



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2018 – 08:21 PM EST

PDB ID : 6BYX
Title : Complex structure of LOR107 mutant (R259N) with tetrasaccharide substrate
Authors : Ulaganathan, T.; Cygler, M.
Deposited on : 2017-12-21
Resolution : 2.21 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-20030736
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-20030736

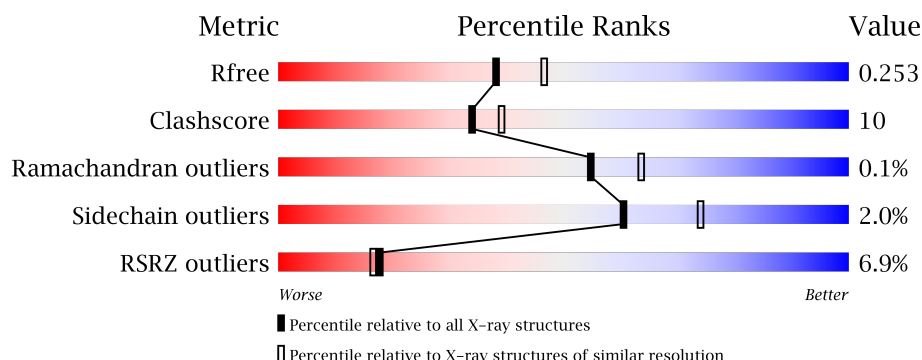
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	506	<div> <div>3%</div> <div>80%</div> <div>14%</div> <div>• 5%</div> </div>
1	B	506	<div> <div>10%</div> <div>75%</div> <div>19%</div> <div>• 5%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	611	-	-	-	X
4	GOL	A	612	-	-	-	X
4	GOL	A	613	-	-	-	X
4	GOL	A	614	-	-	-	X
5	83Y	A	615	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8285 atoms, of which 116 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 Short ulvan lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3812	2426	643	734	9			
1	B	481	Total	C	N	O	S	0	0	0
			3680	2334	622	715	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	initiating methionine	UNP A0A109PTH9
A	259	ASN	ARG	engineered mutation	UNP A0A109PTH9
A	523	LEU	-	expression tag	UNP A0A109PTH9
A	524	GLU	-	expression tag	UNP A0A109PTH9
A	525	HIS	-	expression tag	UNP A0A109PTH9
A	526	HIS	-	expression tag	UNP A0A109PTH9
A	527	HIS	-	expression tag	UNP A0A109PTH9
A	528	HIS	-	expression tag	UNP A0A109PTH9
A	529	HIS	-	expression tag	UNP A0A109PTH9
A	530	HIS	-	expression tag	UNP A0A109PTH9
B	25	MET	-	initiating methionine	UNP A0A109PTH9
B	259	ASN	ARG	engineered mutation	UNP A0A109PTH9
B	523	LEU	-	expression tag	UNP A0A109PTH9
B	524	GLU	-	expression tag	UNP A0A109PTH9
B	525	HIS	-	expression tag	UNP A0A109PTH9
B	526	HIS	-	expression tag	UNP A0A109PTH9
B	527	HIS	-	expression tag	UNP A0A109PTH9
B	528	HIS	-	expression tag	UNP A0A109PTH9
B	529	HIS	-	expression tag	UNP A0A109PTH9
B	530	HIS	-	expression tag	UNP A0A109PTH9

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Ca 2 2	0	0
2	A	2	Total Ca 2 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



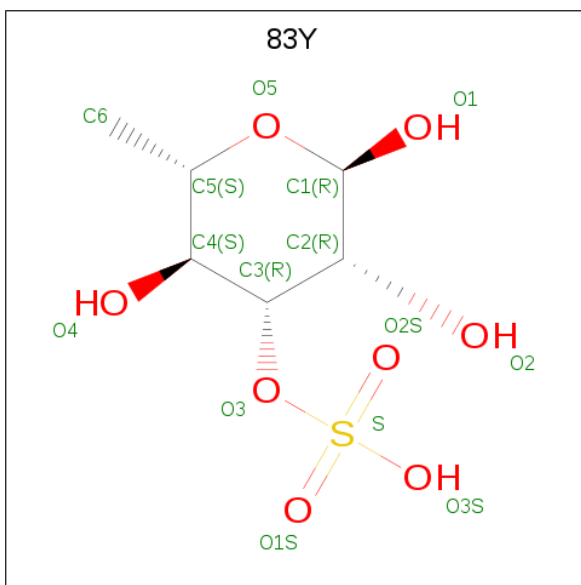
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



