



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:37 AM UTC

PDB ID : 3WT3 / pdb_00003wt3
Title : New crystal form of a hyperthermophilic endocellulase
Authors : Kataoka, M.; Ishikawa, K.
Deposited on : 2014-04-07
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

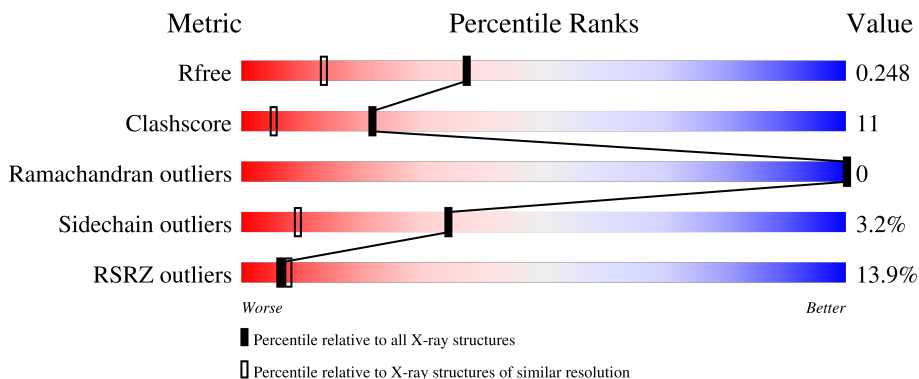
1 Overall quality at a glance

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	510	-	X	-	-
3	GOL	A	511	-	X	-	-
3	GOL	A	512	-	X	-	-
3	GOL	B	503	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5011 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.

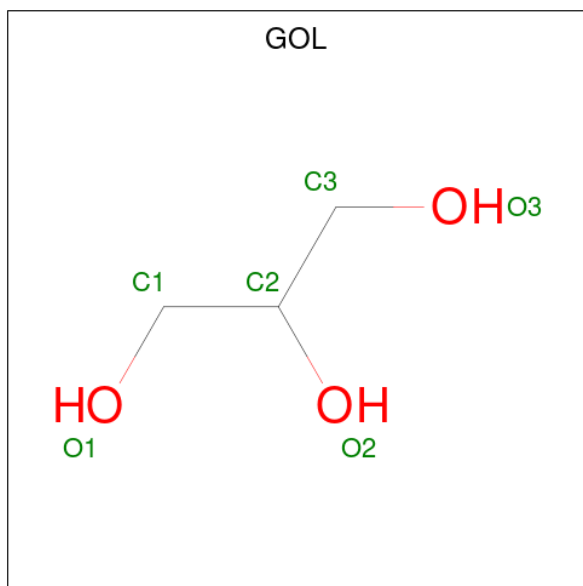
- Molecule 1 is a protein called Endoglucanase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	270	Total 2175	C 1416	N 346	O 411	S 2	0	1	0
1	B	270	Total 2228	C 1446	N 357	O 423	S 2	0	7	0

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

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

- 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	B	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
3	B	1	Total C O 6 3 3	0	0


- Molecule 4 is water.

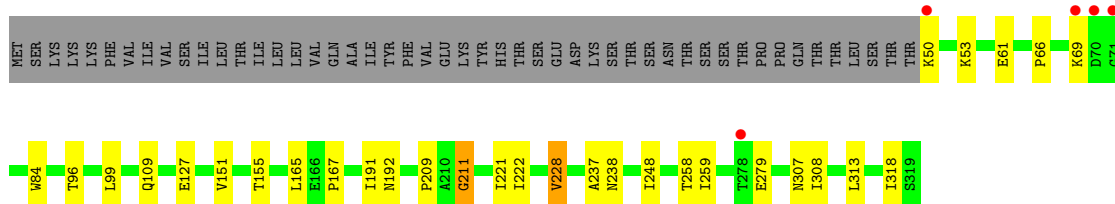
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	312	Total O 319 319	0	6
4	B	197	Total O 201 201	0	4

