



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:03 AM UTC

PDB ID : 6W4Q / pdb_00006w4q
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 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

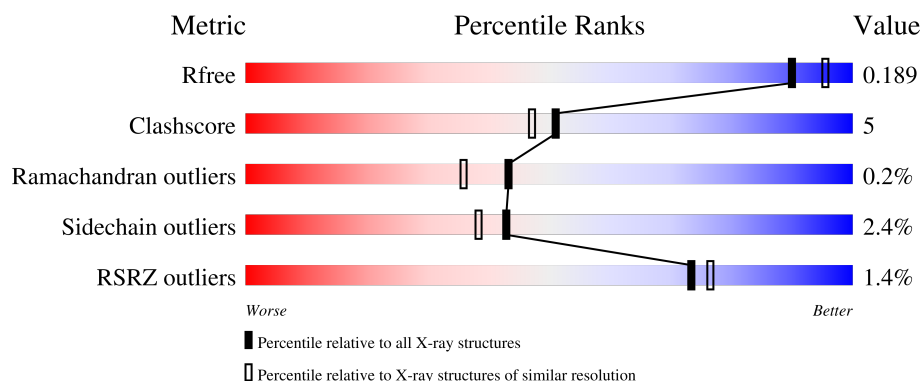
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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	2% 73% 9% 18%
1	B	927	2% 72% 9% 18%
1	C	927	2% 72% 8% 18%
1	D	927	2% 72% 9% 19%
1	E	927	2% 72% 8% 19%

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Mol	Chain	Length	Quality of chain
1	F	927	 71% 9% 19%

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

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

There are 36 discrepancies between the modelled and reference sequences:

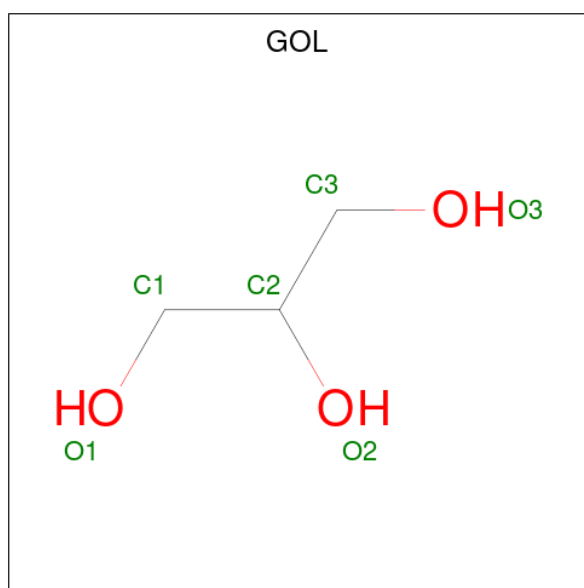
Chain	Residue	Modelled	Actual	Comment	Reference
A	922	HIS	-	expression tag	UNP G3M190
A	923	HIS	-	expression tag	UNP G3M190
A	924	HIS	-	expression tag	UNP G3M190
A	925	HIS	-	expression tag	UNP G3M190
A	926	HIS	-	expression tag	UNP G3M190
A	927	HIS	-	expression tag	UNP G3M190
B	922	HIS	-	expression tag	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 (CCD ID: 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		
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	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		
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		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	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		

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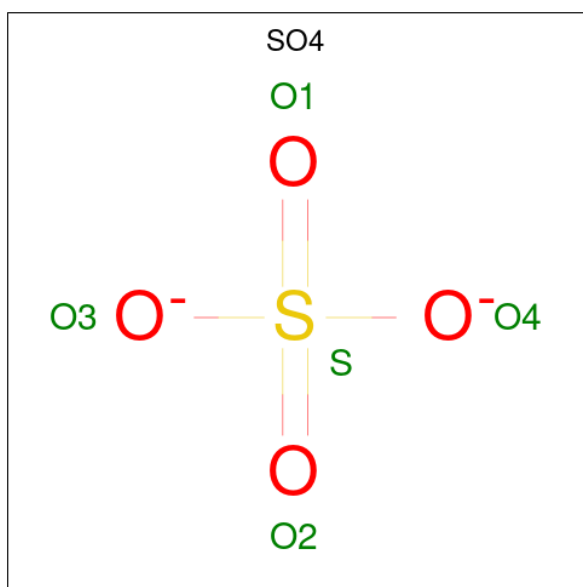
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total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