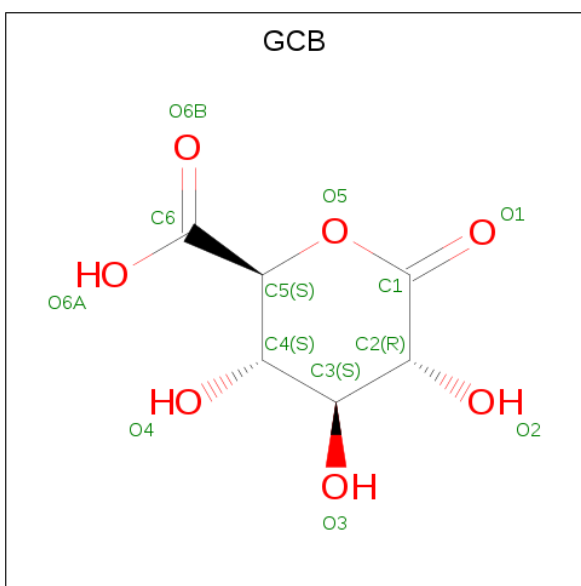
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			6	3	3			
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	O		0	0
			6	3	3			
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is 6-deoxy-3-O-sulfo- α -L-mannopyranose (three-letter code: 83Y) (formula: $C_6H_{12}O_8S$).



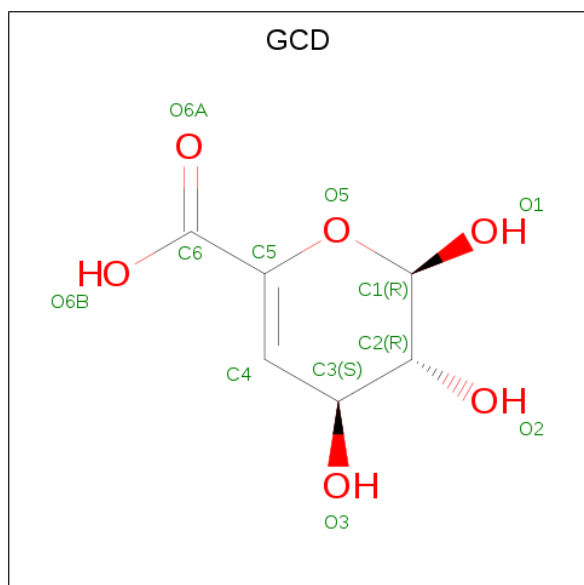
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	O	S	0	0
			23	6	9	7	1		
5	A	1	Total	C	H	O	S	0	0
			23	6	9	7	1		
5	B	1	Total	C	H	O	S	0	0
			23	6	9	7	1		
5	B	1	Total	C	H	O	S	0	0
			23	6	9	7	1		

- Molecule 6 is D-SACCHARIC ACID 1,5-LACTONE (three-letter code: GCB) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			18	6	6	6		
6	B	1	Total	C	H	O	0	0
			18	6	6	6		

- Molecule 7 is 4,5-DEHYDRO-D-GLUCURONIC ACID (three-letter code: GCD) (formula: $C_6H_8O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			18	6	6	6		
7	B	1	Total	C	H	O	0	0
			18	6	6	6		

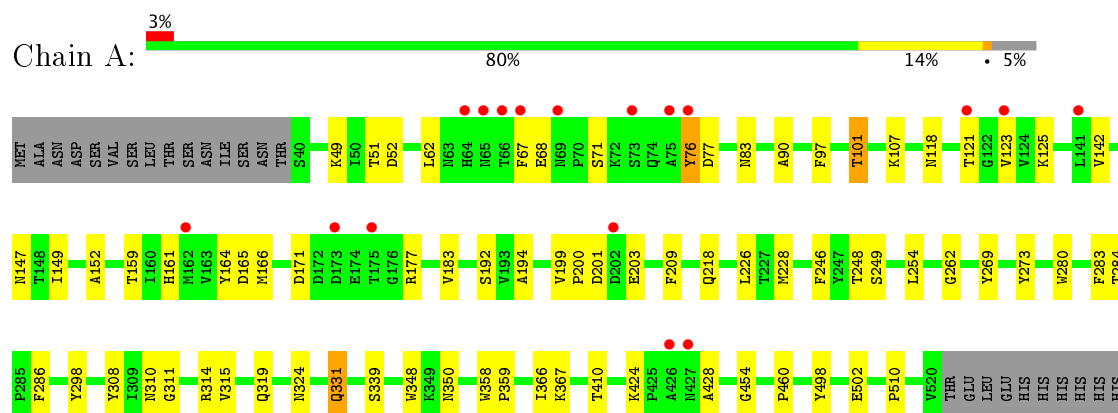
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	259	Total	O	0	0
			259	259		
8	B	206	Total	O	0	0
			206	206		

