



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2023 – 09:44 PM EDT

PDB ID : 6W4Q
Title : Crystal structure of full-length tailspike protein 2 (TSP2, ORF211)) from Escherichia coli O157:H7 bacteriophage CAB120
Authors : Greenfield, J.; Herzberg, O.
Deposited on : 2020-03-11
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

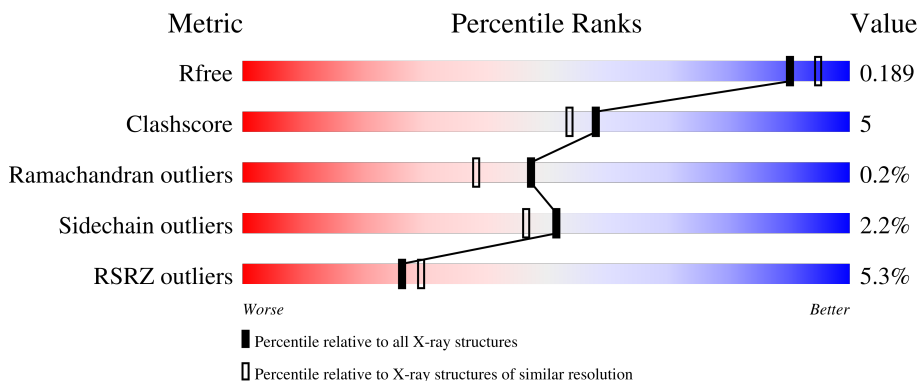
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

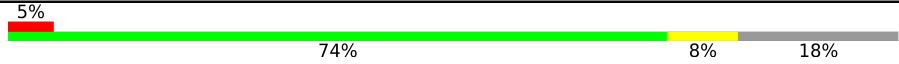

The reported resolution of this entry is 1.90 Å.

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	927	 <p>5% 74% 8% 18%</p>
1	B	927	 <p>3% 73% 8% 18%</p>
1	C	927	 <p>2% 74% 7% 18%</p>
1	D	927	 <p>8% 73% 8% 19%</p>
1	E	927	 <p>6% 73% 8% 19%</p>

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Mol	Chain	Length	Quality of chain
1	F	927	<p>%</p> <p>72% 8% 19%</p>

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	A	1005	-	-	X	-
2	GOL	A	1020	-	-	X	-
2	GOL	B	1004	-	-	X	-
2	GOL	C	1018	-	-	X	-
3	SO4	C	1024	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 38610 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 Tail fiber.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	757	5708	3577	971	1139	21	0	11	0
1	B	756	5697	3571	968	1136	22	0	10	0
1	C	758	5697	3568	970	1138	21	0	7	0
1	D	755	5687	3561	969	1136	21	0	8	0
1	E	754	5663	3543	966	1132	22	0	6	0
1	F	753	5643	3530	962	1129	22	0	3	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	922	HIS	-	expression tag	UNP G3M190
A	923	HIS	-	expression tag	UNP G3M190
A	924	HIS	-	expression tag	UNP G3M190
A	925	HIS	-	expression tag	UNP G3M190
A	926	HIS	-	expression tag	UNP G3M190
A	927	HIS	-	expression tag	UNP G3M190
B	922	HIS	-	expression tag	UNP G3M190
B	923	HIS	-	expression tag	UNP G3M190
B	924	HIS	-	expression tag	UNP G3M190
B	925	HIS	-	expression tag	UNP G3M190
B	926	HIS	-	expression tag	UNP G3M190
B	927	HIS	-	expression tag	UNP G3M190
C	922	HIS	-	expression tag	UNP G3M190
C	923	HIS	-	expression tag	UNP G3M190
C	924	HIS	-	expression tag	UNP G3M190
C	925	HIS	-	expression tag	UNP G3M190
C	926	HIS	-	expression tag	UNP G3M190

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Chain	Residue	Modelled	Actual	Comment	Reference
C	927	HIS	-	expression tag	UNP G3M190
D	922	HIS	-	expression tag	UNP G3M190
D	923	HIS	-	expression tag	UNP G3M190
D	924	HIS	-	expression tag	UNP G3M190
D	925	HIS	-	expression tag	UNP G3M190
D	926	HIS	-	expression tag	UNP G3M190
D	927	HIS	-	expression tag	UNP G3M190
E	922	HIS	-	expression tag	UNP G3M190
E	923	HIS	-	expression tag	UNP G3M190
E	924	HIS	-	expression tag	UNP G3M190
E	925	HIS	-	expression tag	UNP G3M190
E	926	HIS	-	expression tag	UNP G3M190
E	927	HIS	-	expression tag	UNP G3M190
F	922	HIS	-	expression tag	UNP G3M190
F	923	HIS	-	expression tag	UNP G3M190
F	924	HIS	-	expression tag	UNP G3M190
F	925	HIS	-	expression tag	UNP G3M190
F	926	HIS	-	expression tag	UNP G3M190
F	927	HIS	-	expression tag	UNP G3M190

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total 6	C 3	O 3	0	0
2	D	1	Total 6	C 3	O 3	0	0
2	E	1	Total 6	C 3	O 3	0	0
2	E	1	Total 6	C 3	O 3	0	0
2	E	1	Total 6	C 3	O 3	0	0
2	E	1	Total 6	C 3	O 3	0	0
2	E	1	Total 6	C 3	O 3	0	0
2	E	1	Total 6	C 3	O 3	0	0
2	E	1	Total 6	C 3	O 3	0	0
2	E	1	Total 6	C 3	O 3	0	0
2	F	1	Total 6	C 3	O 3	0	0
2	F	1	Total 6	C 3	O 3	0	0
2	F	1	Total 6	C 3	O 3	0	0
2	F	1	Total 6	C 3	O 3	0	0

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



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Cl	0	0
			3	3		
4	B	1	Total	Cl	0	0
			1	1		
4	D	3	Total	Cl	0	0
			3	3		

- Molecule 5 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	1	3		
5	D	1	Total	C	O	0	0
			4	1	3		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0