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

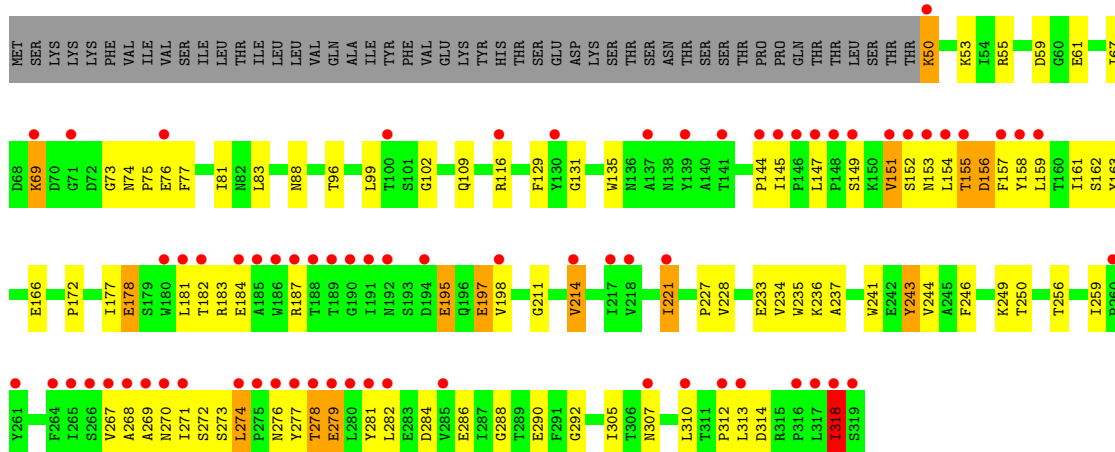
- Molecule 1: Endoglucanase A

Chain A: 



- Molecule 1: Endoglucanase A

Chain B: 



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)	99.8 (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	3.13 (at 1.68Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.181 , 0.218 (Not available) , 0.248	Depositor DCC
R_{free} test set	4096 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtrriage
Anisotropy	0.083	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5011	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage'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	1.62	11/2243 (0.5%)	1.41	0/3079
1	B	1.50	16/2296 (0.7%)	1.43	17/3149 (0.5%)
All	All	1.56	27/4539 (0.6%)	1.42	17/6228 (0.3%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	288	GLY	N-CA	8.51	1.54	1.45
1	A	211	GLY	N-CA	8.11	1.57	1.45
1	A	191	ILE	C-O	7.05	1.31	1.24
1	B	161	ILE	C-O	6.77	1.31	1.24
1	B	305	ILE	N-CA	6.53	1.54	1.46
1	B	197	GLU	N-CA	6.17	1.53	1.46
1	B	149	SER	N-CA	6.16	1.53	1.45
1	B	195	GLU	CA-C	5.92	1.61	1.53
1	A	84	TRP	C-O	5.83	1.31	1.24
1	A	192	ASN	N-CA	5.78	1.52	1.45
1	B	155	THR	CA-C	5.78	1.60	1.52
1	A	167	PRO	C-O	5.74	1.30	1.23
1	A	209	PRO	CA-CB	5.53	1.61	1.53
1	A	248	ILE	CA-CB	5.46	1.59	1.54
1	B	221	ILE	C-O	5.43	1.30	1.23
1	A	127	GLU	C-O	5.41	1.30	1.23
1	B	163	TYR	N-CA	5.41	1.52	1.46
1	B	172	PRO	CA-C	5.37	1.58	1.52
1	B	292	GLY	N-CA	5.37	1.51	1.45
1	B	157	PHE	N-CA	5.36	1.52	1.45
1	A	259	ILE	CA-CB	5.32	1.61	1.54
1	A	165	LEU	N-CA	5.23	1.52	1.46
1	A	66	PRO	C-O	5.20	1.29	1.23
1	B	166	GLU	CA-C	5.09	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	55	ARG	N-CA	5.08	1.52	1.46
1	B	156	ASP	CA-C	5.02	1.60	1.53
1	B	227	PRO	C-O	5.02	1.29	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	SER	N-CA-C	-8.98	101.85	113.17
1	B	154	LEU	CA-C-N	8.31	132.52	120.71
1	B	154	LEU	C-N-CA	8.31	132.52	120.71
1	B	135	TRP	N-CA-C	7.76	122.52	112.89
1	B	155	THR	N-CA-CB	-7.19	98.98	109.83
1	B	318	ILE	N-CA-C	6.80	118.37	108.58
1	B	154	LEU	N-CA-C	5.86	119.03	109.59
1	B	214	VAL	N-CA-C	-5.83	107.01	111.62
1	B	271	ILE	CB-CA-C	5.78	117.29	110.93
1	B	131	GLY	CA-C-N	-5.76	114.99	123.05
1	B	131	GLY	C-N-CA	-5.76	114.99	123.05
1	B	67	ILE	N-CA-C	-5.76	99.17	107.75
1	B	69	LYS	N-CA-C	5.48	116.95	111.09
1	B	278	THR	N-CA-C	-5.47	106.68	113.19
1	B	241	TRP	N-CA-C	-5.34	100.80	108.60
1	B	284	ASP	N-CA-C	5.23	116.23	108.60
1	B	178	GLU	N-CA-C	5.07	117.51	109.50

