



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:12 AM UTC

PDB ID : 4DM2 / pdb_00004dm2
Title : Contribution of disulfide bond toward thermostability in hyperthermostable endocellulase
Authors : Kim, H.-W.; Ishikawa, K.
Deposited on : 2012-02-06
Resolution : 1.95 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

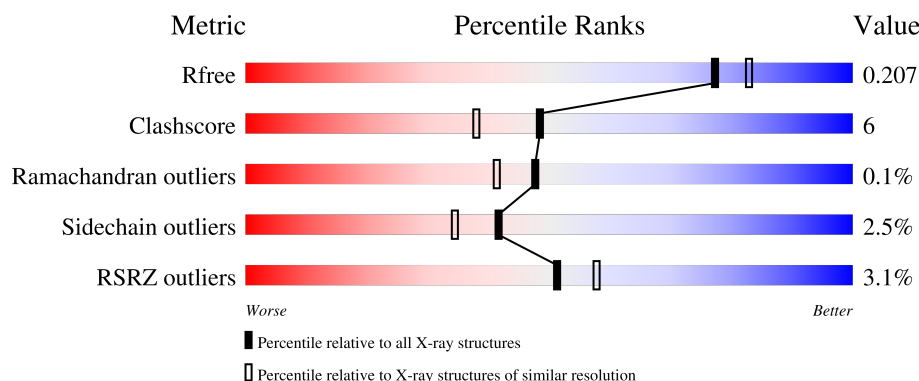
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

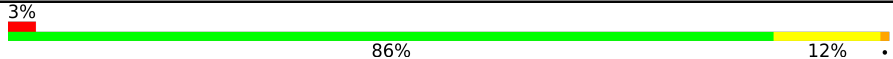
The reported resolution of this entry is 1.95 Å.

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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	377	
1	B	377	
1	C	377	

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
2	GOL	B	502	-	X	X	-
2	GOL	B	503	-	-	X	-
2	GOL	B	505	-	X	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9570 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 458aa long hypothetical endo-1,4-beta-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			3067	2000	500	556	11			
1	B	377	Total	C	N	O	S	0	0	0
			3067	2000	500	556	11			
1	C	377	Total	C	N	O	S	0	0	0
			3067	2000	500	556	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	CYS	PRO	conflict	UNP O58925
A	289	LYS	ARG	conflict	UNP O58925
B	74	CYS	PRO	conflict	UNP O58925
B	289	LYS	ARG	conflict	UNP O58925
C	74	CYS	PRO	conflict	UNP O58925
C	289	LYS	ARG	conflict	UNP O58925

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

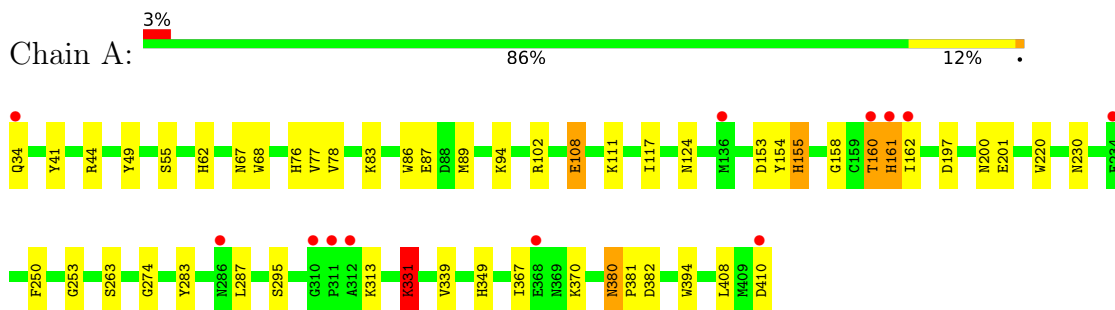
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	116	Total	O	0	0
			116	116		
3	B	111	Total	O	0	0
			111	111		
3	C	106	Total	O	0	0
			106	106		