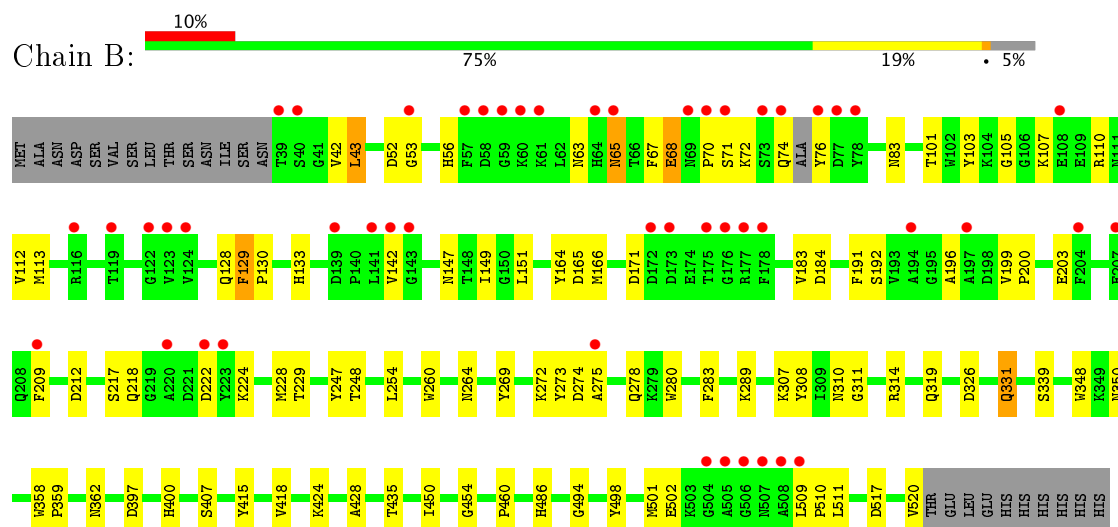
3 Residue-property plots

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: Short ulvan lyase



- Molecule 1: Short ulvan lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.05Å 120.96Å 127.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.89 – 2.21 48.89 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.89-2.21) 97.4 (48.89-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.13rc2_2981: ???)	Depositor
R, R_{free}	0.204 , 0.255 0.201 , 0.253	Depositor DCC
R_{free} test set	2014 reflections (3.18%)	DCC
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8285	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.20 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.9882e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: GOL, GCB, GCD, CA, 83Y, SO4

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	0.44	0/3923	0.59	0/5326
1	B	0.41	0/3783	0.58	0/5144
All	All	0.43	0/7706	0.59	0/10470

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	3812	0	3487	57	0
1	B	3680	0	3224	81	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	30	0	0	1	0
3	B	20	0	0	2	0
4	A	36	40	48	3	0
4	B	18	16	23	3	0
5	A	28	18	0	1	0
5	B	28	18	0	0	0
6	A	12	6	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	12	6	0	0	0
7	A	12	6	6	0	0
7	B	12	6	6	0	0
8	A	259	0	0	6	0
8	B	206	0	0	5	0
All	All	8169	116	6794	139	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 10.