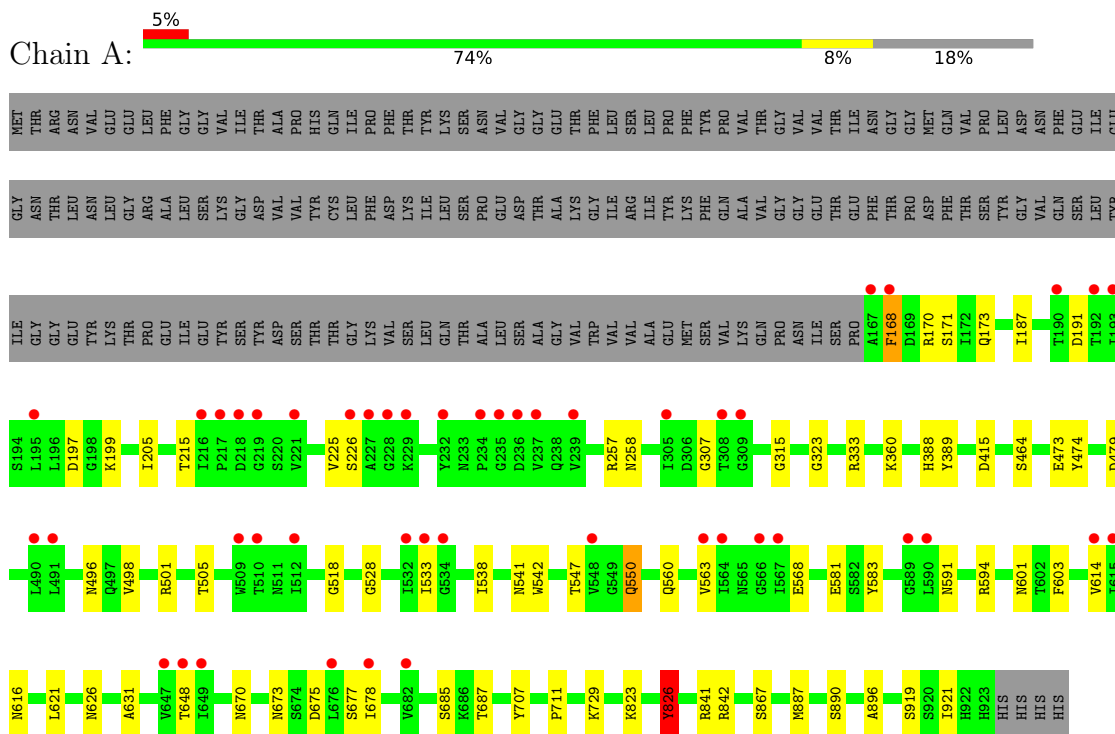
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	802	Total O 802 802	0	0
7	B	793	Total O 793 793	0	0
7	C	759	Total O 759 759	0	0
7	D	502	Total O 502 502	0	0
7	E	504	Total O 504 504	0	0
7	F	527	Total O 527 527	0	0

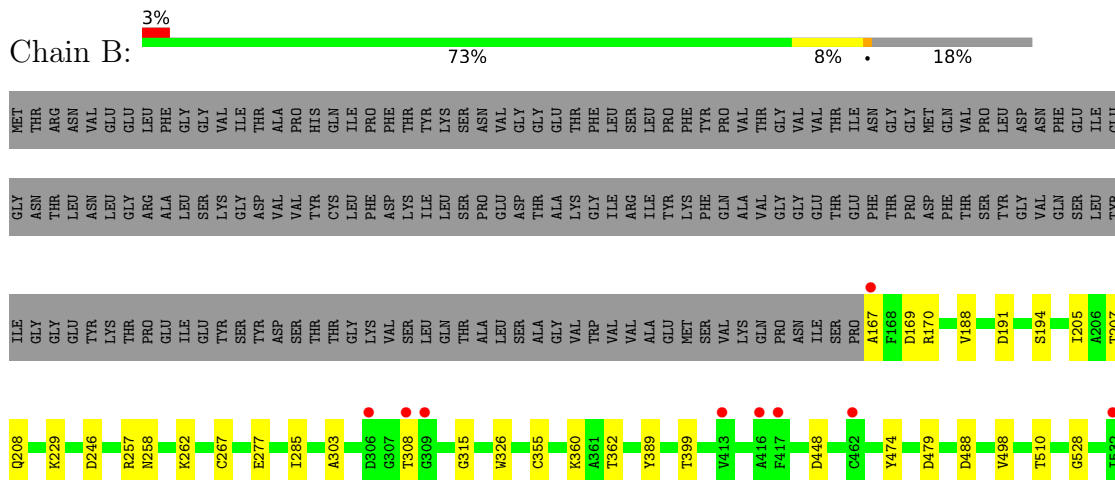
3 Residue-property plots [i](#)

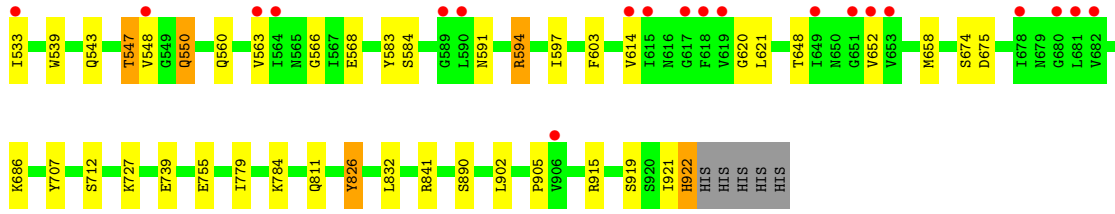
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Tail fiber

