



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:36 AM UTC

PDB ID : 5YMR / pdb_00005ymr
Title : The Crystal Structure of IseG
Authors : Lin, L.; Zhang, J.; Xing, M.; Hua, G.; Guo, C.; Hu, Y.; Wei, Y.; Ang, E.;
Zhao, H.; Zhang, Y.; Yuchi, Z.
Deposited on : 2017-10-22
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

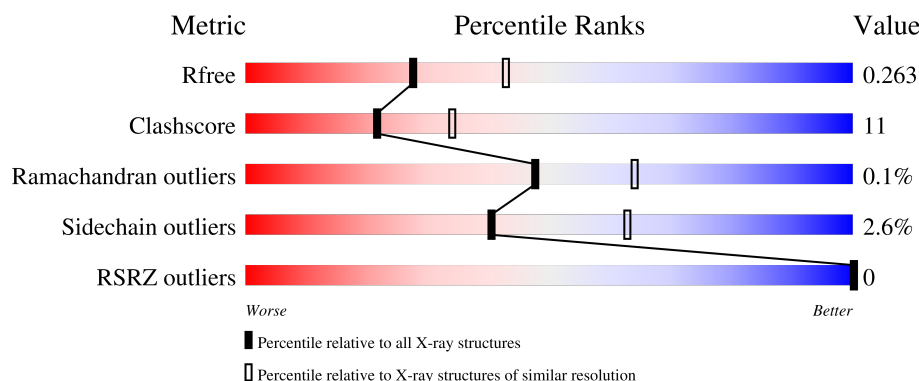
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

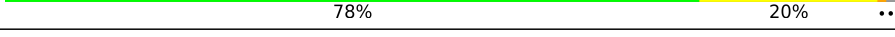
The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	808	 77% 20% ..
1	B	808	 75% 22% ..
1	C	808	 77% 21% ..
1	D	808	 78% 20% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25800 atoms, of which 68 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 Formate acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	798	Total	C	N	O	S	0	0	0
			6251	3980	1062	1177	32			
1	D	798	Total	C	N	O	S	0	0	0
			6232	3970	1059	1171	32			
1	C	797	Total	C	N	O	S	0	0	0
			6229	3961	1061	1175	32			
1	A	798	Total	C	N	O	S	0	0	0
			6219	3962	1052	1173	32			

There are 24 discrepancies between the modelled and reference sequences:

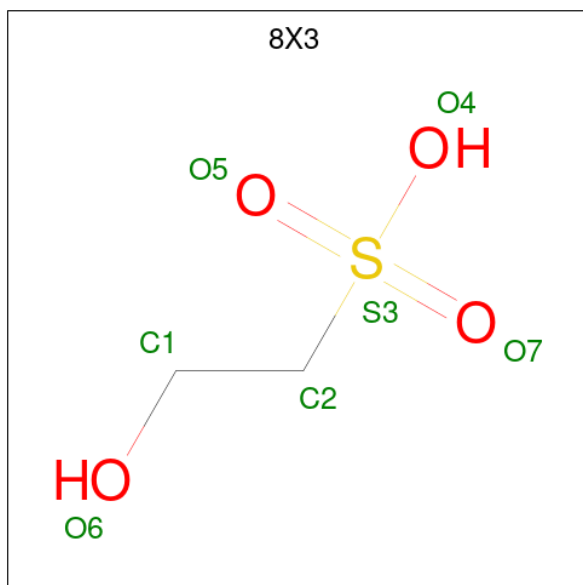
Chain	Residue	Modelled	Actual	Comment	Reference
B	21	SER	-	expression tag	UNP Q727N1
B	22	ASN	-	expression tag	UNP Q727N1
B	23	ALA	-	expression tag	UNP Q727N1
B	133	ALA	GLU	engineered mutation	UNP Q727N1
B	134	ALA	ASP	engineered mutation	UNP Q727N1
B	136	ALA	ARG	engineered mutation	UNP Q727N1
D	21	SER	-	expression tag	UNP Q727N1
D	22	ASN	-	expression tag	UNP Q727N1
D	23	ALA	-	expression tag	UNP Q727N1
D	133	ALA	GLU	engineered mutation	UNP Q727N1
D	134	ALA	ASP	engineered mutation	UNP Q727N1
D	136	ALA	ARG	engineered mutation	UNP Q727N1
C	21	SER	-	expression tag	UNP Q727N1
C	22	ASN	-	expression tag	UNP Q727N1
C	23	ALA	-	expression tag	UNP Q727N1
C	133	ALA	GLU	engineered mutation	UNP Q727N1
C	134	ALA	ASP	engineered mutation	UNP Q727N1
C	136	ALA	ARG	engineered mutation	UNP Q727N1
A	21	SER	-	expression tag	UNP Q727N1
A	22	ASN	-	expression tag	UNP Q727N1
A	23	ALA	-	expression tag	UNP Q727N1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	133	ALA	GLU	engineered mutation	UNP Q727N1
A	134	ALA	ASP	engineered mutation	UNP Q727N1
A	136	ALA	ARG	engineered mutation	UNP Q727N1

- Molecule 2 is 2-hydroxyethylsulfonic acid (CCD ID: 8X3) (formula: $C_2H_6O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	O	S	0	0
			12	2	5	4	1		
2	D	1	Total	C	H	O	S	0	0
			12	2	5	4	1		
2	C	1	Total	C	H	O	S	0	0
			12	2	5	4	1		
2	A	1	Total	C	H	O	S	0	0
			12	2	5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		

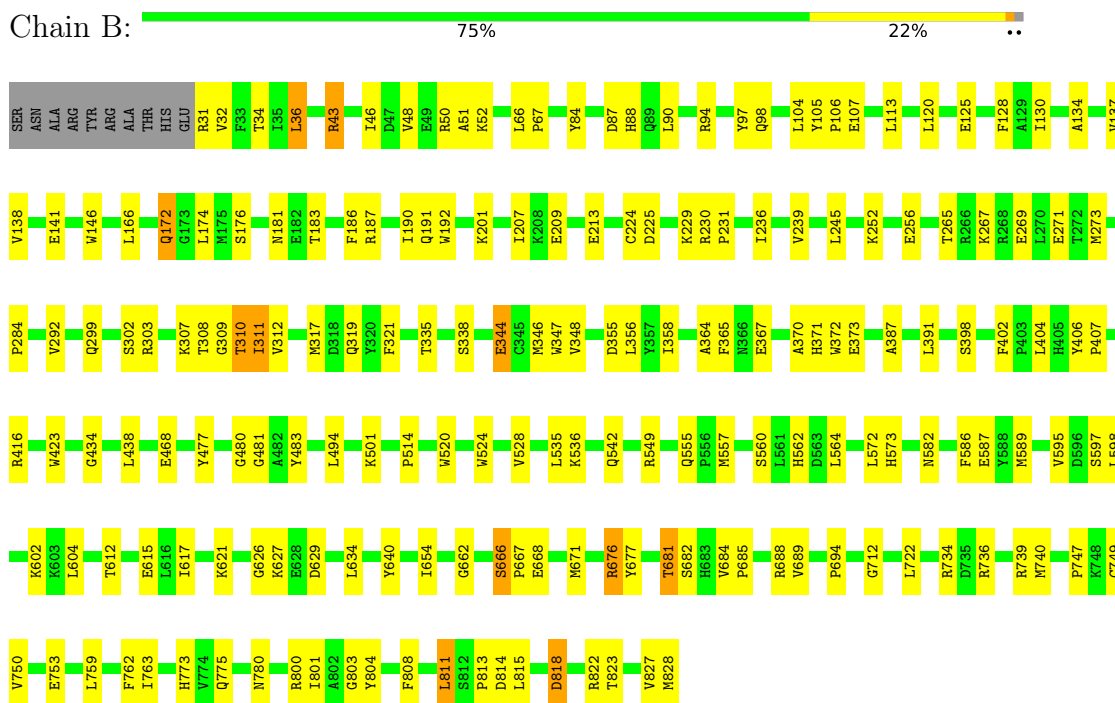
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	204	Total	O	0	0
			204	204		
4	D	154	Total	O	0	0
			154	154		
4	C	161	Total	O	0	0
			161	161		
4	A	218	Total	O	0	0
			218	218		