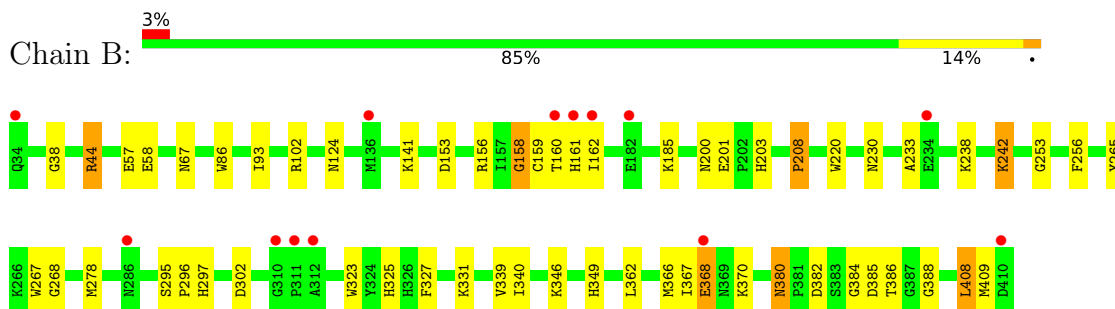
3 Residue-property plots [i](#)

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.

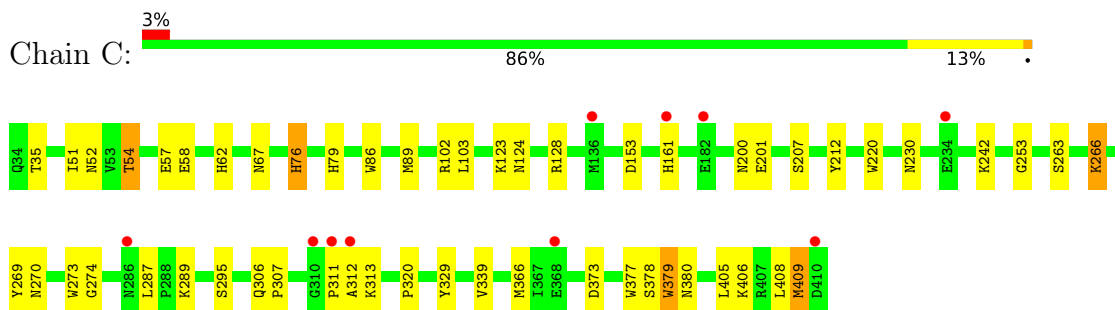
- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase



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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.24Å 58.67Å 138.54Å 90.00° 108.93° 90.00°	Depositor
Resolution (Å)	34.53 – 1.95 34.53 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.9 (34.53-1.95) 99.2 (34.53-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.39 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.166 , 0.207 0.166 , 0.207	Depositor DCC
R_{free} test set	4453 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9570	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
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	1.48	13/3177 (0.4%)	1.19	9/4336 (0.2%)
1	B	1.48	16/3177 (0.5%)	1.22	10/4336 (0.2%)
1	C	1.40	8/3177 (0.3%)	1.13	4/4336 (0.1%)
All	All	1.45	37/9531 (0.4%)	1.18	23/13008 (0.2%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	201	GLU	CA-CB	7.26	1.57	1.52
1	B	93	ILE	N-CA	7.08	1.54	1.46
1	C	76	HIS	ND1-CE1	6.80	1.39	1.32
1	C	379	TRP	C-O	6.77	1.31	1.24
1	A	201	GLU	CA-CB	6.75	1.57	1.52
1	C	287	LEU	N-CA	6.64	1.51	1.45
1	B	162	ILE	CA-CB	6.56	1.60	1.53
1	B	159	CYS	C-O	-6.38	1.15	1.24
1	A	287	LEU	N-CA	6.37	1.51	1.45
1	B	325	HIS	ND1-CE1	6.17	1.38	1.32
1	A	160	THR	CA-C	6.15	1.60	1.52
1	B	388	GLY	N-CA	6.09	1.52	1.44
1	B	349	HIS	CG-CD2	5.97	1.42	1.35
1	B	158	GLY	N-CA	5.77	1.50	1.44
1	C	161	HIS	CG-CD2	5.77	1.42	1.35
1	A	158	GLY	C-O	-5.74	1.16	1.23
1	B	233	ALA	C-O	5.72	1.30	1.24
1	A	41	TYR	C-O	5.58	1.30	1.23
1	A	155	HIS	CG-CD2	5.55	1.42	1.35
1	B	253	GLY	C-O	5.54	1.29	1.23
1	C	79	HIS	CG-CD2	5.51	1.42	1.35
1	C	329	TYR	N-CA	5.44	1.53	1.46
1	A	108	GLU	CD-OE2	5.42	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	103	LEU	C-O	-5.39	1.19	1.24
1	A	162	ILE	CA-CB	5.34	1.61	1.54
1	B	203	HIS	CG-CD2	5.33	1.41	1.35
1	C	161	HIS	ND1-CE1	5.32	1.37	1.32
1	B	38	GLY	CA-C	5.27	1.59	1.51
1	A	161	HIS	CG-CD2	5.26	1.41	1.35
1	B	208	PRO	CA-C	5.24	1.55	1.52
1	B	325	HIS	CG-CD2	5.17	1.41	1.35
1	A	62	HIS	CG-CD2	5.08	1.41	1.35
1	A	349	HIS	CE1-NE2	5.05	1.37	1.32
1	B	296	PRO	CA-C	5.05	1.58	1.52
1	A	154	TYR	N-CA	5.04	1.53	1.46
1	A	161	HIS	N-CA	5.03	1.52	1.46
1	B	161	HIS	CG-CD2	5.00	1.41	1.35