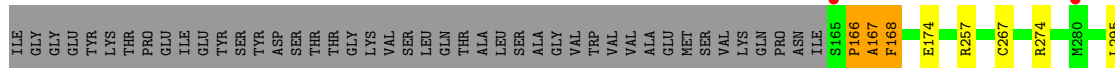
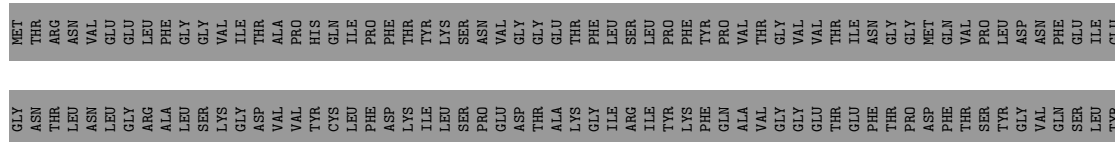
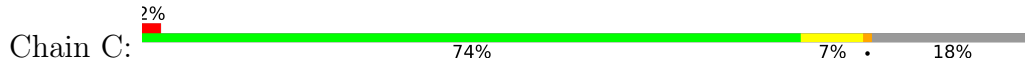


- Molecule 1: Tail fiber

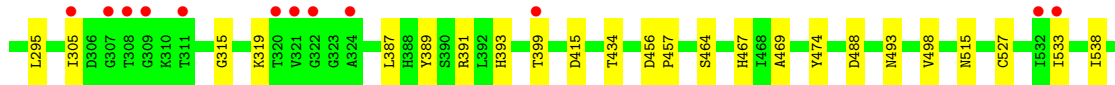
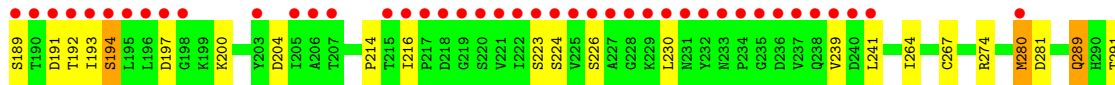
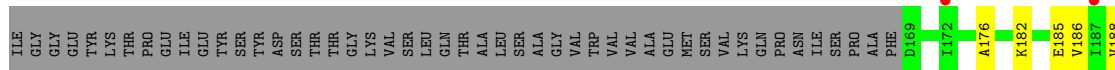
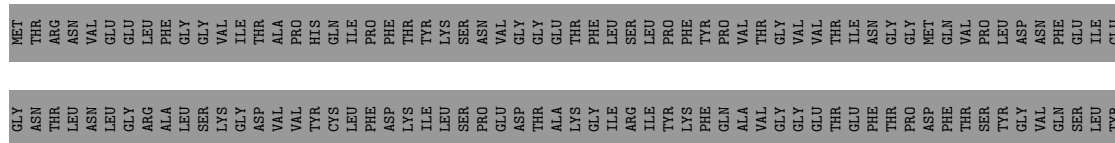


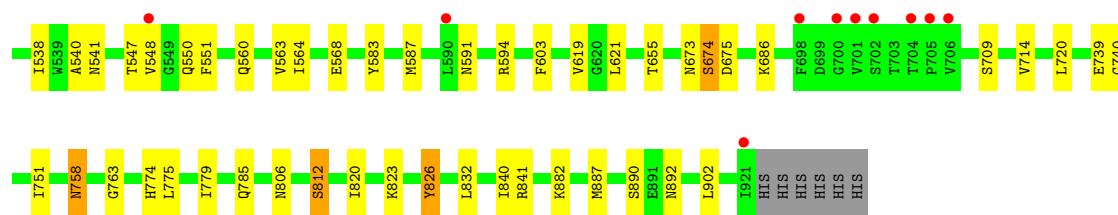


● Molecule 1: Tail fiber



● Molecule 1: Tail fiber





4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.99Å 259.01Å 269.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.36 – 1.90 48.36 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.36-1.90) 99.8 (48.36-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.167 , 0.188 0.169 , 0.189	Depositor DCC
R_{free} test set	23018 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtrriage
Anisotropy	0.131	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.003 for -h,l,k	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	38610	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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: CL, SO4, GOL, CO3, EDO

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	0.60	1/5848 (0.0%)	0.88	5/7962 (0.1%)
1	B	0.59	0/5833	0.90	3/7940 (0.0%)
1	C	0.59	1/5822 (0.0%)	0.92	4/7927 (0.1%)
1	D	0.54	0/5814	0.81	1/7915 (0.0%)
1	E	0.54	0/5783	0.82	3/7872 (0.0%)
1	F	0.52	0/5753	0.82	4/7831 (0.1%)
All	All	0.57	2/34853 (0.0%)	0.86	20/47447 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	473	GLU	CD-OE1	-5.45	1.19	1.25
1	C	174	GLU	CD-OE1	5.10	1.31	1.25

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	493	ASN	CB-CA-C	-10.65	89.10	110.40
1	F	257	ARG	CB-CG-CD	7.65	131.49	111.60
1	A	333	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	B	826	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	A	826	TYR	CB-CG-CD2	-6.21	117.27	121.00

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	5708	0	5592	54	0
1	B	5697	0	5584	62	0
1	C	5697	0	5569	57	0
1	D	5687	0	5559	58	0
1	E	5663	0	5532	46	0
1	F	5643	0	5506	59	0
2	A	150	0	200	27	0
2	B	96	0	128	12	0
2	C	126	0	168	23	0
2	D	30	0	40	3	0
2	E	42	0	56	8	0
2	F	24	0	32	4	0
3	A	25	0	0	0	0
3	B	20	0	0	1	0
3	C	20	0	0	3	0
3	D	20	0	0	1	0
3	E	20	0	0	0	0
3	F	20	0	0	0	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	D	3	0	0	0	0
5	A	4	0	0	0	0
5	D	4	0	0	0	0
6	A	4	0	6	2	0
6	B	4	0	6	0	0
6	C	12	0	18	1	0
7	A	802	0	0	17	1
7	B	793	0	0	17	1
7	C	759	0	0	17	0
7	D	502	0	0	6	0
7	E	504	0	0	8	0
7	F	527	0	0	6	0
All	All	38610	0	33996	332	1

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 5.