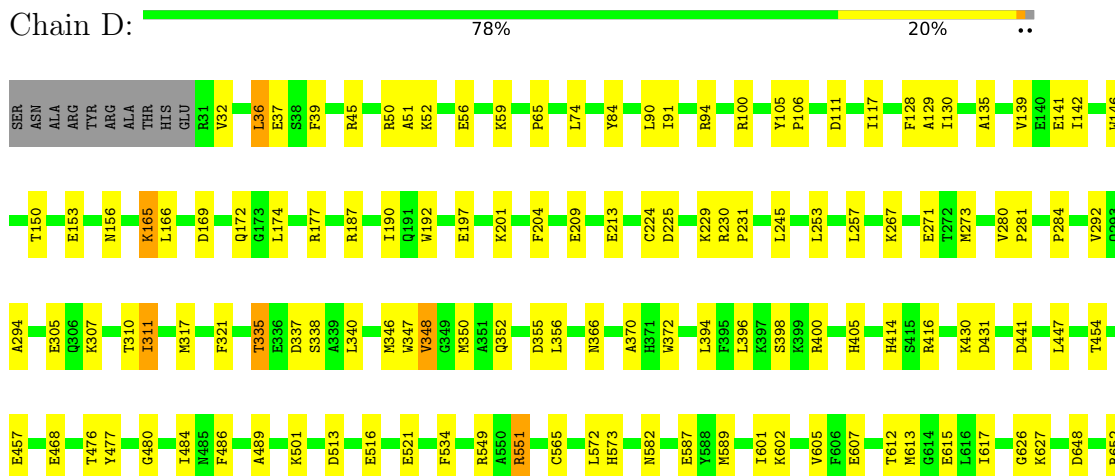
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Formate acetyltransferase



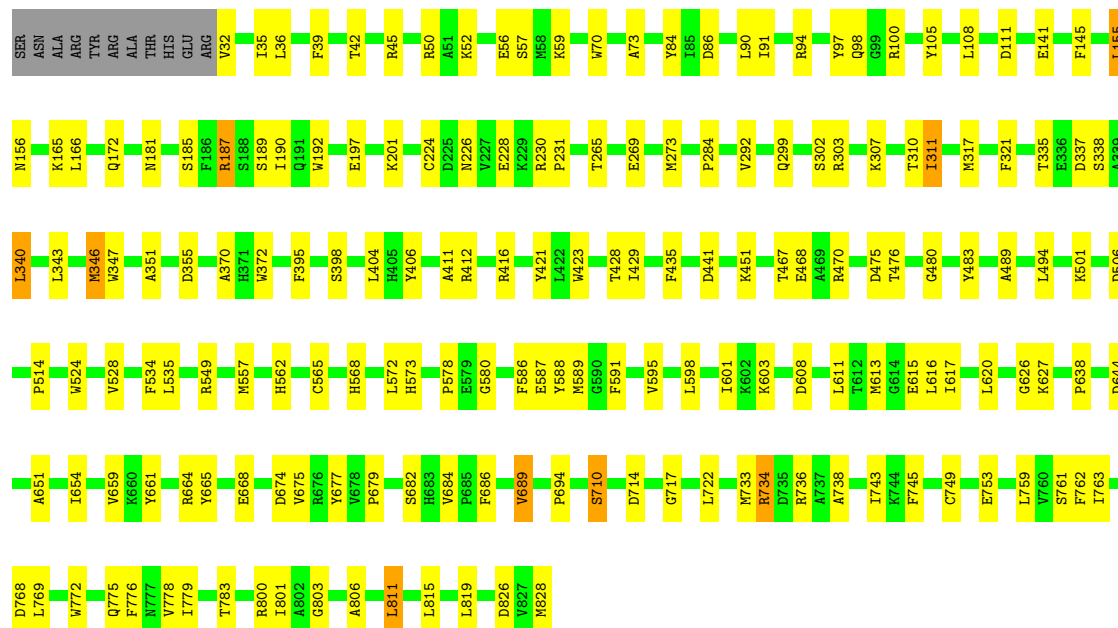
- Molecule 1: Formate acetyltransferase





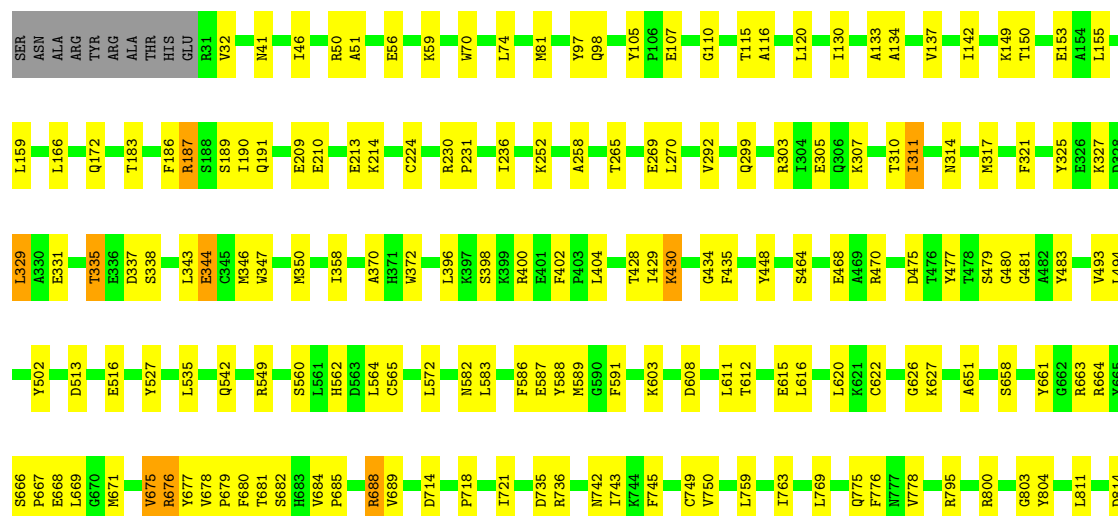
• Molecule 1: Formate acetyltransferase

Chain C: 77% 21% ..



• Molecule 1: Formate acetyltransferase

Chain A: 77% 20% ..



L815	
L819	
D826	
V827	
M828	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.11Å 159.44Å 115.38Å 90.00° 91.66° 90.00°	Depositor
Resolution (Å)	48.27 – 2.40 48.27 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.27-2.40) 87.7 (48.27-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.212 , 0.262 0.213 , 0.263	Depositor DCC
R_{free} test set	15307 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 11.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.033 for l,k,-h 0.087 for h,-k,-l 0.035 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25800	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 8X3, GOL

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	0.38	0/6377	0.54	0/8673
1	B	0.36	0/6409	0.54	0/8713
1	C	0.34	0/6387	0.52	0/8683
1	D	0.34	0/6390	0.53	0/8685
All	All	0.36	0/25563	0.53	0/34754

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6219	0	5936	142	0
1	B	6251	0	5992	137	0
1	C	6229	0	5937	128	0
1	D	6232	0	5965	131	0
2	A	7	5	0	0	0
2	B	7	5	0	0	0
2	C	7	5	0	0	0
2	D	7	5	0	1	0
3	A	12	16	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	16	16	1	0
3	C	6	8	8	0	0
3	D	6	8	8	2	0
4	A	218	0	0	10	0
4	B	204	0	0	2	0
4	C	161	0	0	6	0
4	D	154	0	0	10	0
All	All	25732	68	23878	530	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 11.

