



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:16 AM UTC

PDB ID : 6FLS / pdb_00006fls
Title : Pentapeptide repeat family protein from Clostridium botulinum
Authors : Martinez-Carranza, M.; Stenmark, P.
Deposited on : 2018-01-27
Resolution : 2.80 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

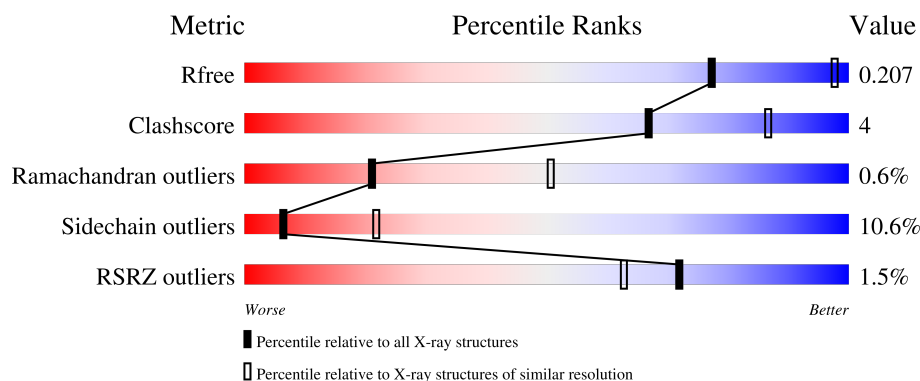
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	239	% 75% 12% • 10%
1	B	239	76% 14% 10%
1	C	239	3% 69% 18% • 10%
1	D	239	% 77% 11% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7204 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 Pentapeptide repeat family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1733	1117	269	334	13			
1	B	216	Total	C	N	O	S	0	0	0
			1733	1117	269	334	13			
1	D	217	Total	C	N	O	S	0	0	0
			1742	1122	271	336	13			
1	C	216	Total	C	N	O	S	0	0	0
			1733	1117	269	334	13			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP A0A0M0A2X5
A	-20	HIS	-	expression tag	UNP A0A0M0A2X5
A	-19	HIS	-	expression tag	UNP A0A0M0A2X5
A	-18	HIS	-	expression tag	UNP A0A0M0A2X5
A	-17	HIS	-	expression tag	UNP A0A0M0A2X5
A	-16	HIS	-	expression tag	UNP A0A0M0A2X5
A	-15	HIS	-	expression tag	UNP A0A0M0A2X5
A	-14	SER	-	expression tag	UNP A0A0M0A2X5
A	-13	SER	-	expression tag	UNP A0A0M0A2X5
A	-12	GLY	-	expression tag	UNP A0A0M0A2X5
A	-11	VAL	-	expression tag	UNP A0A0M0A2X5
A	-10	ASP	-	expression tag	UNP A0A0M0A2X5
A	-9	LEU	-	expression tag	UNP A0A0M0A2X5
A	-8	GLY	-	expression tag	UNP A0A0M0A2X5
A	-7	THR	-	expression tag	UNP A0A0M0A2X5
A	-6	GLU	-	expression tag	UNP A0A0M0A2X5
A	-5	ASN	-	expression tag	UNP A0A0M0A2X5
A	-4	LEU	-	expression tag	UNP A0A0M0A2X5
A	-3	TYR	-	expression tag	UNP A0A0M0A2X5
A	-2	PHE	-	expression tag	UNP A0A0M0A2X5
A	-1	GLN	-	expression tag	UNP A0A0M0A2X5

