



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:56 AM UTC

PDB ID : 3WQ7 / pdb_00003wq7
Title : New crystal form of the hyperthermophilic family 12 endo-cellulase from *Pyrococcus furiosus*
Authors : Kataoka, M.; Ishikawa, K.
Deposited on : 2014-01-23
Resolution : 1.68 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

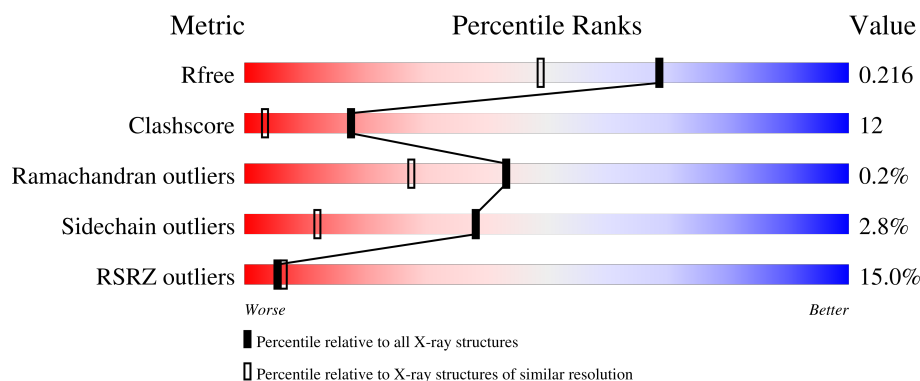
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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

Mol	Chain	Length	Quality of chain
1	A	319	
1	B	319	

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
3	GOL	A	512	-	X	-	-
3	GOL	A	516	-	X	-	-
3	GOL	B	504	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4967 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 Endoglucanase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	3	0
			2195	1427	351	415	2			
1	B	270	Total	C	N	O	S	0	3	0
			2195	1427	351	415	2			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 12 6 6	0	1
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	289	Total O 291 291	0	2
4	B	179	Total O 180 180	0	1