All (139) 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:171:ASP:OD1	1:B:183:VAL:HA	1.77	0.84
1:A:101:THR:HG21	1:A:149:ILE:O	1.82	0.80
1:A:147:ASN:HB3	1:A:165:ASP:HA	1.66	0.77
1:B:501:MET:HE3	1:B:509:LEU:HD12	1.69	0.74
1:A:171:ASP:OD1	1:A:183:VAL:HA	1.89	0.73
1:A:199:VAL:HG22	1:A:200:PRO:HD2	1.70	0.72
1:A:199:VAL:HG22	1:A:203:GLU:HB2	1.71	0.71
1:B:147:ASN:HB3	1:B:165:ASP:HA	1.73	0.71
1:A:90:ALA:HB1	1:A:101:THR:HG22	1.73	0.70
1:A:310:ASN:HB2	1:A:314:ARG:HH21	1.59	0.66
1:A:502:GLU:HB3	1:A:510:PRO:HG2	1.81	0.63
1:A:71:SER:HB3	1:A:77:ASP:OD2	1.99	0.63
1:B:229:THR:HG22	1:B:280:TRP:O	1.99	0.62
1:A:367:LYS:HD3	4:A:610:GOL:H11	1.81	0.62
1:B:128:GLN:O	1:B:129:PHE:HD2	1.83	0.62
1:A:52:ASP:HA	1:A:510:PRO:HB3	1.82	0.62
1:B:101:THR:HG23	1:B:151:LEU:HD22	1.83	0.61
1:A:83:ASN:ND2	3:A:608:SO4:O3	2.34	0.61
1:B:192:SER:HB3	1:B:209:PHE:CE1	2.36	0.60
1:B:192:SER:HA	1:B:209:PHE:HA	1.83	0.60
1:B:310:ASN:HB2	1:B:314:ARG:HH21	1.67	0.60
1:A:76:TYR:HA	1:A:107:LYS:HD2	1.84	0.59
1:B:218:GLN:HB2	8:B:884:HOH:O	2.02	0.59
1:A:121:THR:OG1	1:A:123:VAL:HG12	2.03	0.58
1:A:339:SER:HB2	1:A:348:TRP:CE2	2.39	0.58
1:B:424:LYS:HE3	1:B:428:ALA:O	2.03	0.58
1:B:200:PRO:O	1:B:203:GLU:N	2.36	0.57
1:A:298:TYR:HE2	4:A:614:GOL:H11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ASN:ND2	4:B:609:GOL:H32	2.19	0.57
1:B:128:GLN:O	1:B:129:PHE:CD2	2.58	0.57
1:B:502:GLU:HB3	1:B:510:PRO:HG2	1.87	0.57
1:A:125:LYS:HE2	8:A:928:HOH:O	2.06	0.56
1:A:90:ALA:CB	1:A:101:THR:HG22	2.36	0.56
1:A:101:THR:HG23	1:A:149:ILE:HB	1.88	0.55
1:A:152:ALA:HB2	1:A:246:PHE:CG	2.42	0.55
1:A:49:LYS:NZ	1:A:52:ASP:OD1	2.28	0.55
1:B:128:GLN:O	1:B:129:PHE:HB2	2.06	0.55
1:B:308:TYR:CZ	1:B:311:GLY:HA2	2.41	0.55
1:B:212:ASP:HB3	1:B:222:ASP:CG	2.27	0.55
1:B:228:MET:HE1	1:B:280:TRP:CD2	2.42	0.55
1:A:51:THR:O	1:A:510:PRO:HA	2.07	0.54
1:B:191:PHE:C	1:B:209:PHE:HD1	2.10	0.54
1:B:43:LEU:HD12	1:B:517:ASP:HB3	1.89	0.54
1:A:248:THR:HG22	1:A:254:LEU:HD23	1.90	0.54
1:B:72:LYS:N	8:B:705:HOH:O	2.40	0.54
1:B:308:TYR:OH	1:B:311:GLY:HA2	2.08	0.54
1:B:184:ASP:CB	8:B:899:HOH:O	2.54	0.54
1:B:63:ASN:O	1:B:67:PHE:N	2.41	0.53
1:B:196:ALA:O	1:B:199:VAL:HG22	2.09	0.53
1:B:65:ASN:OD1	1:B:65:ASN:N	2.41	0.53
1:A:107:LYS:HE2	8:A:866:HOH:O	2.08	0.53
1:A:199:VAL:HG22	1:A:200:PRO:CD	2.37	0.52
1:B:339:SER:HB2	1:B:348:TRP:CE2	2.45	0.52
1:B:70:PRO:HB3	1:B:142:VAL:HG23	1.92	0.52
1:B:248:THR:HG22	1:B:254:LEU:HD23	1.91	0.52
1:B:418:VAL:HG21	1:B:435:THR:CG2	2.40	0.51
1:B:164:TYR:O	1:B:166:MET:HG3	2.11	0.51
1:A:118:ASN:HB3	1:A:123:VAL:HG12	1.93	0.50
1:B:199:VAL:HG21	1:B:203:GLU:O	2.11	0.50
1:A:164:TYR:O	1:A:166:MET:HG3	2.12	0.50
1:A:62:LEU:HD13	1:A:67:PHE:HA	1.94	0.50
1:B:112:VAL:O	1:B:128:GLN:O	2.29	0.50
1:B:248:THR:HG22	1:B:254:LEU:CD2	2.42	0.50
1:B:400:HIS:CE1	1:B:450:ILE:HD13	2.47	0.50
1:A:123:VAL:HG11	1:A:201:ASP:OD2	2.12	0.49
1:A:101:THR:CG2	1:A:149:ILE:HB	2.42	0.49
1:B:260:TRP:CH2	1:B:289:LYS:HD2	2.48	0.49
1:B:43:LEU:CD1	1:B:517:ASP:HB3	2.42	0.49
1:A:254:LEU:HB2	1:A:273:TYR:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:HIS:HE1	1:B:501:MET:HE1	1.78	0.48
1:A:67:PHE:CE1	1:A:68:GLU:HG3	2.49	0.48
