



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2017 – 11:41 PM EST

PDB ID : 4LPC
Title : Crystal Structure of E.Coli Branching Enzyme in complex with maltoheptaose
Authors : Feng, L.; Geiger, J.H.
Deposited on : unknown
Resolution : 2.39 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

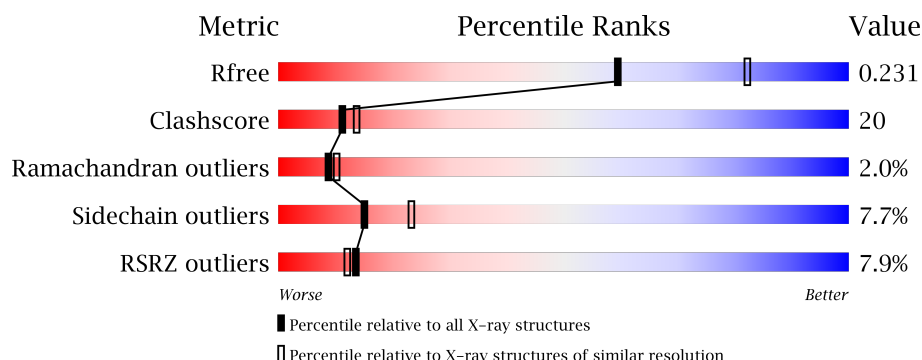
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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 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	612	<div> <div>9%</div> <div>60% 30% 5%</div> </div>
1	B	612	<div> <div>2%</div> <div>67% 24% 6%</div> </div>
1	C	612	<div> <div>17%</div> <div>62% 29% 5%</div> </div>
1	D	612	<div> <div>2%</div> <div>68% 23%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	A	801	-	-	-	X
2	GLC	A	803	-	-	-	X
2	GLC	A	808	-	-	-	X
2	GLC	A	809	-	-	-	X
2	GLC	B	804	-	-	-	X
2	GLC	B	808	-	-	-	X
2	GLC	D	806	-	-	-	X
2	GLC	D	813	-	-	-	X
3	GOL	A	805	-	-	-	X
3	GOL	A	807	-	-	X	X
3	GOL	B	813	-	-	-	X
3	GOL	B	815	-	-	X	-
4	BGC	B	801	-	-	-	X
4	BGC	B	803	-	-	-	X
4	BGC	B	810	-	-	-	X
4	BGC	B	816	-	-	-	X
4	BGC	D	810	-	-	X	X
4	BGC	D	812	-	-	-	X

2 Entry composition [i](#)

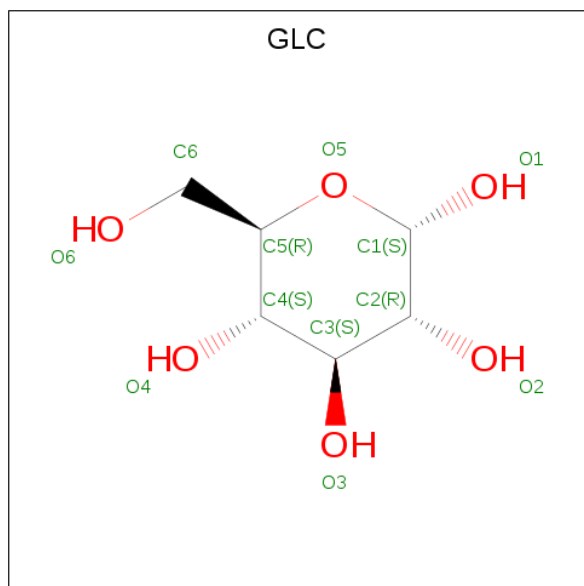
There are 5 unique types of molecules in this entry. The entry contains 20728 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1,4-alpha-glucan branching enzyme GlgB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	5	0
			4870	3109	867	878	16			
1	B	598	Total	C	N	O	S	0	2	0
			4935	3149	880	890	16			
1	C	582	Total	C	N	O	S	0	1	0
			4795	3068	850	861	16			
1	D	588	Total	C	N	O	S	0	4	0
			4867	3108	865	877	17			

- Molecule 2 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			12	6	6		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	C	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



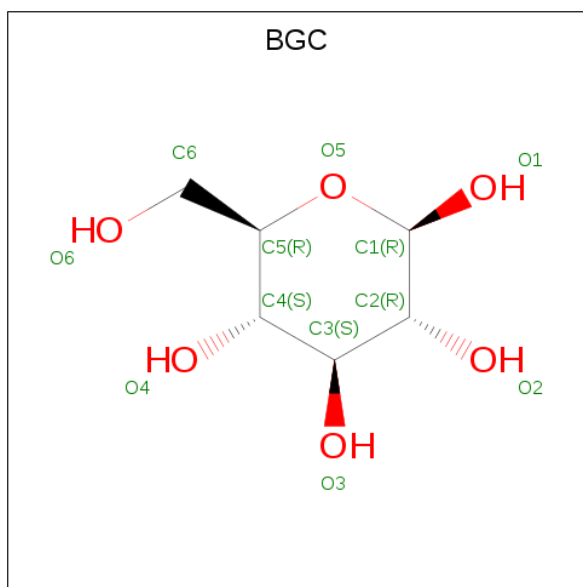
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is BETA-D-GLUCOSE (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	6	6		
4	B	1	Total	C	O	0	0
			12	6	6		
4	B	1	Total	C	O	0	0
			12	6	6		
4	B	1	Total	C	O	0	0
			12	6	6		
4	D	1	Total	C	O	0	0
			12	6	6		
4	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	220	Total	O	0	0
			220	220		

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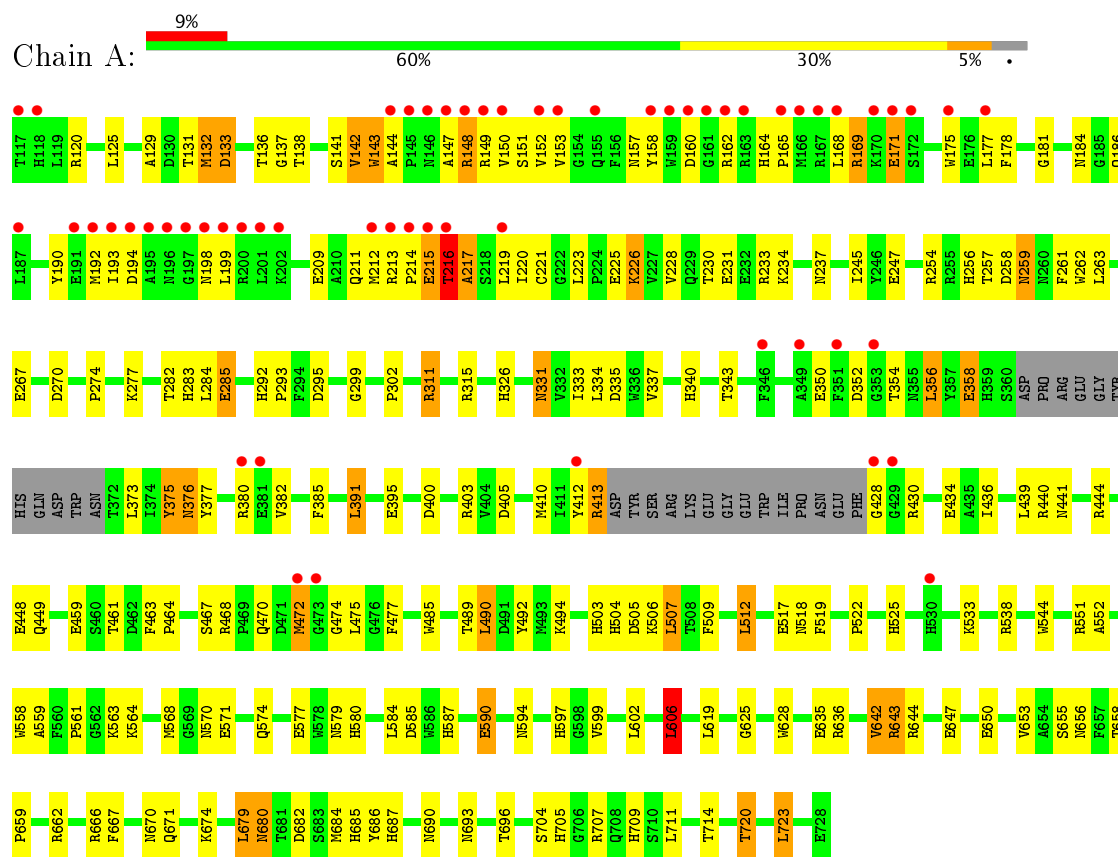
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	329	Total 329	O 329	0	0
5	C	72	Total 72	O 72	0	0
5	D	221	Total 221	O 221	0	0

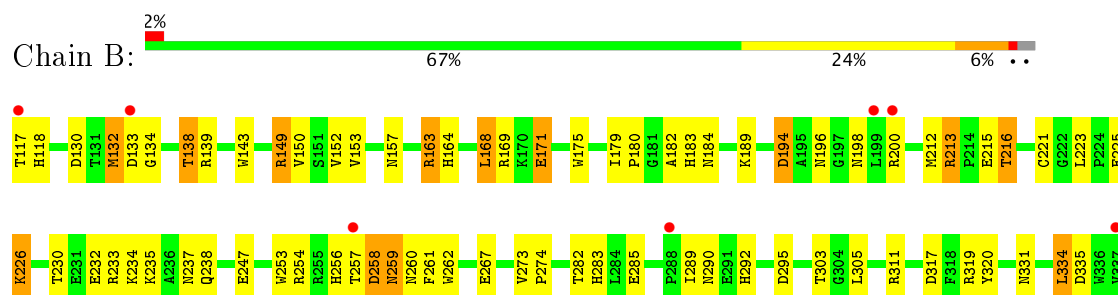
3 Residue-property plots

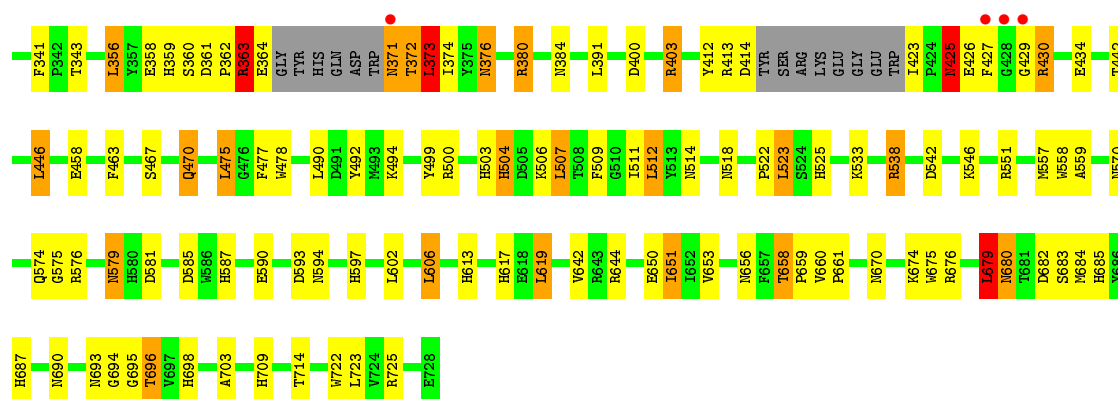
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 1,4-alpha-glucan branching enzyme GlgB