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	134.73Å 62.57Å 86.28Å 90.00° 95.08° 90.00°	Depositor
Resolution (Å)	43.01 – 1.68 43.01 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.01-1.68) 99.9 (43.01-1.68)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 1.68Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.181 , 0.217 0.180 , 0.216	Depositor DCC
R_{free} test set	4096 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4967	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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: CA, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.70	16/2263 (0.7%)	1.46	0/3105
1	B	1.62	18/2263 (0.8%)	1.50	22/3105 (0.7%)
All	All	1.66	34/4526 (0.8%)	1.48	22/6210 (0.4%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	288	GLY	N-CA	9.29	1.55	1.45
1	A	191	ILE	C-O	7.80	1.31	1.24
1	A	211	GLY	N-CA	7.60	1.56	1.45
1	B	149	SER	N-CA	7.22	1.55	1.45
1	B	197	GLU	N-CA	7.17	1.54	1.46
1	A	192	ASN	N-CA	6.68	1.53	1.45
1	B	155	THR	CA-C	6.58	1.61	1.52
1	B	161	ILE	C-O	6.46	1.30	1.24
1	B	195	GLU	CA-C	6.41	1.61	1.52
1	A	84	TRP	C-O	6.01	1.31	1.24
1	A	127	GLU	C-O	6.00	1.30	1.23
1	A	305	ILE	C-O	6.00	1.30	1.24
1	B	221	ILE	C-O	5.94	1.30	1.23
1	B	105	HIS	N-CA	5.93	1.53	1.46
1	B	157	PHE	N-CA	5.85	1.53	1.46
1	A	259	ILE	CA-CB	5.85	1.61	1.54
1	B	163	TYR	N-CA	5.82	1.52	1.46
1	A	311	THR	C-O	-5.75	1.19	1.25
1	B	305	ILE	N-CA	5.75	1.53	1.46
1	B	156	ASP	CA-C	5.61	1.61	1.53
1	B	227	PRO	C-O	5.59	1.29	1.23
1	B	55	ARG	N-CA	5.53	1.52	1.46
1	A	116	ARG	C-O	5.46	1.30	1.24
1	A	243	TYR	N-CA	5.41	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	PRO	C-O	5.39	1.29	1.23
1	A	209	PRO	CA-CB	5.35	1.61	1.53
1	A	65	ALA	N-CA	5.31	1.51	1.46
1	B	107	VAL	N-CA	5.29	1.53	1.46
1	B	166	GLU	CA-C	5.27	1.59	1.52
1	B	292	GLY	N-CA	5.26	1.50	1.45
1	A	128	ILE	CA-C	5.24	1.59	1.52
1	A	113	ILE	CA-CB	5.21	1.60	1.54
1	A	66	PRO	C-O	5.18	1.29	1.23
1	B	172	PRO	CA-C	5.16	1.58	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	SER	N-CA-C	-9.63	101.03	113.17
1	B	154	LEU	CA-C-N	8.18	132.32	120.71
1	B	154	LEU	C-N-CA	8.18	132.32	120.71
1	B	135	TRP	N-CA-C	7.58	122.29	112.89
1	B	241	TRP	N-CA-C	-6.79	99.37	108.74
1	B	133	LYS	CA-C-N	6.59	126.28	119.56
1	B	133	LYS	C-N-CA	6.59	126.28	119.56
1	B	155	THR	N-CA-CB	-6.37	100.21	109.83
1	B	67	ILE	N-CA-C	-6.26	98.85	107.99
1	B	131	GLY	CA-C-N	-6.18	114.47	123.00
1	B	131	GLY	C-N-CA	-6.18	114.47	123.00
1	B	318	ILE	N-CA-C	5.76	116.88	108.58
1	B	164	LYS	N-CA-C	-5.42	98.73	108.48
1	B	68	ASP	CB-CA-C	-5.30	103.85	111.70
1	B	250	THR	CA-C-N	-5.30	114.79	120.03
1	B	250	THR	C-N-CA	-5.30	114.79	120.03
1	B	155	THR	CB-CA-C	5.27	118.47	109.72
1	B	154	LEU	N-CA-C	5.20	117.96	109.59
1	B	100	THR	N-CA-C	5.20	116.75	111.14
1	B	284	ASP	N-CA-C	5.05	115.98	108.60
1	B	303	TRP	CA-CB-CG	5.03	123.16	113.60
1	B	149	SER	N-CA-C	5.00	117.28	109.52

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	2195	0	2128	23	1
1	B	2195	0	2128	77	2
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	90	0	118	13	0
3	B	12	0	14	6	0
4	A	291	0	0	11	1
4	B	180	0	0	20	0
All	All	4967	0	4388	110	2

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 12.