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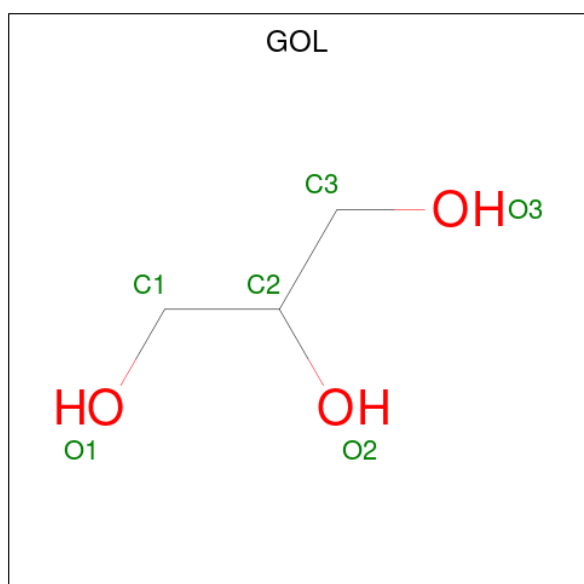
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A0M0A2X5
B	-21	MET	-	initiating methionine	UNP A0A0M0A2X5
B	-20	HIS	-	expression tag	UNP A0A0M0A2X5
B	-19	HIS	-	expression tag	UNP A0A0M0A2X5
B	-18	HIS	-	expression tag	UNP A0A0M0A2X5
B	-17	HIS	-	expression tag	UNP A0A0M0A2X5
B	-16	HIS	-	expression tag	UNP A0A0M0A2X5
B	-15	HIS	-	expression tag	UNP A0A0M0A2X5
B	-14	SER	-	expression tag	UNP A0A0M0A2X5
B	-13	SER	-	expression tag	UNP A0A0M0A2X5
B	-12	GLY	-	expression tag	UNP A0A0M0A2X5
B	-11	VAL	-	expression tag	UNP A0A0M0A2X5
B	-10	ASP	-	expression tag	UNP A0A0M0A2X5
B	-9	LEU	-	expression tag	UNP A0A0M0A2X5
B	-8	GLY	-	expression tag	UNP A0A0M0A2X5
B	-7	THR	-	expression tag	UNP A0A0M0A2X5
B	-6	GLU	-	expression tag	UNP A0A0M0A2X5
B	-5	ASN	-	expression tag	UNP A0A0M0A2X5
B	-4	LEU	-	expression tag	UNP A0A0M0A2X5
B	-3	TYR	-	expression tag	UNP A0A0M0A2X5
B	-2	PHE	-	expression tag	UNP A0A0M0A2X5
B	-1	GLN	-	expression tag	UNP A0A0M0A2X5
B	0	SER	-	expression tag	UNP A0A0M0A2X5
D	-21	MET	-	initiating methionine	UNP A0A0M0A2X5
D	-20	HIS	-	expression tag	UNP A0A0M0A2X5
D	-19	HIS	-	expression tag	UNP A0A0M0A2X5
D	-18	HIS	-	expression tag	UNP A0A0M0A2X5
D	-17	HIS	-	expression tag	UNP A0A0M0A2X5
D	-16	HIS	-	expression tag	UNP A0A0M0A2X5
D	-15	HIS	-	expression tag	UNP A0A0M0A2X5
D	-14	SER	-	expression tag	UNP A0A0M0A2X5
D	-13	SER	-	expression tag	UNP A0A0M0A2X5
D	-12	GLY	-	expression tag	UNP A0A0M0A2X5
D	-11	VAL	-	expression tag	UNP A0A0M0A2X5
D	-10	ASP	-	expression tag	UNP A0A0M0A2X5
D	-9	LEU	-	expression tag	UNP A0A0M0A2X5
D	-8	GLY	-	expression tag	UNP A0A0M0A2X5
D	-7	THR	-	expression tag	UNP A0A0M0A2X5
D	-6	GLU	-	expression tag	UNP A0A0M0A2X5
D	-5	ASN	-	expression tag	UNP A0A0M0A2X5
D	-4	LEU	-	expression tag	UNP A0A0M0A2X5
D	-3	TYR	-	expression tag	UNP A0A0M0A2X5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	PHE	-	expression tag	UNP A0A0M0A2X5
D	-1	GLN	-	expression tag	UNP A0A0M0A2X5
D	0	SER	-	expression tag	UNP A0A0M0A2X5
C	-21	MET	-	initiating methionine	UNP A0A0M0A2X5
C	-20	HIS	-	expression tag	UNP A0A0M0A2X5
C	-19	HIS	-	expression tag	UNP A0A0M0A2X5
C	-18	HIS	-	expression tag	UNP A0A0M0A2X5
C	-17	HIS	-	expression tag	UNP A0A0M0A2X5
C	-16	HIS	-	expression tag	UNP A0A0M0A2X5
C	-15	HIS	-	expression tag	UNP A0A0M0A2X5
C	-14	SER	-	expression tag	UNP A0A0M0A2X5
C	-13	SER	-	expression tag	UNP A0A0M0A2X5
C	-12	GLY	-	expression tag	UNP A0A0M0A2X5
C	-11	VAL	-	expression tag	UNP A0A0M0A2X5
C	-10	ASP	-	expression tag	UNP A0A0M0A2X5
C	-9	LEU	-	expression tag	UNP A0A0M0A2X5
C	-8	GLY	-	expression tag	UNP A0A0M0A2X5
C	-7	THR	-	expression tag	UNP A0A0M0A2X5
C	-6	GLU	-	expression tag	UNP A0A0M0A2X5
C	-5	ASN	-	expression tag	UNP A0A0M0A2X5
C	-4	LEU	-	expression tag	UNP A0A0M0A2X5
C	-3	TYR	-	expression tag	UNP A0A0M0A2X5
C	-2	PHE	-	expression tag	UNP A0A0M0A2X5
C	-1	GLN	-	expression tag	UNP A0A0M0A2X5
C	0	SER	-	expression tag	UNP A0A0M0A2X5