The worst 5 of 332 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:388:HIS:NE2	2:A:1005:GOL:H12	1.70	1.06
2:A:1020:GOL:H12	7:A:1688:HOH:O	1.57	1.02
1:C:497:GLN:OE1	2:C:1021:GOL:H12	1.60	0.98
1:C:257:ARG:HD2	2:C:1009:GOL:H32	1.45	0.97
2:C:1018:GOL:H31	7:C:1687:HOH:O	1.67	0.94

All (1) 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)
7:A:1168:HOH:O	7:B:1680:HOH:O[1_455]	2.06	0.14

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	766/927 (83%)	726 (95%)	39 (5%)	1 (0%)	51 42
1	B	764/927 (82%)	730 (96%)	32 (4%)	2 (0%)	41 31
1	C	763/927 (82%)	727 (95%)	32 (4%)	4 (0%)	29 18
1	D	761/927 (82%)	724 (95%)	36 (5%)	1 (0%)	51 42
1	E	758/927 (82%)	721 (95%)	35 (5%)	2 (0%)	41 31
1	F	754/927 (81%)	718 (95%)	35 (5%)	1 (0%)	51 42
All	All	4566/5562 (82%)	4346 (95%)	209 (5%)	11 (0%)	47 38

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	167	ALA
1	F	315	GLY

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Mol	Chain	Res	Type
1	B	315	GLY
1	C	308	THR
1	C	315	GLY

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	636/770 (83%)	621 (98%)	15 (2%)	49	43
1	B	634/770 (82%)	620 (98%)	14 (2%)	52	47
1	C	633/770 (82%)	622 (98%)	11 (2%)	60	57
1	D	632/770 (82%)	618 (98%)	14 (2%)	52	47
1	E	629/770 (82%)	611 (97%)	18 (3%)	42	35
1	F	625/770 (81%)	613 (98%)	12 (2%)	57	53
All	All	3789/4620 (82%)	3705 (98%)	84 (2%)	52	47

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	272	ASP
1	E	915	ARG
1	E	280	MET
1	E	547	THR
1	F	488	ASP