All (110) 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)
3:A:512:GOL:H31	4:A:889:HOH:O	1.24	1.27
1:B:149:SER:HB2	1:B:154:LEU:HD21	1.31	1.13
1:B:149:SER:CB	1:B:154:LEU:HD21	1.93	0.98
1:A:238[B]:ASN:OD1	4:A:748:HOH:O	1.91	0.88
1:A:183[A]:ARG:HD3	4:A:873:HOH:O	1.75	0.84
1:B:272:SER:OG	1:B:274:LEU:HB2	1.78	0.81
1:B:169:ASN:HA	3:B:503:GOL:H11	1.63	0.81
3:A:507:GOL:O1	4:A:868:HOH:O	2.00	0.78
3:A:512:GOL:C3	4:A:889:HOH:O	2.00	0.78
1:B:76[A]:GLU:HG3	4:B:674:HOH:O	1.83	0.77
1:B:144:PRO:O	4:B:734:HOH:O	2.02	0.76
3:A:514[A]:GOL:O3	4:A:888:HOH:O	2.04	0.76
1:B:156:ASP:O	4:B:667:HOH:O	2.04	0.75
1:B:180:TRP:C	1:B:181:LEU:HD22	2.12	0.75
1:B:88[B]:ASN:ND2	4:B:715:HOH:O	1.95	0.72
1:A:53:LYS:HG2	1:A:96:THR:HG22	1.71	0.71
1:B:76[B]:GLU:HG3	1:B:77:PHE:CD2	2.26	0.70
1:B:61:GLU:OE2	1:B:116[B]:ARG:NH1	2.25	0.69
1:B:154:LEU:HB3	4:B:773:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ALA:HA	1:B:277:TYR:CZ	2.30	0.66
1:A:183[A]:ARG:NH1	1:A:275:PRO:O	2.28	0.66
1:A:279:GLU:OE2	1:A:279:GLU:HA	1.94	0.65
1:B:73:GLY:HA3	4:B:738:HOH:O	1.98	0.64
1:B:50:LYS:HD3	1:B:100:THR:HG23	1.80	0.63
3:A:513:GOL:H32	4:B:779:HOH:O	1.98	0.63
1:B:155:THR:O	4:B:773:HOH:O	2.15	0.63
1:B:184:GLU:O	1:B:281:TYR:CD2	2.52	0.63
1:B:152:SER:HB3	1:B:278:THR:HB	1.80	0.63
1:B:76[A]:GLU:CG	4:B:674:HOH:O	2.45	0.62
1:A:183[A]:ARG:HG2	1:A:280:LEU:HD23	1.82	0.60
1:B:129:PHE:CB	1:B:286:GLU:HG2	2.32	0.60
1:B:233:GLU:O	1:B:246:PHE:HA	2.02	0.59
3:B:504:GOL:H12	4:B:718:HOH:O	2.02	0.58
1:B:150:LYS:O	1:B:154:LEU:HD23	2.02	0.57
1:B:259:ILE:O	1:B:259:ILE:HG13	2.05	0.57
1:B:129:PHE:HB3	1:B:286:GLU:HG2	1.86	0.57
3:B:504:GOL:C1	4:B:718:HOH:O	2.52	0.57
1:B:238:ASN:HB3	4:B:665:HOH:O	2.05	0.56
1:B:149:SER:HB3	1:B:154:LEU:HD21	1.83	0.56
1:B:269:ALA:HA	1:B:277:TYR:CE2	2.41	0.56
1:B:159:LEU:HD13	1:B:310:LEU:HD21	1.88	0.55
1:B:236:LYS:HA	1:B:243:TYR:O	2.08	0.54
1:B:177:ILE:HA	1:B:286:GLU:O	2.09	0.53
1:B:81:ILE:HG22	1:B:83:LEU:HG	1.91	0.53
1:B:198:VAL:HA	1:B:244:VAL:O	2.09	0.52
1:B:76[A]:GLU:CD	4:B:674:HOH:O	2.52	0.52
1:B:151:VAL:CG2	1:B:278:THR:HA	2.40	0.52
1:B:154:LEU:HD12	4:B:773:HOH:O	2.10	0.51
1:B:155:THR:HG23	4:B:773:HOH:O	2.10	0.51
1:A:158:TYR:CE1	3:A:509:GOL:H31	2.46	0.51
1:B:158:TYR:CE2	1:B:313:LEU:HD21	2.46	0.51
1:A:307:ASN:HA	3:A:504:GOL:H31	1.93	0.51
1:B:112:ASN:HD21	3:B:504:GOL:H11	1.74	0.51
1:B:153:ASN:C	1:B:154:LEU:HD22	2.36	0.51
1:B:270:ASN:OD1	1:B:270:ASN:C	2.54	0.51
1:A:118:ARG:CD	4:A:698:HOH:O	2.58	0.50
1:B:194:ASP:O	1:B:274:LEU:HG	2.11	0.50