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

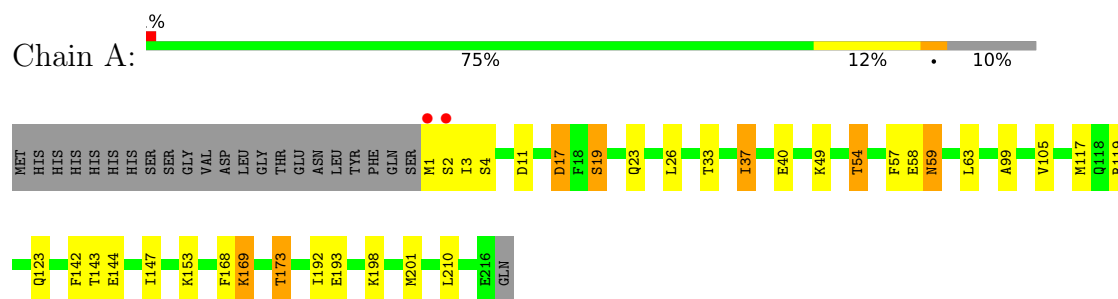
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	51	Total O 51 51	0	0
3	B	47	Total O 47 47	0	0
3	D	54	Total O 54 54	0	0
3	C	21	Total O 21 21	0	0

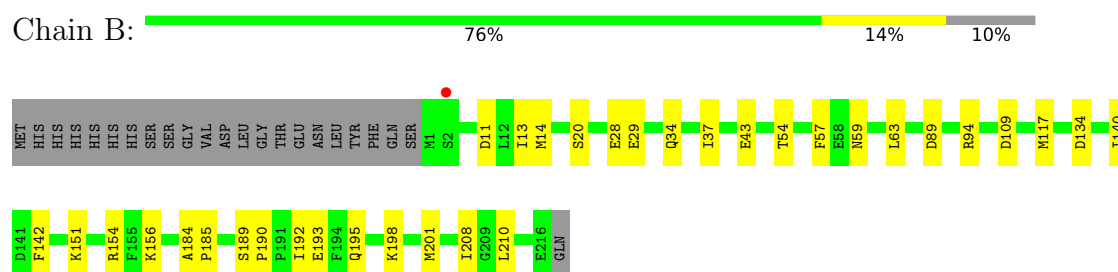
3 Residue-property plots [i](#)

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.

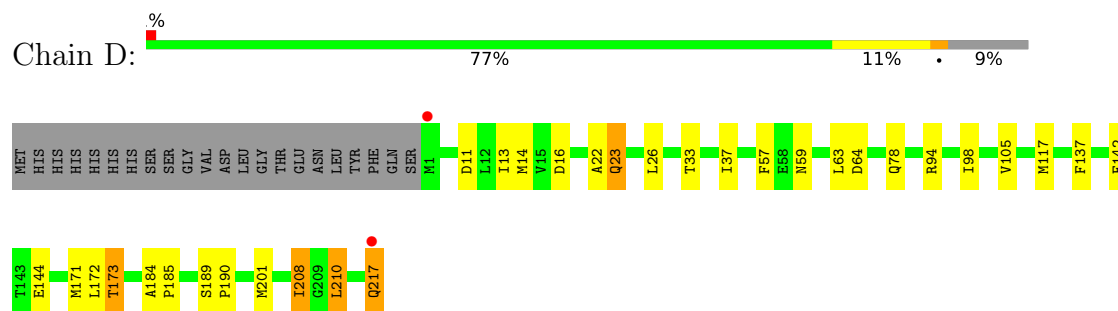
- Molecule 1: Pentapeptide repeat family protein