All (530) 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:B:48:VAL:HG21	1:B:137:VAL:HG21	1.28	1.07
1:C:36:LEU:HD11	1:C:404:LEU:HD11	1.36	1.07
1:D:346:MET:HG2	1:D:350:MET:HE3	1.36	1.06
1:D:659:VAL:HG12	1:D:733:MET:HE2	1.41	1.03
1:A:775:GLN:HE22	1:A:803:GLY:H	1.03	1.01
1:D:347:TRP:HZ3	1:D:398:SER:HG	1.04	0.97
1:B:299:GLN:HG2	1:B:303:ARG:HH12	1.27	0.97
1:D:335:THR:HG22	1:D:337:ASP:H	1.30	0.95
1:D:317:MET:HE2	1:D:321:PHE:HE2	1.28	0.94
1:C:775:GLN:HE22	1:C:803:GLY:H	1.08	0.94
1:C:659:VAL:HG12	1:C:733:MET:HE2	1.47	0.93
1:C:317:MET:HE3	1:C:321:PHE:HE2	1.32	0.93
1:A:46:ILE:HD11	1:A:120:LEU:HD13	1.51	0.92
1:C:32:VAL:HG22	1:C:35:ILE:HG13	1.51	0.92
1:A:187:ARG:HD2	4:A:1169:HOH:O	1.71	0.91
1:D:36:LEU:HD22	1:D:348:VAL:HG23	1.52	0.90
1:B:775:GLN:HE22	1:B:803:GLY:H	1.18	0.89
1:B:299:GLN:HG2	1:B:303:ARG:NH1	1.89	0.86
1:A:347:TRP:HZ3	1:A:398:SER:HG	1.24	0.86
1:A:335:THR:HG22	1:A:338:SER:H	1.37	0.85
1:D:663:ARG:HD2	1:D:733:MET:HE3	1.58	0.85
1:C:335:THR:HG22	1:C:337:ASP:H	1.39	0.85
1:C:317:MET:HE3	1:C:321:PHE:CE2	2.12	0.83
1:D:317:MET:HE2	1:D:321:PHE:CE2	2.12	0.82
1:B:46:ILE:HD12	1:B:130:ILE:HG12	1.62	0.82
1:B:501:LYS:HG2	1:B:689:VAL:HG23	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:VAL:HG13	1:A:346:MET:HE3	1.61	0.82
1:C:501:LYS:HG2	1:C:689:VAL:CG2	2.10	0.82
1:C:668:GLU:HG3	4:C:1033:HOH:O	1.79	0.81
1:C:32:VAL:HG23	1:C:35:ILE:H	1.44	0.81
1:B:365:PHE:C	1:B:681:THR:HG22	2.07	0.80
1:C:299:GLN:HG2	1:C:303:ARG:HH12	1.45	0.80
1:D:335:THR:HG22	1:D:337:ASP:N	1.95	0.80
1:D:292:VAL:HG13	1:D:346:MET:HE3	1.64	0.79
1:B:292:VAL:HG13	1:B:346:MET:HE3	1.64	0.79
1:B:347:TRP:HZ3	1:B:398:SER:HG	1.28	0.79
1:C:317:MET:HE2	1:C:395:PHE:CZ	2.17	0.78
1:A:589:MET:HE2	1:A:682:SER:OG	1.83	0.78
1:D:811:LEU:HG	1:D:815:LEU:HD23	1.67	0.77
1:B:317:MET:HE2	1:B:321:PHE:HE2	1.48	0.77
1:D:292:VAL:HG13	1:D:346:MET:CE	2.16	0.76
1:B:46:ILE:HD11	1:B:120:LEU:HD13	1.68	0.75
1:A:299:GLN:HG2	1:A:303:ARG:HH12	1.52	0.75
1:B:32:VAL:HG11	1:B:344:GLU:HB3	1.67	0.75
1:C:501:LYS:HG2	1:C:689:VAL:HG23	1.70	0.74
1:B:317:MET:HE2	1:B:321:PHE:CE2	2.22	0.74
1:C:36:LEU:HD11	1:C:404:LEU:CD1	2.17	0.73
1:B:299:GLN:CG	1:B:303:ARG:HH12	1.99	0.73
1:A:745:PHE:CZ	1:A:828:MET:HE2	2.24	0.73
1:A:775:GLN:HE22	1:A:803:GLY:N	1.84	0.73
1:C:299:GLN:HG2	1:C:303:ARG:NH1	2.04	0.73
1:A:430:LYS:HE2	1:A:750:VAL:O	1.89	0.72
1:D:659:VAL:HG12	1:D:733:MET:CE	2.16	0.72
1:D:340:LEU:HD13	1:D:394:LEU:HD11	1.70	0.72
1:B:501:LYS:HG2	1:B:689:VAL:CG2	2.18	0.72
1:D:90:LEU:C	1:D:273:MET:HE2	2.15	0.72
1:C:197:GLU:OE2	1:C:201:LYS:HE3	1.89	0.72
1:C:659:VAL:HG12	1:C:733:MET:CE	2.18	0.71
1:A:347:TRP:HZ3	1:A:398:SER:OG	1.71	0.71
1:A:116:ALA:HB1	1:A:120:LEU:CD1	2.20	0.71
1:A:775:GLN:NE2	1:A:803:GLY:H	1.83	0.71
1:D:668:GLU:HB3	1:A:224:CYS:SG	2.30	0.71
1:D:668:GLU:HG3	4:D:1063:HOH:O	1.90	0.70
1:B:589:MET:HE2	1:B:682:SER:OG	1.92	0.70
1:C:317:MET:HE2	1:C:395:PHE:CE2	2.27	0.70
1:D:105:TYR:CD1	1:D:307:LYS:HB2	2.26	0.70
1:D:521:GLU:HG3	4:D:1061:HOH:O	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:GLU:HG3	4:A:1034:HOH:O	1.92	0.69
1:A:292:VAL:HG13	1:A:346:MET:CE	2.22	0.69
1:A:586:PHE:CE2	1:A:675:VAL:HG13	2.28	0.68
1:C:52:LYS:HE3	1:C:141:GLU:OE2	1.93	0.68
1:B:48:VAL:CG2	1:B:137:VAL:HG21	2.15	0.68
1:A:299:GLN:HG2	1:A:303:ARG:NH1	2.08	0.67
1:A:622:CYS:HB3	4:A:1206:HOH:O	1.93	0.67
1:B:105:TYR:CE2	1:B:307:LYS:HB2	2.30	0.67
1:A:483:TYR:CE2	1:A:587:GLU:HG2	2.30	0.67
1:D:501:LYS:HG2	1:D:689:VAL:CG2	2.24	0.67
1:C:335:THR:HG22	1:C:337:ASP:N	2.10	0.67
1:B:612:THR:OG1	1:B:615:GLU:HG3	1.94	0.66
1:C:501:LYS:HG2	1:C:689:VAL:HG22	1.77	0.66
1:B:46:ILE:HD12	1:B:130:ILE:CG1	2.25	0.66
1:D:501:LYS:HG2	1:D:689:VAL:HG22	1.76	0.66
1:C:801:ILE:HD11	1:C:811:LEU:HD21	1.76	0.66
1:A:750:VAL:O	1:A:750:VAL:HG22	1.95	0.66
1:B:347:TRP:HZ3	1:B:398:SER:OG	1.78	0.65
1:D:105:TYR:CE1	1:D:307:LYS:HB2	2.30	0.65
1:D:769:LEU:HD23	1:C:416:ARG:HD2	1.78	0.65
1:D:340:LEU:HD13	1:D:394:LEU:CD1	2.26	0.65
1:C:181:ASN:HA	4:C:1137:HOH:O	1.97	0.65
1:C:811:LEU:HG	1:C:815:LEU:HD23	1.79	0.65
1:A:116:ALA:HB1	1:A:120:LEU:HD12	1.79	0.64
1:A:120:LEU:HD11	1:A:358:ILE:HG22	1.78	0.64
1:B:252:LYS:HE2	1:B:256:GLU:OE2	1.98	0.64
1:C:32:VAL:CG2	1:C:35:ILE:H	2.10	0.64
1:D:209:GLU:O	1:D:213:GLU:HG3	1.98	0.64
1:B:31:ARG:N	1:B:34:THR:HG1	1.96	0.63
1:C:749:CYS:SG	1:C:828:MET:HG3	2.39	0.63
1:B:749:CYS:SG	1:B:828:MET:HE2	2.39	0.63
1:A:155:LEU:HD11	1:A:159:LEU:HD21	1.81	0.63
1:C:32:VAL:CG2	1:C:35:ILE:HG13	2.27	0.63
1:C:423:TRP:HH2	1:C:753:GLU:HG3	1.64	0.62
1:A:115:THR:HG23	4:A:1091:HOH:O	2.00	0.62
1:D:36:LEU:HD22	1:D:348:VAL:CG2	2.26	0.62
1:B:483:TYR:CE2	1:B:587:GLU:HG2	2.35	0.62
1:A:325:TYR:O	1:A:329:LEU:HB2	2.00	0.61
1:A:105:TYR:CD2	1:A:307:LYS:HB2	2.35	0.61
1:C:589:MET:HE2	1:C:682:SER:OG	2.01	0.61
1:D:416:ARG:HE	3:D:902:GOL:H32	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:GLN:CG	1:C:303:ARG:HH12	2.15	0.60
1:A:343:LEU:HB3	1:A:347:TRP:CZ3	2.35	0.60
1:D:801:ILE:HD11	1:D:811:LEU:HD21	1.83	0.60
1:D:612:THR:OG1	1:D:615:GLU:HG3	2.01	0.60
1:D:135:ALA:O	1:D:139:VAL:HG23	2.02	0.59
1:B:750:VAL:HG12	1:B:828:MET:HE1	1.85	0.59
1:D:587:GLU:OE1	1:D:676:ARG:CD	2.50	0.59
1:C:91:ILE:C	1:C:273:MET:HE2	2.28	0.59
1:B:52:LYS:HE3	1:B:141:GLU:OE2	2.02	0.59
1:D:676:ARG:NH2	2:D:901:8X3:O5	2.31	0.58
1:C:428:THR:HG22	1:C:435:PHE:O	2.03	0.58
1:C:565:CYS:SG	1:C:572:LEU:HD13	2.42	0.58
1:B:48:VAL:HG21	1:B:137:VAL:CG2	2.19	0.58
1:B:808:PHE:HA	1:B:811:LEU:HD22	1.84	0.58
1:A:327:LYS:O	1:A:331:GLU:HG3	2.03	0.58
1:A:565:CYS:SG	1:A:572:LEU:HD13	2.43	0.58
1:B:423:TRP:HH2	1:B:753:GLU:HG3	1.68	0.58
1:B:172:GLN:HG3	1:B:174:LEU:HG	1.83	0.58
1:A:314:ASN:HD21	1:A:350:MET:HE1	1.67	0.58
1:A:513:ASP:HB3	1:A:516:GLU:HG3	1.84	0.58
1:A:684:VAL:HG21	1:A:815:LEU:HB2	1.86	0.58
1:D:811:LEU:HG	1:D:815:LEU:CD2	2.33	0.58
1:C:524:TRP:O	1:C:528:VAL:HG23	2.04	0.58
1:B:749:CYS:SG	1:B:828:MET:HB3	2.43	0.58