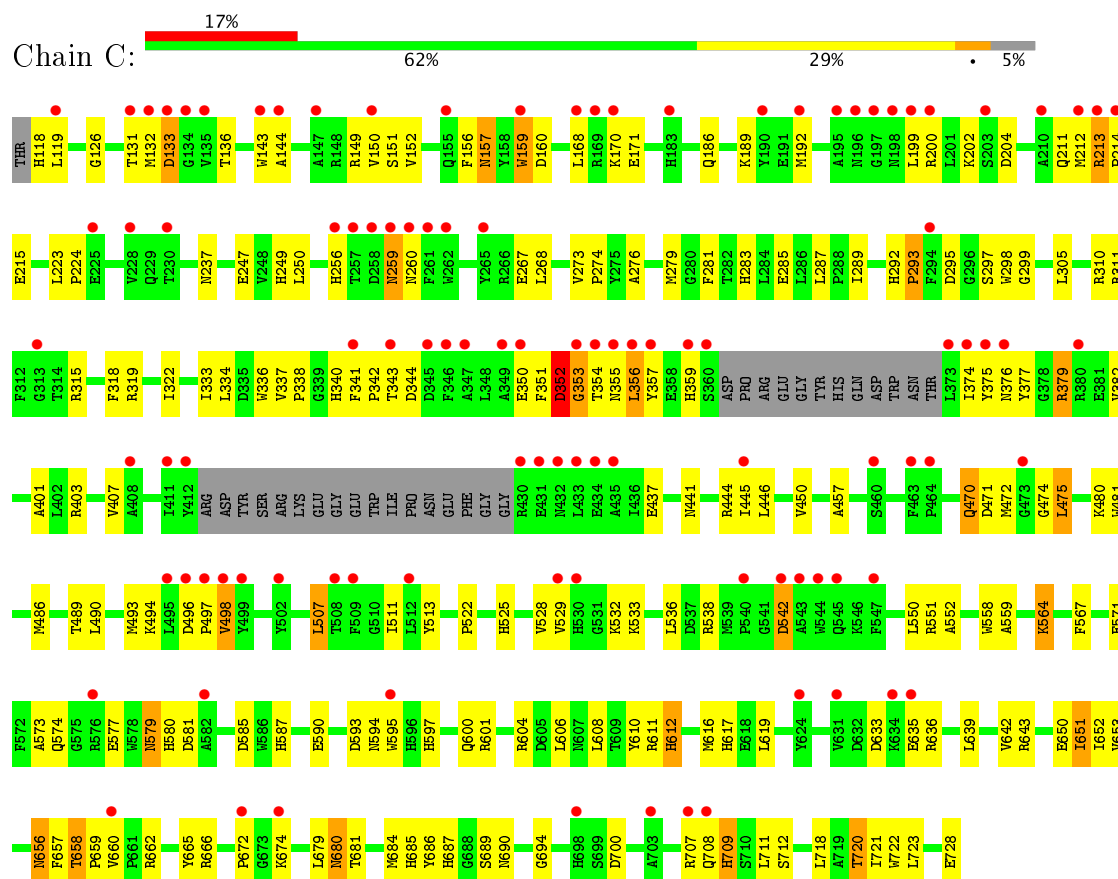


- Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

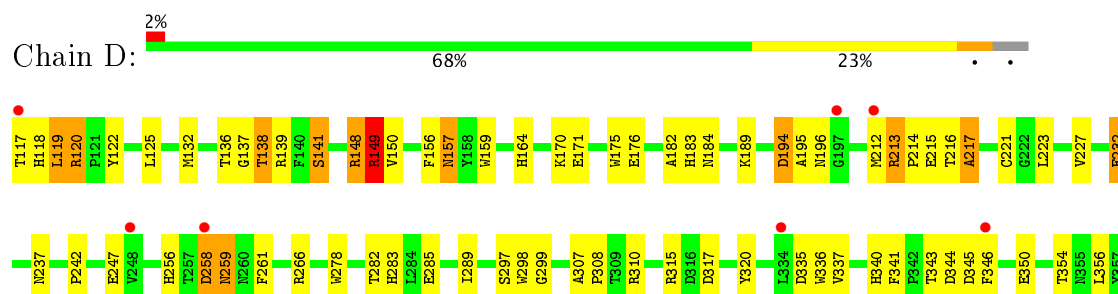


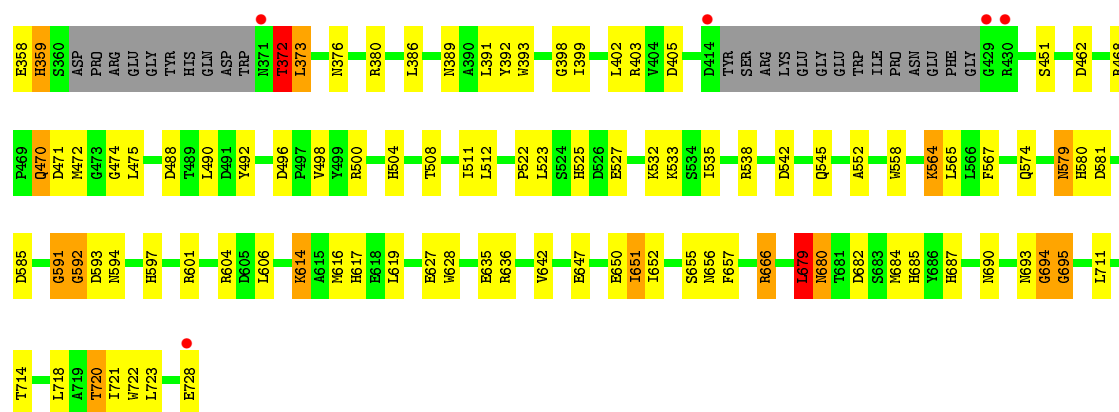


• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB



• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.19Å 103.42Å 185.94Å 90.00° 91.57° 90.00°	Depositor
Resolution (Å)	50.00 – 2.39 41.27 – 2.39	Depositor EDS
% Data completeness (in resolution range)	90.4 (50.00-2.39) 90.4 (41.27-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.183 , 0.234 0.182 , 0.231	Depositor DCC
R_{free} test set	6287 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20728	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: GLC, GOL, BGC

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	0.57	0/5024	0.66	5/6820 (0.1%)
1	B	0.72	1/5092 (0.0%)	0.77	5/6914 (0.1%)
1	C	0.37	0/4948	0.48	0/6719
1	D	0.56	0/5021	0.67	3/6817 (0.0%)
All	All	0.57	1/20085 (0.0%)	0.66	13/27270 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	478	TRP	CB-CG	5.21	1.59	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	538	ARG	NE-CZ-NH2	-9.29	115.65	120.30
1	B	373	LEU	CA-CB-CG	7.06	131.53	115.30
1	A	606	LEU	CA-CB-CG	6.50	130.26	115.30
1	B	723	LEU	CA-CB-CG	6.12	129.39	115.30
1	A	643	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	D	120	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	D	679	LEU	CA-CB-CG	-5.89	101.74	115.30
1	A	606	LEU	CB-CG-CD1	5.62	120.55	111.00
1	B	403	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	723	LEU	CA-CB-CG	5.16	127.17	115.30
1	D	636	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	679	LEU	CA-CB-CG	-5.15	103.46	115.30
1	A	643	ARG	CG-CD-NE	-5.02	101.26	111.80

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	4870	0	4590	218	0
1	B	4935	0	4647	207	0
1	C	4795	0	4527	158	0
1	D	4867	0	4586	180	0
2	A	80	0	72	12	0
2	B	88	0	75	12	0
2	C	23	0	21	0	0
2	D	90	0	80	2	0
3	A	18	0	24	6	0
3	B	30	0	40	12	0
3	D	18	0	24	2	0
4	B	48	0	45	7	0
4	D	24	0	22	7	0
5	A	220	0	0	29	0
5	B	329	0	0	49	0
5	C	72	0	0	14	0
5	D	221	0	0	17	0
All	All	20728	0	18753	768	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 20.

