1-C2	2.97	118.46	109.96
7	A	404	LMT	C2'-C3'-C4'	3.00	116.19	109.60
7	A	404	LMT	O1B-C1B-C2B	3.07	115.56	108.10
7	A	405	LMT	C1-O1'-C1'	3.10	119.36	113.94
7	B	404	LMT	O1'-C1-C2	3.10	118.84	109.96
7	B	404	LMT	C1-O1'-C1'	3.37	119.84	113.94
6	D	402	IVM	O12-C46-C45	5.31	120.56	111.35
6	B	403	IVM	O12-C46-C45	5.31	120.56	111.35
6	A	402	IVM	O12-C46-C45	5.36	120.64	111.35
6	E	402	IVM	O12-C46-C45	5.42	120.75	111.35
6	A	403	IVM	O12-C46-C45	5.46	120.81	111.35
9	C	400	NAG	C1-O5-C5	5.93	119.78	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	402	IVM	4	0
6	A	403	IVM	7	0
7	A	404	LMT	10	0
7	A	405	LMT	3	0
9	B	400	NAG	1	0
4	B	401	GLU	2	0
6	B	403	IVM	5	0
7	B	404	LMT	7	0
9	C	400	NAG	1	0
4	C	401	GLU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	GLU	1	0
6	D	402	IVM	3	0
4	E	401	GLU	1	0
6	E	402	IVM	3	0
8	E	403	OCT	3	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	340/347 (97%)	0.07	5 (1%) 76 76	32, 66, 123, 196	0
1	B	340/347 (97%)	-0.06	4 (1%) 81 81	38, 68, 125, 199	0
1	C	339/347 (97%)	0.12	14 (4%) 41 39	41, 71, 153, 279	0
1	D	340/347 (97%)	-0.09	7 (2%) 67 66	39, 72, 159, 243	0
1	E	340/347 (97%)	0.04	7 (2%) 67 66	36, 69, 142, 210	0
2	F	171/221 (77%)	0.59	21 (12%) 5 5	58, 106, 163, 192	0
2	G	214/221 (96%)	0.33	9 (4%) 40 38	40, 89, 142, 182	0
2	H	221/221 (100%)	-0.07	6 (2%) 58 57	42, 76, 131, 201	0
2	I	192/221 (86%)	0.81	32 (16%) 2 2	57, 110, 171, 201	0
2	J	200/221 (90%)	0.13	10 (5%) 32 32	49, 90, 158, 182	0
3	K	210/210 (100%)	0.14	7 (3%) 50 49	50, 95, 139, 209	0
3	L	210/210 (100%)	0.04	4 (1%) 70 69	38, 73, 114, 159	0
3	M	210/210 (100%)	0.21	13 (6%) 24 24	49, 93, 143, 165	0
3	N	148/210 (70%)	0.92	28 (18%) 2 2	58, 119, 178, 202	0
3	O	195/210 (92%)	0.72	28 (14%) 3 3	63, 113, 167, 190	0
All	All	3670/3890 (94%)	0.20	195 (5%) 30 30	32, 82, 155, 279	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	208	SER	8.7
2	I	212	SER	7.6
2	I	189	SER	7.0
2	I	188	SER	6.8
2	I	213	THR	6.7
3	N	109	LEU	6.5
3	O	207	LYS	6.3

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Mol	Chain	Res	Type	RSRZ
1	C	304	GLY	6.0
3	O	195	SER	5.8
3	N	178	SER	5.5
1	C	303	ALA	5.4
3	O	1	GLN	5.4
2	F	187	SER	5.3
1	C	305	THR	5.2