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	ARG	NE-CZ-NH1	-8.29	113.21	121.50
1	B	160	THR	N-CA-C	6.66	122.07	113.88
1	B	44	ARG	NE-CZ-NH2	6.43	124.99	119.20
1	A	160	THR	N-CA-C	6.34	121.04	113.12
1	C	212	TYR	N-CA-C	6.31	119.14	111.82
1	B	409	MET	CA-C-N	6.16	132.80	121.70
1	B	409	MET	C-N-CA	6.16	132.80	121.70
1	A	331	LYS	CD-CE-NZ	6.14	131.55	111.90
1	A	263	SER	CA-CB-OG	-5.84	99.42	111.10
1	C	409	MET	CA-C-N	5.75	132.05	121.70
1	C	409	MET	C-N-CA	5.75	132.05	121.70
1	A	380	ASN	CB-CA-C	-5.73	100.47	109.52
1	A	55	SER	N-CA-C	-5.67	105.86	112.89
1	C	380	ASN	CB-CA-C	-5.57	100.43	109.56
1	B	368	GLU	CB-CA-C	-5.44	101.75	110.79
1	B	327	PHE	CA-C-N	-5.40	113.37	120.22
1	B	327	PHE	C-N-CA	-5.40	113.37	120.22
1	B	380	ASN	CB-CA-C	-5.35	101.07	109.52
1	B	386	THR	CB-CA-C	-5.33	100.53	109.27
1	A	283	TYR	CA-C-N	-5.25	114.37	119.78
1	A	283	TYR	C-N-CA	-5.25	114.37	119.78
1	A	367	ILE	CA-C-O	-5.22	115.71	121.29
1	A	44	ARG	N-CA-C	-5.08	100.00	108.34

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	3067	0	2906	25	0
1	B	3067	0	2906	33	1
1	C	3067	0	2906	40	0
2	A	6	0	8	0	0
2	B	30	0	37	10	0
3	A	116	0	0	2	2
3	B	111	0	0	1	2
3	C	106	0	0	9	0
All	All	9570	0	8763	99	4

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 6.