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	2175	0	2111	17	0
1	B	2228	0	2156	71	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	60	0	79	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	32	8	0
4	A	319	0	0	9	0
4	B	201	0	0	17	0
All	All	5011	0	4378	96	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (96) 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:511:GOL:H12	4:A:904:HOH:O	1.25	1.31
3:A:509:GOL:H32	4:A:902:HOH:O	1.32	1.22
1:B:88:ASN:HB2	4:B:796:HOH:O	1.58	1.02
1:B:88:ASN:CB	4:B:796:HOH:O	2.18	0.89
1:A:238[B]:ASN:OD1	4:A:752:HOH:O	1.90	0.87
1:B:50:LYS:HA	4:B:774:HOH:O	1.79	0.81
1:B:178:GLU:OE2	3:B:503:GOL:O2	1.98	0.81
1:A:308:ILE:H	3:A:504:GOL:H12	1.48	0.78
1:B:151:VAL:HG13	1:B:318:ILE:HD11	1.69	0.72
1:A:53:LYS:HG2	1:A:96:THR:HG22	1.69	0.72
1:B:144:PRO:O	4:B:777:HOH:O	2.08	0.72
1:B:272:SER:OG	1:B:274:LEU:HB2	1.91	0.70
1:B:151:VAL:CG1	1:B:318:ILE:HD11	2.22	0.69
1:B:53[A]:LYS:HE2	4:B:714:HOH:O	1.93	0.69
3:B:506:GOL:O3	4:B:796:HOH:O	2.10	0.69
3:A:511:GOL:C1	4:A:904:HOH:O	2.04	0.68
1:B:156:ASP:O	4:B:678:HOH:O	2.11	0.67
1:B:102:GLY:O	3:B:504:GOL:H12	1.94	0.67
3:A:509:GOL:O1	3:A:510:GOL:O1	2.13	0.66
1:B:181:LEU:HD13	1:B:282:LEU:HA	1.77	0.65
1:B:76[B]:GLU:HG3	1:B:77:PHE:CD2	2.32	0.64
1:B:183:ARG:O	1:B:281:TYR:HD2	1.80	0.64
1:B:151:VAL:HG13	1:B:318:ILE:CD1	2.29	0.62
1:B:183:ARG:O	1:B:281:TYR:CD2	2.52	0.62
1:B:53[B]:LYS:NZ	4:B:710:HOH:O	2.09	0.62
1:B:129:PHE:CB	1:B:286:GLU:HG2	2.30	0.61
1:B:61:GLU:OE1	1:B:116[B]:ARG:NH2	2.33	0.61
1:B:187:ARG:HH12	1:B:195:GLU:CD	2.07	0.61
1:B:276:ASN:N	4:B:793:HOH:O	2.35	0.60
1:B:307[B]:ASN:HA	3:B:504:GOL:H11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LEU:HD13	1:B:310:LEU:HD21	1.85	0.58
1:B:73:GLY:HA3	4:B:776:HOH:O	2.04	0.58
1:B:147:LEU:HD22	1:B:282:LEU:O	2.03	0.58
1:B:277:TYR:C	1:B:279:GLU:H	2.13	0.57
1:B:236:LYS:HE2	4:B:772:HOH:O	2.04	0.57
1:B:53[B]:LYS:HG2	1:B:96:THR:HG22	1.89	0.55
1:B:259:ILE:O	1:B:259:ILE:HG13	2.05	0.55
1:A:279:GLU:HA	1:A:279:GLU:OE1	2.06	0.55
1:B:233:GLU:O	1:B:246:PHE:HA	2.05	0.55
1:B:221:ILE:CG1	1:B:228:VAL:CG2	2.85	0.55
1:B:158:TYR:CE2	1:B:313:LEU:HD21	2.42	0.55
1:B:277:TYR:C	1:B:279:GLU:N	2.66	0.54
1:B:162:SER:HB2	1:B:307[A]:ASN:HB3	1.88	0.54
1:B:129:PHE:HB3	1:B:286:GLU:HG2	1.90	0.54
1:B:151:VAL:HG13	1:B:318:ILE:CG1	2.38	0.54
1:B:290:GLU:OE2	3:B:503:GOL:H2	2.08	0.53
1:B:109[A]:GLN:HG2	4:B:698:HOH:O	2.09	0.52
3:A:505:GOL:H11	4:A:802[A]:HOH:O	2.10	0.52