All (768) 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:D:212[A]:MET:CE	1:D:213:ARG:HH12	1.14	1.58
1:D:212[A]:MET:CE	1:D:213:ARG:NH1	1.91	1.29
1:D:470:GLN:N	1:D:470:GLN:HE21	1.33	1.26
1:D:212[A]:MET:HG3	1:D:213:ARG:NH1	1.50	1.25
1:B:434:GLU:HG2	5:B:1114:HOH:O	1.35	1.24
1:D:470:GLN:NE2	1:D:470:GLN:H	1.33	1.22
1:B:118:HIS:HB3	5:B:1180:HOH:O	1.40	1.20
1:A:352:ASP:OD2	1:A:354:THR:HG22	1.38	1.19
1:D:212[A]:MET:HE3	1:D:213:ARG:NH1	1.51	1.16
1:D:695:GLY:HA2	5:D:1113:HOH:O	1.47	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:LEU:HD13	4:B:816:BGC:H6C1	1.17	1.13
1:A:214:PRO:HA	1:A:215:GLU:HB3	1.16	1.12
1:D:212[A]:MET:CG	1:D:213:ARG:NH1	2.12	1.11
1:A:214:PRO:CA	1:A:215:GLU:HB3	1.82	1.09
1:B:149:ARG:HG3	1:B:149:ARG:HH21	1.04	1.08
1:C:213:ARG:HB3	1:C:214:PRO:HD3	1.31	1.08
1:C:681:THR:HG22	5:C:916:HOH:O	1.51	1.07
1:B:257:THR:HA	5:B:1045:HOH:O	1.53	1.06
1:B:225:GLU:O	1:B:226:LYS:HB2	1.24	1.04
1:D:149:ARG:HH11	1:D:149:ARG:HG3	1.21	1.03
1:B:470:GLN:HE21	1:B:470:GLN:N	1.54	1.03
1:B:470:GLN:NE2	1:B:470:GLN:H	1.55	1.03
1:C:276:ALA:HA	5:C:971:HOH:O	1.60	1.02
1:A:470:GLN:HA	1:A:474:GLY:HA2	1.46	0.98
1:A:148:ARG:O	1:A:149:ARG:HG2	1.64	0.97
1:A:214:PRO:HA	1:A:215:GLU:CB	1.91	0.97
1:C:470:GLN:H	1:C:470:GLN:HE21	1.02	0.97
1:A:131:THR:HB	1:A:136:THR:HG22	1.43	0.97
1:A:233:ARG:NH1	5:A:1026:HOH:O	1.96	0.97
1:B:225:GLU:O	1:B:226:LYS:CB	2.11	0.96
1:B:364:GLU:HB2	5:B:1207:HOH:O	1.66	0.95
1:B:371:ASN:HB3	1:B:372:THR:HB	1.48	0.95
1:D:266:ARG:HD3	5:D:1017:HOH:O	1.66	0.95
1:A:358:GLU:OE2	1:A:358:GLU:N	1.99	0.95
1:C:213:ARG:CB	1:C:214:PRO:HD3	1.97	0.94
5:A:993:HOH:O	1:D:635[B]:GLU:HG2	1.66	0.94
1:B:658:THR:HG22	1:B:660:VAL:H	1.32	0.93
1:C:281:PHE:HD2	5:C:971:HOH:O	1.51	0.93
1:D:628:TRP:HE1	4:D:810:BGC:C6	1.80	0.93
1:A:259:ASN:HD22	1:A:261:PHE:H	1.14	0.91
1:B:212:MET:O	1:B:213:ARG:HB3	1.69	0.91
1:D:212[A]:MET:HG3	1:D:213:ARG:HH11	1.33	0.90
1:B:380:ARG:HD2	5:B:1203:HOH:O	1.72	0.90
1:D:212[A]:MET:HE2	1:D:213:ARG:HH22	1.35	0.89
1:D:628:TRP:HE1	4:D:810:BGC:H6C2	1.35	0.89
1:B:613:HIS:NE2	3:B:813:GOL:H32	1.86	0.89
1:D:212[A]:MET:SD	1:D:213:ARG:NH1	2.37	0.89
1:C:213:ARG:HB3	1:C:214:PRO:CD	2.02	0.88
1:C:551:ARG:HB3	1:C:681:THR:HG23	1.55	0.88
1:A:628:TRP:HE1	2:A:808:GLC:C6	1.87	0.88
1:C:213:ARG:CB	1:C:214:PRO:CD	2.52	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:GLU:O	1:A:226:LYS:HB2	1.74	0.88
1:B:683:SER:HB2	3:B:815:GOL:H2	1.53	0.88
1:B:171:GLU:HG3	5:B:1169:HOH:O	1.74	0.87
1:B:693:ASN:HD21	1:B:714:THR:H	1.23	0.87
1:B:363:ARG:HD3	1:B:364:GLU:H	1.37	0.87
1:A:209:GLU:HG2	1:A:219:LEU:HD22	1.57	0.87
1:D:693:ASN:HD21	1:D:714:THR:H	1.17	0.87
1:A:709:HIS:HD2	5:A:990:HOH:O	1.57	0.87
1:B:512:LEU:HD13	4:B:816:BGC:C6	2.04	0.86
1:C:606:LEU:HD23	1:C:679:LEU:HD11	1.55	0.86
1:A:551:ARG:HH12	3:A:807:GOL:H11	1.41	0.86
1:C:674:LYS:NZ	5:C:933:HOH:O	2.07	0.86
1:B:149:ARG:HG3	1:B:149:ARG:NH2	1.85	0.86
1:B:335:ASP:OD1	1:B:403:ARG:HD3	1.76	0.86
1:B:138:THR:HG22	1:B:182:ALA:O	1.76	0.86
1:A:209:GLU:HG2	1:A:219:LEU:CD2	2.06	0.85
1:A:151:SER:HB2	1:A:164:HIS:O	1.76	0.85
1:C:470:GLN:N	1:C:470:GLN:HE21	1.75	0.85
1:B:262:TRP:CZ3	1:B:311:ARG:HG2	2.12	0.85
1:D:148:ARG:O	1:D:149:ARG:HB2	1.74	0.85
1:B:371:ASN:CB	1:B:372:THR:HB	2.07	0.84
1:B:576:ARG:HH22	2:B:807:GLC:H62	1.41	0.84
1:D:628:TRP:NE1	4:D:810:BGC:H6C2	1.92	0.84
1:B:512:LEU:CD1	4:B:816:BGC:H6C1	2.06	0.84
1:C:199:LEU:O	1:C:200:ARG:NH1	2.11	0.84
1:A:340:HIS:HE1	1:A:405:ASP:OD2	1.60	0.83
1:A:687:HIS:O	3:A:807:GOL:H31	1.79	0.83
1:A:350:GLU:HA	1:A:354:THR:O	1.78	0.83
1:B:149:ARG:CG	1:B:149:ARG:HH21	1.92	0.82
1:D:216:THR:O	1:D:217:ALA:HB3	1.79	0.82
1:A:628:TRP:HE1	2:A:808:GLC:H61	1.45	0.82
1:A:259:ASN:ND2	1:A:261:PHE:H	1.78	0.82
1:B:694:GLY:HA3	5:B:1054:HOH:O	1.80	0.82
1:A:693:ASN:HD21	1:A:714:THR:H	1.26	0.81
1:A:594:ASN:H	1:A:597:HIS:HD2	1.29	0.81
1:A:225:GLU:O	1:A:226:LYS:CB	2.26	0.81
1:C:658:THR:H	1:C:718:LEU:HD23	1.45	0.81
1:C:684:MET:H	1:C:690:ASN:HD22	1.27	0.81
1:C:340:HIS:HD2	5:C:936:HOH:O	1.62	0.81
1:C:642:VAL:HG13	1:C:650:GLU:HB2	1.62	0.81
1:D:212[A]:MET:CE	1:D:213:ARG:CZ	2.58	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ARG:HD2	5:B:1084:HOH:O	1.81	0.80
1:A:144:ALA:HB1	1:A:352:ASP:HB3	1.63	0.80
1:B:169:ARG:HD3	5:B:1195:HOH:O	1.81	0.80
1:D:212[A]:MET:HE3	1:D:213:ARG:HH12	1.10	0.80
1:D:247:GLU:OE1	1:D:525:HIS:HD2	1.65	0.79
1:D:212[A]:MET:HE2	1:D:213:ARG:NH2	1.96	0.79
1:D:212[A]:MET:HE3	1:D:213:ARG:CZ	2.12	0.79
1:D:216:THR:O	1:D:217:ALA:CB	2.31	0.79
1:C:359:HIS:HB2	1:C:376:ASN:HB2	1.62	0.79
1:D:372:THR:HG23	1:D:372:THR:O	1.83	0.79
1:D:693:ASN:O	1:D:694:GLY:C	2.19	0.79
1:D:594:ASN:H	1:D:597:HIS:HD2	1.30	0.79
1:B:492:TYR:CZ	1:B:500:ARG:HG2	2.18	0.79
3:B:815:GOL:H12	5:B:1035:HOH:O	1.83	0.78
1:A:262:TRP:CZ3	1:A:311:ARG:HG2	2.17	0.78
1:D:593:ASP:OD2	1:D:687:HIS:HE1	1.66	0.78
1:A:551:ARG:HH12	3:A:807:GOL:C1	1.97	0.78
1:D:138:THR:HG23	1:D:182:ALA:O	1.85	0.78
1:D:212[A]:MET:HE2	1:D:213:ARG:HH12	1.44	0.77
1:B:371:ASN:HD22	1:B:371:ASN:C	1.87	0.77
1:A:628:TRP:NE1	2:A:808:GLC:H62	1.99	0.77
1:B:362:PRO:CA	1:B:363:ARG:HB2	2.15	0.77
1:B:494:LYS:HD2	1:B:538:ARG:HG2	1.65	0.77
1:B:371:ASN:CA	1:B:372:THR:HB	2.15	0.77
1:A:680:ASN:HD22	1:A:682:ASP:H	1.32	0.76
1:B:518:ASN:HD21	2:B:802:GLC:H62	1.50	0.76
1:D:213:ARG:N	1:D:214:PRO:HD2	1.99	0.76
1:B:371:ASN:O	1:B:371:ASN:ND2	2.18	0.76
1:C:657:PHE:O	1:C:658:THR:HB	1.86	0.76
1:A:132:MET:HE3	1:A:132:MET:HA	1.66	0.76
1:D:373:LEU:H	1:D:373:LEU:CD2	2.00	0.75
1:C:250:LEU:HD22	1:C:268:LEU:HD13	1.67	0.75
1:B:295:ASP:OD2	1:B:311:ARG:NH2	2.20	0.74
1:D:149:ARG:HH11	1:D:149:ARG:CG	2.00	0.74
1:C:249:HIS:HB2	1:C:287:LEU:HD22	1.69	0.74
1:D:149:ARG:HG3	1:D:149:ARG:NH1	2.01	0.74
1:B:414:ASP:OD1	5:B:1131:HOH:O	2.06	0.74
1:C:289:ILE:HG13	1:C:334:LEU:HD11	1.69	0.74
1:A:533:LYS:O	1:A:538:ARG:NH2	2.21	0.73
1:D:337:VAL:O	1:D:337:VAL:HG23	1.89	0.73
1:D:258:ASP:HB2	5:D:979:HOH:O	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:THR:CB	1:A:136:THR:HG22	2.20	0.72
1:D:138:THR:CG2	1:D:182:ALA:O	2.38	0.72
1:A:680:ASN:ND2	1:A:682:ASP:H	1.88	0.72
1:A:655:SER:OG	1:A:720:THR:HB	1.87	0.72
1:D:278:TRP:O	1:D:604:ARG:HD2	1.88	0.72
1:B:725:ARG:HD3	5:B:1062:HOH:O	1.90	0.71
1:A:292:HIS:O	1:A:311:ARG:NH1	2.23	0.71
1:A:590[A]:GLU:OE2	1:B:676:ARG:NH2	2.23	0.71
1:B:143:TRP:CH2	1:B:356:LEU:HD22	2.25	0.71
1:B:644:ARG:HG2	1:B:650:GLU:HG2	1.72	0.71
1:D:614:LYS:HE3	5:D:997:HOH:O	1.91	0.71
1:A:147:ALA:O	1:A:148:ARG:CB	2.37	0.71
1:A:211:GLN:HE21	1:A:215:GLU:H	1.37	0.70
1:B:117:THR:OG1	1:B:118:HIS:N	2.23	0.70
1:D:212[A]:MET:HE2	1:D:213:ARG:NH1	2.03	0.70
1:B:362:PRO:CB	1:B:363:ARG:HB2	2.21	0.70
1:C:564:LYS:HE2	1:C:610:TYR:CE1	2.26	0.70
1:A:132:MET:CE	1:A:132:MET:HA	2.22	0.70
1:B:683:SER:HB2	3:B:815:GOL:C2	2.22	0.70
1:C:351:PHE:O	1:C:352:ASP:HB3	1.92	0.70
1:A:262:TRP:CH2	1:A:311:ARG:HG2	2.27	0.70
1:D:373:LEU:H	1:D:373:LEU:HD22	1.56	0.70
2:B:807:GLC:H4	2:B:808:GLC:O2	1.90	0.69
1:C:118:HIS:N	5:C:935:HOH:O	2.23	0.69
1:C:496:ASP:O	1:C:498:VAL:N	2.25	0.69
1:D:237:ASN:ND2	1:D:283:HIS:HE1	1.91	0.69
1:D:373:LEU:N	1:D:373:LEU:CD2	2.56	0.69
1:D:647:GLU:OE1	5:D:938:HOH:O	2.10	0.69
1:A:594:ASN:H	1:A:597:HIS:CD2	2.10	0.69
1:D:212[A]:MET:CE	1:D:213:ARG:HH22	2.06	0.69
1:A:259:ASN:HD22	1:A:261:PHE:N	1.88	0.69
1:C:651:ILE:HD13	1:C:722:TRP:HB3	1.74	0.69
1:A:216:THR:O	1:A:217:ALA:C	2.31	0.69
1:B:130:ASP:OD1	1:B:139:ARG:NH1	2.18	0.69
1:D:232:GLU:H	1:D:232:GLU:CD	1.94	0.68
1:C:237:ASN:ND2	1:C:283:HIS:HE1	1.91	0.68
1:C:494:LYS:HD3	1:C:538:ARG:HG2	1.76	0.68
1:A:587:HIS:NE2	5:A:949:HOH:O	2.27	0.68
1:B:413:ARG:O	1:B:414:ASP:HB2	1.92	0.68
1:A:215:GLU:O	1:A:216:THR:HG23	1.93	0.68
1:B:594:ASN:H	1:B:597:HIS:HD2	1.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212[A]:MET:CE	1:D:213:ARG:NH2	2.57	0.68
1:A:282:THR:OG1	1:A:283:HIS:HD2	1.76	0.68
1:B:371:ASN:N	1:B:372:THR:HB	2.07	0.68
1:D:628:TRP:HE1	4:D:810:BGC:H6C1	1.59	0.68
1:B:364:GLU:CB	5:B:1207:HOH:O	2.33	0.68
1:D:373:LEU:N	1:D:373:LEU:HD22	2.09	0.68
1:D:574:GLN:NE2	1:D:585:ASP:H	1.90	0.68
1:B:132:MET:HA	1:B:132:MET:CE	2.24	0.68
1:C:657:PHE:O	1:C:658:THR:CB	2.42	0.67
1:B:194:ASP:HB3	1:B:196:ASN:H	1.58	0.67
1:A:302:PRO:HG3	1:A:337:VAL:HG21	1.76	0.67
1:A:444:ARG:HA	5:A:1087:HOH:O	1.95	0.67
1:A:142:VAL:O	1:A:143:TRP:HB2	1.95	0.67
1:D:247:GLU:OE1	1:D:525:HIS:CD2	2.48	0.67
1:A:149:ARG:HA	1:A:175:TRP:CH2	2.30	0.66
1:A:343:THR:HG22	1:A:373:LEU:HD12	1.77	0.66
1:A:642:VAL:HG13	1:A:650:GLU:HB2	1.76	0.66
1:A:544:TRP:HB2	3:A:807:GOL:H2	1.78	0.66
1:D:237:ASN:HD22	1:D:283:HIS:HE1	1.40	0.66
1:A:214:PRO:CA	1:A:215:GLU:CB	2.60	0.66
1:A:650:GLU:OE2	1:A:670:ASN:HB2	1.96	0.66
1:B:423:ILE:N	5:B:1223:HOH:O	2.26	0.66
1:A:410:MET:HE1	1:A:439:LEU:HD21	1.78	0.66
1:B:189:LYS:NZ	1:B:216:THR:HG22	2.10	0.66
1:B:658:THR:CG2	1:B:660:VAL:H	2.07	0.66
1:D:117:THR:HG21	5:D:1077:HOH:O	1.94	0.66
1:B:376:ASN:ND2	5:B:1018:HOH:O	2.23	0.66
1:C:352:ASP:OD2	1:C:353:GLY:N	2.29	0.66
1:C:635:GLU:HB3	5:C:912:HOH:O	1.96	0.65
1:D:194:ASP:HB3	1:D:196:ASN:H	1.60	0.65
1:A:335:ASP:OD1	1:A:403:ARG:HD3	1.96	0.65
1:B:292:HIS:O	1:B:311:ARG:NH1	2.29	0.65
1:B:617:HIS:HE1	5:B:1086:HOH:O	1.78	0.65
1:C:470:GLN:HA	1:C:474:GLY:HA2	1.78	0.65
1:D:594:ASN:H	1:D:597:HIS:CD2	2.12	0.65
1:B:593:ASP:OD2	1:B:687:HIS:CE1	2.49	0.65
1:C:279:MET:HB2	5:C:971:HOH:O	1.96	0.65
1:C:375:TYR:O	1:C:376:ASN:HB3	1.95	0.65
1:C:728:GLU:OE2	1:D:256:HIS:HD2	1.80	0.65
1:A:181:GLY:HA2	5:A:967:HOH:O	1.96	0.65
1:B:262:TRP:CH2	1:B:311:ARG:HG2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ARG:H	1:B:430:ARG:HD2	1.62	0.65
1:A:168:LEU:HD12	1:A:175:TRP:CZ2	2.31	0.65
1:A:503:HIS:HB3	1:A:506:LYS:HD2	1.79	0.65
1:B:189:LYS:CE	1:B:216:THR:HG22	2.26	0.65
1:C:708:GLN:O	1:C:709:HIS:HB2	1.97	0.65
1:B:533:LYS:O	1:B:538:ARG:NH2	2.30	0.64
1:D:593:ASP:OD2	1:D:687:HIS:CE1	2.50	0.64
1:B:593:ASP:OD2	1:B:687:HIS:HE1	1.80	0.64
2:B:804:GLC:H61	2:B:805:GLC:H2	1.80	0.64
1:D:693:ASN:ND2	1:D:714:THR:H	1.93	0.64
1:B:149:ARG:HD2	1:B:149:ARG:C	2.18	0.64
1:B:171:GLU:CG	5:B:1169:HOH:O	2.40	0.64
1:B:149:ARG:HD2	1:B:150:VAL:N	2.13	0.64
1:B:685[B]:HIS:CD2	5:B:1098:HOH:O	2.51	0.64
1:B:212:MET:O	1:B:213:ARG:CB	2.43	0.63
1:B:477:PHE:O	4:B:801:BGC:H6C2	1.98	0.63
1:A:684:MET:H	1:A:690:ASN:HD22	1.47	0.63
1:D:117:THR:N	5:D:1031:HOH:O	2.31	0.63
1:B:579:ASN:HD22	1:B:581:ASP:H	1.47	0.63
1:B:613:HIS:CE1	3:B:813:GOL:H32	2.33	0.63
1:B:644:ARG:CG	1:B:650:GLU:HG2	2.28	0.63
1:C:711:LEU:O	1:C:712:SER:HB3	1.99	0.62
1:D:616:MET:SD	1:D:651:ILE:HG12	2.39	0.62
1:A:628:TRP:NE1	2:A:808:GLC:C6	2.57	0.62
1:C:356:LEU:O	1:C:357:TYR:HB2	1.98	0.62
1:D:372:THR:CG2	1:D:372:THR:O	2.47	0.62
1:B:153:VAL:HA	1:B:157:ASN:HD22	1.65	0.62
1:C:611:ARG:O	1:C:612:HIS:CB	2.46	0.62
1:D:558:TRP:HA	1:D:564:LYS:HE3	1.80	0.62
1:B:587:HIS:O	1:B:590:GLU:HG2	2.00	0.62
1:A:148:ARG:HB3	1:A:193:ILE:O	1.99	0.62
1:A:352:ASP:OD2	1:A:354:THR:CG2	2.31	0.62
1:B:371:ASN:N	1:B:372:THR:O	2.33	0.62
1:D:728:GLU:HG2	5:D:1050:HOH:O	2.00	0.62
1:A:256:HIS:HB2	1:A:259:ASN:HD21	1.64	0.61
1:B:282:THR:OG1	1:B:283:HIS:HD2	1.84	0.61
1:A:152:VAL:O	1:A:157:ASN:ND2	2.34	0.61
1:B:371:ASN:N	1:B:372:THR:CB	2.63	0.61
1:A:413:ARG:HD3	1:A:430:ARG:HH12	1.64	0.61
1:D:680:ASN:C	1:D:680:ASN:HD22	2.04	0.61