1:B:103:TYR:CE1	1:B:149:ILE:HG13	2.49	0.47
1:B:273:TYR:CE2	1:B:275:ALA:HA	2.49	0.47
1:A:358:TRP:CD1	1:A:359:PRO:HA	2.49	0.47
1:B:43:LEU:HD12	1:B:43:LEU:O	2.15	0.47
1:B:362:ASN:HD22	4:B:607:GOL:H32	1.79	0.47
1:A:310:ASN:HB2	1:A:314:ARG:NH2	2.28	0.46
1:B:326:ASP:HA	3:B:604:SO4:O2	2.15	0.46
1:B:42:VAL:HA	1:B:517:ASP:O	2.15	0.46
1:A:218:GLN:HG3	8:A:773:HOH:O	2.15	0.46
1:B:110:ARG:HB3	1:B:133:HIS:HB3	1.96	0.46
1:B:56:HIS:ND1	1:B:501:MET:HE1	2.31	0.45
1:B:128:GLN:O	1:B:129:PHE:CB	2.64	0.45
1:B:358:TRP:HA	1:B:359:PRO:C	2.36	0.45
1:B:418:VAL:HG21	1:B:435:THR:HG21	1.97	0.45
1:B:273:TYR:HB2	1:B:280:TRP:CH2	2.52	0.45
1:B:319:GLN:O	1:B:331:GLN:HA	2.17	0.45
1:B:454:GLY:O	1:B:460:PRO:HA	2.16	0.45
1:A:308:TYR:CZ	1:A:311:GLY:HA2	2.52	0.45
1:A:319:GLN:O	1:A:331:GLN:HA	2.16	0.45
1:B:149:ILE:HG23	1:B:164:TYR:HB3	1.99	0.45
1:A:62:LEU:HD12	1:A:142:VAL:HG22	1.99	0.45
1:B:53:GLY:O	1:B:105:GLY:N	2.48	0.45
1:B:71:SER:O	1:B:107:LYS:NZ	2.42	0.45
1:B:228:MET:CB	1:B:280:TRP:HB2	2.47	0.44
1:A:269:TYR:HB3	1:A:283:PHE:HB3	1.98	0.44
1:B:407:SER:HB2	1:B:415:TYR:CD1	2.53	0.44
1:B:502:GLU:CB	1:B:510:PRO:HG2	2.48	0.44
1:B:52:ASP:HA	1:B:510:PRO:HB3	2.00	0.44
1:B:196:ALA:HA	1:B:199:VAL:HG13	1.99	0.44
1:A:199:VAL:CG2	1:A:203:GLU:HB2	2.44	0.44
1:B:74:GLN:N	8:B:722:HOH:O	2.51	0.43
1:A:350:ASN:HB3	1:A:366:ILE:HG22	2.00	0.43
1:B:501:MET:HA	1:B:511:LEU:HD23	2.00	0.43
1:A:248:THR:HG22	1:A:254:LEU:CD2	2.49	0.43
1:B:254:LEU:HB2	1:B:273:TYR:HB3	2.01	0.43
1:B:362:ASN:HD21	4:B:609:GOL:H32	1.81	0.43
1:A:358:TRP:HA	1:A:359:PRO:C	2.38	0.43
1:A:298:TYR:CE2	4:A:614:GOL:H11	2.51	0.43
1:B:68:GLU:H	1:B:68:GLU:CD	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:THR:HG22	1:A:194:ALA:HA	2.01	0.43
1:B:129:PHE:HA	1:B:130:PRO:HD3	1.89	0.43
1:A:159:THR:OG1	1:A:161:HIS:NE2	2.51	0.42
1:B:113:MET:SD	1:B:128:GLN:HG3	2.58	0.42
1:B:269:TYR:HB3	1:B:283:PHE:HB3	2.02	0.42
1:B:56:HIS:HE1	1:B:83:ASN:HD22	1.67	0.42
1:A:424:LYS:HE3	1:A:428:ALA:O	2.20	0.42
1:B:164:TYR:OH	1:B:224:LYS:HG2	2.20	0.42
1:B:70:PRO:HB3	1:B:142:VAL:CG2	2.50	0.42
1:A:262:GLY:HA2	8:A:898:HOH:O	2.20	0.41
1:B:212:ASP:O	1:B:217:SER:HB2	2.20	0.41
1:B:264:ASN:ND2	3:B:606:SO4:O3	2.48	0.41
1:B:272:LYS:HG2	1:B:273:TYR:N	2.35	0.41
1:B:274:ASP:O	1:B:278:GLN:N	2.53	0.41
1:B:350:ASN:HB2	8:B:767:HOH:O	2.20	0.41
1:A:97:PHE:O	8:A:701:HOH:O	2.22	0.41
1:B:494:GLY:HA3	1:B:520:VAL:HB	2.02	0.41
1:B:418:VAL:CG2	1:B:435:THR:HB	2.50	0.41
1:A:454:GLY:O	1:A:460:PRO:HA	2.20	0.41
1:B:56:HIS:CG	1:B:501:MET:CE	3.04	0.41
1:A:324:ASN:HA	8:A:816:HOH:O	2.21	0.41
1:A:339:SER:HB2	1:A:348:TRP:CD2	2.56	0.41
1:A:192:SER:HA	1:A:209:PHE:HA	2.03	0.40
1:B:247:TYR:CZ	1:B:307:LYS:HA	2.57	0.40
1:A:228:MET:HE1	1:A:280:TRP:CD2	2.56	0.40
5:A:615:83Y:C6	6:A:616:GCB:O5	2.69	0.40
1:A:125:LYS:HD2	1:A:125:LYS:HA	1.76	0.40
1:A:286:PHE:CZ	1:A:315:VAL:HG11	2.57	0.40
1:A:249:SER:HA	1:A:308:TYR:CE2	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	479/506 (95%)	455 (95%)	24 (5%)	0	100	100
1	B	477/506 (94%)	450 (94%)	26 (6%)	1 (0%)	51	58
All	All	956/1012 (94%)	905 (95%)	50 (5%)	1 (0%)	55	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	129	PHE