All (99) 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:C:266:LYS:H	1:C:266:LYS:CD	1.65	1.09
1:C:128:ARG:HD3	3:C:521:HOH:O	1.51	1.07
1:C:52:ASN:HB2	3:C:501:HOH:O	1.59	1.01
1:C:266:LYS:HD3	1:C:266:LYS:N	1.71	1.01
1:C:266:LYS:H	1:C:266:LYS:HD3	0.86	1.00
1:B:385:ASP:OD2	2:B:503:GOL:H12	1.67	0.95
1:C:406:LYS:HA	1:C:409:MET:HE3	1.53	0.90
1:A:67:ASN:HD21	1:A:102:ARG:HH11	1.24	0.86
1:C:67:ASN:HD21	1:C:102:ARG:HH11	1.19	0.85
1:C:128:ARG:CD	3:C:521:HOH:O	2.20	0.79
1:B:238:LYS:O	1:B:242:LYS:HD2	1.83	0.78
1:B:67:ASN:HD21	1:B:102:ARG:HH11	1.31	0.78
1:C:270:ASN:HD22	1:C:306:GLN:HE22	1.34	0.75
1:B:102:ARG:HH22	1:B:200:ASN:HD22	1.36	0.74
1:B:346:LYS:HZ1	2:B:502:GOL:H11	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:NH1	1:B:58:GLU:OE1	2.22	0.72
1:B:346:LYS:NZ	2:B:502:GOL:H11	2.04	0.71
1:C:67:ASN:ND2	1:C:102:ARG:HH11	1.90	0.69
1:A:102:ARG:HH22	1:A:200:ASN:HD22	1.38	0.69
1:A:67:ASN:ND2	1:A:102:ARG:HH11	1.89	0.69
1:B:331:LYS:HE3	1:B:370:LYS:O	1.92	0.69
1:A:160:THR:OG1	1:A:161:HIS:HD2	1.78	0.66
1:B:86:TRP:H	1:B:124:ASN:HD21	1.44	0.65
1:C:102:ARG:HH22	1:C:200:ASN:HD22	1.46	0.63
1:C:266:LYS:CD	1:C:266:LYS:N	2.39	0.61
1:B:67:ASN:ND2	1:B:102:ARG:HH11	1.98	0.60
1:C:52:ASN:CB	3:C:501:HOH:O	2.31	0.60
1:C:86:TRP:HD1	1:C:124:ASN:HD22	1.50	0.59
1:C:406:LYS:CA	1:C:409:MET:HE3	2.30	0.59
1:C:270:ASN:HD22	1:C:306:GLN:NE2	1.99	0.59
1:A:102:ARG:HH22	1:A:200:ASN:ND2	2.00	0.58
1:B:86:TRP:HD1	1:B:124:ASN:HD22	1.50	0.58
1:A:86:TRP:H	1:A:124:ASN:HD21	1.51	0.58
1:A:49:TYR:OH	1:C:54:THR:HG21	2.02	0.58
1:B:86:TRP:H	1:B:124:ASN:ND2	2.01	0.57
1:B:102:ARG:HH22	1:B:200:ASN:ND2	1.99	0.57
1:C:51:ILE:HG12	1:C:58:GLU:HG3	1.85	0.57
1:C:406:LYS:HA	1:C:409:MET:CE	2.31	0.56
1:B:384:GLY:CA	2:B:505:GOL:H31	2.36	0.55
1:C:52:ASN:CG	3:C:501:HOH:O	2.48	0.55
1:C:86:TRP:H	1:C:124:ASN:HD21	1.52	0.55
1:A:67:ASN:HD21	1:A:102:ARG:HD3	1.72	0.55
2:B:503:GOL:O1	2:B:505:GOL:H11	2.08	0.54
1:B:385:ASP:CG	2:B:503:GOL:H12	2.34	0.52
1:C:263:SER:HB3	1:C:269:TYR:OH	2.09	0.52
1:B:67:ASN:HD21	1:B:102:ARG:HD3	1.73	0.52
1:C:123:LYS:HE3	3:C:514:HOH:O	2.11	0.51
1:C:102:ARG:HH22	1:C:200:ASN:ND2	2.07	0.51
1:B:302:ASP:HA	2:B:502:GOL:H31	1.94	0.50
1:B:156:ARG:HB3	1:B:158:GLY:O	2.12	0.50
1:C:123:LYS:CE	3:C:514:HOH:O	2.60	0.49
1:C:62:HIS:HA	1:C:373:ASP:OD1	2.12	0.49
1:C:311:PRO:C	1:C:313:LYS:H	2.20	0.49
1:B:86:TRP:N	1:B:124:ASN:HD21	2.09	0.49
1:A:86:TRP:HD1	1:A:124:ASN:HD22	1.60	0.49
2:B:503:GOL:O1	2:B:505:GOL:C1	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:TRP:H	1:A:124:ASN:ND2	2.10	0.48
1:C:306:GLN:HE21	1:C:307:PRO:HD2	1.79	0.47
1:A:34:GLN:NE2	3:A:703:HOH:O	2.46	0.47
1:A:253:GLY:O	1:A:274:GLY:HA2	2.15	0.47
1:B:384:GLY:HA3	2:B:505:GOL:H31	1.97	0.47
1:B:367:ILE:HG13	1:B:408:LEU:CD1	2.45	0.46
1:C:220:TRP:CE2	1:C:230:ASN:HB3	2.51	0.46
1:A:220:TRP:CE2	1:A:230:ASN:HB3	2.51	0.46
1:B:265:TYR:CE2	1:B:267:TRP:HB2	2.51	0.46
1:C:76:HIS:HE1	3:C:538:HOH:O	1.98	0.46
1:A:381:PRO:HD2	1:A:394:TRP:CZ2	2.51	0.46
1:B:368:GLU:HG3	3:B:676:HOH:O	2.15	0.46
1:C:52:ASN:OD1	1:C:52:ASN:C	2.59	0.46
1:C:253:GLY:O	1:C:274:GLY:HA2	2.16	0.45
1:C:86:TRP:H	1:C:124:ASN:ND2	2.13	0.45
1:B:380:ASN:HB3	1:B:382:ASP:OD1	2.17	0.45
1:C:366:MET:HE2	1:C:408:LEU:HD21	1.99	0.45
1:A:76:HIS:HE1	1:A:108:GLU:OE1	2.00	0.45
1:A:197:ASP:HA	1:A:250:PHE:HB2	1.98	0.45
1:C:89:MET:CG	1:C:379:TRP:HE1	2.30	0.44
1:B:208:PRO:HD3	1:B:256:PHE:CE2	2.52	0.44
1:C:405:LEU:HG	1:C:409:MET:HE2	1.99	0.44
1:B:220:TRP:CE2	1:B:230:ASN:HB3	2.53	0.43
1:B:268:GLY:HA2	1:B:278:MET:HE1	2.00	0.43
1:B:200:ASN:ND2	1:B:297:HIS:HE1	2.17	0.43
1:C:52:ASN:ND2	3:C:501:HOH:O	2.51	0.43
1:A:295:SER:HA	1:A:339:VAL:O	2.19	0.42
1:A:68:TRP:CZ2	1:A:89:MET:HE3	2.54	0.42
1:B:346:LYS:NZ	2:B:502:GOL:C1	2.79	0.42
1:B:323:TRP:CH2	1:B:362:LEU:HA	2.55	0.42
1:A:331:LYS:HE2	1:A:370:LYS:O	2.20	0.42
1:C:201:GLU:HB3	1:C:273:TRP:HB3	2.01	0.42
1:C:295:SER:HA	1:C:339:VAL:O	2.20	0.42
1:A:77:VAL:O	1:A:78:VAL:C	2.63	0.42
1:A:155:HIS:HA	1:A:200:ASN:HB3	2.02	0.41
1:A:160:THR:OG1	1:A:161:HIS:CD2	2.67	0.41
1:B:295:SER:HA	1:B:339:VAL:O	2.22	0.40
1:A:86:TRP:CE2	1:A:87:GLU:HG3	2.56	0.40
1:A:380:ASN:HB3	1:A:382:ASP:OD1	2.21	0.40
1:A:34:GLN:HG3	3:A:601:HOH:O	2.21	0.40
1:B:102:ARG:NH2	1:B:200:ASN:HD22	2.11	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ILE:HD12	1:B:366:MET:HE3	2.02	0.40
1:C:377:TRP:HA	1:C:378:SER:HA	1.85	0.40