1:B:76[B]:GLU:CG	1:B:77:PHE:CD2	2.96	0.49
3:A:516:GOL:H31	1:B:298:SER:HB3	1.93	0.49
1:B:221:ILE:CG1	1:B:228:VAL:CG2	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:516:GOL:C1	4:B:612:HOH:O	2.60	0.49
1:B:277:TYR:C	1:B:279:GLU:H	2.22	0.48
1:B:216:GLU:OE2	1:B:249:LYS:NZ	2.45	0.48
1:B:234:VAL:HG22	1:B:246:PHE:CD2	2.48	0.48
1:B:151:VAL:HB	1:B:318:ILE:HD11	1.94	0.48
1:A:308:ILE:H	3:A:504:GOL:C1	2.27	0.48
1:A:50:LYS:N	4:A:774:HOH:O	2.46	0.48
1:B:50:LYS:HD3	1:B:100:THR:CG2	2.42	0.47
1:B:53:LYS:HG2	1:B:96:THR:HG22	1.96	0.47
1:A:211:GLY:HA3	1:A:237:ALA:HB2	1.96	0.47
1:B:221:ILE:HG13	1:B:228:VAL:HG22	1.97	0.47
1:A:308:ILE:H	3:A:504:GOL:H12	1.81	0.46
1:B:187:ARG:HH22	1:B:195:GLU:CD	2.23	0.46
1:B:221:ILE:HG12	1:B:228:VAL:CG2	2.46	0.46
1:B:187:ARG:HH21	1:B:187:ARG:HG2	1.81	0.45
1:A:118:ARG:HD2	4:A:698:HOH:O	2.17	0.45
1:A:118:ARG:NH1	4:A:866:HOH:O	2.50	0.45
1:B:277:TYR:C	1:B:277:TYR:CD1	2.95	0.45
1:B:178:GLU:HB3	1:B:286:GLU:HB2	1.98	0.44
1:B:236:LYS:HE2	4:B:703:HOH:O	2.17	0.44
1:A:151:VAL:HB	1:A:318:ILE:HD12	2.00	0.44
1:B:69:LYS:HB3	1:B:76[A]:GLU:OE2	2.17	0.44
1:B:136:ASN:O	4:B:638:HOH:O	2.20	0.44
1:B:235:TRP:O	1:B:244:VAL:HA	2.17	0.44
1:B:183:ARG:HH21	1:B:194:ASP:HB2	1.83	0.44
1:B:277:TYR:C	1:B:279:GLU:N	2.76	0.44
1:B:180:TRP:O	1:B:181:LEU:HD22	2.18	0.43
1:A:69:LYS:HG2	4:A:688:HOH:O	2.18	0.43
1:B:217:ILE:HD13	1:B:267:VAL:HG21	2.00	0.43
1:B:221:ILE:HG12	1:B:228:VAL:HG23	2.01	0.42
1:B:70:ASP:OD1	1:B:72:ASP:HB3	2.20	0.42
1:B:158:TYR:CD2	1:B:313:LEU:HD21	2.54	0.42
1:B:74:ASN:HA	1:B:75:PRO:HD3	1.91	0.42
1:B:267:VAL:O	1:B:268:ALA:C	2.63	0.42
1:B:211:GLY:HA3	1:B:237:ALA:HB2	2.03	0.41
1:A:209:PRO:HA	3:A:513:GOL:H31	2.01	0.41
1:B:133:LYS:HA	1:B:134:PRO:HD2	1.88	0.41
3:B:504:GOL:H11	4:B:718:HOH:O	2.19	0.41
1:A:222:ILE:HB	1:A:258:THR:HB	2.01	0.41
1:A:313:LEU:HD23	1:A:313:LEU:HA	1.84	0.41
1:B:181:LEU:HD13	1:B:282:LEU:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:516:GOL:H11	1:B:296:THR:HG23	2.02	0.41
1:B:221:ILE:HG13	1:B:228:VAL:CG2	2.51	0.41
1:B:178:GLU:OE2	1:B:199:MET:HE3	2.21	0.40
1:B:145:ILE:HD13	1:B:312:PRO:HG3	2.01	0.40
3:B:503:GOL:C3	4:B:762:HOH:O	2.69	0.40
1:A:69:LYS:HA	1:A:69:LYS:HD2	1.95	0.40
1:A:181:LEU:HA	1:A:281:TYR:O	2.22	0.40
1:A:183[A]:ARG:NH2	1:A:194:ASP:O	2.55	0.40
1:B:66:PRO:HB2	1:B:75:PRO:HG3	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88[B]:ASN:ND2	4:A:720:HOH:O[4_555]	2.05	0.15
1:A:61[A]:GLU:OE1	1:B:168:LYS:NZ[4_555]	2.09	0.11