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

Mol	Chain	Res	Type
1	D	806	ASN
1	E	661	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 117 ligands modelled in this entry, 7 are monoatomic - leaving 110 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
2	GOL	B	1013	-	5,5,5	0.11	0	5,5,5	0.38	0
2	GOL	A	1018	-	5,5,5	0.21	0	5,5,5	0.23	0
6	EDO	A	1035	-	3,3,3	0.34	0	2,2,2	0.50	0
3	SO4	B	1001	-	4,4,4	0.36	0	6,6,6	0.63	0
3	SO4	C	1023	-	4,4,4	0.42	0	6,6,6	0.56	0
2	GOL	A	1021	-	5,5,5	0.13	0	5,5,5	0.43	0
3	SO4	F	1006	-	4,4,4	0.29	0	6,6,6	0.17	0
2	GOL	B	1006	-	5,5,5	0.23	0	5,5,5	0.47	0
2	GOL	B	1008	-	5,5,5	0.44	0	5,5,5	1.69	1 (20%)
3	SO4	C	1025	-	4,4,4	0.35	0	6,6,6	0.47	0
2	GOL	C	1016	-	5,5,5	0.12	0	5,5,5	0.32	0
2	GOL	A	1015	-	5,5,5	0.11	0	5,5,5	0.53	0
2	GOL	D	1011	-	5,5,5	0.17	0	5,5,5	0.31	0
2	GOL	C	1018	-	5,5,5	0.39	0	5,5,5	1.01	0
2	GOL	A	1006	-	5,5,5	0.08	0	5,5,5	0.42	0
2	GOL	A	1019	-	5,5,5	0.15	0	5,5,5	0.34	0
3	SO4	A	1032	-	4,4,4	0.43	0	6,6,6	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	E	1002	-	5,5,5	0.24	0	5,5,5	0.57	0
2	GOL	E	1008	-	5,5,5	0.24	0	5,5,5	0.59	0
2	GOL	A	1008	-	5,5,5	0.40	0	5,5,5	0.76	0
2	GOL	A	1011	-	5,5,5	0.61	0	5,5,5	1.03	0
2	GOL	C	1009	-	5,5,5	0.24	0	5,5,5	0.50	0
2	GOL	C	1017	-	5,5,5	0.25	0	5,5,5	0.86	0
2	GOL	C	1013	-	5,5,5	0.12	0	5,5,5	0.94	0
2	GOL	A	1020	-	5,5,5	0.32	0	5,5,5	0.84	0
2	GOL	C	1004	-	5,5,5	0.16	0	5,5,5	0.58	0
6	EDO	C	1026	-	3,3,3	0.30	0	2,2,2	1.42	0
2	GOL	E	1004	-	5,5,5	0.21	0	5,5,5	0.42	0
2	GOL	B	1007	-	5,5,5	0.24	0	5,5,5	0.39	0
3	SO4	E	1011	-	4,4,4	0.29	0	6,6,6	0.29	0
2	GOL	D	1001	-	5,5,5	0.10	0	5,5,5	0.79	0
2	GOL	A	1022	-	5,5,5	0.15	0	5,5,5	0.35	0
2	GOL	B	1010	-	5,5,5	0.10	0	5,5,5	0.28	0
2	GOL	A	1003	-	5,5,5	0.23	0	5,5,5	1.64	1 (20%)
2	GOL	A	1016	-	5,5,5	0.10	0	5,5,5	0.44	0
2	GOL	C	1022	-	5,5,5	0.45	0	5,5,5	0.86	0
3	SO4	D	1003	-	4,4,4	0.33	0	6,6,6	0.16	0
2	GOL	E	1005	-	5,5,5	0.11	0	5,5,5	0.60	0
2	GOL	C	1008	-	5,5,5	0.11	0	5,5,5	0.43	0
3	SO4	B	1019	-	4,4,4	0.40	0	6,6,6	0.21	0
2	GOL	E	1007	-	5,5,5	0.11	0	5,5,5	0.42	0
3	SO4	E	1009	-	4,4,4	0.40	0	6,6,6	0.16	0
2	GOL	D	1009	-	5,5,5	0.37	0	5,5,5	0.62	0
2	GOL	B	1016	-	5,5,5	0.22	0	5,5,5	0.65	0
2	GOL	B	1011	-	5,5,5	0.24	0	5,5,5	0.70	0
2	GOL	C	1005	-	5,5,5	0.31	0	5,5,5	1.33	1 (20%)
2	GOL	C	1012	-	5,5,5	0.23	0	5,5,5	0.42	0
3	SO4	D	1004	-	4,4,4	0.26	0	6,6,6	0.40	0
2	GOL	B	1014	-	5,5,5	0.45	0	5,5,5	0.94	0
2	GOL	B	1003	-	5,5,5	0.22	0	5,5,5	0.32	0
2	GOL	C	1020	-	5,5,5	0.10	0	5,5,5	0.33	0
3	SO4	C	1002	-	4,4,4	0.35	0	6,6,6	0.30	0
2	GOL	B	1002	-	5,5,5	0.26	0	5,5,5	1.22	1 (20%)
3	SO4	A	1027	-	4,4,4	0.41	0	6,6,6	0.38	0
3	SO4	D	1012	-	4,4,4	0.37	0	6,6,6	0.37	0
2	GOL	D	1010	-	5,5,5	0.39	0	5,5,5	0.72	0
2	GOL	D	1002	-	5,5,5	0.35	0	5,5,5	0.66	0
2	GOL	A	1033	-	5,5,5	0.15	0	5,5,5	0.26	0
3	SO4	A	1034	-	4,4,4	0.47	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	1017	-	5,5,5	0.10	0	5,5,5	0.32	0
2	GOL	C	1007	-	5,5,5	0.11	0	5,5,5	0.52	0
2	GOL	F	1003	-	5,5,5	0.19	0	5,5,5	0.71	0
2	GOL	B	1012	-	5,5,5	0.16	0	5,5,5	0.49	0
6	EDO	B	1022	-	3,3,3	0.29	0	2,2,2	0.67	0
2	GOL	A	1014	-	5,5,5	0.15	0	5,5,5	0.52	0
2	GOL	B	1005	-	5,5,5	0.25	0	5,5,5	1.07	0
2	GOL	F	1001	-	5,5,5	0.20	0	5,5,5	0.39	0
2	GOL	A	1002	-	5,5,5	0.42	0	5,5,5	0.60	0
3	SO4	D	1013	-	4,4,4	0.40	0	6,6,6	0.30	0
2	GOL	E	1006	-	5,5,5	0.13	0	5,5,5	0.24	0
3	SO4	E	1001	-	4,4,4	0.29	0	6,6,6	0.45	0
2	GOL	F	1002	-	5,5,5	0.10	0	5,5,5	0.69	0
6	EDO	C	1027	-	3,3,3	0.24	0	2,2,2	1.74	0
2	GOL	A	1010	-	5,5,5	0.13	0	5,5,5	0.31	0
2	GOL	A	1009	-	5,5,5	0.17	0	5,5,5	0.80	0
3	SO4	B	1020	-	4,4,4	0.21	0	6,6,6	0.46	0
5	CO3	A	1031	-	2,3,3	0.58	0	2,3,3	0.43	0
3	SO4	A	1025	-	4,4,4	0.40	0	6,6,6	0.42	0
3	SO4	B	1018	-	4,4,4	0.30	0	6,6,6	0.45	0
5	CO3	D	1007	-	2,3,3	0.75	0	2,3,3	0.26	0
2	GOL	C	1010	-	5,5,5	0.17	0	5,5,5	0.39	0
3	SO4	E	1010	-	4,4,4	0.27	0	6,6,6	0.19	0
2	GOL	C	1021	-	5,5,5	0.50	0	5,5,5	0.97	0