1:B:81:ILE:HG22	1:B:83:LEU:HG	1.91	0.51
1:B:221:ILE:HG12	1:B:228:VAL:HG23	1.93	0.50
1:B:269:ALA:HA	1:B:277:TYR:CZ	2.47	0.50
1:B:221:ILE:HG13	1:B:228:VAL:HG22	1.94	0.50
1:A:308:ILE:H	3:A:504:GOL:C1	2.21	0.49
1:B:221:ILE:HG13	1:B:228:VAL:CG2	2.43	0.49
1:B:152:SER:HB3	1:B:278:THR:HB	1.95	0.48
1:B:236:LYS:HA	1:B:243:TYR:O	2.12	0.48
1:A:211:GLY:HA3	1:A:237:ALA:HB2	1.95	0.48
1:B:234:VAL:HG22	1:B:246:PHE:CD2	2.49	0.48
1:B:277:TYR:C	1:B:277:TYR:CD1	2.92	0.47
1:B:211:GLY:HA3	1:B:237:ALA:HB2	1.96	0.47
1:A:53:LYS:HE3	4:A:879:HOH:O	2.15	0.47
1:B:197:GLU:OE2	3:B:503:GOL:H12	2.15	0.47
3:A:508:GOL:H12	4:A:651:HOH:O	2.16	0.46
1:B:221:ILE:HG12	1:B:228:VAL:CG2	2.45	0.46
1:B:145:ILE:HD13	1:B:312:PRO:HG3	1.96	0.46
1:B:151:VAL:HG13	1:B:318:ILE:HG13	1.97	0.46
1:B:177:ILE:HA	1:B:286:GLU:O	2.16	0.46
1:B:314:ASP:N	4:B:781[A]:HOH:O	2.43	0.46
1:B:50:LYS:HD2	1:B:99:LEU:HD22	1.97	0.46
1:B:88:ASN:HB3	4:B:796:HOH:O	2.00	0.46
3:B:505:GOL:H11	4:B:747:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLU:CD	4:A:893:HOH:O	2.60	0.45
1:A:109:GLN:HG2	4:A:877:HOH:O	2.16	0.45
1:A:222:ILE:HD11	3:A:507:GOL:H11	1.98	0.45
1:B:59:ASP:OD2	4:B:715:HOH:O	2.21	0.45
1:B:198:VAL:HA	1:B:244:VAL:O	2.17	0.44
1:B:187:ARG:HG2	1:B:187:ARG:HH11	1.82	0.44
1:B:182[A]:THR:HG23	1:B:184:GLU:O	2.17	0.44
1:A:155:THR:OG1	1:A:313:LEU:O	2.36	0.43
1:A:221:ILE:HG13	1:A:228:VAL:HG13	1.99	0.43
1:B:187:ARG:NH1	1:B:195:GLU:OE1	2.38	0.43
1:B:267:VAL:O	1:B:268:ALA:C	2.61	0.42
1:B:235:TRP:O	1:B:244:VAL:HA	2.19	0.42
1:A:238[B]:ASN:OD1	1:A:238[B]:ASN:C	2.62	0.42
1:A:307:ASN:HA	3:A:504:GOL:H31	2.01	0.42
1:B:76[B]:GLU:CG	1:B:77:PHE:CD2	3.01	0.42
1:B:102:GLY:O	3:B:504:GOL:C1	2.64	0.42
1:B:310:LEU:HA	1:B:310:LEU:HD23	1.70	0.42
1:B:182[A]:THR:CG2	1:B:184:GLU:O	2.68	0.42
1:B:162:SER:OG	1:B:256:THR:HG23	2.21	0.41
1:A:151:VAL:HB	1:A:318:ILE:HD12	2.02	0.41
1:B:50:LYS:HG2	4:B:774:HOH:O	2.21	0.41
1:B:74:ASN:HA	1:B:75:PRO:HD3	1.86	0.41
1:A:222:ILE:HB	1:A:258:THR:HB	2.02	0.40
1:A:69:LYS:CE	1:A:99:LEU:O	2.69	0.40
1:B:129:PHE:HB2	1:B:286:GLU:HG2	2.03	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	269/319 (84%)	261 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	275/319 (86%)	261 (95%)	14 (5%)	0	100	100
All	All	544/638 (85%)	522 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	237/284 (84%)	235 (99%)	2 (1%)	73	59
1	B	243/284 (86%)	230 (95%)	13 (5%)	20	2
All	All	480/568 (84%)	465 (97%)	15 (3%)	34	10