1:A:337:VAL:HG23	1:A:337:VAL:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:601:ARG:HD2	1:D:685[A]:HIS:NE2	2.16	0.60
1:D:642:VAL:HG22	1:D:650:GLU:HB3	1.82	0.60
1:A:214:PRO:CB	1:A:215:GLU:HB3	2.31	0.60
1:B:259:ASN:HB2	1:B:261:PHE:CE2	2.37	0.60
1:B:247:GLU:OE1	1:B:525:HIS:HD2	1.84	0.60
1:C:728:GLU:O	2:D:804:GLC:O4	2.19	0.60
3:B:815:GOL:C1	5:B:1035:HOH:O	2.46	0.60
1:A:216:THR:O	1:A:217:ALA:O	2.20	0.60
1:D:359:HIS:HD2	1:D:376:ASN:HA	1.67	0.60
1:A:151:SER:CB	1:A:164:HIS:O	2.48	0.60
1:A:209:GLU:HG2	1:A:219:LEU:HD23	1.84	0.60
1:B:680:ASN:HD22	1:B:680:ASN:C	2.04	0.60
1:C:131:THR:OG1	1:C:136:THR:HG22	2.02	0.60
1:A:247:GLU:OE1	1:A:525:HIS:HD2	1.85	0.60
1:B:362:PRO:HA	1:B:363:ARG:HB2	1.83	0.60
1:C:551:ARG:HB3	1:C:681:THR:CG2	2.30	0.60
1:B:551:ARG:NH2	5:B:986:HOH:O	2.35	0.59
1:C:593:ASP:OD2	1:C:687:HIS:HE1	1.84	0.59
1:C:489:THR:HG22	1:C:507:LEU:HD12	1.84	0.59
1:A:233:ARG:HG2	1:A:331:ASN:HD21	1.68	0.59
1:A:168:LEU:C	1:A:168:LEU:HD23	2.23	0.59
1:D:684:MET:H	1:D:690:ASN:ND2	2.00	0.59
1:B:504:HIS:HD2	5:B:908:HOH:O	1.86	0.59
1:C:574:GLN:NE2	1:C:585:ASP:H	2.01	0.59
1:D:679:LEU:HG	1:D:680:ASN:N	2.17	0.59
1:B:189:LYS:HE2	1:B:216:THR:HG22	1.82	0.59
1:B:658:THR:HG23	1:B:659:PRO:HD2	1.85	0.59
1:C:665:TYR:O	1:C:712:SER:HA	2.02	0.59
1:A:137:GLY:HA2	5:A:1089:HOH:O	2.01	0.59
2:B:805:GLC:H62	2:B:806:GLC:O2	2.03	0.59
1:A:551:ARG:NH1	3:A:807:GOL:H11	2.15	0.59
1:B:512:LEU:HD22	2:B:817:GLC:H62	1.84	0.59
1:C:157:ASN:C	1:C:157:ASN:HD22	2.06	0.59
3:B:812:GOL:H31	5:B:942:HOH:O	2.03	0.58
1:C:635:GLU:HG3	1:C:636:ARG:HG3	1.84	0.58
1:B:425:ASN:ND2	1:B:429:GLY:H	2.01	0.58
1:B:138:THR:CG2	1:B:182:ALA:O	2.51	0.58
1:D:512:LEU:HD21	4:D:810:BGC:H5	1.84	0.58
1:D:212[A]:MET:HE2	1:D:213:ARG:CZ	2.29	0.58
1:B:683:SER:CB	3:B:815:GOL:H2	2.29	0.58
1:C:202:LYS:HD2	1:C:351:PHE:CD1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:ASN:C	1:A:680:ASN:HD22	2.07	0.58
1:C:604:ARG:NH2	5:C:910:HOH:O	2.37	0.58
1:B:574:GLN:NE2	1:B:585:ASP:H	2.02	0.58
1:B:613:HIS:NE2	3:B:813:GOL:C3	2.64	0.58
1:B:693:ASN:ND2	1:B:714:THR:H	1.96	0.58
1:C:513:TYR:HB2	5:C:939:HOH:O	2.03	0.58
1:A:132:MET:HB2	1:A:178:PHE:CE1	2.39	0.57
1:D:340:HIS:HE1	1:D:405:ASP:OD2	1.87	0.57
1:A:129:ALA:HA	1:A:138:THR:HG22	1.86	0.57
1:D:504:HIS:HD2	5:D:960:HOH:O	1.87	0.57
1:A:147:ALA:O	1:A:148:ARG:HB2	2.04	0.57
1:B:651:ILE:CD1	1:B:722:TRP:HB3	2.34	0.57
1:A:233:ARG:HD3	1:A:326:HIS:CD2	2.39	0.57
1:A:144:ALA:HB1	1:A:352:ASP:CB	2.32	0.57
1:D:212[A]:MET:HG3	1:D:213:ARG:HB2	1.85	0.57
1:D:508:THR:O	4:D:810:BGC:O6	2.20	0.57
1:A:635[A]:GLU:N	1:A:635[A]:GLU:OE2	2.32	0.57
1:A:150:VAL:HG13	1:A:192:MET:HB3	1.87	0.57
1:B:138:THR:HG23	1:B:182:ALA:HB3	1.87	0.57
1:C:694:GLY:O	1:D:591:GLY:HA2	2.05	0.57
1:A:590[A]:GLU:OE1	1:B:695:GLY:O	2.23	0.57
1:A:636:ARG:HG2	1:A:662:ARG:CZ	2.35	0.56
1:D:468:ARG:O	1:D:474:GLY:HA3	2.05	0.56
1:C:295:ASP:OD2	1:C:311:ARG:NH2	2.38	0.56
1:A:558:TRP:HA	1:A:564:LYS:HE3	1.88	0.56
1:B:685[B]:HIS:HD2	5:B:1098:HOH:O	1.88	0.56
1:D:132:MET:SD	1:D:139:ARG:NH1	2.79	0.56
1:B:194:ASP:HB2	1:B:198:ASN:H	1.69	0.56
1:C:525:HIS:HB3	1:C:567:PHE:CE1	2.41	0.56
3:D:808:GOL:H11	5:D:933:HOH:O	2.05	0.56
1:A:693:ASN:ND2	1:A:714:THR:H	1.99	0.56
1:B:134:GLY:N	5:B:1060:HOH:O	2.37	0.56
1:A:211:GLN:NE2	1:A:215:GLU:H	2.02	0.56
1:C:150:VAL:HG22	1:C:192:MET:HG3	1.87	0.56
1:A:237:ASN:ND2	1:A:283:HIS:HE1	2.03	0.56
1:C:608:LEU:O	1:C:611:ARG:O	2.24	0.56
1:A:436:ILE:O	1:A:440:ARG:HG3	2.06	0.56
1:A:679:LEU:HG	1:A:680:ASN:N	2.20	0.56
1:D:680:ASN:ND2	1:D:682:ASP:H	2.04	0.55
1:C:289:ILE:HG13	1:C:334:LEU:CD1	2.35	0.55
1:D:451:SER:HB3	5:D:1092:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:492:TYR:CZ	1:D:500:ARG:HG2	2.41	0.55
1:D:642:VAL:CG2	1:D:650:GLU:HB3	2.35	0.55
1:A:709:HIS:CD2	5:A:990:HOH:O	2.42	0.55
1:C:132:MET:O	1:C:133:ASP:HB2	2.05	0.55
1:B:373:LEU:HA	5:B:1164:HOH:O	2.06	0.55
1:D:399:ILE:HD11	1:D:402:LEU:HD21	1.89	0.55
1:C:700:ASP:O	1:C:709:HIS:HA	2.07	0.55
1:B:380:ARG:HD3	1:B:384:ASN:HD21	1.71	0.55
1:C:606:LEU:HD23	1:C:679:LEU:CD1	2.32	0.55
1:C:610:TYR:O	1:C:617:HIS:HD2	1.90	0.55
1:C:149:ARG:NH1	1:C:151:SER:HB2	2.22	0.55
1:C:336:TRP:CZ3	1:C:338:PRO:HG3	2.41	0.55
1:A:574:GLN:NE2	1:A:585:ASP:H	2.05	0.54
1:A:468:ARG:CZ	2:A:804:GLC:H61	2.37	0.54
1:C:480:LYS:HD3	1:C:481:TRP:O	2.07	0.54
1:A:704:SER:OG	1:A:705:HIS:CD2	2.60	0.54
1:C:351:PHE:O	1:C:352:ASP:CB	2.55	0.54
3:B:812:GOL:C3	5:B:942:HOH:O	2.55	0.54
1:C:494:LYS:CD	1:C:538:ARG:HG2	2.35	0.54
1:A:428:GLY:HA2	5:A:1040:HOH:O	2.08	0.54
1:A:504:HIS:HD2	5:A:989:HOH:O	1.89	0.54
1:A:505:ASP:HB3	5:A:1051:HOH:O	2.06	0.54
1:C:213:ARG:HB2	1:C:214:PRO:CD	2.37	0.54
1:A:171:GLU:CD	1:A:171:GLU:H	2.10	0.54
1:B:579:ASN:ND2	1:B:581:ASP:H	2.04	0.54
1:C:342:PRO:O	1:C:344:ASP:N	2.32	0.54
1:D:685[A]:HIS:CE1	5:D:1036:HOH:O	2.60	0.54
1:A:143:TRP:CH2	1:A:356:LEU:HD22	2.42	0.54
1:B:425:ASN:HD22	1:B:427:PHE:H	1.56	0.54
1:B:680:ASN:HB3	3:B:815:GOL:O2	2.07	0.54
1:C:379:ARG:HB3	1:C:382:VAL:HG23	1.89	0.54
1:D:148:ARG:NH1	1:D:195:ALA:O	2.41	0.54
1:C:273:VAL:HB	1:C:274:PRO:HD3	1.90	0.53
1:C:536:LEU:HD22	1:C:573:ALA:HB1	1.90	0.53
1:A:142:VAL:O	1:A:143:TRP:CB	2.53	0.53
1:B:594:ASN:H	1:B:597:HIS:CD2	2.26	0.53
1:A:157:ASN:O	1:A:158:TYR:HB2	2.07	0.53
1:C:379:ARG:NH2	5:C:921:HOH:O	2.41	0.53
1:A:643:ARG:NH2	5:A:994:HOH:O	2.40	0.53
1:B:363:ARG:HD3	1:B:364:GLU:N	2.16	0.53
1:D:594:ASN:N	1:D:597:HIS:HD2	2.01	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:LYS:HD2	1:A:696:THR:HG21	1.91	0.53
1:D:680:ASN:HD22	1:D:682:ASP:H	1.55	0.53
1:D:684:MET:H	1:D:690:ASN:HD22	1.54	0.53
1:B:442:THR:HG22	1:B:446:LEU:HD22	1.90	0.53
1:B:237:ASN:HD22	1:B:283:HIS:HE1	1.57	0.52
1:C:496:ASP:C	1:C:498:VAL:H	2.12	0.52
1:C:281:PHE:CD2	5:C:971:HOH:O	2.40	0.52
1:D:118:HIS:CD2	1:D:119:LEU:HD13	2.44	0.52
1:D:157:ASN:OD1	1:D:164:HIS:HD2	1.93	0.52
1:A:428:GLY:HA2	5:A:981:HOH:O	2.08	0.52
1:B:237:ASN:ND2	1:B:283:HIS:HE1	2.06	0.52
1:B:512:LEU:HD22	2:B:817:GLC:C6	2.39	0.52
1:D:216:THR:HG22	1:D:217:ALA:N	2.24	0.52
1:A:147:ALA:O	1:A:148:ARG:HB3	2.10	0.52
1:C:633:ASP:OD2	1:C:665:TYR:OH	2.19	0.52
1:A:459:GLU:OE1	1:A:461:THR:O	2.26	0.52
1:A:587:HIS:HA	1:A:590[B]:GLU:HG3	1.90	0.52
1:A:277:LYS:NZ	5:A:1112:HOH:O	2.43	0.52
1:A:410:MET:HE3	1:A:439:LEU:HD11	1.90	0.52
1:B:343:THR:HG22	1:B:373:LEU:HD21	1.92	0.52
1:C:247:GLU:OE1	1:C:525:HIS:CD2	2.63	0.52
1:C:529:VAL:O	1:C:532:LYS:HB2	2.10	0.52
1:C:143:TRP:CH2	1:C:356:LEU:HD21	2.45	0.52
1:C:407:VAL:HG21	1:C:457:ALA:HB1	1.92	0.52
1:C:486:MET:O	1:C:490:LEU:HB2	2.10	0.52
1:A:490:LEU:O	1:A:494:LYS:HG3	2.10	0.52
1:B:362:PRO:HA	1:B:363:ARG:CB	2.38	0.52
1:A:391:LEU:O	1:A:395:GLU:HB2	2.09	0.51
1:A:552:ALA:O	1:A:720:THR:CG2	2.58	0.51
1:A:667:PHE:HA	1:A:705:HIS:CD2	2.45	0.51
1:A:358:GLU:H	1:A:358:GLU:CD	2.03	0.51
1:D:335:ASP:OD1	1:D:403:ARG:HD3	2.10	0.51
1:C:256:HIS:HE1	1:C:267:GLU:OE1	1.93	0.51
1:A:666:ARG:HA	1:A:711:LEU:O	2.09	0.51
1:A:169:ARG:HB2	1:A:169:ARG:NH1	2.26	0.51
1:A:468:ARG:NH1	2:A:804:GLC:H61	2.25	0.51
1:B:651:ILE:HD11	1:B:722:TRP:HB3	1.92	0.51
1:C:359:HIS:CB	1:C:376:ASN:HB2	2.36	0.51
1:A:602:LEU:HG	1:A:606:LEU:HD22	1.92	0.51
1:D:393:TRP:HB3	1:D:399:ILE:HG12	1.93	0.51
1:C:658:THR:HG22	1:C:660:VAL:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ARG:NH1	5:A:1065:HOH:O	2.42	0.50
1:B:118:HIS:CB	5:B:1180:HOH:O	2.24	0.50
1:C:237:ASN:HD21	1:C:283:HIS:HE1	1.56	0.50
1:C:550:LEU:CD2	1:C:573:ALA:HB2	2.41	0.50
1:D:350:GLU:HA	1:D:354:THR:O	2.10	0.50
1:D:488:ASP:OD2	5:D:1015:HOH:O	2.19	0.50
1:D:728:GLU:CG	5:D:1050:HOH:O	2.58	0.50
1:A:209:GLU:HB3	1:A:221:CYS:SG	2.51	0.50
1:B:233:ARG:NH1	1:B:400:ASP:OD2	2.42	0.50
1:C:611:ARG:O	1:C:612:HIS:HB3	2.10	0.50
1:A:509:PHE:HA	2:A:809:GLC:H62	1.93	0.50
1:B:709:HIS:HD2	5:B:1000:HOH:O	1.94	0.50
1:C:474:GLY:O	1:C:475:LEU:HB2	2.12	0.50
1:C:685[A]:HIS:CE1	1:D:685[A]:HIS:HD2	2.29	0.50
1:A:684:MET:H	1:A:690:ASN:ND2	2.08	0.50
1:B:260:ASN:HA	5:B:1065:HOH:O	2.10	0.50
1:B:117:THR:HB	5:B:1069:HOH:O	2.10	0.50
1:B:477:PHE:O	4:B:801:BGC:C6	2.60	0.50
1:B:362:PRO:HB2	1:B:363:ARG:HB2	1.93	0.50
1:C:298:TRP:HE1	1:C:580:HIS:CD2	2.30	0.50
1:A:149:ARG:HA	1:A:175:TRP:CZ3	2.46	0.50
1:C:525:HIS:HB3	1:C:567:PHE:CD1	2.47	0.50
1:D:216:THR:CG2	1:D:217:ALA:N	2.74	0.50
1:D:282:THR:OG1	1:D:283:HIS:HD2	1.95	0.50
1:A:233:ARG:HG2	1:A:331:ASN:ND2	2.26	0.50
1:B:157:ASN:OD1	1:B:164:HIS:HD2	1.95	0.50
1:B:494:LYS:CD	1:B:538:ARG:HG2	2.39	0.50
1:B:579:ASN:C	1:B:579:ASN:HD22	2.16	0.50
1:C:297:SER:C	1:C:299:GLY:H	2.15	0.50
1:C:437:GLU:HA	1:C:437:GLU:OE2	2.11	0.50
1:C:616:MET:SD	1:C:651:ILE:HG12	2.51	0.50
1:D:679:LEU:HG	1:D:680:ASN:H	1.76	0.49
1:A:704:SER:OG	1:A:705:HIS:HD2	1.95	0.49
1:B:189:LYS:HZ1	1:B:216:THR:HG22	1.77	0.49
1:C:403:ARG:NE	1:C:481:TRP:CZ2	2.80	0.49
1:D:652:ILE:HB	1:D:723:LEU:HB2	1.94	0.49
1:B:117:THR:N	5:B:1057:HOH:O	2.45	0.49
1:B:523:LEU:HD22	1:B:557:MET:SD	2.53	0.49
1:C:558:TRP:HA	1:C:564:LYS:HE3	1.94	0.49
1:C:642:VAL:CG1	1:C:650:GLU:HB2	2.38	0.49
1:D:242:PRO:HB3	1:D:617:HIS:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:ARG:NH1	5:D:1017:HOH:O	2.36	0.49
1:A:684:MET:HG3	1:A:685[A]:HIS:N	2.24	0.49
1:D:221:CYS:HB2	5:D:1052:HOH:O	2.12	0.49
1:D:399:ILE:HD11	1:D:402:LEU:CD2	2.42	0.49
1:A:157:ASN:OD1	1:A:164:HIS:CD2	2.65	0.49
1:A:254[B]:ARG:HD3	1:A:263:LEU:HD11	1.94	0.49
1:A:194:ASP:OD2	1:A:198:ASN:N	2.37	0.49
1:C:159:TRP:HZ3	1:C:189:LYS:HB2	1.77	0.49
1:C:551:ARG:NH1	1:C:681:THR:O	2.46	0.49
1:C:680:ASN:HD22	1:C:680:ASN:C	2.15	0.49
1:A:148:ARG:O	1:A:149:ARG:CG	2.50	0.49
1:C:672:PRO:HB3	1:C:709:HIS:CD2	2.47	0.49
1:D:120:ARG:HG2	1:D:122:TYR:OH	2.12	0.49
1:A:684:MET:HG3	1:A:685[B]:HIS:N	2.25	0.49
1:B:132:MET:HA	1:B:132:MET:HE2	1.92	0.49
1:B:143:TRP:CZ3	1:B:356:LEU:HD22	2.48	0.49
1:C:444:ARG:NH2	1:C:445:ILE:HG13	2.27	0.49
1:D:156:PHE:CD2	1:D:157:ASN:HB2	2.48	0.49
1:A:165:PRO:O	1:A:177:LEU:HD22	2.13	0.49
1:B:512:LEU:CD1	4:B:816:BGC:C6	2.81	0.49
1:A:334:LEU:HD12	1:A:335:ASP:N	2.28	0.48
1:D:213:ARG:N	1:D:214:PRO:CD	2.57	0.48
1:B:679:LEU:HG	1:B:680:ASN:N	2.27	0.48
1:C:550:LEU:HD21	1:C:573:ALA:HB2	1.93	0.48
1:D:212[B]:MET:HG2	1:D:212[B]:MET:O	2.13	0.48
1:A:382:VAL:O	1:A:385:PHE:HB3	2.13	0.48
1:B:373:LEU:CD2	5:B:1031:HOH:O	2.61	0.48
1:B:551:ARG:HG2	1:B:602:LEU:HD23	1.95	0.48
1:C:658:THR:H	1:C:718:LEU:CD2	2.21	0.48
1:C:681:THR:CG2	5:C:916:HOH:O	2.28	0.48
1:A:302:PRO:HG3	1:A:337:VAL:CG2	2.41	0.48
1:A:494:LYS:HD3	1:A:538:ARG:HG2	1.94	0.48
1:C:643:ARG:O	1:C:650:GLU:HA	2.14	0.48
1:D:565:LEU:C	1:D:565:LEU:HD23	2.34	0.48
1:A:561:PRO:HA	1:A:643:ARG:NH2	2.29	0.48
1:B:303:THR:O	5:B:1146:HOH:O	2.20	0.48
1:C:213:ARG:HB2	1:C:214:PRO:HD3	1.93	0.48
1:D:655:SER:OG	1:D:720:THR:HB	2.14	0.48
1:B:371:ASN:HB3	1:B:372:THR:CB	2.34	0.48
1:A:245:ILE:CG2	1:A:285:GLU:HB2	2.44	0.48
1:A:120:ARG:NH2	1:A:449:GLN:OE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:ASP:O	1:D:320:TYR:HB3	2.13	0.48
1:D:693:ASN:O	1:D:694:GLY:O	2.31	0.48
1:B:183:HIS:HD2	1:B:184:ASN:O	1.97	0.47
1:C:571:GLU:O	1:C:600:GLN:HA	2.14	0.47
1:D:535:ILE:HA	1:D:538:ARG:HD2	1.96	0.47
1:A:142:VAL:HG22	1:A:190:TYR:CZ	2.48	0.47
1:D:261:PHE:HA	3:D:809:GOL:O2	2.14	0.47
1:A:413:ARG:HH11	1:A:430:ARG:HH12	1.60	0.47
1:B:403:ARG:NH2	5:B:1085:HOH:O	2.46	0.47
1:C:156:PHE:HB3	1:C:186:GLN:NE2	2.29	0.47