3	SO4	F	1007	-	4,4,4	0.27	0	6,6,6	0.18	0
2	GOL	A	1004	-	5,5,5	0.21	0	5,5,5	0.67	0
2	GOL	C	1011	-	5,5,5	0.08	0	5,5,5	0.42	0
2	GOL	B	1004	-	5,5,5	0.08	0	5,5,5	0.40	0
2	GOL	C	1015	-	5,5,5	0.15	0	5,5,5	0.31	0
2	GOL	C	1003	-	5,5,5	0.46	0	5,5,5	1.36	0
2	GOL	C	1014	-	5,5,5	0.09	0	5,5,5	0.34	0
3	SO4	C	1024	-	4,4,4	0.29	0	6,6,6	0.36	0
2	GOL	F	1004	-	5,5,5	0.17	0	5,5,5	0.50	0
2	GOL	A	1001	-	5,5,5	0.49	0	5,5,5	0.84	0
2	GOL	E	1003	-	5,5,5	0.15	0	5,5,5	0.32	0
6	EDO	C	1028	-	3,3,3	0.13	0	2,2,2	0.68	0
3	SO4	F	1005	-	4,4,4	0.18	0	6,6,6	0.44	0
2	GOL	A	1024	-	5,5,5	0.18	0	5,5,5	0.59	0
2	GOL	A	1007	-	5,5,5	0.11	0	5,5,5	0.41	0
2	GOL	C	1019	-	5,5,5	0.14	0	5,5,5	0.44	0
2	GOL	A	1013	-	5,5,5	0.24	0	5,5,5	1.28	1 (20%)
2	GOL	C	1001	-	5,5,5	0.16	0	5,5,5	0.50	0
2	GOL	A	1005	-	5,5,5	0.43	0	5,5,5	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	1012	-	5,5,5	0.55	0	5,5,5	0.88	0
3	SO4	A	1026	-	4,4,4	0.31	0	6,6,6	0.64	0
2	GOL	C	1006	-	5,5,5	0.31	0	5,5,5	0.98	0
2	GOL	B	1009	-	5,5,5	0.16	0	5,5,5	0.45	0
2	GOL	B	1015	-	5,5,5	0.22	0	5,5,5	0.54	0
2	GOL	A	1023	-	5,5,5	0.27	0	5,5,5	1.10	0
2	GOL	A	1017	-	5,5,5	0.19	0	5,5,5	0.23	0
3	SO4	F	1008	-	4,4,4	0.31	0	6,6,6	0.16	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	1013	-	-	0/4/4/4	-
2	GOL	A	1018	-	-	2/4/4/4	-
6	EDO	A	1035	-	-	1/1/1/1	-
2	GOL	A	1021	-	-	0/4/4/4	-
2	GOL	B	1006	-	-	0/4/4/4	-
2	GOL	B	1008	-	-	0/4/4/4	-
2	GOL	C	1016	-	-	0/4/4/4	-
2	GOL	A	1015	-	-	1/4/4/4	-
2	GOL	D	1011	-	-	4/4/4/4	-
2	GOL	C	1018	-	-	2/4/4/4	-
2	GOL	A	1006	-	-	3/4/4/4	-
2	GOL	A	1019	-	-	4/4/4/4	-
2	GOL	E	1002	-	-	0/4/4/4	-
2	GOL	E	1008	-	-	0/4/4/4	-
2	GOL	A	1008	-	-	4/4/4/4	-
2	GOL	A	1011	-	-	2/4/4/4	-
2	GOL	C	1009	-	-	1/4/4/4	-
2	GOL	C	1017	-	-	2/4/4/4	-
2	GOL	C	1013	-	-	2/4/4/4	-
2	GOL	A	1020	-	-	4/4/4/4	-
2	GOL	C	1004	-	-	0/4/4/4	-
6	EDO	C	1026	-	-	1/1/1/1	-
2	GOL	E	1004	-	-	2/4/4/4	-
2	GOL	B	1007	-	-	0/4/4/4	-
2	GOL	D	1001	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	1022	-	-	2/4/4/4	-
2	GOL	B	1010	-	-	3/4/4/4	-
2	GOL	A	1003	-	-	3/4/4/4	-
2	GOL	A	1016	-	-	4/4/4/4	-
2	GOL	C	1022	-	-	4/4/4/4	-
2	GOL	E	1005	-	-	2/4/4/4	-
2	GOL	C	1008	-	-	2/4/4/4	-
2	GOL	E	1007	-	-	2/4/4/4	-
2	GOL	D	1009	-	-	0/4/4/4	-
2	GOL	B	1016	-	-	1/4/4/4	-
2	GOL	B	1011	-	-	0/4/4/4	-
2	GOL	C	1005	-	-	2/4/4/4	-
2	GOL	C	1012	-	-	4/4/4/4	-
2	GOL	B	1014	-	-	2/4/4/4	-
2	GOL	B	1003	-	-	0/4/4/4	-
2	GOL	C	1020	-	-	3/4/4/4	-
2	GOL	B	1002	-	-	4/4/4/4	-
2	GOL	D	1010	-	-	0/4/4/4	-
2	GOL	D	1002	-	-	0/4/4/4	-
2	GOL	A	1033	-	-	4/4/4/4	-
2	GOL	B	1017	-	-	4/4/4/4	-
2	GOL	C	1007	-	-	2/4/4/4	-
2	GOL	F	1003	-	-	3/4/4/4	-
2	GOL	B	1012	-	-	2/4/4/4	-
6	EDO	B	1022	-	-	1/1/1/1	-
2	GOL	A	1014	-	-	2/4/4/4	-
2	GOL	B	1005	-	-	2/4/4/4	-
2	GOL	F	1001	-	-	2/4/4/4	-
2	GOL	A	1002	-	-	0/4/4/4	-
2	GOL	E	1006	-	-	2/4/4/4	-
6	EDO	C	1027	-	-	1/1/1/1	-
2	GOL	F	1002	-	-	2/4/4/4	-
2	GOL	A	1010	-	-	4/4/4/4	-
2	GOL	A	1009	-	-	2/4/4/4	-
2	GOL	C	1010	-	-	2/4/4/4	-
2	GOL	C	1021	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	1004	-	-	0/4/4/4	-
2	GOL	C	1011	-	-	0/4/4/4	-
2	GOL	B	1004	-	-	0/4/4/4	-
2	GOL	C	1015	-	-	4/4/4/4	-
2	GOL	C	1003	-	-	4/4/4/4	-
2	GOL	C	1014	-	-	1/4/4/4	-
2	GOL	F	1004	-	-	2/4/4/4	-
2	GOL	A	1001	-	-	0/4/4/4	-
2	GOL	E	1003	-	-	3/4/4/4	-
6	EDO	C	1028	-	-	1/1/1/1	-
2	GOL	A	1024	-	-	3/4/4/4	-
2	GOL	A	1007	-	-	0/4/4/4	-
2	GOL	C	1019	-	-	2/4/4/4	-
2	GOL	A	1013	-	-	2/4/4/4	-
2	GOL	C	1001	-	-	1/4/4/4	-
2	GOL	A	1005	-	-	3/4/4/4	-
2	GOL	A	1012	-	-	2/4/4/4	-
2	GOL	C	1006	-	-	3/4/4/4	-
2	GOL	B	1009	-	-	0/4/4/4	-
2	GOL	B	1015	-	-	2/4/4/4	-
2	GOL	A	1023	-	-	4/4/4/4	-
2	GOL	A	1017	-	-	0/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1008	GOL	O2-C2-C3	-2.87	96.49	109.12
2	A	1003	GOL	O2-C2-C1	2.71	121.08	109.12
2	A	1013	GOL	O2-C2-C3	2.31	119.28	109.12
2	C	1005	GOL	O3-C3-C2	-2.28	99.25	110.20
2	B	1002	GOL	O2-C2-C3	2.22	118.89	109.12