1:C:589:MET:HE1	1:C:679:PRO:CB	2.34	0.58
1:B:494:LEU:O	1:B:514:PRO:HG3	2.04	0.57
1:C:165:LYS:HD2	1:C:506:ASP:O	2.04	0.57
1:D:626:GLY:O	1:D:627:LYS:HD3	2.05	0.57
1:A:314:ASN:HD21	1:A:350:MET:CE	2.17	0.57
1:A:688:ARG:HD2	1:A:814:ASP:OD2	2.03	0.57
1:C:201:LYS:O	1:C:284:PRO:HB3	2.04	0.57
1:A:183:THR:HA	1:A:186:PHE:CE1	2.39	0.57
1:A:658:SER:CB	1:A:675:VAL:HG11	2.35	0.57
1:A:589:MET:HE1	1:A:679:PRO:CB	2.34	0.57
1:B:230:ARG:HB3	1:B:231:PRO:HD3	1.86	0.57
1:C:775:GLN:NE2	1:C:803:GLY:H	1.90	0.56
1:B:818:ASP:O	1:B:822:ARG:HG3	2.05	0.56
1:B:36:LEU:HD13	1:B:348:VAL:HG23	1.87	0.56
1:D:430:LYS:HE2	1:D:756:SER:OG	2.05	0.56
1:C:86:ASP:HB3	4:C:1098:HOH:O	2.06	0.56
1:C:684:VAL:HG21	1:C:815:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:801:ILE:HD11	1:B:811:LEU:HD21	1.88	0.56
1:D:659:VAL:CG1	1:D:733:MET:HE2	2.26	0.56
1:C:317:MET:HE2	1:C:395:PHE:HZ	1.67	0.56
1:A:658:SER:HB3	1:A:675:VAL:CG1	2.35	0.56
1:C:659:VAL:CG1	1:C:733:MET:HE2	2.28	0.56
1:D:489:ALA:HB2	1:D:534:PHE:CE2	2.41	0.56
1:A:105:TYR:CE2	1:A:307:LYS:HB2	2.41	0.56
1:B:201:LYS:O	1:B:284:PRO:HB3	2.05	0.55
1:C:489:ALA:HB2	1:C:534:PHE:CE2	2.42	0.55
1:B:107:GLU:HA	1:B:146:TRP:CZ3	2.42	0.55
1:D:652:ARG:NE	4:D:1002:HOH:O	2.33	0.55
1:B:209:GLU:O	1:B:213:GLU:HG3	2.06	0.55
1:A:310:THR:HB	1:A:372:TRP:HB2	1.87	0.55
1:D:454:THR:OG1	1:D:457:GLU:HG3	2.06	0.55
1:B:46:ILE:HD12	1:B:130:ILE:CD1	2.37	0.55
1:A:56:GLU:HA	1:A:59:LYS:HE2	1.88	0.55
1:C:265:THR:O	1:C:269:GLU:HG3	2.07	0.55
1:B:367:GLU:H	1:B:681:THR:HG21	1.71	0.55
1:A:335:THR:CG2	1:A:337:ASP:H	2.19	0.55
1:B:344:GLU:HG3	1:B:402:PHE:CD1	2.40	0.55
1:A:612:THR:OG1	1:A:615:GLU:HG3	2.07	0.55
1:B:265:THR:O	1:B:269:GLU:HG3	2.07	0.54
1:D:190:ILE:HG23	1:D:480:GLY:HA2	1.89	0.54
1:A:41:ASN:HB2	1:A:795:ARG:HH12	1.73	0.54
1:A:230:ARG:HB3	1:A:231:PRO:HD3	1.88	0.54
1:B:105:TYR:CD2	1:B:307:LYS:HB2	2.42	0.54
1:B:598:LEU:HD12	1:B:654:ILE:HD11	1.90	0.54
1:A:616:LEU:O	1:A:620:LEU:HG	2.07	0.54
1:B:434:GLY:HA3	1:B:800:ARG:HB2	1.90	0.54
1:B:775:GLN:HE22	1:B:803:GLY:N	1.98	0.54
1:A:396:LEU:O	1:A:400:ARG:HG3	2.07	0.54
1:A:314:ASN:ND2	1:A:350:MET:HE1	2.22	0.54
1:B:827:VAL:O	1:B:828:MET:C	2.50	0.54
1:C:598:LEU:HD12	1:C:654:ILE:HD11	1.90	0.54
1:A:611:LEU:HD23	1:A:611:LEU:N	2.22	0.54
1:A:714:ASP:OD1	1:A:714:ASP:N	2.38	0.54
1:B:759:LEU:O	1:B:763:ILE:HG13	2.07	0.54
1:D:91:ILE:N	1:D:273:MET:HE2	2.23	0.54
1:C:50:ARG:HD3	1:C:50:ARG:C	2.32	0.54
1:B:292:VAL:HG13	1:B:346:MET:CE	2.37	0.53
1:B:681:THR:HG23	1:B:681:THR:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ALA:O	1:B:137:VAL:HG22	2.09	0.53
1:B:662:GLY:O	1:B:666:SER:HB2	2.08	0.53
1:D:589:MET:HE1	1:D:679:PRO:CB	2.39	0.53
1:C:302:SER:HB2	1:C:557:MET:HE1	1.89	0.53
1:A:470:ARG:HH11	1:A:475:ASP:HB3	1.74	0.53
1:D:587:GLU:OE1	1:D:676:ARG:HD3	2.07	0.53
1:D:775:GLN:HE22	1:D:803:GLY:HA2	1.73	0.53
1:A:116:ALA:HB1	1:A:120:LEU:HD11	1.91	0.53
1:D:36:LEU:HD13	1:D:39:PHE:CZ	2.44	0.53
1:C:84:TYR:CD2	1:C:94:ARG:HD3	2.44	0.53
1:D:230:ARG:HB3	1:D:231:PRO:HD3	1.91	0.52
1:D:52:LYS:HE2	1:D:141:GLU:OE2	2.10	0.52
1:D:245:LEU:C	1:D:245:LEU:HD23	2.34	0.52
1:D:648:ASP:OD2	1:D:724:SER:OG	2.26	0.52
1:D:660:LYS:HA	1:D:733:MET:HE1	1.91	0.52
1:A:327:LYS:HD2	4:A:1214:HOH:O	2.08	0.52
1:C:230:ARG:HB3	1:C:231:PRO:HD3	1.91	0.52
1:D:56:GLU:HA	1:D:59:LYS:HE2	1.92	0.52
1:D:416:ARG:HE	3:D:902:GOL:C3	2.23	0.52
1:C:90:LEU:C	1:C:273:MET:HE3	2.35	0.52
1:A:210:GLU:OE2	1:A:214:LYS:NZ	2.39	0.52
1:A:591:PHE:CZ	1:A:651:ALA:HB1	2.45	0.52
1:D:549:ARG:HH22	1:D:573:HIS:CE1	2.28	0.52
1:D:50:ARG:C	1:D:50:ARG:HD3	2.35	0.51
1:B:236:ILE:O	1:B:239:VAL:HG12	2.10	0.51
1:D:370:ALA:HB1	1:D:372:TRP:CH2	2.46	0.51
1:C:335:THR:N	1:C:338:SER:OG	2.31	0.51
1:A:317:MET:O	1:A:321:PHE:HB2	2.10	0.51
1:B:481:GLY:HA2	1:B:542:GLN:OE1	2.09	0.51
1:D:224:CYS:SG	1:A:668:GLU:HB3	2.51	0.51
1:A:663:ARG:HB2	1:A:735:ASP:CG	2.35	0.51
1:B:90:LEU:C	1:B:273:MET:HE2	2.36	0.51
1:C:588:TYR:HB3	1:C:677:TYR:CE2	2.46	0.51
1:D:447:LEU:HD11	1:D:736:ARG:NH1	2.25	0.51
1:C:111:ASP:N	1:C:111:ASP:OD1	2.43	0.51
1:B:225:ASP:HA	1:B:229:LYS:HB2	1.91	0.51
1:B:668:GLU:HB3	1:C:224:CYS:SG	2.51	0.51
1:D:117:ILE:HD12	1:D:130:ILE:HD13	1.93	0.51
1:C:470:ARG:HH11	1:C:475:ASP:HB3	1.76	0.51
1:B:370:ALA:HB1	1:B:372:TRP:CH2	2.45	0.51
1:C:429:ILE:HD13	1:C:776:PHE:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ALA:HB1	1:A:372:TRP:CH2	2.46	0.51
1:D:605:VAL:HG11	1:D:613:MET:HE2	1.93	0.50
1:C:589:MET:HG3	1:C:686:PHE:CE2	2.46	0.50
1:A:335:THR:HG23	1:A:337:ASP:H	1.76	0.50
1:A:335:THR:H	1:A:338:SER:HG	1.59	0.50
1:D:718:PRO:CG	1:D:828:MET:HA	2.41	0.50
1:B:307:LYS:NZ	1:B:355:ASP:OD1	2.41	0.50
1:A:587:GLU:OE1	1:A:676:ARG:HD2	2.11	0.50
1:D:150:THR:HG23	1:D:153:GLU:OE2	2.11	0.50
1:D:477:TYR:CZ	1:D:671:MET:HE1	2.45	0.50
1:C:568:HIS:CG	1:C:578:PRO:HG2	2.47	0.50
1:C:743:ILE:O	1:C:776:PHE:HA	2.12	0.50
1:C:745:PHE:O	1:C:778:VAL:HA	2.11	0.50
1:A:335:THR:HG22	1:A:338:SER:N	2.16	0.50
1:B:626:GLY:O	1:B:627:LYS:HD3	2.12	0.50
1:D:416:ARG:HD2	1:C:769:LEU:HD23	1.93	0.50
1:B:722:LEU:HD11	1:B:762:PHE:CZ	2.46	0.49
1:C:105:TYR:CE1	1:C:307:LYS:HB2	2.47	0.49
1:A:470:ARG:NH1	1:A:475:ASP:HB3	2.28	0.49
1:A:587:GLU:OE1	1:A:676:ARG:CD	2.60	0.49
1:D:681:THR:O	1:D:685:PRO:HD2	2.12	0.49
1:C:292:VAL:HG13	1:C:346:MET:HE3	1.93	0.49
1:C:611:LEU:HB2	1:C:615:GLU:OE2	2.12	0.49
1:B:775:GLN:NE2	1:B:803:GLY:H	1.99	0.49
1:D:613:MET:O	1:D:617:ILE:HG12	2.12	0.49
1:C:801:ILE:HD11	1:C:806:ALA:HB3	1.94	0.49
1:A:718:PRO:CG	1:A:828:MET:HA	2.43	0.49
1:D:727:ASN:CB	4:D:1136:HOH:O	2.59	0.49
1:C:351:ALA:HA	1:C:406:TYR:CZ	2.47	0.49
1:D:652:ARG:NH2	4:D:1002:HOH:O	2.45	0.49
1:C:108:LEU:HD11	1:C:185:SER:C	2.37	0.49
1:D:414:HIS:HB3	1:D:441:ASP:HB2	1.94	0.49
1:C:759:LEU:O	1:C:763:ILE:HG13	2.13	0.49
1:B:740:MET:HE1	1:B:803:GLY:N	2.28	0.49
1:D:201:LYS:O	1:D:284:PRO:HB3	2.12	0.49
1:C:155:LEU:O	1:C:155:LEU:HD22	2.13	0.49
1:B:302:SER:HB2	1:B:557:MET:HE1	1.94	0.48