1:D:635[B]:GLU:H	1:D:635[B]:GLU:CD	2.17	0.47
1:A:132:MET:CE	1:A:132:MET:CA	2.91	0.47
1:A:169:ARG:HG3	1:A:171:GLU:OE2	2.14	0.47
1:B:467:SER:HA	1:B:477:PHE:O	2.14	0.47
1:B:658:THR:HG22	1:B:660:VAL:N	2.15	0.47
1:D:655:SER:HB3	1:D:657:PHE:CE1	2.50	0.47
1:A:230:THR:O	1:A:234:LYS:HG3	2.14	0.47
1:B:503:HIS:HB3	1:B:506:LYS:HD2	1.96	0.47
1:A:168:LEU:HD12	1:A:175:TRP:CE2	2.49	0.47
1:B:559:ALA:HB1	1:B:653:VAL:HG21	1.97	0.47
1:C:528:VAL:O	1:C:577:GLU:HB2	2.15	0.47
1:D:591:GLY:O	1:D:592:GLY:O	2.32	0.47
1:D:693:ASN:HD21	1:D:714:THR:N	1.98	0.47
1:A:494:LYS:CD	1:A:538:ARG:HG2	2.45	0.47
1:B:200:ARG:HA	5:B:1208:HOH:O	2.13	0.47
1:B:617:HIS:CE1	5:B:1086:HOH:O	2.61	0.47
1:C:552:ALA:HA	1:C:720:THR:HG22	1.96	0.47
1:D:232:GLU:N	1:D:232:GLU:CD	2.67	0.47
1:B:341:PHE:CZ	1:B:358:GLU:HB3	2.49	0.47
1:B:570:ASN:ND2	5:B:1014:HOH:O	2.48	0.47
1:B:658:THR:HG23	1:B:659:PRO:CD	2.44	0.47
1:D:189:LYS:CE	1:D:216:THR:HG22	2.45	0.47
1:A:157:ASN:OD1	1:A:164:HIS:HD2	1.98	0.47
1:A:153:VAL:HA	1:A:157:ASN:HD22	1.80	0.46
1:B:117:THR:CB	5:B:1069:HOH:O	2.62	0.46
1:B:256:HIS:HE1	1:B:267:GLU:OE2	1.98	0.46
1:B:285:GLU:OE1	1:B:403:ARG:HD2	2.14	0.46
1:C:666:ARG:HA	1:C:712:SER:HA	1.96	0.46
1:D:297:SER:C	1:D:299:GLY:H	2.17	0.46
1:D:532:LYS:O	1:D:533:LYS:HB2	2.15	0.46
1:A:475:LEU:HD12	1:A:475:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:ARG:CD	5:A:1107:HOH:O	2.62	0.46
1:B:680:ASN:HD22	1:B:682:ASP:H	1.62	0.46
1:B:680:ASN:ND2	1:B:682:ASP:H	2.13	0.46
1:D:593:ASP:HA	1:D:597:HIS:CD2	2.50	0.46
1:A:580:HIS:HD2	5:A:980:HOH:O	1.98	0.46
1:B:693:ASN:HD21	1:B:714:THR:N	2.02	0.46
1:C:680:ASN:HA	1:C:721:ILE:HG22	1.96	0.46
1:A:231:GLU:HG3	5:A:1029:HOH:O	2.15	0.46
1:A:580:HIS:CD2	5:A:980:HOH:O	2.67	0.46
1:D:525:HIS:HB3	1:D:567:PHE:CE1	2.51	0.46
1:C:152:VAL:HG12	1:C:156:PHE:HZ	1.81	0.46
1:A:258:ASP:HB3	5:A:1111:HOH:O	2.14	0.46
1:A:233:ARG:HD2	1:A:400:ASP:OD2	2.14	0.46
1:D:149:ARG:CG	1:D:149:ARG:NH1	2.65	0.46
1:A:133:ASP:N	1:A:133:ASP:OD2	2.48	0.46
1:A:428:GLY:CA	5:A:981:HOH:O	2.61	0.46
1:C:211:GLN:HB3	1:C:215:GLU:HB2	1.98	0.46
1:C:587:HIS:HA	1:C:590:GLU:HG2	1.97	0.46
1:A:570:ASN:ND2	5:A:906:HOH:O	2.48	0.46
1:B:684:MET:H	1:B:690:ASN:ND2	2.14	0.46
1:A:441:ASN:OD1	1:A:444:ARG:NH1	2.49	0.46
1:A:577:GLU:CD	5:A:1086:HOH:O	2.54	0.46
1:B:380:ARG:HD3	1:B:384:ASN:ND2	2.30	0.46
1:C:494:LYS:CG	1:C:538:ARG:HG2	2.46	0.46
1:B:238:GLN:HG2	5:B:1186:HOH:O	2.15	0.46
1:C:202:LYS:HD2	1:C:351:PHE:HD1	1.80	0.46
1:C:636:ARG:HG2	1:C:662:ARG:CZ	2.46	0.46
1:B:675:TRP:O	1:B:696:THR:HA	2.15	0.45
1:D:579:ASN:ND2	1:D:581:ASP:H	2.14	0.45
1:B:289:ILE:HD12	1:B:289:ILE:C	2.36	0.45
1:D:141:SER:HA	1:D:175:TRP:O	2.16	0.45
1:B:213:ARG:NH1	1:B:295:ASP:OD2	2.49	0.45
1:C:285:GLU:HA	1:C:333:ILE:O	2.15	0.45
1:C:341:PHE:CG	1:C:342:PRO:HD2	2.51	0.45
1:C:489:THR:O	1:C:493:MET:HG2	2.17	0.45
1:D:159:TRP:CD1	2:D:805:GLC:H61	2.51	0.45
1:B:168:LEU:HG	1:B:175:TRP:CE2	2.52	0.45
1:B:256:HIS:CE1	1:B:267:GLU:OE2	2.70	0.45
1:B:373:LEU:CD2	1:B:373:LEU:H	2.29	0.45
1:C:686:TYR:O	1:C:687:HIS:HB2	2.17	0.45
1:D:259:ASN:HB3	1:D:261:PHE:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:GLN:O	5:A:1105:HOH:O	2.21	0.45
1:B:163:ARG:CD	5:B:1084:HOH:O	2.53	0.45
1:A:178:PHE:O	1:A:178:PHE:CD1	2.70	0.45
1:A:270:ASP:O	1:A:274:PRO:HG2	2.16	0.45
1:A:658:THR:HB	1:A:659:PRO:HD2	1.98	0.45
1:D:552:ALA:O	1:D:720:THR:CG2	2.65	0.45
1:A:285:GLU:HG3	1:A:333:ILE:CG2	2.47	0.45
1:A:295:ASP:OD2	1:A:311:ARG:NH2	2.40	0.45
1:B:425:ASN:HD21	1:B:429:GLY:H	1.65	0.45
1:D:627:GLU:HB3	1:D:642:VAL:HG12	1.98	0.45
1:A:247:GLU:OE1	1:A:525:HIS:CD2	2.68	0.45
1:C:707:ARG:NH1	5:C:919:HOH:O	2.50	0.45
1:A:517:GLU:HB2	1:A:519:PHE:CZ	2.51	0.45
1:B:412:TYR:CD2	1:B:430:ARG:HG2	2.52	0.45
1:A:186:GLN:O	1:A:220:ILE:HG13	2.17	0.45
1:C:259:ASN:O	1:C:260:ASN:HB3	2.17	0.45
1:B:149:ARG:CG	1:B:149:ARG:NH2	2.62	0.44
1:C:450:VAL:HG23	1:C:450:VAL:O	2.16	0.44
1:C:559:ALA:HB1	1:C:653:VAL:HG21	1.98	0.44
1:B:463:PHE:CE2	1:B:475:LEU:HD13	2.52	0.44
1:C:333:ILE:HG12	1:C:401:ALA:HB3	1.97	0.44
2:B:804:GLC:H4	2:B:805:GLC:H2	1.66	0.44
1:C:375:TYR:O	1:C:376:ASN:CB	2.64	0.44
1:C:564:LYS:HD2	1:C:564:LYS:N	2.32	0.44
1:D:212[A]:MET:HB2	1:D:310:ARG:HG2	1.99	0.44
1:A:168:LEU:HD23	1:A:169:ARG:C	2.38	0.44
1:A:237:ASN:HD22	1:A:283:HIS:HE1	1.66	0.44
1:A:512:LEU:CD1	2:A:808:GLC:H5	2.47	0.44
1:C:658:THR:HA	1:C:659:PRO:HD3	1.77	0.44
1:C:636:ARG:HG2	1:C:662:ARG:NH2	2.33	0.44
1:A:125:LEU:HA	1:A:141:SER:HB2	1.98	0.44
1:A:412:TYR:O	5:A:992:HOH:O	2.21	0.44
1:B:319:ARG:NH1	5:B:971:HOH:O	2.50	0.44
1:C:126:GLY:HA2	1:C:204:ASP:OD2	2.17	0.44
1:C:318:PHE:O	1:C:322:ILE:HG12	2.18	0.44
1:C:525:HIS:CD2	1:C:525:HIS:H	2.36	0.44
1:A:467:SER:HA	1:A:477:PHE:O	2.17	0.44
1:A:644:ARG:HD2	5:A:1107:HOH:O	2.17	0.44
1:A:643:ARG:O	1:A:650:GLU:HA	2.17	0.44
1:B:458:GLU:HG3	5:B:1085:HOH:O	2.18	0.44
1:C:639:LEU:HD13	1:C:657:PHE:HE1	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:807:GOL:H32	5:A:1078:HOH:O	2.17	0.44
1:B:259:ASN:ND2	1:B:259:ASN:H	2.15	0.44
1:B:619:LEU:HA	5:B:1012:HOH:O	2.17	0.44
1:D:148:ARG:O	1:D:149:ARG:CB	2.56	0.44
1:A:444:ARG:O	1:A:448:GLU:HG3	2.18	0.44
1:A:650:GLU:HG2	1:A:671:GLN:OE1	2.18	0.44
1:B:694:GLY:CA	5:B:1054:HOH:O	2.54	0.44
1:D:341:PHE:CZ	1:D:358:GLU:HB3	2.53	0.44
1:D:136:THR:HG22	1:D:137:GLY:N	2.33	0.43
1:C:375:TYR:HB2	1:C:377:TYR:CZ	2.53	0.43
1:C:594:ASN:H	1:C:597:HIS:HD2	1.66	0.43
1:D:227:VAL:HG11	1:D:398:GLY:HA3	2.00	0.43
1:B:371:ASN:N	1:B:372:THR:CA	2.81	0.43
1:A:211:GLN:HE21	1:A:216:THR:H	1.66	0.43
1:B:259:ASN:HB2	1:B:261:PHE:CD2	2.53	0.43
1:B:509:PHE:HA	2:B:817:GLC:H62	1.99	0.43
1:D:496:ASP:OD1	1:D:498:VAL:HG22	2.19	0.43
1:A:292:HIS:CG	1:A:299:GLY:HA2	2.54	0.43
1:A:492:TYR:CZ	1:A:507:LEU:HD22	2.52	0.43
1:A:563:LYS:C	1:A:564:LYS:HD3	2.39	0.43
1:D:258:ASP:O	1:D:259:ASN:HB2	2.17	0.43
1:A:254[B]:ARG:HE	2:A:802:GLC:C6	2.31	0.43
1:A:644:ARG:NH2	1:A:650:GLU:OE1	2.51	0.43
1:B:230:THR:O	1:B:234:LYS:HG3	2.19	0.43
1:D:527:GLU:O	1:D:538:ARG:NH2	2.51	0.43
1:D:597:HIS:HB3	1:D:601:ARG:NH1	2.33	0.43
1:A:485:TRP:CE2	1:A:489:THR:HG21	2.54	0.43
1:B:179:ILE:HA	1:B:180:PRO:HD2	1.92	0.43
1:B:507:LEU:HA	1:B:507:LEU:HD12	1.77	0.43
1:D:389:ASN:O	1:D:392:TYR:HB3	2.19	0.43
1:A:284:LEU:HD12	1:A:284:LEU:HA	1.78	0.43
1:B:152:VAL:O	1:B:157:ASN:ND2	2.51	0.43
1:B:359:HIS:HE1	1:B:361:ASP:OD1	2.01	0.43
1:B:542:ASP:O	1:B:546:LYS:HG3	2.19	0.43
1:C:684:MET:HB2	1:C:690:ASN:HB2	2.00	0.43
1:C:684:MET:H	1:C:690:ASN:ND2	2.05	0.43
1:D:597:HIS:HB3	1:D:601:ARG:HH12	1.84	0.43
1:A:259:ASN:ND2	1:A:261:PHE:HB2	2.34	0.43
1:A:262:TRP:CH2	1:A:311:ARG:CG	3.01	0.43
1:A:144:ALA:CB	1:A:352:ASP:HB3	2.43	0.43
1:C:144:ALA:HB1	1:C:352:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:TRP:HE1	1:D:580:HIS:CD2	2.36	0.43
1:D:511:ILE:HB	4:D:810:BGC:H6C1	2.00	0.43
1:D:532:LYS:O	1:D:533:LYS:CB	2.67	0.43
1:A:686:TYR:O	1:A:687:HIS:HB2	2.17	0.42
1:D:336:TRP:HZ2	1:D:386:LEU:O	2.02	0.42
1:D:721:ILE:HD12	1:D:723:LEU:HD21	2.00	0.42
1:B:670:ASN:HB3	5:B:1063:HOH:O	2.19	0.42
1:D:542:ASP:OD1	1:D:545:GLN:HG3	2.19	0.42
1:A:184:ASN:HA	1:A:220:ILE:O	2.19	0.42
1:A:376:ASN:C	1:A:376:ASN:HD22	2.22	0.42
1:A:340:HIS:CE1	1:A:405:ASP:OD2	2.53	0.42
1:A:705:HIS:HE1	5:A:985:HOH:O	2.02	0.42
1:B:575:GLY:HA3	2:B:804:GLC:H5	2.02	0.42
1:A:157:ASN:HB3	1:A:160:ASP:H	1.84	0.42
1:C:437:GLU:O	1:C:441:ASN:HB2	2.20	0.42
1:D:285:GLU:OE1	1:D:403:ARG:HD2	2.19	0.42
1:D:666:ARG:HA	1:D:711:LEU:O	2.19	0.42
1:B:373:LEU:HD22	5:B:1031:HOH:O	2.20	0.42
1:D:344:ASP:O	1:D:346:PHE:N	2.53	0.42
1:B:258:ASP:HB2	5:B:1070:HOH:O	2.19	0.42
1:B:317:ASP:O	1:B:320:TYR:HB3	2.19	0.42
1:B:363:ARG:CD	1:B:364:GLU:H	2.22	0.42
1:D:343:THR:HG22	1:D:373:LEU:HD21	2.02	0.42
1:A:169:ARG:HB2	1:A:169:ARG:CZ	2.49	0.42
1:A:254[B]:ARG:HE	2:A:802:GLC:H62	1.85	0.42
1:B:463:PHE:HE2	1:B:475:LEU:HD13	1.85	0.42
1:C:341:PHE:CD2	1:C:342:PRO:HD2	2.55	0.42
1:D:183:HIS:HD2	1:D:184:ASN:O	2.02	0.42
1:D:341:PHE:O	1:D:343:THR:HG23	2.20	0.42
1:D:718:LEU:HD23	1:D:718:LEU:HA	1.83	0.42
1:D:651:ILE:HD13	1:D:722:TRP:HB3	2.01	0.42
1:B:690:ASN:ND2	3:B:815:GOL:O3	2.45	0.41
1:D:215:GLU:O	1:D:216:THR:HB	2.20	0.41
1:B:380:ARG:HE	1:B:380:ARG:HB2	1.71	0.41
1:A:625:GLY:O	1:A:643:ARG:HD2	2.20	0.41
1:C:656:ASN:ND2	1:C:656:ASN:C	2.73	0.41
1:B:273:VAL:HB	1:B:274:PRO:HD3	2.01	0.41
1:B:642:VAL:HG13	1:B:650:GLU:HB3	2.02	0.41
1:B:518:ASN:ND2	2:B:802:GLC:H62	2.25	0.41
1:A:568:MET:HG3	1:A:584:LEU:HD11	2.03	0.41
1:A:559:ALA:HB1	1:A:653:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ARG:HH12	1:C:151:SER:HB2	1.85	0.41
1:C:494:LYS:HG2	1:C:538:ARG:HG2	2.02	0.41
1:C:593:ASP:OD2	1:C:687:HIS:CE1	2.70	0.41
1:C:684:MET:HB2	1:C:690:ASN:ND2	2.35	0.41
1:D:307:ALA:HA	1:D:308:PRO:HD3	1.87	0.41
1:A:162:ARG:HB2	1:A:162:ARG:HE	1.62	0.41
1:A:705:HIS:O	5:A:1065:HOH:O	2.22	0.41
1:B:232:GLU:O	1:B:235:LYS:HB3	2.20	0.41
1:B:334:LEU:HD12	1:B:335:ASP:N	2.36	0.41
1:B:343:THR:HG22	1:B:373:LEU:CD2	2.50	0.41
1:C:249:HIS:CB	1:C:287:LEU:HD22	2.46	0.41
1:C:608:LEU:HD23	1:C:608:LEU:HA	1.87	0.41
1:C:551:ARG:C	1:C:681:THR:HG21	2.41	0.41
1:D:212[A]:MET:CG	1:D:213:ARG:HH11	2.09	0.41
1:B:157:ASN:OD1	1:B:164:HIS:CD2	2.73	0.41
1:B:602:LEU:HG	1:B:606:LEU:HD22	2.01	0.41
1:D:120:ARG:HG2	1:D:122:TYR:CZ	2.55	0.41
1:B:414:ASP:CG	5:B:1131:HOH:O	2.54	0.41
1:D:373:LEU:H	1:D:373:LEU:HD23	1.79	0.41
1:A:470:GLN:C	1:A:472:MET:H	2.23	0.41
1:A:518:ASN:HD21	2:A:804:GLC:H62	1.86	0.41
1:B:499:TYR:O	1:B:503:HIS:HD2	2.03	0.41
1:B:514:ASN:ND2	5:B:958:HOH:O	2.51	0.41
1:B:674:LYS:HG2	1:B:698:HIS:HD2	1.85	0.41
1:C:292:HIS:HA	1:C:293:PRO:HD3	1.89	0.41
1:D:289:ILE:HD12	1:D:289:ILE:C	2.42	0.41
1:A:148:ARG:O	1:A:148:ARG:HG2	2.20	0.41
1:A:214:PRO:HB3	1:A:215:GLU:HB3	2.02	0.41
1:A:468:ARG:NH1	2:A:804:GLC:C6	2.84	0.41
1:B:606:LEU:HD13	1:B:679:LEU:HD11	2.03	0.41
1:A:213:ARG:NH1	1:A:293:PRO:O	2.53	0.41
4:B:803:BGC:H6	2:B:804:GLC:C2	2.34	0.41
1:A:693:ASN:HD21	1:A:714:THR:N	2.03	0.40
1:D:564:LYS:HD2	1:D:564:LYS:N	2.36	0.40
1:B:363:ARG:HA	1:B:364:GLU:OE1	2.21	0.40
1:C:224:PRO:HB2	1:C:319:ARG:HH22	1.87	0.40
1:C:579:ASN:HD21	1:C:581:ASP:HB3	1.86	0.40
1:C:601:ARG:CZ	1:D:685[B]:HIS:HE2	2.34	0.40
1:D:125:LEU:HA	1:D:125:LEU:HD23	1.77	0.40
1:D:183:HIS:CD2	1:D:184:ASN:O	2.74	0.40
1:D:405:ASP:N	1:D:405:ASP:OD1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:HIS:HE1	1:A:267:GLU:OE2	2.03	0.40
1:B:362:PRO:CA	1:B:363:ARG:CB	2.88	0.40
1:C:157:ASN:O	1:C:160:ASP:HB2	2.21	0.40
1:C:354:THR:O	1:C:356:LEU:N	2.54	0.40
1:D:237:ASN:ND2	1:D:283:HIS:CE1	2.81	0.40
1:C:652:ILE:O	1:C:722:TRP:HA	2.22	0.40
1:D:149:ARG:HD2	1:D:150:VAL:N	2.36	0.40
1:D:538:ARG:NH1	5:D:1079:HOH:O	2.54	0.40
1:D:721:ILE:CD1	1:D:723:LEU:HD21	2.51	0.40
1:A:375:TYR:HB2	1:A:377:TYR:CZ	2.57	0.40
1:A:463:PHE:HA	1:A:464:PRO:HD3	1.92	0.40
1:A:571:GLU:O	1:A:599:VAL:HG12	2.21	0.40
1:B:253:TRP:CE3	1:B:254[A]:ARG:HG3	2.56	0.40
1:B:660:VAL:HA	1:B:661:PRO:HD3	1.95	0.40
1:D:139:ARG:HD3	1:D:176:GLU:OE1	2.22	0.40
1:D:212[A]:MET:HA	1:D:213:ARG:HA	1.89	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	586/612 (96%)	546 (93%)	31 (5%)	9 (2%)	12	16
1	B	594/612 (97%)	566 (95%)	18 (3%)	10 (2%)	11	13
1	C	577/612 (94%)	512 (89%)	49 (8%)	16 (3%)	6	5
1	D	586/612 (96%)	545 (93%)	29 (5%)	12 (2%)	9	10
All	All	2343/2448 (96%)	2169 (93%)	127 (5%)	47 (2%)	9	10