1	E	340	HIS	5.1
1	A	340	HIS	4.9
3	N	120	LEU	4.9
3	K	188	TRP	4.8
3	O	120	LEU	4.8
2	F	132	PRO	4.8
2	I	146	THR	4.7
2	I	173	HIS	4.7
2	H	140	GLN	4.6
2	H	137	SER	4.5
2	F	178	VAL	4.4
1	C	1	SER	4.4
1	C	83	HIS	4.3
1	C	308	TRP	4.3
1	C	68	VAL	4.3
3	M	195	SER	4.2
2	F	149	CYS	4.2
2	I	191	THR	4.2
2	I	192	VAL	4.2
3	O	183	LEU	4.1
2	I	209	PRO	4.1
3	O	179	SER	4.0
2	F	150	LEU	3.9
2	F	161	VAL	3.9
3	O	117	SER	3.9
1	C	239	ARG	3.9
2	G	168	LEU	3.9
3	N	138	THR	3.9
1	D	80	THR	3.8
3	N	123	PRO	3.8
2	I	143	SER	3.7
3	N	116	PRO	3.7
2	I	214	LYS	3.7
3	N	179	SER	3.7
1	C	80	THR	3.7

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Mol	Chain	Res	Type	RSRZ
2	I	144	MET	3.7
3	N	140	THR	3.7
2	G	197	TRP	3.7
2	I	147	LEU	3.6
2	G	169	SER	3.6
1	D	304	GLY	3.6
2	F	131	TYR	3.5
3	O	151	TRP	3.5
3	N	19	THR	3.5
3	N	167	PRO	3.5
3	N	177	ALA	3.4
3	M	209	LEU	3.4
3	N	115	SER	3.4
3	O	194	TYR	3.4
3	N	137	CYS	3.4
2	I	190	VAL	3.4
3	N	171	SER	3.4
3	O	121	PHE	3.4
3	O	206	GLU	3.4
2	F	175	PHE	3.4
2	I	193	PRO	3.4
3	N	90	CYS	3.3
2	I	145	VAL	3.3
2	I	207	ALA	3.3
3	N	122	PRO	3.3
2	I	125	THR	3.2
2	J	170	SER	3.2
2	I	124	LYS	3.1
1	E	14	TYR	3.1
1	B	308	TRP	3.1
1	A	339	GLY	3.1
3	O	177	ALA	3.1
1	C	338	PHE	3.1
2	F	206	VAL	3.1
2	J	167	SER	3.0
3	L	1	GLN	3.0
3	O	119	THR	3.0
3	O	135	LEU	3.0
2	H	136	GLY	3.0
2	F	12	VAL	3.0
2	F	174	THR	3.0
2	I	134	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	J	168	LEU	2.9
3	M	120	LEU	2.9
3	N	108	VAL	2.9
2	H	42	GLY	2.9
2	G	201	THR	2.9
2	I	206	VAL	2.9
2	I	187	SER	2.9
2	I	25	SER	2.9
2	G	167	SER	2.9
3	N	141	ASP	2.8
3	O	196	CYS	2.8
1	E	307	GLU	2.8
2	F	151	VAL	2.8
1	C	301	ALA	2.8
2	G	1	GLU	2.7
3	M	14	PRO	2.7
2	F	11	LEU	2.7
3	O	118	VAL	2.7
1	C	311	ILE	2.7
3	L	191	HIS	2.6
3	O	138	THR	2.6
3	O	178	SER	2.6
2	I	84	LEU	2.6
3	K	1	GLN	2.6
2	F	156	PRO	2.6
2	J	209	PRO	2.6
3	N	117	SER	2.5
2	I	1	GLU	2.5
1	A	83	HIS	2.5
2	I	26	GLY	2.5
3	M	208	SER	2.5
3	N	112	PRO	2.5
3	O	188	TRP	2.5
3	N	144	PRO	2.5
3	N	18	VAL	2.5
3	M	192	SER	2.5
2	I	211	SER	2.4
3	K	194	TYR	2.4
2	H	139	ALA	2.4
2	J	203	THR	2.4
1	C	16	PHE	2.4
1	D	305	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	N	121	PHE	2.4
2	I	210	ALA	2.4
2	G	198	PRO	2.3
3	N	114	SER	2.3