1:B:677:TYR:CD1	1:B:739:ARG:HG2	2.48	0.48
1:D:335:THR:CG2	1:D:337:ASP:H	2.14	0.48
1:A:149:LYS:O	3:A:903:GOL:O3	2.30	0.48
1:A:292:VAL:CG1	1:A:346:MET:HE3	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:GLY:HA2	1:A:542:GLN:OE1	2.14	0.48
1:A:675:VAL:HG22	4:A:1180:HOH:O	2.12	0.48
1:A:350:MET:HE3	4:A:1004:HOH:O	2.13	0.48
1:D:551:ARG:NH2	4:D:1005:HOH:O	2.38	0.48
1:A:172:GLN:HG2	4:A:1155:HOH:O	2.12	0.48
1:D:156:ASN:ND2	1:D:172:GLN:HA	2.28	0.48
1:D:190:ILE:CG2	1:D:480:GLY:HA2	2.42	0.48
1:C:299:GLN:NE2	1:C:303:ARG:HH22	2.11	0.48
1:C:801:ILE:CD1	1:C:811:LEU:HD21	2.43	0.48
1:D:759:LEU:O	1:D:763:ILE:HG13	2.13	0.48
1:B:595:VAL:HG11	1:B:640:TYR:HB2	1.95	0.48
1:D:601:ILE:HD11	1:D:694:PRO:HG2	1.95	0.48
1:D:745:PHE:O	1:D:778:VAL:HA	2.14	0.48
1:B:604:LEU:CD1	1:B:634:LEU:HA	2.43	0.48
1:B:747:PRO:HD2	1:B:780:ASN:ND2	2.29	0.47
1:D:100:ARG:HG2	1:D:352:GLN:HA	1.96	0.47
1:C:613:MET:O	1:C:617:ILE:HG12	2.13	0.47
1:D:111:ASP:HB3	4:D:1081:HOH:O	2.13	0.47
1:C:105:TYR:CD1	1:C:307:LYS:HB2	2.48	0.47
1:A:50:ARG:HB2	1:A:81:MET:HE1	1.95	0.47
1:D:513:ASP:HB3	1:D:516:GLU:HG3	1.96	0.47
1:A:676:ARG:HD3	1:A:678:VAL:HB	1.96	0.47
1:A:742:ASN:O	1:A:743:ILE:HD13	2.14	0.47
1:B:120:LEU:HD11	1:B:358:ILE:HG22	1.97	0.47
1:D:292:VAL:CG1	1:D:346:MET:HE3	2.41	0.47
1:D:317:MET:O	1:D:321:PHE:HB2	2.15	0.47
1:C:187:ARG:HG3	1:C:189:SER:O	2.15	0.47
1:C:616:LEU:O	1:C:620:LEU:HG	2.13	0.47
1:D:280:VAL:HB	1:D:294:ALA:HB2	1.96	0.47
1:D:45:ARG:HA	1:D:129:ALA:O	2.15	0.47
1:D:74:LEU:HD21	1:D:305:GLU:HA	1.97	0.47
1:D:310:THR:O	1:D:311:ILE:HB	2.15	0.47
1:D:335:THR:H	1:D:338:SER:HG	1.60	0.47
1:D:468:GLU:HG2	1:D:676:ARG:HH21	1.80	0.47
1:D:714:ASP:OD1	1:D:714:ASP:N	2.45	0.47
1:A:335:THR:HG22	1:A:337:ASP:N	2.29	0.47
1:A:428:THR:HG22	1:A:435:PHE:O	2.15	0.47
1:A:815:LEU:O	1:A:819:LEU:HD13	2.15	0.47
1:B:712:GLY:HA2	1:B:823:THR:OG1	2.15	0.47
1:D:818:ASP:O	1:D:822:ARG:HG3	2.15	0.47
1:C:192:TRP:CZ2	1:C:572:LEU:HD21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:745:PHE:CZ	1:C:828:MET:HE3	2.50	0.47
1:C:717:GLY:HA3	4:C:1015:HOH:O	2.14	0.47
1:A:46:ILE:CD1	1:A:120:LEU:HD13	2.36	0.47
1:A:493:VAL:HG21	1:A:527:TYR:HA	1.97	0.47
1:B:319:GLN:NE2	1:B:387:ALA:HB1	2.30	0.47
1:C:626:GLY:O	1:C:627:LYS:HD3	2.15	0.47
1:A:347:TRP:HD1	1:A:350:MET:SD	2.38	0.47
1:A:658:SER:HB3	1:A:675:VAL:HG11	1.96	0.47
1:B:36:LEU:HD11	1:B:404:LEU:HD11	1.97	0.46
1:B:311:ILE:HB	1:B:373:GLU:HG3	1.97	0.46
1:B:347:TRP:CZ2	1:B:407:PRO:HG3	2.50	0.46
1:A:430:LYS:HE2	1:A:750:VAL:HG22	1.97	0.46
1:B:299:GLN:CD	1:B:303:ARG:HH12	2.23	0.46
1:C:42:THR:O	1:C:100:ARG:NH1	2.41	0.46
1:B:310:THR:HB	1:B:372:TRP:HB2	1.97	0.46
1:D:169:ASP:HB2	1:D:177:ARG:HG3	1.96	0.46
1:D:311:ILE:HD11	1:D:355:ASP:HB2	1.97	0.46
1:D:366:ASN:HB3	1:D:370:ALA:HB3	1.96	0.46
1:C:311:ILE:HD11	1:C:355:ASP:HB2	1.98	0.46
1:A:721:ILE:HD12	1:A:743:ILE:HD12	1.98	0.46
1:B:128:PHE:CD2	1:B:356:LEU:HD13	2.51	0.46
1:B:555:GLN:OE1	1:B:572:LEU:HD23	2.15	0.46
1:C:36:LEU:HD12	1:C:39:PHE:CZ	2.50	0.46
1:B:224:CYS:SG	1:C:668:GLU:HB3	2.56	0.46
1:D:307:LYS:HE3	1:D:356:LEU:O	2.16	0.46
1:D:468:GLU:CG	1:D:676:ARG:HH21	2.29	0.46
1:A:434:GLY:HA3	1:A:800:ARG:HB2	1.98	0.46
1:D:187:ARG:HD2	4:D:1072:HOH:O	2.16	0.46
1:D:346:MET:HG2	1:D:350:MET:CE	2.26	0.46
1:B:468:GLU:N	1:B:468:GLU:CD	2.74	0.46
1:D:65:PRO:HG3	4:D:1125:HOH:O	2.15	0.46
1:A:190:ILE:HG23	1:A:480:GLY:HA2	1.98	0.46
1:A:402:PHE:CE2	1:A:404:LEU:HB2	2.51	0.46
1:B:50:ARG:HD3	1:B:50:ARG:C	2.41	0.46
1:B:51:ALA:HB2	1:B:104:LEU:HB2	1.98	0.46
1:B:617:ILE:HG22	1:B:621:LYS:HD3	1.98	0.46
1:D:32:VAL:O	1:D:36:LEU:HB2	2.15	0.46
1:C:343:LEU:HB3	1:C:347:TRP:CH2	2.51	0.46
1:A:265:THR:O	1:A:269:GLU:HG3	2.16	0.46
1:B:549:ARG:HH22	1:B:573:HIS:CE1	2.34	0.45
1:A:562:HIS:CE1	1:A:564:LEU:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:VAL:HG21	1:B:344:GLU:HG2	1.98	0.45
1:C:317:MET:O	1:C:321:PHE:HB2	2.16	0.45
1:A:130:ILE:HD11	1:A:134:ALA:CB	2.46	0.45
1:A:663:ARG:HB2	1:A:735:ASP:OD1	2.17	0.45
1:B:684:VAL:HG21	1:B:815:LEU:HB2	1.98	0.45
1:D:192:TRP:CZ2	1:D:572:LEU:HD21	2.51	0.45
1:B:402:PHE:CE2	1:B:404:LEU:HB2	2.51	0.45
1:B:524:TRP:O	1:B:528:VAL:HG23	2.16	0.45
1:D:800:ARG:NH2	1:D:805:SER:OG	2.44	0.45
1:C:340:LEU:HD21	1:C:398:SER:HA	1.98	0.45
1:A:97:TYR:CG	1:A:98:GLN:N	2.84	0.45
1:A:429:ILE:HD13	1:A:776:PHE:CD2	2.51	0.45
1:B:97:TYR:CG	1:B:98:GLN:N	2.85	0.45
1:D:602:LYS:HE2	1:D:607:GLU:OE2	2.17	0.45
1:B:416:ARG:HD3	1:A:769:LEU:HD23	1.97	0.45
1:B:828:MET:O	1:B:828:MET:CG	2.65	0.45
1:C:595:VAL:HG21	1:C:651:ALA:HB2	1.97	0.45
1:A:343:LEU:HB3	1:A:347:TRP:CH2	2.51	0.45
1:D:292:VAL:HG13	1:D:346:MET:HE1	1.97	0.45
1:A:130:ILE:CD1	1:A:134:ALA:HB3	2.47	0.45
1:A:344:GLU:HG2	1:A:402:PHE:CD1	2.52	0.45
1:A:588:TYR:HB3	1:A:677:TYR:CE2	2.52	0.45
1:D:204:PHE:HD2	1:D:281:PRO:HB2	1.81	0.45
1:A:110:GLY:HA2	4:A:1187:HOH:O	2.17	0.45
1:A:745:PHE:O	1:A:778:VAL:HA	2.16	0.45
1:C:190:ILE:HG23	1:C:480:GLY:HA2	1.99	0.45
1:A:258:ALA:HB2	1:A:270:LEU:CB	2.46	0.45
1:A:479:SER:OG	1:A:549:ARG:NH1	2.47	0.45
1:B:477:TYR:CZ	1:B:671:MET:HE1	2.52	0.45
1:B:520:TRP:CE2	1:B:602:LYS:HD2	2.52	0.45
1:C:714:ASP:OD1	1:C:714:ASP:N	2.36	0.45
1:A:626:GLY:O	1:A:627:LYS:HD3	2.17	0.45
1:B:84:TYR:CD1	1:B:94:ARG:HD3	2.52	0.44
1:D:267:LYS:O	1:D:271:GLU:HG3	2.17	0.44
1:A:32:VAL:HG11	1:A:344:GLU:HB3	1.99	0.44
1:A:669:LEU:HB2	1:A:671:MET:HG2	1.99	0.44
1:D:317:MET:HE1	1:D:346:MET:SD	2.57	0.44
1:A:603:LYS:HE3	1:A:608:ASP:OD2	2.17	0.44
1:B:43:ARG:HH11	1:B:43:ARG:CB	2.30	0.44
1:B:245:LEU:C	1:B:245:LEU:HD23	2.42	0.44
1:B:800:ARG:HD3	1:B:804:TYR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:VAL:HG23	1:C:35:ILE:N	2.24	0.44
1:C:549:ARG:HH22	1:C:573:HIS:CE1	2.36	0.44
1:A:335:THR:CG2	1:A:337:ASP:N	2.80	0.44
1:A:658:SER:HB3	1:A:675:VAL:HG13	1.98	0.44
1:B:113:LEU:HD13	1:B:138:VAL:HG13	1.99	0.44
1:B:172:GLN:HG3	1:B:174:LEU:CD1	2.47	0.44
1:B:308:THR:HG21	1:B:312:VAL:HA	1.99	0.44
1:D:800:ARG:HD2	1:D:804:TYR:O	2.17	0.44