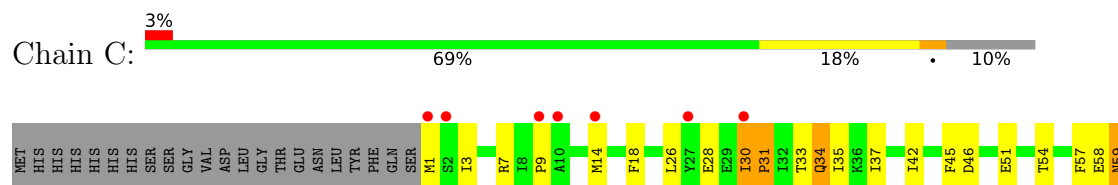
- Molecule 1: Pentapeptide repeat family protein



- Molecule 1: Pentapeptide repeat family protein



- Molecule 1: Pentapeptide repeat family protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.75Å 108.47Å 112.89Å 90.00° 94.60° 90.00°	Depositor
Resolution (Å)	112.53 – 2.80 112.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (112.53-2.80) 89.8 (112.53-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.170 , 0.205 0.179 , 0.207	Depositor DCC
R_{free} test set	3079 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7204	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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	0.79	0/1772	0.96	2/2393 (0.1%)
1	B	0.75	0/1772	0.92	0/2393
1	C	0.82	0/1772	1.01	3/2393 (0.1%)
1	D	0.76	0/1781	0.98	3/2405 (0.1%)
All	All	0.78	0/7097	0.97	8/9584 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	30	ILE	CA-C-N	6.65	128.16	119.84
1	C	30	ILE	C-N-CA	6.65	128.16	119.84
1	A	173	THR	CB-CA-C	-6.37	100.29	109.84
1	A	54	THR	CB-CA-C	6.08	120.36	111.73
1	C	31	PRO	CA-N-CD	-5.72	103.99	112.00
1	D	208	ILE	CA-C-N	5.28	126.79	120.13
1	D	208	ILE	C-N-CA	5.28	126.79	120.13
1	D	137	PHE	CA-CB-CG	5.06	118.86	113.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	94	ARG	Sidechain
1	C	119	ARG	Sidechain
1	C	94	ARG	Sidechain
1	D	94	ARG	Sidechain

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	1733	0	1679	11	0
1	B	1733	0	1679	8	0
1	C	1733	0	1679	21	0
1	D	1742	0	1687	11	0
2	A	48	0	64	1	0
2	B	18	0	24	0	0
2	C	6	0	8	0	0
2	D	18	0	24	0	0
3	A	51	0	0	1	0
3	B	47	0	0	0	0
3	C	21	0	0	1	0
3	D	54	0	0	0	0
All	All	7204	0	6844	51	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 4.