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	271/319 (85%)	262 (97%)	9 (3%)	0	100	100
1	B	271/319 (85%)	250 (92%)	20 (7%)	1 (0%)	30	13
All	All	542/638 (85%)	512 (94%)	29 (5%)	1 (0%)	43	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	89	ALA

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	239/284 (84%)	239 (100%)	0	100	100
1	B	239/284 (84%)	226 (95%)	13 (5%)	20	2
All	All	478/568 (84%)	465 (97%)	13 (3%)	38	13

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	68	ASP
1	B	153	ASN
1	B	154	LEU
1	B	155	THR
1	B	184	GLU
1	B	208	GLN
1	B	214	VAL
1	B	243	TYR
1	B	249	LYS
1	B	250	THR
1	B	270	ASN
1	B	274	LEU
1	B	318	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	169	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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	GOL	A	512	-	5,5,5	1.05	0	5,5,5	3.37	3 (60%)
3	GOL	B	504	-	5,5,5	1.30	1 (20%)	5,5,5	1.41	0
3	GOL	A	506	-	5,5,5	0.54	0	5,5,5	0.63	0
3	GOL	A	511	-	5,5,5	0.67	0	5,5,5	0.88	0
3	GOL	A	516	-	5,5,5	2.08	2 (40%)	5,5,5	2.94	2 (40%)
3	GOL	A	508	-	5,5,5	1.00	0	5,5,5	1.44	1 (20%)
3	GOL	A	503	-	5,5,5	0.38	0	5,5,5	0.86	0
3	GOL	A	513	-	5,5,5	0.98	0	5,5,5	1.34	1 (20%)
3	GOL	A	507	-	5,5,5	0.46	0	5,5,5	2.36	3 (60%)
3	GOL	A	509	-	5,5,5	0.52	0	5,5,5	1.23	1 (20%)
3	GOL	A	510	-	5,5,5	1.36	1 (20%)	5,5,5	1.18	0
3	GOL	A	514[A]	-	5,5,5	0.48	0	5,5,5	1.75	1 (20%)
3	GOL	A	514[B]	-	5,5,5	0.58	0	5,5,5	0.49	0
3	GOL	A	504	-	5,5,5	0.64	0	5,5,5	1.02	0
3	GOL	B	503	-	5,5,5	0.39	0	5,5,5	0.82	0
3	GOL	A	515	-	5,5,5	0.41	0	5,5,5	2.07	2 (40%)
3	GOL	A	505	-	5,5,5	0.56	0	5,5,5	2.02	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	512	-	-	3/4/4/4	-
3	GOL	B	504	-	-	2/4/4/4	-
3	GOL	A	506	-	-	1/4/4/4	-
3	GOL	A	511	-	-	0/4/4/4	-
3	GOL	A	516	-	-	4/4/4/4	-
3	GOL	A	508	-	-	4/4/4/4	-
3	GOL	A	503	-	-	2/4/4/4	-
3	GOL	A	513	-	-	3/4/4/4	-
3	GOL	A	507	-	-	2/4/4/4	-
3	GOL	A	509	-	-	2/4/4/4	-
3	GOL	A	510	-	-	4/4/4/4	-
3	GOL	A	514[A]	-	-	0/4/4/4	-
3	GOL	A	514[B]	-	-	2/4/4/4	-
3	GOL	A	504	-	-	1/4/4/4	-
3	GOL	B	503	-	-	2/4/4/4	-
3	GOL	A	515	-	-	1/4/4/4	-
3	GOL	A	505	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	516	GOL	C1-C2	-3.53	1.38	1.51
3	A	510	GOL	O2-C2	2.73	1.51	1.43
3	A	516	GOL	O3-C3	-2.52	1.31	1.42
3	B	504	GOL	O2-C2	-2.37	1.36	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	516	GOL	O1-C1-C2	-6.04	83.20	110.38
3	A	512	GOL	O2-C2-C1	-5.59	86.01	109.18
3	A	507	GOL	O3-C3-C2	-3.92	92.75	110.38
3	A	505	GOL	O2-C2-C3	-3.88	93.12	109.18
3	A	512	GOL	O2-C2-C3	-3.51	94.65	109.18
3	A	512	GOL	C3-C2-C1	3.42	124.33	111.80
3	A	515	GOL	O1-C1-C2	-3.29	95.57	110.38
3	A	514[A]	GOL	C3-C2-C1	-3.18	100.15	111.80
3	A	515	GOL	O3-C3-C2	-3.06	96.58	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	508	GOL	O1-C1-C2	2.80	122.96	110.38
3	A	516	GOL	O2-C2-C1	-2.35	99.44	109.18
3	A	507	GOL	O2-C2-C1	2.33	118.81	109.18
3	A	513	GOL	O2-C2-C3	-2.30	99.65	109.18
3	A	509	GOL	O1-C1-C2	-2.24	100.29	110.38
3	A	507	GOL	C3-C2-C1	-2.03	104.37	111.80