There are no chirality outliers.

5 of 150 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1005	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	A	1006	GOL	C1-C2-C3-O3
2	A	1008	GOL	O1-C1-C2-O2
2	A	1008	GOL	O1-C1-C2-C3
2	A	1008	GOL	C1-C2-C3-O3

There are no ring outliers.

51 monomers are involved in 83 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1018	GOL	1	0
6	A	1035	EDO	2	0
3	B	1001	SO4	1	0
2	A	1021	GOL	3	0
2	B	1008	GOL	3	0
3	C	1025	SO4	1	0
2	C	1018	GOL	4	0
2	E	1008	GOL	1	0
2	A	1008	GOL	2	0
2	A	1011	GOL	2	0
2	C	1009	GOL	2	0
2	C	1017	GOL	1	0
2	C	1013	GOL	1	0
2	A	1020	GOL	4	0
6	C	1026	EDO	1	0
2	E	1004	GOL	1	0
2	B	1007	GOL	1	0
2	A	1022	GOL	3	0
2	B	1010	GOL	1	0
2	A	1016	GOL	1	0
2	C	1022	GOL	1	0
2	E	1005	GOL	1	0
2	C	1008	GOL	2	0
2	E	1007	GOL	2	0
2	C	1005	GOL	1	0
2	C	1020	GOL	1	0
3	D	1012	SO4	1	0
2	D	1010	GOL	3	0
2	A	1033	GOL	1	0
2	B	1012	GOL	1	0
2	A	1014	GOL	1	0
2	E	1006	GOL	1	0
2	F	1002	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1009	GOL	1	0
2	C	1010	GOL	2	0
2	C	1021	GOL	3	0
2	B	1004	GOL	4	0
2	C	1015	GOL	1	0
2	C	1003	GOL	2	0
2	C	1014	GOL	1	0
3	C	1024	SO4	2	0
2	F	1004	GOL	3	0
2	E	1003	GOL	2	0
2	A	1024	GOL	1	0
2	A	1007	GOL	1	0
2	A	1013	GOL	1	0
2	C	1001	GOL	1	0
2	A	1005	GOL	4	0
2	A	1012	GOL	1	0
2	B	1009	GOL	1	0
2	B	1015	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	757/927 (81%)	-0.00	47 (6%) 20 23	18, 25, 61, 89	0
1	B	756/927 (81%)	-0.02	29 (3%) 40 43	19, 26, 46, 96	0
1	C	758/927 (81%)	-0.19	19 (2%) 57 60	20, 27, 47, 88	0
1	D	755/927 (81%)	0.29	77 (10%) 6 8	27, 37, 77, 121	0
1	E	754/927 (81%)	0.11	57 (7%) 13 15	24, 37, 74, 114	1 (0%)
1	F	753/927 (81%)	-0.14	13 (1%) 70 72	27, 38, 56, 88	0
All	All	4533/5562 (81%)	0.01	242 (5%) 26 29	18, 33, 61, 121	1 (0%)

The worst 5 of 242 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	237	VAL	8.2
1	D	216	ILE	7.0
1	D	235	GLY	6.6
1	D	232	TYR	6.3
1	D	222	ILE	6.3