All (51) 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:A:143:THR:HG22	1:A:144:GLU:HG3	1.83	0.58
1:A:19:SER:HB2	3:A:402:HOH:O	2.06	0.55
1:A:37:ILE:HD13	1:A:57:PHE:CE2	2.41	0.55
1:C:33:THR:O	1:C:35:ILE:HG23	2.07	0.55
1:A:153:LYS:HA	2:A:302:GOL:H2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:PHE:HA	1:C:165:ASN:HD21	1.76	0.51
1:C:162:PHE:CA	1:C:165:ASN:HD21	2.24	0.51
1:C:58:GLU:HG2	1:C:59:ASN:HD22	1.77	0.48
1:C:123:GLN:HG2	1:C:124:TYR:CD2	2.49	0.48
1:D:37:ILE:HD13	1:D:57:PHE:CD2	2.48	0.47
1:D:189:SER:HA	1:D:190:PRO:C	2.39	0.47
1:B:37:ILE:HD13	1:B:57:PHE:CE2	2.49	0.47
1:A:99:ALA:HA	1:A:119:ARG:O	2.15	0.47
1:D:78:GLN:HE21	1:D:98:ILE:HG21	1.80	0.47
1:C:42:ILE:CG2	1:C:45:PHE:HB2	2.45	0.47
1:C:187:VAL:HG11	1:C:194:PHE:CE2	2.50	0.47
1:A:59:ASN:HD22	1:A:59:ASN:N	2.13	0.46
1:A:123:GLN:HG2	1:A:143:THR:HB	1.98	0.46
1:C:58:GLU:HG2	1:C:59:ASN:ND2	2.31	0.45
1:C:86:ASN:OD1	1:C:88:THR:HG22	2.17	0.45
1:A:17:ASP:C	1:A:17:ASP:OD1	2.59	0.45
1:A:168:PHE:CZ	1:A:169:LYS:HE2	2.52	0.44
1:C:33:THR:HG22	1:C:34:GLN:CG	2.47	0.44
1:B:37:ILE:HD13	1:B:57:PHE:CD2	2.53	0.44
1:D:16:ASP:OD1	1:D:16:ASP:N	2.50	0.44
1:C:88:THR:HG21	3:C:406:HOH:O	2.17	0.44
1:C:18:PHE:CE1	1:C:37:ILE:HD11	2.53	0.44
1:C:88:THR:O	1:C:89:ASP:HB2	2.17	0.43
1:B:134:ASP:OD1	1:B:154:ARG:HD2	2.17	0.43
1:B:117:MET:HB3	1:B:140:ILE:HD11	2.01	0.43
1:D:217:GLN:O	1:D:217:GLN:HG2	2.19	0.43
1:B:189:SER:HA	1:B:190:PRO:C	2.44	0.43
1:B:184:ALA:N	1:B:185:PRO:CD	2.82	0.43
1:D:22:ALA:O	1:D:23:GLN:C	2.61	0.43
1:D:184:ALA:N	1:D:185:PRO:CD	2.82	0.43
1:C:46:ASP:OD1	1:C:46:ASP:C	2.61	0.43
1:D:184:ALA:HA	1:D:210:LEU:HD11	2.01	0.42
1:A:201:MET:HE2	1:A:201:MET:HB2	1.90	0.42
1:C:59:ASN:HD22	1:C:59:ASN:N	2.18	0.42
1:C:78:GLN:HG3	1:C:79:ASN:HD22	1.84	0.42
1:B:34:GLN:HA	1:B:54:THR:O	2.20	0.41
1:B:43:GLU:HG2	1:B:63:LEU:HB2	2.02	0.41
1:C:152:LEU:CD1	1:C:152:LEU:N	2.84	0.41
1:D:172:LEU:O	1:D:173:THR:C	2.61	0.41
1:C:93:GLU:O	1:C:94:ARG:C	2.63	0.41
1:D:210:LEU:HD23	1:D:210:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:MET:HE2	1:D:201:MET:HB2	2.00	0.41
1:C:117:MET:HB3	1:C:140:ILE:HD11	2.03	0.41
1:C:173:THR:HG23	1:C:196:GLY:HA3	2.03	0.40
1:A:37:ILE:HG22	1:A:40:GLU:HG3	2.03	0.40
1:C:9:PRO:HG2	1:C:34:GLN:HE22	1.85	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	214/239 (90%)	207 (97%)	6 (3%)	1 (0%)	24	55
1	B	214/239 (90%)	207 (97%)	6 (3%)	1 (0%)	24	55
1	C	214/239 (90%)	191 (89%)	21 (10%)	2 (1%)	14	41
1	D	215/239 (90%)	207 (96%)	7 (3%)	1 (0%)	24	55
All	All	857/956 (90%)	812 (95%)	40 (5%)	5 (1%)	21	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	64	ASP
1	D	11	ASP
1	A	147	ILE
1	B	11	ASP
1	C	147	ILE

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	195/216 (90%)	170 (87%)	25 (13%)	4	15
1	B	195/216 (90%)	177 (91%)	18 (9%)	8	27
1	C	195/216 (90%)	172 (88%)	23 (12%)	5	17
1	D	196/216 (91%)	179 (91%)	17 (9%)	9	30
All	All	781/864 (90%)	698 (89%)	83 (11%)	6	22