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

Mol	Chain	Res	Type
1	A	50	LYS
1	A	228	VAL
1	B	50	LYS
1	B	69	LYS
1	B	151	VAL
1	B	153	ASN
1	B	155	THR
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	279	GLU
1	B	318	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	B	504	-	5,5,5	0.44	0	5,5,5	0.79	0
3	GOL	A	508	-	5,5,5	0.78	0	5,5,5	1.11	0
3	GOL	A	512	-	5,5,5	1.69	1 (20%)	5,5,5	3.04	3 (60%)
3	GOL	B	503	-	5,5,5	0.56	0	5,5,5	1.76	2 (40%)
3	GOL	B	506	-	5,5,5	0.62	0	5,5,5	0.98	0
3	GOL	A	507	-	5,5,5	0.51	0	5,5,5	1.06	1 (20%)
3	GOL	A	504	-	5,5,5	0.58	0	5,5,5	0.99	0
3	GOL	A	506	-	5,5,5	0.47	0	5,5,5	1.78	2 (40%)
3	GOL	A	510	-	5,5,5	1.21	0	5,5,5	2.13	3 (60%)
3	GOL	A	503	-	5,5,5	2.14	2 (40%)	5,5,5	1.37	1 (20%)
3	GOL	A	505	-	5,5,5	1.12	0	5,5,5	1.47	1 (20%)
3	GOL	A	509	-	5,5,5	0.91	0	5,5,5	1.30	1 (20%)
3	GOL	B	505	-	5,5,5	0.66	0	5,5,5	1.20	0
3	GOL	A	511	-	5,5,5	0.96	0	5,5,5	3.53	3 (60%)