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	GOL	O1-C1-C2-O2
3	A	503	GOL	O1-C1-C2-C3
3	A	505	GOL	C1-C2-C3-O3
3	A	507	GOL	C1-C2-C3-O3
3	A	508	GOL	O1-C1-C2-C3
3	A	510	GOL	C1-C2-C3-O3
3	A	512	GOL	O1-C1-C2-C3
3	A	512	GOL	C1-C2-C3-O3
3	A	513	GOL	C1-C2-C3-O3
3	A	513	GOL	O2-C2-C3-O3
3	A	514[B]	GOL	C1-C2-C3-O3
3	A	516	GOL	O1-C1-C2-C3
3	A	516	GOL	C1-C2-C3-O3
3	B	503	GOL	C1-C2-C3-O3
3	A	508	GOL	O1-C1-C2-O2
3	A	516	GOL	O1-C1-C2-O2
3	A	505	GOL	O1-C1-C2-C3
3	A	508	GOL	C1-C2-C3-O3
3	A	509	GOL	C1-C2-C3-O3
3	A	510	GOL	O1-C1-C2-C3
3	B	504	GOL	C1-C2-C3-O3
3	A	505	GOL	O1-C1-C2-O2
3	A	505	GOL	O2-C2-C3-O3
3	A	512	GOL	O2-C2-C3-O3
3	A	516	GOL	O2-C2-C3-O3
3	B	503	GOL	O2-C2-C3-O3
3	A	509	GOL	O2-C2-C3-O3
3	A	514[B]	GOL	O2-C2-C3-O3
3	A	510	GOL	O2-C2-C3-O3
3	A	515	GOL	O1-C1-C2-O2
3	B	504	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	508	GOL	O2-C2-C3-O3
3	A	510	GOL	O1-C1-C2-O2
3	A	507	GOL	O2-C2-C3-O3
3	A	504	GOL	O2-C2-C3-O3
3	A	513	GOL	O1-C1-C2-O2
3	A	506	GOL	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	512	GOL	2	0
3	B	504	GOL	4	0
3	A	516	GOL	3	0
3	A	513	GOL	2	0
3	A	507	GOL	1	0
3	A	509	GOL	1	0
3	A	514[A]	GOL	1	0
3	A	504	GOL	3	0
3	B	503	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	270/319 (84%)	-0.47	4 (1%) 72 80	9, 16, 32, 68	3 (1%)
1	B	270/319 (84%)	1.20	77 (28%) 1 2	10, 33, 54, 76	3 (1%)
All	All	540/638 (84%)	0.37	81 (15%) 5 6	9, 21, 50, 76	6 (1%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	TRP	5.6
1	B	277	TYR	5.2
1	B	181	LEU	4.8
1	B	267	VAL	4.7
1	B	157	PHE	4.5
1	B	316	PRO	4.2
1	B	155	THR	4.2
1	B	182	THR	3.9
1	A	71	GLY	3.8
1	B	280	LEU	3.8
1	B	151	VAL	3.7
1	B	146	PRO	3.7
1	B	154	LEU	3.7
1	B	180	TRP	3.6
1	B	281	TYR	3.6
1	B	185	ALA	3.5
1	B	189	THR	3.5
1	B	188	THR	3.4
1	B	278	THR	3.4
1	B	274	LEU	3.2
1	B	214	VAL	3.2
1	B	130	TYR	3.2
1	B	269	ALA	3.2
1	B	158	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	50	LYS	3.1
1	B	285	VAL	3.1
1	B	268	ALA	3.1