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	SER
1	A	3	ILE
1	A	4	SER
1	A	11	ASP
1	A	17	ASP
1	A	19	SER
1	A	23	GLN
1	A	26	LEU
1	A	33	THR
1	A	37	ILE
1	A	49	LYS
1	A	54	THR
1	A	58	GLU
1	A	59	ASN
1	A	63	LEU
1	A	105	VAL
1	A	117	MET
1	A	142	PHE
1	A	169	LYS
1	A	173	THR
1	A	192	ILE
1	A	193	GLU
1	A	198	LYS
1	A	210	LEU
1	B	13	ILE
1	B	14	MET
1	B	20	SER

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Mol	Chain	Res	Type
1	B	28	GLU
1	B	29	GLU
1	B	59	ASN
1	B	89	ASP
1	B	109	ASP
1	B	142	PHE
1	B	151	LYS
1	B	156	LYS
1	B	192	ILE
1	B	193	GLU
1	B	195	GLN
1	B	198	LYS
1	B	201	MET
1	B	208	ILE
1	B	210	LEU
1	D	13	ILE
1	D	14	MET
1	D	23	GLN
1	D	26	LEU
1	D	33	THR
1	D	59	ASN
1	D	63	LEU
1	D	64	ASP
1	D	105	VAL
1	D	117	MET
1	D	142	PHE
1	D	144	GLU
1	D	171	MET
1	D	173	THR
1	D	208	ILE
1	D	210	LEU
1	D	217	GLN
1	C	1	MET
1	C	3	ILE
1	C	7	ARG
1	C	14	MET
1	C	26	LEU
1	C	28	GLU
1	C	30	ILE
1	C	31	PRO
1	C	34	GLN
1	C	51	GLU

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Mol	Chain	Res	Type
1	C	54	THR
1	C	57	PHE
1	C	59	ASN
1	C	89	ASP
1	C	93	GLU
1	C	142	PHE
1	C	144	GLU
1	C	151	LYS
1	C	169	LYS
1	C	179	LYS
1	C	192	ILE
1	C	193	GLU
1	C	210	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	59	ASN
1	A	79	ASN
1	A	96	GLN
1	A	159	ASN
1	B	5	ASN
1	B	78	GLN
1	B	165	ASN
1	D	34	GLN
1	D	78	GLN
1	D	79	ASN
1	C	34	GLN
1	C	59	ASN
1	C	79	ASN
1	C	118	GLN
1	C	159	ASN
1	C	165	ASN
1	C	195	GLN

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](#)