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	TRP
1	A	148	ARG
1	A	215	GLU
1	A	226	LYS
1	B	194	ASP
1	B	213	ARG
1	B	226	LYS
1	C	213	ARG
1	C	343	THR
1	C	352	ASP
1	C	612	HIS
1	C	658	THR
1	D	149	ARG
1	D	194	ASP
1	D	213	ARG
1	D	259	ASN
1	D	694	GLY
1	A	142	VAL
1	A	216	THR
1	A	217	ALA
1	A	375	TYR
1	C	355	ASN
1	D	217	ALA
1	D	345	ASP
1	D	372	THR
1	D	522	PRO
1	D	591	GLY
1	D	592	GLY
1	A	522	PRO
1	B	363	ARG
1	C	472	MET
1	C	497	PRO
1	C	522	PRO
1	B	221	CYS
1	B	372	THR
1	B	425	ASN
1	B	696	THR
1	C	293	PRO
1	C	542	ASP
1	B	703	ALA
1	C	159	TRP
1	C	533	LYS
1	C	709	HIS

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Mol	Chain	Res	Type
1	D	695	GLY
1	B	522	PRO
1	C	374	ILE
1	C	353	GLY

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	503/521 (96%)	465 (92%)	38 (8%)	15	24
1	B	510/521 (98%)	464 (91%)	46 (9%)	11	16
1	C	495/521 (95%)	460 (93%)	35 (7%)	17	27
1	D	503/521 (96%)	467 (93%)	36 (7%)	17	26
All	All	2011/2084 (96%)	1856 (92%)	155 (8%)	15	23

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	MET
1	A	133	ASP
1	A	169	ARG
1	A	171	GLU
1	A	199	LEU
1	A	212	MET
1	A	216	THR
1	A	223	LEU
1	A	228	VAL
1	A	257	THR
1	A	259	ASN
1	A	285	GLU
1	A	311	ARG
1	A	315	ARG
1	A	331	ASN
1	A	356	LEU
1	A	358	GLU

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Mol	Chain	Res	Type
1	A	376	ASN
1	A	380	ARG
1	A	391	LEU
1	A	413	ARG
1	A	434	GLU
1	A	472	MET
1	A	490	LEU
1	A	507	LEU
1	A	512	LEU
1	A	579	ASN
1	A	590[A]	GLU
1	A	590[B]	GLU
1	A	606	LEU
1	A	619	LEU
1	A	642	VAL
1	A	647	GLU
1	A	656	ASN
1	A	679	LEU
1	A	680	ASN
1	A	720	THR
1	A	723	LEU
1	B	132	MET
1	B	133	ASP
1	B	138	THR
1	B	149	ARG
1	B	163	ARG
1	B	168	LEU
1	B	171	GLU
1	B	215	GLU
1	B	216	THR
1	B	223	LEU
1	B	258	ASP
1	B	259	ASN
1	B	290	ASN
1	B	305	LEU
1	B	331	ASN
1	B	334	LEU
1	B	356	LEU
1	B	360	SER
1	B	363	ARG
1	B	371	ASN
1	B	373	LEU