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	393/434 (91%)	385 (98%)	8 (2%)	60	74
1	B	355/434 (82%)	348 (98%)	7 (2%)	60	74
All	All	748/868 (86%)	733 (98%)	15 (2%)	60	74

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	TYR
1	A	101	THR
1	A	177	ARG
1	A	226	LEU
1	A	284	THR
1	A	331	GLN
1	A	410	THR
1	A	498	TYR
1	B	43	LEU
1	B	65	ASN
1	B	68	GLU
1	B	76	TYR
1	B	331	GLN
1	B	397	ASP
1	B	498	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	83	ASN

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](#)

Of 31 ligands modelled in this entry, 4 are monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	603	-	4,4,4	0.16	0	6,6,6	0.18	0
3	SO4	A	604	-	4,4,4	0.22	0	6,6,6	0.19	0
3	SO4	A	605	-	4,4,4	0.17	0	6,6,6	0.12	0
3	SO4	A	606	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	A	607	-	4,4,4	0.18	0	6,6,6	0.23	0
3	SO4	A	608	-	4,4,4	0.15	0	6,6,6	0.06	0
4	GOL	A	609	-	5,5,5	0.88	0	5,5,5	0.93	0
4	GOL	A	610	-	5,5,5	0.51	0	5,5,5	0.87	0
4	GOL	A	611	-	5,5,5	1.02	0	5,5,5	0.91	0
4	GOL	A	612	-	5,5,5	0.80	0	5,5,5	0.54	0
4	GOL	A	613	-	5,5,5	0.68	0	5,5,5	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	614	-	5,5,5	1.62	1 (20%)	5,5,5	1.32	1 (20%)
5	83Y	A	615	6	14,14,15	1.88	3 (21%)	15,21,23	1.78	4 (26%)
6	GCB	A	616	5	9,12,13	3.51	4 (44%)	10,17,19	3.33	3 (30%)
5	83Y	A	617	7,6	14,14,15	1.57	3 (21%)	15,21,23	1.38	2 (13%)
7	GCD	A	618	5	9,12,12	1.47	2 (22%)	10,17,17	2.58	5 (50%)
3	SO4	B	603	-	4,4,4	0.10	0	6,6,6	0.23	0
3	SO4	B	604	-	4,4,4	0.25	0	6,6,6	0.24	0
3	SO4	B	605	-	4,4,4	0.18	0	6,6,6	0.18	0
3	SO4	B	606	-	4,4,4	0.17	0	6,6,6	0.06	0
4	GOL	B	607	-	5,5,5	0.68	0	5,5,5	0.99	0
4	GOL	B	608	-	5,5,5	1.22	1 (20%)	5,5,5	1.27	1 (20%)
4	GOL	B	609	-	5,5,5	1.49	2 (40%)	5,5,5	1.21	0
5	83Y	B	610	6	14,14,15	1.82	4 (28%)	15,21,23	1.09	2 (13%)
6	GCB	B	611	5	9,12,13	3.63	5 (55%)	10,17,19	3.55	3 (30%)
5	83Y	B	612	7,6	14,14,15	1.48	3 (21%)	15,21,23	1.20	1 (6%)
7	GCD	B	613	5	9,12,12	1.46	1 (11%)	10,17,17	1.27	1 (10%)