1	A	278	THR	3.0
1	B	271	ILE	3.0
1	B	282	LEU	3.0
1	B	275	PRO	3.0
1	B	218	VAL	2.9
1	B	99	LEU	2.9
1	B	148	PRO	2.9
1	B	147	LEU	2.9
1	B	139	TYR	2.8
1	B	187	ARG	2.8
1	B	265	ILE	2.8
1	B	318	ILE	2.8
1	B	149	SER	2.7
1	B	319	SER	2.7
1	B	317	LEU	2.6
1	B	100	THR	2.6
1	B	69	LYS	2.5
1	B	159	LEU	2.5
1	B	76[A]	GLU	2.5
1	B	192	ASN	2.5
1	B	191	ILE	2.5
1	B	312	PRO	2.5
1	B	190	GLY	2.5
1	B	270	ASN	2.5
1	A	50	LYS	2.5
1	B	184	GLU	2.5
1	B	266	SER	2.5
1	B	75	PRO	2.4
1	B	264	PHE	2.4
1	B	137	ALA	2.4
1	B	261	TYR	2.4
1	B	198	VAL	2.4
1	B	307	ASN	2.4
1	B	217	ILE	2.4
1	B	228	VAL	2.3
1	B	71	GLY	2.3
1	B	141	THR	2.3
1	B	145	ILE	2.3
1	B	144	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	313	LEU	2.2
1	B	276	ASN	2.2
1	B	284	ASP	2.1
1	B	102	GLY	2.1
1	B	310	LEU	2.1
1	A	70	ASP	2.1
1	B	68	ASP	2.1
1	B	152	SER	2.1
1	B	194	ASP	2.1
1	B	221	ILE	2.1
1	B	227	PRO	2.1
1	B	153	ASN	2.0
1	B	263	ALA	2.0
1	B	193	SER	2.0
1	B	309	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	508	6/6	0.71	0.22	25,34,36,37	6
3	GOL	A	503	6/6	0.82	0.22	52,55,58,60	0
3	GOL	A	506	6/6	0.86	0.18	32,37,46,47	6
3	GOL	A	504	6/6	0.86	0.16	38,44,46,51	0
3	GOL	A	507	6/6	0.87	0.17	24,33,36,42	6
3	GOL	A	515	6/6	0.87	0.18	30,32,32,37	6
3	GOL	B	503	6/6	0.87	0.17	30,34,36,38	6
3	GOL	A	505	6/6	0.88	0.14	17,31,38,38	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	511	6/6	0.88	0.16	33,43,44,46	6
3	GOL	B	504	6/6	0.88	0.14	24,27,28,31	6
2	CA	B	501	1/1	0.90	0.11	63,63,63,63	0
3	GOL	A	510	6/6	0.91	0.14	22,34,39,43	6
3	GOL	A	509	6/6	0.92	0.12	22,42,44,52	0
3	GOL	A	516	6/6	0.94	0.10	15,23,29,29	0
3	GOL	A	512	6/6	0.95	0.10	14,25,29,30	0
3	GOL	A	513	6/6	0.95	0.09	12,29,33,34	0
3	GOL	A	514[A]	6/6	0.96	0.06	15,18,20,22	6
3	GOL	A	514[B]	6/6	0.96	0.06	19,20,24,29	6
2	CA	B	502	1/1	0.99	0.08	26,26,26,26	1
2	CA	A	502	1/1	0.99	0.06	23,23,23,23	1
2	CA	A	501	1/1	0.99	0.08	35,35,35,35	1

6.5 Other polymers [i](#)

There are no such residues in this entry.