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	B	504	-	-	2/4/4/4	-
3	GOL	A	508	-	-	2/4/4/4	-
3	GOL	A	512	-	-	4/4/4/4	-
3	GOL	B	503	-	-	4/4/4/4	-
3	GOL	B	506	-	-	2/4/4/4	-
3	GOL	A	507	-	-	0/4/4/4	-
3	GOL	A	504	-	-	2/4/4/4	-
3	GOL	A	506	-	-	1/4/4/4	-
3	GOL	A	510	-	-	4/4/4/4	-
3	GOL	A	503	-	-	2/4/4/4	-
3	GOL	A	505	-	-	2/4/4/4	-
3	GOL	A	509	-	-	0/4/4/4	-
3	GOL	B	505	-	-	4/4/4/4	-
3	GOL	A	511	-	-	3/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	GOL	O1-C1	3.40	1.56	1.42
3	A	512	GOL	C1-C2	-3.06	1.40	1.51
3	A	503	GOL	O3-C3	2.38	1.52	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	511	GOL	O2-C2-C3	-5.93	84.62	109.18
3	A	512	GOL	O1-C1-C2	-5.25	86.74	110.38
3	A	511	GOL	O2-C2-C1	-3.91	93.00	109.18
3	A	512	GOL	O3-C3-C2	-3.60	94.15	110.38
3	A	511	GOL	C3-C2-C1	3.26	123.74	111.80
3	A	510	GOL	O2-C2-C3	-3.07	96.48	109.18
3	A	505	GOL	C3-C2-C1	-3.02	100.74	111.80
3	A	506	GOL	O1-C1-C2	-2.99	96.93	110.38
3	B	503	GOL	O3-C3-C2	-2.82	97.69	110.38
3	A	510	GOL	C3-C2-C1	2.65	121.52	111.80
3	B	503	GOL	O2-C2-C1	2.38	119.03	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	509	GOL	C3-C2-C1	-2.37	103.11	111.80
3	A	503	GOL	C3-C2-C1	2.35	120.41	111.80
3	A	510	GOL	O1-C1-C2	-2.28	100.09	110.38
3	A	506	GOL	O3-C3-C2	-2.21	100.41	110.38
3	A	507	GOL	O1-C1-C2	-2.17	100.60	110.38
3	A	512	GOL	O2-C2-C1	-2.11	100.43	109.18