3	O	184	THR	2.3
3	O	116	PRO	2.3
3	K	197	GLN	2.3
3	N	166	GLN	2.3
1	B	340	HIS	2.3
1	D	307	GLU	2.3
1	E	308	TRP	2.3
3	M	205	VAL	2.3
1	E	9	LEU	2.3
2	H	138	ALA	2.3
3	O	181	LEU	2.3
3	O	136	VAL	2.2
2	J	169	SER	2.2
3	M	207	LYS	2.2
3	M	122	PRO	2.2
3	M	194	TYR	2.2
2	F	130	VAL	2.2
3	M	13	SER	2.2
3	O	205	VAL	2.2
2	F	162	THR	2.2
2	F	128	PRO	2.2
3	O	131	ASN	2.2
1	E	8	HIS	2.2
2	I	175	PHE	2.2
3	N	139	ILE	2.2
3	N	183	LEU	2.2
3	M	196	CYS	2.2
2	I	208	HIS	2.2
2	F	186	LEU	2.1
2	J	147	LEU	2.1
2	F	173	HIS	2.1
2	I	127	PRO	2.1
3	K	199	THR	2.1
3	N	77	ILE	2.1
1	A	24	ASN	2.1
1	D	303	ALA	2.1
3	K	149	VAL	2.1
2	J	44	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
3	O	44	HIS	2.1
3	L	181	LEU	2.1
3	K	192	SER	2.1
3	M	210	SER	2.1
1	B	307	GLU	2.1
3	L	160	GLN	2.0
1	E	338	PHE	2.0
1	B	62	LYS	2.0
1	D	23	ASP	2.0
2	F	17	SER	2.0
2	G	146	THR	2.0
3	O	26	THR	2.0
2	J	166	GLY	2.0
1	C	23	ASP	2.0
2	J	43	LYS	2.0
2	F	153	GLY	2.0
1	A	307	GLU	2.0
1	D	104	ASP	2.0
2	G	145	VAL	2.0
2	I	24	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
9	NAG	B	400	14/15	0.83	0.60	11.51	138,141,143,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	OCT	D	403	8/8	0.82	0.60	9.71	59,59,59,59	0
4	GLU	A	401	10/10	0.90	0.36	6.65	73,74,77,78	0
8	OCT	B	405	8/8	0.84	0.31	5.15	60,60,60,60	0
4	GLU	D	401	10/10	0.91	0.34	4.79	66,67,69,69	0
10	UND	B	406	11/11	0.59	0.49	4.56	60,60,60,60	0
9	NAG	E	400	14/15	0.82	0.34	3.64	172,176,179,180	0
6	IVM	E	402	62/62	0.91	0.31	2.70	65,69,73,75	0
9	NAG	C	400	14/15	0.77	0.35	2.48	128,132,137,137	0
6	IVM	B	403	62/62	0.89	0.29	2.31	60,68,83,84	0
7	LMT	A	405	27/35	0.58	0.60	2.26	143,143,143,143	0
4	GLU	B	401	10/10	0.90	0.27	1.78	67,68,71,71	0
6	IVM	A	402	62/62	0.87	0.25	1.01	55,58,69,70	0
6	IVM	A	403	62/62	0.90	0.25	0.99	70,73,80,81	0
4	GLU	C	401	10/10	0.92	0.23	0.93	74,76,79,80	0
6	IVM	D	402	62/62	0.90	0.23	0.87	61,70,84,85	0
7	LMT	A	404	26/35	0.86	0.26	-0.13	106,106,106,106	0
4	GLU	E	401	10/10	0.95	0.20	-0.40	66,67,69,70	0
5	CL	B	402	1/1	0.83	1.02	-	72,72,72,72	0
8	OCT	E	403	8/8	0.74	0.39	-	79,79,79,79	0
7	LMT	B	404	26/35	0.76	0.39	-	145,145,145,145	0

6.5 Other polymers

There are no such residues in this entry.