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Mol	Chain	Res	Type
1	B	374	ILE
1	B	376	ASN
1	B	380	ARG
1	B	391	LEU
1	B	425	ASN
1	B	426	GLU
1	B	430	ARG
1	B	446	LEU
1	B	470	GLN
1	B	475	LEU
1	B	490	LEU
1	B	504	HIS
1	B	507	LEU
1	B	511	ILE
1	B	512	LEU
1	B	523	LEU
1	B	558	TRP
1	B	579	ASN
1	B	606	LEU
1	B	619	LEU
1	B	651	ILE
1	B	656	ASN
1	B	658	THR
1	B	679	LEU
1	B	680	ASN
1	C	119	LEU
1	C	133	ASP
1	C	157	ASN
1	C	168	LEU
1	C	170	LYS
1	C	171	GLU
1	C	212	MET
1	C	223	LEU
1	C	259	ASN
1	C	305	LEU
1	C	310	ARG
1	C	315	ARG
1	C	337	VAL
1	C	350	GLU
1	C	352	ASP
1	C	356	LEU
1	C	379	ARG

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Mol	Chain	Res	Type
1	C	446	LEU
1	C	470	GLN
1	C	471	ASP
1	C	475	LEU
1	C	498	VAL
1	C	507	LEU
1	C	511	ILE
1	C	542	ASP
1	C	564	LYS
1	C	579	ASN
1	C	595	TRP
1	C	619	LEU
1	C	651	ILE
1	C	656	ASN
1	C	680	ASN
1	C	689	SER
1	C	720	THR
1	C	723	LEU
1	D	119	LEU
1	D	138	THR
1	D	141	SER
1	D	148	ARG
1	D	149	ARG
1	D	157	ASN
1	D	170	LYS
1	D	171	GLU
1	D	223	LEU
1	D	232	GLU
1	D	258	ASP
1	D	315	ARG
1	D	356	LEU
1	D	359	HIS
1	D	372	THR
1	D	373	LEU
1	D	380	ARG
1	D	391	LEU
1	D	462	ASP
1	D	470	GLN
1	D	471	ASP
1	D	472	MET
1	D	475	LEU
1	D	490	LEU

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Mol	Chain	Res	Type
1	D	523	LEU
1	D	564	LYS
1	D	579	ASN
1	D	606	LEU
1	D	614	LYS
1	D	619	LEU
1	D	651	ILE
1	D	656	ASN
1	D	666	ARG
1	D	679	LEU
1	D	680	ASN
1	D	720	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	157	ASN
1	A	164	HIS
1	A	211	GLN
1	A	237	ASN
1	A	256	HIS
1	A	259	ASN
1	A	260	ASN
1	A	283	HIS
1	A	331	ASN
1	A	340	HIS
1	A	355	ASN
1	A	376	ASN
1	A	384	ASN
1	A	504	HIS
1	A	525	HIS
1	A	570	ASN
1	A	574	GLN
1	A	579	ASN
1	A	597	HIS
1	A	617	HIS
1	A	656	ASN
1	A	680	ASN
1	A	690	ASN
1	A	693	ASN
1	A	705	HIS

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Mol	Chain	Res	Type
1	A	708	GLN
1	A	709	HIS
1	B	157	ASN
1	B	164	HIS
1	B	183	HIS
1	B	198	ASN
1	B	237	ASN
1	B	256	HIS
1	B	259	ASN
1	B	283	HIS
1	B	331	ASN
1	B	340	HIS
1	B	359	HIS
1	B	371	ASN
1	B	376	ASN
1	B	384	ASN
1	B	425	ASN
1	B	470	GLN
1	B	501	GLN
1	B	504	HIS
1	B	514	ASN
1	B	525	HIS
1	B	545	GLN
1	B	570	ASN
1	B	574	GLN
1	B	579	ASN
1	B	597	HIS
1	B	617	HIS
1	B	656	ASN
1	B	680	ASN
1	B	687	HIS
1	B	690	ASN
1	B	693	ASN
1	B	705	HIS
1	C	157	ASN
1	C	164	HIS
1	C	183	HIS
1	C	186	GLN
1	C	211	GLN
1	C	229	GLN
1	C	237	ASN
1	C	256	HIS

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Mol	Chain	Res	Type
1	C	259	ASN
1	C	283	HIS
1	C	301	GLN
1	C	331	ASN
1	C	355	ASN
1	C	470	GLN
1	C	525	HIS
1	C	545	GLN
1	C	570	ASN
1	C	574	GLN
1	C	579	ASN
1	C	580	HIS
1	C	597	HIS
1	C	612	HIS
1	C	613	HIS
1	C	617	HIS
1	C	656	ASN
1	C	680	ASN
1	C	687	HIS
1	C	690	ASN
1	C	693	ASN
1	C	705	HIS
1	C	709	HIS
1	D	118	HIS
1	D	164	HIS
1	D	183	HIS
1	D	237	ASN
1	D	256	HIS
1	D	260	ASN
1	D	283	HIS
1	D	290	ASN
1	D	331	ASN
1	D	340	HIS
1	D	359	HIS
1	D	443	ASN
1	D	470	GLN
1	D	525	HIS
1	D	545	GLN
1	D	570	ASN
1	D	574	GLN
1	D	579	ASN
1	D	597	HIS

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Mol	Chain	Res	Type
1	D	617	HIS
1	D	656	ASN
1	D	680	ASN
1	D	687	HIS
1	D	690	ASN
1	D	693	ASN
1	D	705	HIS
1	D	708	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

42 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLC	A	801	2	12,12,12	0.51	0	17,17,17	0.84	0
2	GLC	A	802	2	11,11,12	0.50	0	13,15,17	1.26	1 (7%)
2	GLC	A	803	2	12,12,12	0.73	0	17,17,17	1.20	2 (11%)
2	GLC	A	804	2	11,11,12	0.48	0	13,15,17	2.13	1 (7%)
3	GOL	A	805	-	5,5,5	0.47	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	806	-	5,5,5	0.24	0	5,5,5	0.42	0
3	GOL	A	807	-	5,5,5	0.44	0	5,5,5	0.79	0
2	GLC	A	808	2	12,12,12	0.48	0	17,17,17	1.72	4 (23%)
2	GLC	A	809	2	11,11,12	0.77	0	13,15,17	0.86	0
2	GLC	A	810	2	11,11,12	0.60	0	13,15,17	1.61	4 (30%)
4	BGC	B	801	2	12,12,12	0.78	0	17,17,17	1.66	4 (23%)
2	GLC	B	802	4	11,11,12	0.41	0	13,15,17	2.18	2 (15%)
4	BGC	B	803	2	12,12,12	0.45	0	17,17,17	2.00	6 (35%)
2	GLC	B	804	2,4	11,11,12	0.49	0	13,15,17	1.74	3 (23%)
2	GLC	B	805	2	11,11,12	0.58	0	13,15,17	1.11	1 (7%)
2	GLC	B	806	2	11,11,12	0.58	0	13,15,17	1.41	2 (15%)
2	GLC	B	807	2	11,11,12	0.64	0	13,15,17	2.21	5 (38%)
2	GLC	B	808	2	11,11,12	0.61	0	13,15,17	1.39	2 (15%)
2	GLC	B	809	2	11,11,12	0.66	0	13,15,17	1.33	2 (15%)
4	BGC	B	810	-	12,12,12	0.50	0	17,17,17	0.90	1 (5%)
3	GOL	B	811	-	5,5,5	0.44	0	5,5,5	0.20	0
3	GOL	B	812	-	5,5,5	0.40	0	5,5,5	0.63	0
3	GOL	B	813	-	5,5,5	0.53	0	5,5,5	0.83	0
3	GOL	B	814	-	5,5,5	0.37	0	5,5,5	0.35	0
3	GOL	B	815	-	5,5,5	0.41	0	5,5,5	0.51	0
4	BGC	B	816	2	12,12,12	0.59	0	17,17,17	1.22	2 (11%)
2	GLC	B	817	4	11,11,12	0.80	0	13,15,17	1.21	1 (7%)
2	GLC	C	801	2	12,12,12	0.56	0	17,17,17	0.54	0
2	GLC	C	802	2	11,11,12	0.67	0	13,15,17	1.02	1 (7%)
2	GLC	D	801	2	12,12,12	0.65	0	17,17,17	1.45	3 (17%)
2	GLC	D	802	2	11,11,12	0.77	0	13,15,17	1.96	2 (15%)
2	GLC	D	803	2	11,11,12	0.58	0	13,15,17	1.21	1 (7%)
2	GLC	D	804	2	11,11,12	0.78	0	13,15,17	1.42	2 (15%)
2	GLC	D	805	2	12,12,12	0.51	0	17,17,17	0.82	0
2	GLC	D	806	2	11,11,12	0.56	0	13,15,17	1.47	3 (23%)
3	GOL	D	807	-	5,5,5	0.30	0	5,5,5	0.31	0
3	GOL	D	808	-	5,5,5	0.29	0	5,5,5	0.41	0
3	GOL	D	809	-	5,5,5	0.32	0	5,5,5	0.43	0
4	BGC	D	810	2	12,12,12	0.69	0	17,17,17	2.13	5 (29%)
2	GLC	D	811	4	11,11,12	0.58	0	13,15,17	1.76	2 (15%)
4	BGC	D	812	2	12,12,12	0.53	0	17,17,17	1.59	3 (17%)
2	GLC	D	813	4	11,11,12	0.52	0	13,15,17	1.69	2 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	A	801	2	-	0/2/22/22	0/1/1/1
2	GLC	A	802	2	-	0/2/19/22	0/1/1/1
2	GLC	A	803	2	-	0/2/22/22	0/1/1/1
2	GLC	A	804	2	-	0/2/19/22	0/1/1/1
3	GOL	A	805	-	-	0/4/4/4	0/0/0/0
3	GOL	A	806	-	-	0/4/4/4	0/0/0/0
3	GOL	A	807	-	-	0/4/4/4	0/0/0/0
2	GLC	A	808	2	-	0/2/22/22	0/1/1/1
2	GLC	A	809	2	-	0/2/19/22	0/1/1/1
2	GLC	A	810	2	-	0/2/19/22	0/1/1/1
4	BGC	B	801	2	-	0/2/22/22	0/1/1/1
2	GLC	B	802	4	-	0/2/19/22	0/1/1/1
4	BGC	B	803	2	-	0/2/22/22	0/1/1/1
2	GLC	B	804	2,4	-	0/2/19/22	0/1/1/1
2	GLC	B	805	2	-	0/2/19/22	0/1/1/1
2	GLC	B	806	2	-	0/2/19/22	0/1/1/1
2	GLC	B	807	2	-	0/2/19/22	0/1/1/1
2	GLC	B	808	2	-	0/2/19/22	0/1/1/1
2	GLC	B	809	2	-	0/2/19/22	0/1/1/1
4	BGC	B	810	-	-	0/2/22/22	0/1/1/1
3	GOL	B	811	-	-	0/4/4/4	0/0/0/0
3	GOL	B	812	-	-	0/4/4/4	0/0/0/0
3	GOL	B	813	-	-	0/4/4/4	0/0/0/0
3	GOL	B	814	-	-	0/4/4/4	0/0/0/0
3	GOL	B	815	-	-	0/4/4/4	0/0/0/0
4	BGC	B	816	2	-	0/2/22/22	0/1/1/1
2	GLC	B	817	4	-	0/2/19/22	0/1/1/1
2	GLC	C	801	2	-	0/2/22/22	0/1/1/1
2	GLC	C	802	2	-	0/2/19/22	0/1/1/1
2	GLC	D	801	2	-	0/2/22/22	0/1/1/1
2	GLC	D	802	2	-	0/2/19/22	0/1/1/1
2	GLC	D	803	2	-	0/2/19/22	0/1/1/1
2	GLC	D	804	2	-	0/2/19/22	0/1/1/1
2	GLC	D	805	2	-	0/2/22/22	0/1/1/1
2	GLC	D	806	2	-	0/2/19/22	0/1/1/1
3	GOL	D	807	-	-	0/4/4/4	0/0/0/0
3	GOL	D	808	-	-	0/4/4/4	0/0/0/0
3	GOL	D	809	-	-	0/4/4/4	0/0/0/0
4	BGC	D	810	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	D	811	4	-	0/2/19/22	0/1/1/1
4	BGC	D	812	2	-	0/2/22/22	0/1/1/1
2	GLC	D	813	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	BGC	O5-C1-C2	-4.54	102.52	110.04
4	B	803	BGC	C4-C3-C2	-4.42	103.04	110.84
4	D	810	BGC	C1-C2-C3	-4.20	103.06	110.65
2	B	808	GLC	O5-C1-C2	-3.68	105.02	110.79
4	D	812	BGC	C4-C3-C2	-3.49	104.69	110.84
4	D	810	BGC	O5-C1-C2	-3.47	104.28	110.04
2	B	807	GLC	C3-C4-C5	-3.45	104.14	110.22
2	A	810	GLC	O5-C1-C2	-3.42	105.43	110.79
2	B	804	GLC	C3-C4-C5	-2.96	105.00	110.22
4	B	801	BGC	C1-O5-C5	-2.78	108.38	113.39
2	B	802	GLC	C2-C3-C4	-2.68	106.20	110.88
2	D	813	GLC	C2-C3-C4	-2.61	106.32	110.88
2	D	806	GLC	C1-C2-C3	-2.51	106.47	109.65
2	B	805	GLC	C3-C4-C5	-2.49	105.83	110.22
2	A	808	GLC	C4-C3-C2	-2.35	106.69	110.84
2	B	809	GLC	C2-C3-C4	-2.27	106.91	110.88
4	B	816	BGC	C1-C2-C3	-2.11	106.83	110.65
2	D	806	GLC	C2-C3-C4	-2.11	107.20	110.88
4	B	816	BGC	O4-C4-C3	-2.10	105.78	110.36
4	B	801	BGC	O4-C4-C5	-2.10	104.00	109.28
2	B	817	GLC	O5-C1-C2	-2.01	107.65	110.79
2	B	808	GLC	O2-C2-C1	2.02	113.28	109.18
4	B	810	BGC	O4-C4-C5	2.04	114.42	109.28
2	D	806	GLC	O2-C2-C3	2.04	114.19	110.17
2	A	810	GLC	C3-C4-C5	2.07	113.87	110.22
2	B	807	GLC	O4-C4-C3	2.08	114.88	110.36
2	B	806	GLC	O4-C4-C3	2.08	114.88	110.36
4	B	801	BGC	C4-C3-C2	2.11	114.56	110.84
4	D	812	BGC	O2-C2-C1	2.17	114.27	109.75
4	D	810	BGC	O2-C2-C1	2.18	114.28	109.75
2	D	801	GLC	C3-C4-C5	2.21	114.11	110.22
2	A	810	GLC	O2-C2-C3	2.26	114.61	110.17
2	A	810	GLC	C1-O5-C5	2.26	115.28	112.17
4	B	803	BGC	O3-C3-C4	2.29	115.33	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	804	GLC	O4-C4-C5	2.46	115.47	109.28
4	D	812	BGC	O4-C4-C3	2.52	115.84	110.36
2	A	803	GLC	C4-C3-C2	2.56	115.35	110.84
2	B	807	GLC	O5-C1-C2	2.57	114.82	110.79
2	A	802	GLC	C1-O5-C5	2.57	115.71	112.17
4	B	803	BGC	O4-C4-C5	2.59	115.82	109.28
4	B	803	BGC	O2-C2-C1	2.68	115.31	109.75
4	B	803	BGC	O4-C4-C3	2.68	116.19	110.36
2	A	808	GLC	O5-C1-C2	2.68	114.49	110.04
2	C	802	GLC	C1-O5-C5	2.71	115.91	112.17
2	D	801	GLC	C1-C2-C3	2.79	115.69	110.65
2	D	811	GLC	C3-C4-C5	2.79	115.14	110.22
2	D	804	GLC	C1-O5-C5	2.80	116.02	112.17
2	A	803	GLC	C1-C2-C3	2.84	115.78	110.65
2	B	809	GLC	C1-O5-C5	2.84	116.08	112.17
2	A	808	GLC	O5-C5-C4	3.02	115.22	109.66
2	B	806	GLC	C1-O5-C5	3.20	116.57	112.17
4	D	810	BGC	C3-C4-C5	3.21	115.87	110.22
2	D	803	GLC	C1-O5-C5	3.32	116.74	112.17
4	B	803	BGC	C1-O5-C5	3.50	119.70	113.39
2	D	802	GLC	C2-C3-C4	3.52	117.02	110.88
2	D	804	GLC	C1-C2-C3	3.75	114.41	109.65
2	D	801	GLC	C4-C3-C2	3.80	117.53	110.84
2	B	807	GLC	C1-C2-C3	3.80	114.47	109.65
2	B	804	GLC	C1-O5-C5	3.98	117.66	112.17
2	D	813	GLC	C1-O5-C5	4.26	118.04	112.17
4	D	810	BGC	O5-C5-C4	4.35	117.67	109.66
2	B	807	GLC	C1-O5-C5	4.43	118.28	112.17
2	A	808	GLC	C1-O5-C5	4.63	121.75	113.39
2	D	802	GLC	C1-C2-C3	5.32	116.39	109.65
2	D	811	GLC	C1-O5-C5	5.41	119.63	112.17
2	A	804	GLC	C1-O5-C5	6.59	121.25	112.17
2	B	802	GLC	C1-O5-C5	7.00	121.81	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	GLC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	804	GLC	4	0
3	A	807	GOL	6	0
2	A	808	GLC	5	0
2	A	809	GLC	1	0
4	B	801	BGC	2	0
2	B	802	GLC	2	0
4	B	803	BGC	1	0
2	B	804	GLC	4	0
2	B	805	GLC	3	0
2	B	806	GLC	1	0
2	B	807	GLC	2	0
2	B	808	GLC	1	0
3	B	812	GOL	2	0
3	B	813	GOL	3	0
3	B	815	GOL	7	0
4	B	816	BGC	4	0
2	B	817	GLC	3	0
2	D	804	GLC	1	0
2	D	805	GLC	1	0
3	D	808	GOL	1	0
3	D	809	GOL	1	0
4	D	810	BGC	7	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	587/612 (95%)	0.28	58 (9%) 8 7	25, 48, 124, 144	1 (0%)
1	B	598/612 (97%)	-0.11	11 (1%) 69 66	21, 38, 63, 77	5 (0%)
1	C	582/612 (95%)	0.86	106 (18%) 1 1	57, 88, 123, 143	2 (0%)
1	D	588/612 (96%)	0.06	12 (2%) 65 63	35, 49, 70, 86	3 (0%)
All	All	2355/2448 (96%)	0.27	187 (7%) 13 12	21, 51, 114, 144	11 (0%)