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	GOL	C1-C2-C3-O3
3	A	505	GOL	O1-C1-C2-C3
3	A	508	GOL	O1-C1-C2-C3
3	A	510	GOL	C1-C2-C3-O3
3	A	511	GOL	O1-C1-C2-C3
3	A	511	GOL	C1-C2-C3-O3
3	A	512	GOL	O1-C1-C2-O2
3	A	512	GOL	O1-C1-C2-C3
3	A	512	GOL	C1-C2-C3-O3
3	A	512	GOL	O2-C2-C3-O3
3	B	503	GOL	O1-C1-C2-O2
3	B	503	GOL	O1-C1-C2-C3
3	B	503	GOL	C1-C2-C3-O3
3	B	503	GOL	O2-C2-C3-O3
3	B	504	GOL	C1-C2-C3-O3
3	B	505	GOL	C1-C2-C3-O3
3	A	503	GOL	O1-C1-C2-C3
3	A	510	GOL	O1-C1-C2-C3
3	B	506	GOL	O1-C1-C2-C3
3	A	505	GOL	O1-C1-C2-O2
3	A	508	GOL	O1-C1-C2-O2
3	A	510	GOL	O1-C1-C2-O2
3	A	510	GOL	O2-C2-C3-O3
3	B	504	GOL	O2-C2-C3-O3
3	A	511	GOL	O1-C1-C2-O2
3	B	505	GOL	O2-C2-C3-O3
3	B	506	GOL	O1-C1-C2-O2
3	A	504	GOL	O2-C2-C3-O3
3	A	506	GOL	O1-C1-C2-O2
3	B	505	GOL	O1-C1-C2-C3
3	A	503	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	505	GOL	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	504	GOL	3	0
3	A	508	GOL	1	0
3	B	503	GOL	3	0
3	B	506	GOL	1	0
3	A	507	GOL	1	0
3	A	504	GOL	3	0
3	A	510	GOL	1	0
3	A	505	GOL	1	0
3	A	509	GOL	2	0
3	B	505	GOL	1	0
3	A	511	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%)	-0.45	5 (1%) 66 74	9, 16, 32, 69	1 (0%)
1	B	270/319 (84%)	1.18	70 (25%) 1 2	8, 32, 55, 77	7 (2%)
All	All	540/638 (84%)	0.36	75 (13%) 6 8	8, 21, 51, 77	8 (1%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	TRP	5.5
1	B	182[A]	THR	5.5
1	B	277	TYR	5.2
1	B	157	PHE	4.5
1	B	155	THR	4.4
1	B	267	VAL	4.2
1	B	185	ALA	4.0
1	B	281	TYR	4.0
1	B	316	PRO	3.9
1	B	280	LEU	3.8
1	B	319	SER	3.7
1	B	151	VAL	3.7
1	B	146	PRO	3.6
1	B	278	THR	3.6
1	B	154	LEU	3.6
1	B	181	LEU	3.6
1	B	180	TRP	3.4
1	B	269	ALA	3.4
1	A	71	GLY	3.3
1	B	274	LEU	3.3
1	B	189	THR	3.3
1	B	188	THR	3.2
1	B	130	TYR	3.1
1	B	270	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	214	VAL	3.1
1	B	285	VAL	3.0
1	B	282	LEU	3.0
1	B	317	LEU	3.0
1	A	278	THR	2.9
1	B	158	TYR	2.9
1	B	187	ARG	2.8
1	B	69	LYS	2.8
1	B	271	ILE	2.8
1	B	318	ILE	2.8
1	B	152	SER	2.8
1	B	268	ALA	2.8
1	B	100	THR	2.7
1	B	266	SER	2.7
1	B	275	PRO	2.7
1	B	312	PRO	2.6
1	B	198	VAL	2.6
1	B	265	ILE	2.6
1	B	149	SER	2.6
1	B	148	PRO	2.6
1	B	307[A]	ASN	2.6
1	B	141	THR	2.5
1	B	139	TYR	2.5
1	B	192	ASN	2.5
1	A	50	LYS	2.5
1	B	50	LYS	2.4
1	A	70	ASP	2.4
1	B	261	TYR	2.4
1	B	218	VAL	2.4
1	B	147	LEU	2.4
1	B	71	GLY	2.3
1	B	264	PHE	2.3
1	B	191	ILE	2.3
1	B	116[A]	ARG	2.3
1	B	217	ILE	2.3
1	B	144	PRO	2.3
1	B	159	LEU	2.3
1	B	194	ASP	2.2
1	B	76[A]	GLU	2.1
1	B	184	GLU	2.1
1	B	190	GLY	2.1
1	B	260	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	153	ASN	2.1
1	B	137	ALA	2.1
1	B	279	GLU	2.1
1	B	310	LEU	2.1
1	B	145	ILE	2.1
1	B	276	ASN	2.0
1	B	313	LEU	2.0
1	B	221	ILE	2.0
1	A	69	LYS	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
2	CA	B	502	1/1	0.80	0.17	64,64,64,64	0
3	GOL	A	508	6/6	0.83	0.17	39,51,57,61	0
3	GOL	B	504	6/6	0.83	0.18	42,44,47,48	6
3	GOL	A	503	6/6	0.84	0.19	23,34,43,45	0
3	GOL	B	503	6/6	0.86	0.15	28,42,47,56	0
3	GOL	A	506	6/6	0.87	0.15	40,45,47,49	0
3	GOL	A	504	6/6	0.87	0.16	40,48,49,57	0
3	GOL	B	506	6/6	0.87	0.14	40,43,51,60	0
3	GOL	A	510	6/6	0.88	0.14	20,25,28,28	6
3	GOL	B	505	6/6	0.89	0.14	30,30,37,43	6
3	GOL	A	505	6/6	0.89	0.14	21,36,46,49	0
3	GOL	A	511	6/6	0.93	0.11	10,21,22,25	6
3	GOL	A	507	6/6	0.94	0.10	23,39,44,51	0
3	GOL	A	512	6/6	0.94	0.12	13,20,27,31	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	A	509	6/6	0.96	0.10	10,26,29,30	6
2	CA	B	501	1/1	0.96	0.07	52,52,52,52	1
2	CA	A	501	1/1	0.98	0.10	34,34,34,34	1
2	CA	A	502	1/1	0.99	0.09	21,21,21,21	1

6.5 Other polymers [i](#)

There are no such residues in this entry.