15 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	303	-	5,5,5	0.80	0	5,5,5	0.58	0
2	GOL	A	304	-	5,5,5	0.39	0	5,5,5	0.58	0
2	GOL	A	306	-	5,5,5	0.40	0	5,5,5	0.61	0
2	GOL	A	303	-	5,5,5	0.21	0	5,5,5	0.67	0
2	GOL	A	308	-	5,5,5	0.35	0	5,5,5	0.42	0
2	GOL	D	302	-	5,5,5	0.43	0	5,5,5	0.34	0
2	GOL	D	301	-	5,5,5	0.84	0	5,5,5	1.12	0
2	GOL	A	302	-	5,5,5	0.87	0	5,5,5	0.93	0
2	GOL	A	307	-	5,5,5	0.68	0	5,5,5	0.73	0
2	GOL	B	301	-	5,5,5	0.66	0	5,5,5	0.49	0
2	GOL	B	302	-	5,5,5	0.84	0	5,5,5	0.89	0
2	GOL	A	305	-	5,5,5	0.42	0	5,5,5	0.73	0
2	GOL	A	301	-	5,5,5	0.53	0	5,5,5	1.00	0
2	GOL	C	301	-	5,5,5	0.77	0	5,5,5	1.11	0
2	GOL	D	303	-	5,5,5	0.17	0	5,5,5	0.39	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	303	-	-	2/4/4/4	-
2	GOL	A	304	-	-	0/4/4/4	-
2	GOL	A	306	-	-	2/4/4/4	-
2	GOL	A	303	-	-	4/4/4/4	-
2	GOL	A	308	-	-	4/4/4/4	-
2	GOL	D	302	-	-	2/4/4/4	-
2	GOL	D	301	-	-	2/4/4/4	-
2	GOL	A	302	-	-	2/4/4/4	-
2	GOL	A	307	-	-	2/4/4/4	-
2	GOL	B	301	-	-	2/4/4/4	-
2	GOL	B	302	-	-	3/4/4/4	-
2	GOL	A	305	-	-	4/4/4/4	-
2	GOL	A	301	-	-	2/4/4/4	-
2	GOL	C	301	-	-	0/4/4/4	-
2	GOL	D	303	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	GOL	O1-C1-C2-C3
2	A	303	GOL	O1-C1-C2-C3
2	A	303	GOL	C1-C2-C3-O3
2	A	305	GOL	O1-C1-C2-C3
2	A	306	GOL	C1-C2-C3-O3
2	A	308	GOL	C1-C2-C3-O3
2	B	301	GOL	C1-C2-C3-O3
2	B	303	GOL	O1-C1-C2-O2
2	B	303	GOL	O1-C1-C2-C3
2	D	302	GOL	O1-C1-C2-C3
2	A	305	GOL	O1-C1-C2-O2
2	A	306	GOL	O2-C2-C3-O3
2	D	302	GOL	O1-C1-C2-O2
2	A	301	GOL	O1-C1-C2-C3
2	A	305	GOL	C1-C2-C3-O3
2	A	307	GOL	C1-C2-C3-O3
2	A	308	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	B	302	GOL	C1-C2-C3-O3
2	D	301	GOL	O1-C1-C2-C3
2	A	302	GOL	O1-C1-C2-O2
2	A	303	GOL	O1-C1-C2-O2
2	A	303	GOL	O2-C2-C3-O3
2	A	305	GOL	O2-C2-C3-O3
2	A	307	GOL	O2-C2-C3-O3
2	A	308	GOL	O1-C1-C2-O2
2	A	308	GOL	O2-C2-C3-O3
2	B	301	GOL	O2-C2-C3-O3
2	B	302	GOL	O2-C2-C3-O3
2	D	301	GOL	O1-C1-C2-O2
2	A	301	GOL	O1-C1-C2-O2
2	B	302	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	GOL	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	216/239 (90%)	-0.45	2 (0%) 81 74	37, 54, 76, 127	0
1	B	216/239 (90%)	-0.50	1 (0%) 87 82	43, 54, 73, 118	0
1	C	216/239 (90%)	0.15	8 (3%) 45 36	43, 66, 109, 134	0
1	D	217/239 (90%)	-0.36	2 (0%) 81 74	36, 56, 79, 126	0
All	All	865/956 (90%)	-0.29	13 (1%) 72 63	36, 57, 89, 134	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	5.1
1	A	1	MET	3.8
1	C	14	MET	3.4
1	D	1	MET	3.2
1	C	27	TYR	3.0
1	C	10	ALA	3.0
1	A	2	SER	2.9
1	C	9	PRO	2.9
1	C	30	ILE	2.4
1	C	156	LYS	2.3
1	D	217	GLN	2.2
1	C	2	SER	2.2
1	B	2	SER	2.1

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	C	301	6/6	0.85	0.21	79,89,93,97	0
2	GOL	A	308	6/6	0.86	0.18	85,100,106,114	0
2	GOL	A	303	6/6	0.89	0.23	92,99,106,117	0
2	GOL	B	301	6/6	0.90	0.19	81,86,91,93	0
2	GOL	A	307	6/6	0.90	0.18	70,73,84,85	0
2	GOL	A	302	6/6	0.91	0.18	68,80,84,88	0
2	GOL	B	302	6/6	0.91	0.18	81,92,97,100	0
2	GOL	A	305	6/6	0.91	0.18	72,95,97,103	0
2	GOL	A	306	6/6	0.92	0.15	78,80,81,81	0
2	GOL	B	303	6/6	0.92	0.15	78,86,93,93	0
2	GOL	D	303	6/6	0.92	0.18	91,96,98,100	0
2	GOL	A	304	6/6	0.92	0.16	82,89,90,91	0
2	GOL	D	302	6/6	0.94	0.17	80,94,97,101	0
2	GOL	D	301	6/6	0.96	0.10	66,71,73,75	0
2	GOL	A	301	6/6	0.98	0.10	61,63,67,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.