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	360	SER	8.3
1	A	201	LEU	7.1
1	C	213	ARG	7.0
1	A	159	TRP	6.6
1	A	195	ALA	6.2
1	A	428	GLY	5.8
1	C	199	LEU	5.7
1	C	212	MET	5.7
1	C	132	MET	5.7
1	C	499	TYR	5.7
1	C	498	VAL	5.7
1	A	149	ARG	5.6
1	C	261	PHE	5.5
1	C	433	LEU	5.4
1	C	134	GLY	5.4
1	C	502	TYR	5.2
1	C	294	PHE	5.1
1	C	133	ASP	5.0
1	A	147	ALA	5.0
1	C	131	THR	5.0
1	A	196	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	145	PRO	4.8
1	A	170	LYS	4.7
1	C	258	ASP	4.7
1	C	512	LEU	4.7
1	A	199	LEU	4.6
1	A	193	ILE	4.6
1	A	175	TRP	4.5
1	C	228	VAL	4.4
1	C	196	ASN	4.4
1	A	429	GLY	4.4
1	C	257	THR	4.3
1	C	431	GLU	4.3
1	C	508	THR	4.3
1	C	374	ILE	4.3
1	C	359	HIS	4.2
1	A	150	VAL	4.2
1	D	117	THR	4.1
1	C	430	ARG	4.1
1	A	146	ASN	4.0
1	A	200	ARG	4.0
1	B	427	PHE	4.0
1	A	158	TYR	3.9
1	C	373	LEU	3.9
1	A	212	MET	3.8
1	C	159	TRP	3.8
1	A	171	GLU	3.8
1	C	543	ALA	3.8
1	C	529	VAL	3.7
1	C	214	PRO	3.7
1	A	215	GLU	3.6
1	C	260	ASN	3.6
1	C	168	LEU	3.6
1	C	341	PHE	3.6
1	C	210	ALA	3.6
1	D	371	ASN	3.6
1	C	135	VAL	3.6
1	C	530	HIS	3.6
1	C	346	PHE	3.6
1	A	153	VAL	3.6
1	C	473	GLY	3.6
1	C	703	ALA	3.5
1	A	191	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	412	TYR	3.5
1	A	194	ASP	3.3
1	C	411	ILE	3.3
1	D	258	ASP	3.3
1	D	212[A]	MET	3.3
1	A	346	PHE	3.2
1	D	429	GLY	3.2
1	C	509	PHE	3.2
1	D	728	GLU	3.1
1	B	371	ASN	3.1
1	C	256	HIS	3.1
1	C	349	ALA	3.1
1	C	355	ASN	3.1
1	D	346	PHE	3.1
1	D	430	ARG	3.1
1	B	199	LEU	3.0
1	C	198	ASN	3.0
1	C	259	ASN	3.0
1	A	118	HIS	3.0
1	A	197	GLY	3.0
1	A	117	THR	3.0
1	C	169	ARG	3.0
1	A	472	MET	3.0
1	A	380	ARG	3.0
1	C	353	GLY	2.9
1	A	148	ARG	2.9
1	A	216	THR	2.9
1	C	707	ARG	2.9
1	C	660	VAL	2.9
1	C	624	TYR	2.9
1	C	496	ASP	2.8
1	C	354	THR	2.8
1	C	203	SER	2.8
1	A	167	ARG	2.8
1	C	375	TYR	2.8
1	C	595	TRP	2.8
1	A	162	ARG	2.7
1	C	576	ARG	2.7
1	C	144	ALA	2.7
1	A	168	LEU	2.7
1	B	429	GLY	2.7
1	C	350	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	347	ALA	2.7
1	D	197	GLY	2.7
1	C	635	GLU	2.7
1	C	460	SER	2.6
1	C	542	ASP	2.6
1	C	195	ALA	2.6
1	C	547	PHE	2.6
1	A	166	MET	2.6
1	C	230	THR	2.6
1	C	708	GLN	2.6
1	C	143	TRP	2.6
1	C	200	ARG	2.6
1	A	160	ASP	2.6
1	C	540	PRO	2.6
1	C	343	THR	2.5
1	C	634	LYS	2.5
1	C	225	GLU	2.5
1	A	351	PHE	2.5
1	A	144	ALA	2.5
1	C	183	HIS	2.5
1	C	197	GLY	2.5
1	C	380	ARG	2.5
1	A	219	LEU	2.5
1	C	495	LEU	2.5
1	A	165	PRO	2.4
1	A	412	TYR	2.4
1	A	353	GLY	2.4
1	C	445	ILE	2.4
1	C	150	VAL	2.4
1	C	170	LYS	2.4
1	A	177	LEU	2.4
1	C	432	ASN	2.4
1	A	163	ARG	2.4
1	B	337	VAL	2.4
1	B	133	ASP	2.4
1	C	497	PRO	2.4
1	A	172	SER	2.4
1	A	530	HIS	2.4
1	A	192	MET	2.4
1	A	349	ALA	2.4
1	A	213	ARG	2.3
1	C	357	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	672	PRO	2.3
1	C	582	ALA	2.3
1	A	152	VAL	2.3
1	C	147	ALA	2.3
1	C	356	LEU	2.3
1	C	119	LEU	2.3
1	C	190	TYR	2.3
1	C	265	TYR	2.3
1	A	202	LYS	2.3
1	C	674	LYS	2.3
1	C	155	GLN	2.3
1	C	545	GLN	2.3
1	A	198	ASN	2.3
1	A	214	PRO	2.3
1	B	117	THR	2.3
1	C	408	ALA	2.3
1	A	187	LEU	2.2
1	C	345	ASP	2.2
1	C	464	PRO	2.2
1	C	698	HIS	2.2
1	C	262	TRP	2.2
1	A	161	GLY	2.2
1	B	200	ARG	2.2
1	C	435	ALA	2.2
1	C	313	GLY	2.2
1	C	631	VAL	2.1
1	C	544	TRP	2.1
1	D	414	ASP	2.1
1	D	334	LEU	2.1
1	D	248	VAL	2.1
1	C	434	GLU	2.1
1	B	257	THR	2.1
1	A	473	GLY	2.1
1	B	288	PRO	2.1
1	B	428	GLY	2.0
1	A	381	GLU	2.0
1	C	463	PHE	2.0
1	C	192	MET	2.0
1	C	376	ASN	2.0
1	A	155	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GLC	B	804	11/12	0.83	0.34	10.13	90,91,93,93	1
4	BGC	B	801	12/12	0.84	0.23	9.31	82,84,86,89	0
2	GLC	D	813	11/12	0.68	0.39	8.32	106,107,108,109	1
2	GLC	B	808	11/12	0.90	0.24	7.50	74,76,78,79	0
4	BGC	D	812	12/12	0.64	0.31	7.26	104,106,106,106	0
3	GOL	A	807	6/6	0.92	0.24	6.48	62,63,63,65	0
4	BGC	D	810	12/12	0.86	0.27	5.93	65,69,71,73	0
3	GOL	B	813	6/6	0.89	0.21	5.34	47,51,53,55	0
4	BGC	B	803	12/12	0.85	0.20	4.64	82,86,87,88	0
2	GLC	A	809	11/12	0.86	0.23	3.51	75,78,81,85	0
4	BGC	B	816	12/12	0.90	0.22	3.42	59,69,70,71	0
2	GLC	A	801	12/12	0.96	0.21	3.34	66,68,69,70	0
2	GLC	A	808	12/12	0.89	0.21	3.26	72,76,77,79	0
4	BGC	B	810	12/12	0.80	0.28	3.22	85,87,89,89	0
2	GLC	D	806	11/12	0.83	0.30	3.02	83,84,85,86	0
2	GLC	A	803	12/12	0.83	0.20	2.97	91,92,92,93	0
3	GOL	A	805	6/6	0.97	0.14	2.29	53,57,59,60	0
3	GOL	B	815	6/6	0.87	0.21	1.93	49,53,53,54	0
2	GLC	A	802	11/12	0.95	0.21	1.93	64,69,70,71	0
2	GLC	C	802	11/12	0.89	0.28	1.40	83,84,85,85	0
2	GLC	D	803	11/12	0.94	0.17	1.06	72,74,76,78	0
3	GOL	A	806	6/6	0.95	0.13	0.93	36,38,40,41	0
3	GOL	B	812	6/6	0.96	0.15	0.50	45,48,49,50	0
2	GLC	B	809	11/12	0.89	0.16	0.44	62,69,72,72	0
2	GLC	D	804	11/12	0.92	0.16	-0.04	64,70,71,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	B	814	6/6	0.92	0.12	-0.33	72,72,73,74	0
2	GLC	D	805	12/12	0.91	0.14	-0.81	77,79,81,81	0
3	GOL	D	808	6/6	0.92	0.12	-0.83	55,59,59,60	0
3	GOL	D	807	6/6	0.95	0.09	-1.65	50,51,52,53	0
2	GLC	D	802	11/12	0.87	0.35	-	83,91,92,93	0
2	GLC	A	804	11/12	0.84	0.23	-	90,90,91,92	0
3	GOL	D	809	6/6	0.58	0.27	-	85,86,88,89	0
2	GLC	B	817	11/12	0.85	0.32	-	69,71,73,74	0
2	GLC	B	805	11/12	0.22	0.68	-	95,96,97,97	11
2	GLC	C	801	12/12	0.91	0.28	-	84,85,86,86	0
2	GLC	D	801	12/12	0.80	0.43	-	95,98,98,99	0
2	GLC	B	802	11/12	0.72	0.31	-	86,87,88,89	0
3	GOL	B	811	6/6	0.96	0.12	-	47,49,53,55	0
2	GLC	B	807	11/12	0.64	0.34	-	83,87,89,89	4
2	GLC	B	806	11/12	0.55	0.57	-	92,94,95,95	10
2	GLC	D	811	11/12	0.86	0.32	-	68,70,71,73	0
2	GLC	A	810	11/12	0.82	0.30	-	88,90,91,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.