All (4) 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)
3:A:612:HOH:O	3:A:677:HOH:O[4_556]	1.37	0.83
3:B:627:HOH:O	3:B:676:HOH:O[4_555]	1.71	0.49
3:A:603:HOH:O	3:A:684:HOH:O[4_556]	1.78	0.42
1:B:368:GLU:OE1	3:B:627:HOH:O[4_545]	2.12	0.08

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	375/377 (100%)	364 (97%)	11 (3%)	0	100	100
1	B	375/377 (100%)	368 (98%)	7 (2%)	0	100	100
1	C	375/377 (100%)	368 (98%)	6 (2%)	1 (0%)	36	28
All	All	1125/1131 (100%)	1100 (98%)	24 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	312	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	324/324 (100%)	315 (97%)	9 (3%)	38	30
1	B	324/324 (100%)	318 (98%)	6 (2%)	50	45
1	C	324/324 (100%)	315 (97%)	9 (3%)	38	30
All	All	972/972 (100%)	948 (98%)	24 (2%)	42	34

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LYS
1	A	94	LYS
1	A	111	LYS
1	A	117	ILE
1	A	153	ASP
1	A	313	LYS
1	A	331	LYS
1	A	408	LEU
1	A	410	ASP
1	B	57	GLU
1	B	141	LYS
1	B	153	ASP
1	B	185	LYS
1	B	242	LYS
1	B	408	LEU
1	C	35	THR
1	C	54	THR
1	C	57	GLU
1	C	153	ASP
1	C	207	SER
1	C	242	LYS
1	C	266	LYS
1	C	289	LYS
1	C	320	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN

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Mol	Chain	Res	Type
1	A	67	ASN
1	A	76	HIS
1	A	124	ASN
1	A	161	HIS
1	A	200	ASN
1	A	270	ASN
1	A	359	GLN
1	A	360	ASN
1	B	34	GLN
1	B	67	ASN
1	B	76	HIS
1	B	124	ASN
1	B	200	ASN
1	B	224	ASN
1	B	286	ASN
1	C	67	ASN
1	C	76	HIS
1	C	124	ASN
1	C	200	ASN
1	C	270	ASN
1	C	306	GLN
1	C	359	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	GOL	B	505	-	5,5,5	1.56	1 (20%)	5,5,5	4.62	2 (40%)
2	GOL	B	503	-	5,5,5	1.02	0	5,5,5	2.94	3 (60%)
2	GOL	B	504	-	5,5,5	0.95	0	5,5,5	0.85	0
2	GOL	B	502	-	5,5,5	0.55	0	5,5,5	1.81	2 (40%)
2	GOL	A	501	-	5,5,5	1.04	0	5,5,5	1.58	0
2	GOL	B	501	-	5,5,5	0.36	0	5,5,5	0.72	0

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	GOL	B	505	-	-	3/4/4/4	-
2	GOL	B	503	-	-	2/4/4/4	-
2	GOL	B	504	-	-	0/4/4/4	-
2	GOL	B	502	-	-	4/4/4/4	-
2	GOL	A	501	-	-	2/4/4/4	-
2	GOL	B	501	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	505	GOL	C1-C2	-2.25	1.43	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	505	GOL	O1-C1-C2	-9.59	67.21	110.38
2	B	503	GOL	O2-C2-C1	-4.76	89.47	109.18
2	B	503	GOL	O3-C3-C2	-3.96	92.56	110.38
2	B	502	GOL	C3-C2-C1	3.28	123.84	111.80
2	B	505	GOL	O2-C2-C3	2.85	120.98	109.18
2	B	502	GOL	O1-C1-C2	2.24	120.46	110.38
2	B	503	GOL	C3-C2-C1	2.17	119.74	111.80

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	C1-C2-C3-O3
2	B	503	GOL	C1-C2-C3-O3
2	B	505	GOL	O1-C1-C2-C3
2	B	502	GOL	O1-C1-C2-C3
2	B	502	GOL	C1-C2-C3-O3
2	B	505	GOL	C1-C2-C3-O3
2	B	502	GOL	O1-C1-C2-O2
2	B	502	GOL	O2-C2-C3-O3
2	B	505	GOL	O1-C1-C2-O2
2	A	501	GOL	O2-C2-C3-O3
2	B	503	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	505	GOL	4	0
2	B	503	GOL	4	0
2	B	502	GOL	4	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	377/377 (100%)	-0.39	12 (3%)	50	56	2, 11, 25, 58	8 (2%)
1	B	377/377 (100%)	-0.36	13 (3%)	48	54	3, 12, 23, 50	10 (2%)
1	C	377/377 (100%)	-0.21	10 (2%)	56	62	3, 15, 29, 40	9 (2%)
All	All	1131/1131 (100%)	-0.32	35 (3%)	51	58	2, 13, 27, 58	27 (2%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	311	PRO	9.5
1	C	312	ALA	8.7
1	A	312	ALA	7.0
1	C	310	GLY	7.0
1	B	312	ALA	6.9
1	A	311	PRO	6.6
1	A	310	GLY	6.4
1	B	311	PRO	6.1
1	B	161	HIS	6.0
1	A	162	ILE	5.8
1	C	161	HIS	5.6
1	B	310	GLY	5.5
1	A	286	ASN	5.2
1	B	160	THR	5.2
1	A	410	ASP	4.8
1	B	34	GLN	4.8
1	C	368	GLU	4.6
1	A	136	MET	4.6
1	C	136	MET	4.5
1	A	34	GLN	4.5
1	B	368	GLU	4.4
1	B	136	MET	4.4
1	A	161	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	286	ASN	4.2
1	A	368	GLU	4.2
1	B	182	GLU	4.0
1	C	286	ASN	4.0
1	A	234	GLU	3.9
1	C	182	GLU	3.7
1	B	234	GLU	3.7
1	C	410	ASP	3.4
1	A	160	THR	3.3
1	C	234	GLU	3.3
1	B	162	ILE	3.1
1	B	410	ASP	2.7

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	GOL	A	501	6/6	0.85	0.12	21,25,27,29	0
2	GOL	B	503	6/6	0.85	0.13	17,24,25,26	0
2	GOL	B	502	6/6	0.86	0.15	19,26,28,36	0
2	GOL	B	501	6/6	0.91	0.10	19,29,33,36	0
2	GOL	B	505	6/6	0.91	0.14	12,14,22,34	0
2	GOL	B	504	6/6	0.94	0.07	19,20,21,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.