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	SO4	A	603	-	-	0/0/0/0	0/0/0/0
3	SO4	A	604	-	-	0/0/0/0	0/0/0/0
3	SO4	A	605	-	-	0/0/0/0	0/0/0/0
3	SO4	A	606	-	-	0/0/0/0	0/0/0/0
3	SO4	A	607	-	-	0/0/0/0	0/0/0/0
3	SO4	A	608	-	-	0/0/0/0	0/0/0/0
4	GOL	A	609	-	-	0/4/4/4	0/0/0/0
4	GOL	A	610	-	-	0/4/4/4	0/0/0/0
4	GOL	A	611	-	-	0/4/4/4	0/0/0/0
4	GOL	A	612	-	-	0/4/4/4	0/0/0/0
4	GOL	A	613	-	-	0/4/4/4	0/0/0/0
4	GOL	A	614	-	-	0/4/4/4	0/0/0/0
5	83Y	A	615	6	-	0/5/21/25	0/1/1/1
6	GCB	A	616	5	-	0/0/20/24	0/1/1/1
5	83Y	A	617	7,6	-	0/5/21/25	0/1/1/1
7	GCD	A	618	5	-	0/0/20/20	0/1/1/1
3	SO4	B	603	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	604	-	-	0/0/0/0	0/0/0/0
3	SO4	B	605	-	-	0/0/0/0	0/0/0/0
3	SO4	B	606	-	-	0/0/0/0	0/0/0/0
4	GOL	B	607	-	-	0/4/4/4	0/0/0/0
4	GOL	B	608	-	-	0/4/4/4	0/0/0/0
4	GOL	B	609	-	-	0/4/4/4	0/0/0/0
5	83Y	B	610	6	-	0/5/21/25	0/1/1/1
6	GCB	B	611	5	-	0/0/20/24	0/1/1/1
5	83Y	B	612	7,6	-	0/5/21/25	0/1/1/1
7	GCD	B	613	5	-	0/0/20/20	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	615	83Y	O3-C3	-4.88	1.39	1.47
5	B	610	83Y	O3-C3	-4.18	1.40	1.47
5	A	617	83Y	O3-C3	-3.78	1.41	1.47
6	B	611	GCB	O5-C5	-3.50	1.39	1.46
5	B	612	83Y	O3-C3	-3.40	1.41	1.47
6	B	611	GCB	C3-C2	-3.26	1.49	1.52
6	A	616	GCB	O5-C5	-2.83	1.40	1.46
5	B	610	83Y	O5-C5	-2.55	1.40	1.44
5	B	610	83Y	O3-S	-2.50	1.49	1.56
5	A	617	83Y	O5-C5	-2.50	1.40	1.44
5	A	615	83Y	O5-C5	-2.43	1.40	1.44
6	B	611	GCB	C4-C3	-2.43	1.48	1.52
5	B	612	83Y	O3-S	-2.39	1.49	1.56
5	A	617	83Y	O3-S	-2.33	1.50	1.56
4	B	608	GOL	O2-C2	-2.31	1.36	1.43
5	B	610	83Y	O5-C1	-2.28	1.39	1.43
4	B	609	GOL	O2-C2	-2.21	1.36	1.43
7	A	618	GCD	C1-C2	-2.18	1.48	1.52
6	A	616	GCB	C2-C1	-2.04	1.48	1.52
5	B	612	83Y	O5-C5	-2.03	1.40	1.44
5	A	615	83Y	O3-S	-2.03	1.51	1.56
4	B	609	GOL	C1-C2	2.24	1.60	1.52
7	A	618	GCD	O5-C5	2.56	1.42	1.37
4	A	614	GOL	C1-C2	2.81	1.62	1.52
7	B	613	GCD	O5-C5	3.48	1.44	1.37
6	B	611	GCB	O5-C1	3.52	1.40	1.34
6	A	616	GCB	O5-C1	4.71	1.42	1.34
6	A	616	GCB	O1-C1	8.04	1.41	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	611	GCB	O1-C1	8.22	1.42	1.21