1:B:90:LEU:HG	3:B:902:GOL:H2	2.00	0.44
1:C:535:LEU:HD13	1:C:661:TYR:CG	2.53	0.44
1:C:722:LEU:HD11	1:C:762:PHE:CZ	2.52	0.44
1:A:299:GLN:CG	1:A:303:ARG:HH12	2.26	0.44
1:B:172:GLN:HG3	1:B:174:LEU:CG	2.48	0.44
1:B:367:GLU:HG3	1:B:681:THR:HG21	1.99	0.44
1:C:226:ASN:O	1:C:231:PRO:HD3	2.17	0.44
1:D:156:ASN:HD21	1:D:172:GLN:HA	1.82	0.43
1:A:448:TYR:CZ	1:A:583:LEU:HD13	2.53	0.43
1:B:468:GLU:CG	1:B:676:ARG:HH21	2.32	0.43
1:D:718:PRO:HG2	1:D:828:MET:HA	1.99	0.43
1:C:589:MET:HE1	1:C:679:PRO:HB3	2.00	0.43
1:D:128:PHE:CD2	1:D:356:LEU:HD13	2.53	0.43
1:D:416:ARG:NH1	4:D:1024:HOH:O	2.52	0.43
1:C:638:PRO:HB3	1:C:644:ASP:OD2	2.19	0.43
1:B:666:SER:N	1:B:667:PRO:CD	2.81	0.43
1:D:679:PRO:O	1:D:680:PHE:HB2	2.18	0.43
1:A:666:SER:N	1:A:667:PRO:CD	2.81	0.43
1:B:46:ILE:HD12	1:B:130:ILE:HD11	2.00	0.43
1:C:591:PHE:CZ	1:C:651:ALA:HB1	2.54	0.43
1:C:759:LEU:HA	1:C:828:MET:HE1	2.01	0.43
1:A:477:TYR:HB2	1:A:582:ASN:HA	2.00	0.43
1:C:411:ALA:HB1	1:C:421:TYR:OH	2.18	0.43
1:A:51:ALA:CB	1:A:142:ILE:HD13	2.48	0.43
1:B:176:SER:HB2	4:B:1110:HOH:O	2.18	0.43
1:C:710:SER:HB3	4:C:1124:HOH:O	2.18	0.43
1:A:429:ILE:HD13	1:A:776:PHE:HD2	1.83	0.43
1:B:309:GLY:C	1:B:310:THR:HG23	2.43	0.43
1:D:225:ASP:HA	1:D:229:LYS:HB2	2.00	0.43
1:D:684:VAL:HB	1:D:685:PRO:CD	2.49	0.43
1:C:562:HIS:HB3	1:C:565:CYS:HB2	2.00	0.43
1:C:467:THR:O	1:C:772:TRP:NE1	2.51	0.43
1:A:50:ARG:HD3	1:A:50:ARG:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD21	1:A:305:GLU:HA	2.00	0.43
1:A:750:VAL:O	1:A:750:VAL:CG2	2.66	0.43
1:B:813:PRO:HD2	4:B:1156:HOH:O	2.18	0.43
1:D:476:THR:OG1	1:D:582:ASN:OD1	2.23	0.43
1:D:798:ILE:CG2	1:D:805:SER:HB3	2.49	0.43
1:C:57:SER:CB	1:C:73:ALA:HA	2.49	0.43
1:B:190:ILE:HG23	1:B:480:GLY:HA2	2.01	0.42
1:B:267:LYS:O	1:B:271:GLU:HG3	2.18	0.42
1:D:396:LEU:O	1:D:400:ARG:HG3	2.19	0.42
1:A:759:LEU:O	1:A:763:ILE:HG13	2.20	0.42
1:C:603:LYS:HE3	1:C:608:ASP:OD2	2.19	0.42
1:A:370:ALA:HA	1:A:804:TYR:CE2	2.53	0.42
1:B:183:THR:HA	1:B:186:PHE:CE2	2.54	0.42
1:B:688:ARG:HD3	1:B:814:ASP:OD2	2.19	0.42
1:A:191:GLN:HB2	1:A:464:SER:OG	2.18	0.42
1:B:125:GLU:HG2	1:B:367:GLU:OE2	2.19	0.42
1:B:207:ILE:HG21	1:B:560:SER:HB2	2.02	0.42
1:B:423:TRP:CH2	1:B:753:GLU:HG3	2.50	0.42
1:D:106:PRO:HB2	1:D:146:TRP:CD1	2.55	0.42
1:D:197:GLU:OE2	1:D:201:LYS:HE3	2.19	0.42
1:C:416:ARG:NH1	4:C:1023:HOH:O	2.52	0.42
1:B:310:THR:HB	1:B:372:TRP:HE3	1.84	0.42
1:B:335:THR:H	1:B:338:SER:HB3	1.83	0.42
1:D:416:ARG:HD3	1:C:768:ASP:O	2.20	0.42
1:D:468:GLU:CD	1:D:468:GLU:N	2.77	0.42
1:D:484:ILE:HB	1:D:486:PHE:CE2	2.55	0.42
1:C:483:TYR:CE2	1:C:587:GLU:HG2	2.55	0.42
1:A:310:THR:O	1:A:311:ILE:HB	2.19	0.42
1:B:66:LEU:HB3	1:B:67:PRO:HD3	2.02	0.42
1:B:192:TRP:CZ2	1:B:572:LEU:HD21	2.55	0.42
1:B:535:LEU:HD21	1:B:586:PHE:CE2	2.54	0.42
1:B:371:HIS:CE1	1:B:406:TYR:CE2	3.08	0.42
1:A:107:GLU:HB2	4:A:1024:HOH:O	2.18	0.42
1:A:236:ILE:HD12	1:A:560:SER:HB3	2.02	0.42
1:B:438:LEU:O	1:B:773:HIS:HA	2.20	0.42
1:B:597:SER:HB3	1:B:694:PRO:HD2	2.01	0.42
1:C:468:GLU:N	1:C:468:GLU:CD	2.78	0.42
1:C:476:THR:HG21	1:C:580:GLY:HA3	2.02	0.42
1:B:364:ALA:O	1:B:681:THR:CG2	2.68	0.42
1:B:477:TYR:HB2	1:B:582:ASN:HA	2.02	0.42
1:D:253:LEU:O	1:D:257:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:GLU:HA	1:C:59:LYS:HE2	2.02	0.42
1:C:224:CYS:O	1:C:228:GLU:HB2	2.20	0.42
1:B:87:ASP:O	1:B:88:HIS:HB2	2.19	0.41
1:B:562:HIS:CE1	1:B:564:LEU:HB2	2.54	0.41
1:B:587:GLU:OE1	1:B:676:ARG:CD	2.68	0.41
1:D:51:ALA:CB	1:D:142:ILE:HD13	2.50	0.41
1:C:156:ASN:ND2	1:C:172:GLN:HA	2.35	0.41
1:A:150:THR:HG23	1:A:153:GLU:OE2	2.19	0.41
1:A:502:TYR:OH	1:A:689:VAL:HG21	2.20	0.41
1:A:745:PHE:CE1	1:A:828:MET:HE2	2.54	0.41
1:D:565:CYS:SG	1:D:572:LEU:HD13	2.60	0.41
1:C:370:ALA:HB1	1:C:372:TRP:CH2	2.55	0.41
1:A:468:GLU:CD	1:A:468:GLU:N	2.77	0.41
1:A:681:THR:O	1:A:685:PRO:HD2	2.20	0.41
1:B:364:ALA:O	1:B:681:THR:HG23	2.20	0.41
1:A:209:GLU:O	1:A:213:GLU:HG3	2.20	0.41
1:A:658:SER:HB2	1:A:675:VAL:HG11	1.99	0.41
1:D:84:TYR:CG	1:D:94:ARG:HD3	2.55	0.41
1:C:310:THR:HB	1:C:372:TRP:CE3	2.55	0.41
1:C:470:ARG:NH1	1:C:475:ASP:HB3	2.34	0.41
1:C:586:PHE:CZ	1:C:675:VAL:HB	2.55	0.41
1:C:601:ILE:HD11	1:C:694:PRO:HG2	2.02	0.41
1:A:513:ASP:HB3	1:A:516:GLU:CG	2.50	0.41
1:B:292:VAL:CG1	1:B:346:MET:HE3	2.44	0.41
1:D:722:LEU:HD11	1:D:762:PHE:CZ	2.55	0.41
1:C:734:ARG:H	1:C:734:ARG:HG3	1.58	0.41
1:C:775:GLN:CD	1:C:800:ARG:HD2	2.45	0.41
1:A:130:ILE:HD11	1:A:134:ALA:HB3	2.03	0.41
1:A:679:PRO:O	1:A:680:PHE:HB2	2.21	0.41
1:A:721:ILE:CD1	1:A:743:ILE:HD12	2.50	0.41
1:C:738:ALA:HA	1:C:772:TRP:CD2	2.56	0.41
1:D:405:HIS:HB3	1:D:798:ILE:HD13	2.01	0.41
1:C:299:GLN:CD	1:C:303:ARG:HH12	2.28	0.41
1:D:165:LYS:HB3	1:D:165:LYS:HE3	1.65	0.41
1:C:97:TYR:CG	1:C:98:GLN:N	2.89	0.41
1:A:749:CYS:HB2	1:A:826:ASP:HA	2.02	0.41
1:B:106:PRO:HB2	1:B:146:TRP:CD1	2.56	0.41
1:B:684:VAL:HB	1:B:685:PRO:CD	2.51	0.41
1:D:684:VAL:HG21	1:D:815:LEU:HB2	2.02	0.41
1:D:726:PHE:CD1	1:D:726:PHE:C	2.98	0.41
1:A:133:ALA:O	1:A:137:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:LYS:HA	1:C:145:PHE:CE1	2.56	0.41
1:C:494:LEU:O	1:C:514:PRO:HG3	2.21	0.41
1:A:800:ARG:HD3	1:A:804:TYR:O	2.21	0.41
1:B:604:LEU:HD12	1:B:634:LEU:HD23	2.03	0.40
1:C:664:ARG:HG2	1:C:665:TYR:CE2	2.55	0.40
1:D:663:ARG:HB2	1:D:735:ASP:CG	2.47	0.40
1:C:412:ARG:HH21	1:C:441:ASP:CG	2.29	0.40
1:C:451:LYS:NZ	1:C:674:ASP:OD2	2.53	0.40
1:A:611:LEU:HD23	1:A:611:LEU:H	1.84	0.40
1:B:391:LEU:HA	1:B:391:LEU:HD12	1.86	0.40
1:A:187:ARG:HG3	1:A:189:SER:O	2.22	0.40
1:A:535:LEU:HD13	1:A:661:TYR:CG	2.57	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	796/808 (98%)	775 (97%)	20 (2%)	1 (0%)	48	64
1	B	796/808 (98%)	771 (97%)	24 (3%)	1 (0%)	48	64
1	C	795/808 (98%)	771 (97%)	23 (3%)	1 (0%)	48	64
1	D	796/808 (98%)	773 (97%)	22 (3%)	1 (0%)	48	64
All	All	3183/3232 (98%)	3090 (97%)	89 (3%)	4 (0%)	48	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	311	ILE
1	D	311	ILE
1	C	311	ILE