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 monosaccharides 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	B	1013	6/6	0.71	0.29	82,84,96,96	0
2	GOL	C	1001	6/6	0.72	0.34	55,67,73,74	0
2	GOL	A	1008	6/6	0.73	0.22	47,58,62,67	0
2	GOL	C	1011	6/6	0.73	0.28	56,74,80,81	0
2	GOL	C	1021	6/6	0.73	0.31	29,53,56,56	0
2	GOL	C	1009	6/6	0.78	0.21	61,70,75,75	0
2	GOL	B	1017	6/6	0.78	0.12	59,64,71,82	0
2	GOL	A	1012	6/6	0.78	0.18	45,49,56,57	0
2	GOL	C	1017	6/6	0.80	0.18	46,62,75,79	0
2	GOL	B	1006	6/6	0.80	0.52	65,83,86,86	0
2	GOL	D	1010	6/6	0.80	0.18	41,56,58,58	0
2	GOL	A	1022	6/6	0.81	0.27	64,68,74,83	0
2	GOL	C	1018	6/6	0.81	0.18	41,45,57,60	0
2	GOL	A	1023	6/6	0.81	0.12	60,63,65,68	0
2	GOL	C	1013	6/6	0.81	0.13	52,54,66,66	0
4	CL	B	1021	1/1	0.82	0.14	71,71,71,71	0
2	GOL	B	1014	6/6	0.83	0.15	49,60,61,62	0
2	GOL	B	1015	6/6	0.83	0.46	60,66,71,77	0
2	GOL	A	1019	6/6	0.83	0.20	63,75,82,99	0
2	GOL	E	1002	6/6	0.84	0.14	67,68,71,71	0
2	GOL	E	1003	6/6	0.84	0.17	48,58,61,63	0
2	GOL	C	1008	6/6	0.84	0.21	59,71,75,80	0
2	GOL	A	1024	6/6	0.85	0.18	50,59,70,74	0
2	GOL	A	1014	6/6	0.86	0.22	58,68,73,78	0
2	GOL	E	1004	6/6	0.86	0.18	50,55,66,68	0
2	GOL	E	1008	6/6	0.86	0.31	56,70,74,87	0
2	GOL	A	1007	6/6	0.86	0.15	51,59,64,69	0
2	GOL	A	1010	6/6	0.87	0.17	59,62,70,80	0
2	GOL	A	1021	6/6	0.87	0.38	54,70,80,83	0
2	GOL	B	1010	6/6	0.88	0.18	60,71,75,80	0
2	GOL	B	1012	6/6	0.88	0.19	67,74,85,87	0
2	GOL	A	1005	6/6	0.88	0.13	40,40,49,49	0
2	GOL	F	1003	6/6	0.88	0.12	43,57,61,70	0
2	GOL	B	1007	6/6	0.88	0.18	48,61,67,78	0
5	CO3	A	1031	4/4	0.88	0.14	55,59,62,67	0
2	GOL	A	1020	6/6	0.89	0.31	50,64,67,81	0
2	GOL	C	1005	6/6	0.89	0.15	38,40,41,45	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	A	1017	6/6	0.89	0.18	48,66,68,78	0
2	GOL	B	1011	6/6	0.89	0.18	45,50,59,62	0
2	GOL	A	1015	6/6	0.89	0.15	52,66,73,75	0
2	GOL	C	1012	6/6	0.89	0.14	47,54,61,66	0
2	GOL	C	1015	6/6	0.90	0.21	62,69,77,78	0
2	GOL	A	1004	6/6	0.90	0.17	30,59,66,68	0
2	GOL	A	1011	6/6	0.90	0.18	34,41,48,54	0
2	GOL	C	1014	6/6	0.90	0.39	47,64,70,89	0
6	EDO	B	1022	4/4	0.90	0.47	58,58,62,64	0
6	EDO	C	1028	4/4	0.90	0.08	56,59,64,71	0
2	GOL	A	1006	6/6	0.91	0.11	50,63,66,68	0
2	GOL	F	1002	6/6	0.91	0.13	51,62,65,67	0
2	GOL	A	1033	6/6	0.91	0.10	51,57,65,65	0
2	GOL	F	1004	6/6	0.91	0.12	48,56,64,65	0
3	SO4	A	1026	5/5	0.91	0.15	20,25,37,38	5
3	SO4	F	1008	5/5	0.91	0.14	70,88,95,111	0
2	GOL	D	1011	6/6	0.91	0.13	55,65,73,85	0
2	GOL	C	1007	6/6	0.91	0.10	49,56,65,68	0
2	GOL	B	1005	6/6	0.91	0.14	43,49,51,53	0
2	GOL	C	1020	6/6	0.91	0.15	52,67,70,74	0
2	GOL	B	1016	6/6	0.92	0.24	38,45,58,63	0
2	GOL	C	1016	6/6	0.92	0.14	45,58,69,85	0
3	SO4	D	1004	5/5	0.92	0.14	67,78,85,118	0
2	GOL	B	1008	6/6	0.92	0.17	32,43,48,55	0
2	GOL	B	1009	6/6	0.92	0.12	57,63,69,74	0
2	GOL	A	1003	6/6	0.92	0.14	33,37,43,43	0
2	GOL	C	1006	6/6	0.92	0.22	41,51,54,58	0
6	EDO	C	1026	4/4	0.92	0.16	35,63,63,63	0
2	GOL	A	1009	6/6	0.92	0.19	57,61,70,71	0
2	GOL	C	1010	6/6	0.93	0.23	62,66,69,76	0
6	EDO	A	1035	4/4	0.93	0.12	44,47,56,60	0
2	GOL	B	1004	6/6	0.93	0.21	47,59,62,63	0
2	GOL	D	1001	6/6	0.93	0.13	50,58,61,64	0
2	GOL	A	1018	6/6	0.93	0.20	48,51,58,71	0
3	SO4	D	1003	5/5	0.94	0.11	36,37,39,48	5
2	GOL	C	1022	6/6	0.94	0.15	32,41,55,65	0
3	SO4	E	1011	5/5	0.94	0.14	75,81,92,111	0
2	GOL	A	1013	6/6	0.94	0.13	36,39,44,48	0
2	GOL	E	1007	6/6	0.94	0.17	40,58,61,73	0
2	GOL	D	1002	6/6	0.94	0.24	43,53,56,60	0
2	GOL	D	1009	6/6	0.94	0.14	41,47,50,55	0
2	GOL	C	1019	6/6	0.94	0.29	46,61,65,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	B	1002	6/6	0.94	0.09	40,42,50,51	0
6	EDO	C	1027	4/4	0.94	0.08	46,53,54,60	0
2	GOL	A	1016	6/6	0.94	0.18	38,50,60,68	0
3	SO4	B	1020	5/5	0.95	0.10	21,23,31,32	5
2	GOL	E	1006	6/6	0.95	0.14	42,58,64,71	0
2	GOL	F	1001	6/6	0.95	0.15	41,50,53,56	0
3	SO4	D	1012	5/5	0.95	0.11	34,42,43,51	5
3	SO4	E	1010	5/5	0.95	0.15	67,86,95,102	0
2	GOL	A	1001	6/6	0.95	0.12	34,37,38,42	0
3	SO4	F	1005	5/5	0.95	0.12	42,46,49,52	5
3	SO4	F	1007	5/5	0.95	0.11	55,55,58,66	5
4	CL	D	1006	1/1	0.96	0.18	56,56,56,56	0
2	GOL	B	1003	6/6	0.96	0.08	36,38,39,41	0
5	CO3	D	1007	4/4	0.96	0.10	67,69,79,84	0
2	GOL	A	1002	6/6	0.96	0.30	25,26,27,28	6
3	SO4	C	1024	5/5	0.96	0.10	35,37,44,49	5
2	GOL	E	1005	6/6	0.96	0.18	52,55,61,65	0
2	GOL	C	1003	6/6	0.96	0.19	32,34,40,41	0
2	GOL	C	1004	6/6	0.96	0.08	29,38,43,50	0
3	SO4	E	1001	5/5	0.97	0.08	41,50,55,65	5
3	SO4	E	1009	5/5	0.97	0.09	50,53,57,65	5
4	CL	A	1030	1/1	0.97	0.05	61,61,61,61	0
3	SO4	A	1027	5/5	0.97	0.07	53,56,59,74	0
3	SO4	B	1001	5/5	0.97	0.08	33,34,44,51	5
3	SO4	C	1025	5/5	0.97	0.10	55,56,69,91	0
3	SO4	A	1032	5/5	0.98	0.18	52,63,77,78	0
3	SO4	B	1018	5/5	0.98	0.06	46,50,67,71	0
3	SO4	B	1019	5/5	0.98	0.08	58,59,65,82	0
3	SO4	A	1034	5/5	0.98	0.07	30,34,39,44	5
3	SO4	F	1006	5/5	0.98	0.15	64,71,86,92	0
3	SO4	C	1002	5/5	0.98	0.09	44,45,49,55	0
3	SO4	D	1013	5/5	0.98	0.15	61,73,80,92	0
4	CL	A	1029	1/1	0.98	0.13	40,40,40,40	0
3	SO4	C	1023	5/5	0.98	0.10	41,47,54,62	5
4	CL	D	1008	1/1	0.99	0.12	41,41,41,41	0
3	SO4	A	1025	5/5	0.99	0.08	45,54,65,70	0
4	CL	D	1005	1/1	1.00	0.14	30,30,30,30	0
4	CL	A	1028	1/1	1.00	0.16	22,22,22,22	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.