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	616	GCB	O5-C1-C2	-8.43	105.99	119.17
6	B	611	GCB	O5-C1-O1	-8.42	105.89	118.51
6	B	611	GCB	O5-C1-C2	-5.69	110.28	119.17
7	A	618	GCD	O2-C2-C1	-4.90	99.57	109.75
7	A	618	GCD	O5-C5-C4	-4.67	117.78	124.31
6	A	616	GCB	O1-C1-C2	-4.62	106.30	121.81
6	B	611	GCB	O1-C1-C2	-4.19	107.74	121.81
5	A	615	83Y	O5-C5-C4	-3.75	103.26	109.10
6	A	616	GCB	O5-C1-O1	-3.23	113.67	118.51
5	A	615	83Y	O2-C2-C1	-2.98	103.56	109.75
5	B	610	83Y	C1-C2-C3	-2.80	105.62	110.66
5	A	615	83Y	O3-C3-C4	-2.76	102.46	108.34
4	A	614	GOL	C3-C2-C1	-2.42	101.92	111.52
4	B	608	GOL	C3-C2-C1	-2.40	101.96	111.52
5	B	610	83Y	O5-C1-C2	-2.22	106.35	110.04
7	B	613	GCD	O5-C5-C4	-2.20	121.23	124.31
5	A	617	83Y	O2-C2-C3	2.25	114.95	109.28
7	A	618	GCD	C2-C3-C4	2.32	115.96	111.90
7	A	618	GCD	C1-C2-C3	2.46	115.09	110.65
7	A	618	GCD	O1-C1-O5	2.50	113.42	110.28
5	B	612	83Y	O3-C3-C2	2.79	110.64	106.77
5	A	615	83Y	C4-C3-C2	3.19	115.50	110.75
5	A	617	83Y	O3-C3-C2	3.49	111.62	106.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	608	SO4	1	0
4	A	610	GOL	1	0
4	A	614	GOL	2	0
5	A	615	83Y	1	0
6	A	616	GCB	1	0
3	B	604	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	606	SO4	1	0
4	B	607	GOL	1	0
4	B	609	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	481/506 (95%)	0.04	17 (3%) 44 42	26, 44, 71, 103	0
1	B	481/506 (95%)	0.49	49 (10%) 7 7	25, 52, 110, 141	0
All	All	962/1012 (95%)	0.27	66 (6%) 18 16	25, 47, 101, 141	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	PRO	6.7
1	B	506	GLY	5.3
1	B	176	GLY	5.2
1	A	69	ASN	4.9
1	B	220	ALA	4.6
1	B	73	SER	4.5
1	B	78	TYR	4.5
1	B	123	VAL	4.3
1	B	59	GLY	4.3
1	B	76	TYR	4.3
1	B	69	ASN	4.2
1	B	275	ALA	4.1
1	B	74	GLN	4.0
1	A	75	ALA	3.9
1	B	204	PHE	3.9
1	A	175	THR	3.9
1	B	178	PHE	3.9
1	B	71	SER	3.7
1	B	39	THR	3.7
1	B	53	GLY	3.6
1	B	177	ARG	3.6
1	B	142	VAL	3.6
1	B	508	ALA	3.6
1	B	60	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	141	LEU	3.5
1	B	507	ASN	3.5
1	A	426	ALA	3.4
1	A	67	PHE	3.4
1	B	139	ASP	3.4
1	B	61	LYS	3.3
1	A	73	SER	3.3
1	B	197	ALA	3.2
1	B	58	ASP	3.2
1	B	77	ASP	3.2
1	A	121	THR	3.2
1	B	505	ALA	3.1
1	B	173	ASP	2.9
1	B	108	GLU	2.9
1	B	124	VAL	2.9
1	B	222	ASP	2.8
1	A	123	VAL	2.7
1	A	64	HIS	2.7
1	A	141	LEU	2.7
1	A	202	ASP	2.6
1	B	116	ARG	2.6
1	B	509	LEU	2.6
1	B	64	HIS	2.5
1	A	65	ASN	2.5
1	A	66	THR	2.5
1	A	76	TYR	2.5
1	B	175	THR	2.4
1	A	173	ASP	2.4
1	B	504	GLY	2.4
1	B	65	ASN	2.4
1	B	40	SER	2.3
1	B	207	GLU	2.3
1	B	223	TYR	2.3
1	B	122	GLY	2.3
1	B	57	PHE	2.3
1	B	172	ASP	2.2
1	B	143	GLY	2.1
1	B	119	THR	2.1
1	A	427	ASN	2.1
1	B	209	PHE	2.0
1	B	194	ALA	2.0
1	A	162	MET	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
4	GOL	A	612	6/6	0.60	0.40	18.01	50,78,93,96	0
4	GOL	A	614	6/6	0.58	0.31	12.39	44,69,83,84	0
4	GOL	A	613	6/6	0.94	0.14	4.18	32,52,67,67	0
4	GOL	A	611	6/6	0.67	0.23	3.24	60,78,91,100	0
5	83Y	A	615	14/15	0.75	0.27	2.39	88,107,118,124	0
3	SO4	B	605	5/5	0.96	0.15	1.39	55,75,81,85	0
5	83Y	B	612	14/15	0.86	0.17	1.17	56,75,88,93	0
5	83Y	A	617	14/15	0.83	0.16	0.96	59,73,85,88	0
3	SO4	B	603	5/5	0.99	0.14	0.11	54,55,57,66	0
6	GCB	A	616	12/13	0.83	0.14	-0.08	58,69,77,79	0
3	SO4	A	607	5/5	0.98	0.10	-0.98	48,48,55,56	0
3	SO4	A	604	5/5	0.97	0.10	-1.27	62,73,75,75	0
6	GCB	B	611	12/13	0.85	0.12	-1.47	54,72,86,98	0
2	CA	B	601	1/1	0.98	0.08	-2.12	38,38,38,38	0
2	CA	B	602	1/1	0.94	0.06	-2.64	55,55,55,55	0
2	CA	A	602	1/1	0.99	0.04	-3.52	37,37,37,37	0
2	CA	A	601	1/1	0.98	0.05	-4.06	43,43,43,43	0
3	SO4	A	606	5/5	0.87	0.34	-	110,114,115,119	0
3	SO4	A	603	5/5	0.96	0.18	-	63,69,73,74	0
4	GOL	B	608	6/6	0.72	0.22	-	72,90,109,109	0
3	SO4	A	608	5/5	0.76	0.38	-	137,139,142,143	0
5	83Y	B	610	14/15	0.72	0.24	-	95,114,125,132	0
3	SO4	B	604	5/5	0.97	0.13	-	56,63,68,69	0
7	GCD	B	613	12/12	0.83	0.19	-	59,78,98,103	0
3	SO4	A	605	5/5	0.90	0.14	-	113,117,119,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	B	609	6/6	0.77	0.48	-	37,57,72,72	0
4	GOL	B	607	6/6	0.74	0.46	-	70,81,84,84	0
4	GOL	A	610	6/6	0.64	0.29	-	79,97,114,116	0
4	GOL	A	609	6/6	0.71	0.37	-	72,82,87,92	0
7	GCD	A	618	12/12	0.92	0.11	-	52,76,92,100	0
3	SO4	B	606	5/5	0.82	0.24	-	129,130,131,131	0

6.5 Other polymers [i](#)

There are no such residues in this entry.