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Mol	Chain	Res	Type
1	A	311	ILE

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	642/680 (94%)	627 (98%)	15 (2%)	44	66
1	B	649/680 (95%)	631 (97%)	18 (3%)	38	60
1	C	642/680 (94%)	625 (97%)	17 (3%)	40	63
1	D	643/680 (95%)	626 (97%)	17 (3%)	40	63
All	All	2576/2720 (95%)	2509 (97%)	67 (3%)	40	63

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	36	LEU
1	B	43	ARG
1	B	166	LEU
1	B	172	GLN
1	B	181	ASN
1	B	187	ARG
1	B	191	GLN
1	B	310	THR
1	B	344	GLU
1	B	536	LYS
1	B	629	ASP
1	B	666	SER
1	B	676	ARG
1	B	681	THR
1	B	734	ARG
1	B	736	ARG
1	B	811	LEU
1	B	818	ASP
1	D	36	LEU
1	D	37	GLU

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Mol	Chain	Res	Type
1	D	165	LYS
1	D	166	LEU
1	D	174	LEU
1	D	335	THR
1	D	348	VAL
1	D	431	ASP
1	D	551	ARG
1	D	664	ARG
1	D	676	ARG
1	D	689	VAL
1	D	754	GLU
1	D	757	GLN
1	D	800	ARG
1	D	811	LEU
1	D	828	MET
1	C	45	ARG
1	C	70	TRP
1	C	155	LEU
1	C	166	LEU
1	C	187	ARG
1	C	340	LEU
1	C	346	MET
1	C	689	VAL
1	C	710	SER
1	C	734	ARG
1	C	736	ARG
1	C	761	SER
1	C	779	ILE
1	C	783	THR
1	C	811	LEU
1	C	819	LEU
1	C	826	ASP
1	A	70	TRP
1	A	166	LEU
1	A	187	ARG
1	A	252	LYS
1	A	329	LEU
1	A	335	THR
1	A	344	GLU
1	A	430	LYS
1	A	494	LEU
1	A	664	ARG

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Mol	Chain	Res	Type
1	A	675	VAL
1	A	676	ARG
1	A	688	ARG
1	A	736	ARG
1	A	811	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	80	ASN
1	B	366	ASN
1	B	673	ASN
1	B	727	ASN
1	D	80	ASN
1	D	156	ASN
1	D	825	HIS
1	C	80	ASN
1	C	88	HIS
1	C	299	GLN
1	C	541	GLN
1	C	673	ASN
1	A	283	ASN
1	A	306	GLN
1	A	319	GLN
1	A	547	ASN
1	A	673	ASN
1	A	723	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	C	902	-	5,5,5	0.34	0	5,5,5	0.54	0
3	GOL	B	903	-	5,5,5	0.50	0	5,5,5	0.83	0
3	GOL	D	902	-	5,5,5	0.44	0	5,5,5	0.82	0
3	GOL	A	903	-	5,5,5	0.32	0	5,5,5	0.62	0
2	8X3	B	901	-	6,6,6	2.13	1 (16%)	7,8,8	1.85	1 (14%)
3	GOL	A	902	-	5,5,5	0.51	0	5,5,5	0.68	0
2	8X3	C	901	-	6,6,6	3.06	1 (16%)	7,8,8	1.33	1 (14%)
2	8X3	A	901	-	6,6,6	3.96	2 (33%)	7,8,8	0.95	0
3	GOL	B	902	-	5,5,5	0.50	0	5,5,5	0.52	0
2	8X3	D	901	-	6,6,6	2.01	1 (16%)	7,8,8	1.31	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	902	-	-	2/4/4/4	-
3	GOL	B	903	-	-	0/4/4/4	-
3	GOL	D	902	-	-	4/4/4/4	-
3	GOL	A	903	-	-	2/4/4/4	-
2	8X3	B	901	-	-	4/4/4/4	-
3	GOL	A	902	-	-	2/4/4/4	-
2	8X3	C	901	-	-	4/4/4/4	-
2	8X3	A	901	-	-	3/4/4/4	-
3	GOL	B	902	-	-	3/4/4/4	-
2	8X3	D	901	-	-	4/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	8X3	C2-S3	9.29	1.90	1.77
2	C	901	8X3	C2-S3	7.32	1.87	1.77
2	B	901	8X3	C2-S3	4.75	1.84	1.77
2	D	901	8X3	C2-S3	4.64	1.84	1.77
2	A	901	8X3	C2-C1	2.26	1.55	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	8X3	O7-S3-C2	-4.02	100.66	106.73
2	D	901	8X3	O7-S3-C2	-2.56	102.86	106.73
2	C	901	8X3	O6-C1-C2	-2.10	104.77	109.82

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	8X3	C1-C2-S3-O4
2	B	901	8X3	C1-C2-S3-O5
2	B	901	8X3	C1-C2-S3-O7
2	D	901	8X3	C1-C2-S3-O4
2	D	901	8X3	C1-C2-S3-O5
2	D	901	8X3	C1-C2-S3-O7
2	C	901	8X3	C1-C2-S3-O7
2	A	901	8X3	C1-C2-S3-O4
2	A	901	8X3	C1-C2-S3-O7
3	B	902	GOL	O1-C1-C2-C3
3	D	902	GOL	O1-C1-C2-C3
3	D	902	GOL	C1-C2-C3-O3
3	C	902	GOL	O1-C1-C2-C3
3	A	902	GOL	O1-C1-C2-C3
3	A	903	GOL	C1-C2-C3-O3
3	D	902	GOL	O1-C1-C2-O2
3	D	902	GOL	O2-C2-C3-O3
3	C	902	GOL	O1-C1-C2-O2
3	A	903	GOL	O2-C2-C3-O3
3	B	902	GOL	O1-C1-C2-O2
3	A	902	GOL	O1-C1-C2-O2
2	D	901	8X3	O6-C1-C2-S3
2	C	901	8X3	C1-C2-S3-O4
2	C	901	8X3	C1-C2-S3-O5
2	A	901	8X3	C1-C2-S3-O5

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Mol	Chain	Res	Type	Atoms
3	B	902	GOL	C1-C2-C3-O3
2	B	901	8X3	O6-C1-C2-S3
2	C	901	8X3	O6-C1-C2-S3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	902	GOL	2	0
3	A	903	GOL	1	0
3	B	902	GOL	1	0
2	D	901	8X3	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	798/808 (98%)	-1.64	0 100 100	14, 22, 34, 52	0
1	B	798/808 (98%)	-1.62	0 100 100	15, 24, 40, 54	0
1	C	797/808 (98%)	-1.55	0 100 100	18, 29, 45, 57	0
1	D	798/808 (98%)	-1.56	0 100 100	19, 28, 43, 56	0
All	All	3191/3232 (98%)	-1.59	0 100 100	14, 25, 42, 57	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	C	902	6/6	0.98	0.05	37,45,51,62	0
3	GOL	B	903	6/6	0.99	0.03	30,39,47,52	0
3	GOL	D	902	6/6	0.99	0.03	28,35,42,45	0
3	GOL	B	902	6/6	0.99	0.03	29,35,43,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	902	6/6	0.99	0.04	23,33,44,44	0
3	GOL	A	903	6/6	0.99	0.05	32,41,48,49	0
2	8X3	C	901	7/7	1.00	0.02	17,25,30,30	0
2	8X3	A	901	7/7	1.00	0.02	13,19,24,24	0
2	8X3	B	901	7/7	1.00	0.04	15,19,23,23	0
2	8X3	D	901	7/7	1.00	0.03	17,25,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.