- Molecule 3 is SULFATE ION (CCD ID: 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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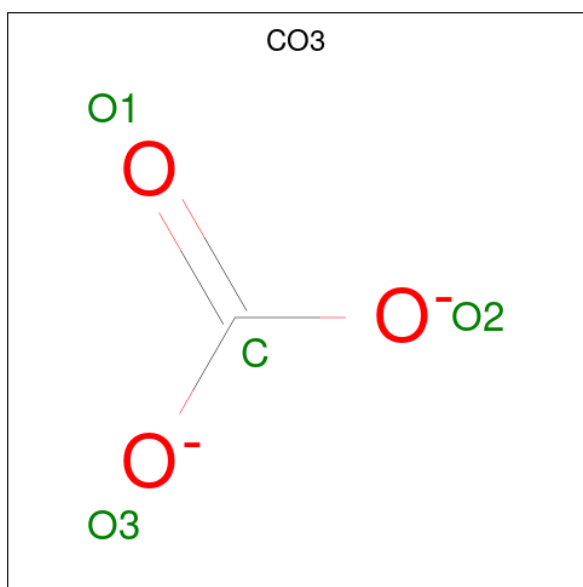
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

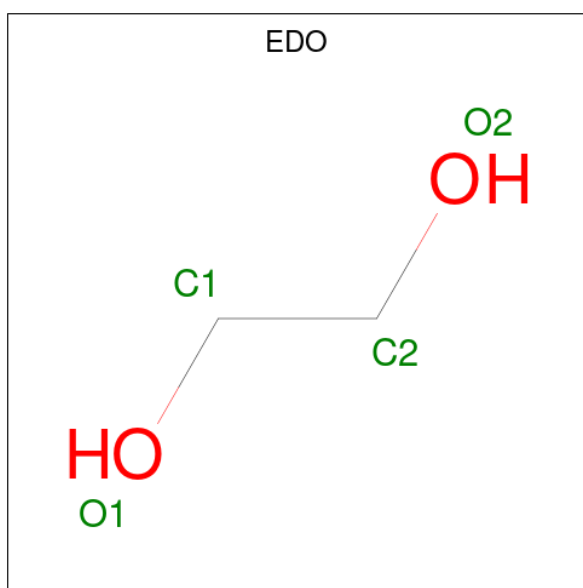
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Cl 3 3	0	0
4	B	1	Total Cl 1 1	0	0
4	D	3	Total Cl 3 3	0	0

- Molecule 5 is CARBONATE ION (CCD ID: 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 (CCD ID: EDO) (formula: C₂H₆O₂).



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	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		

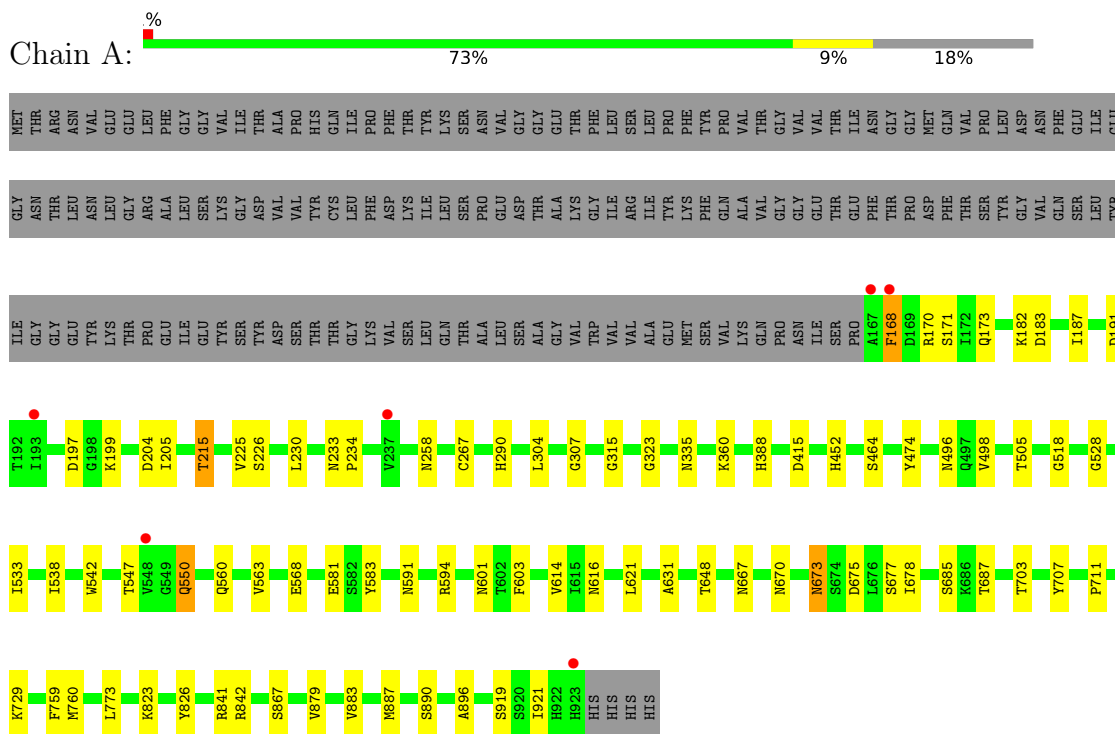
- Molecule 7 is water.

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

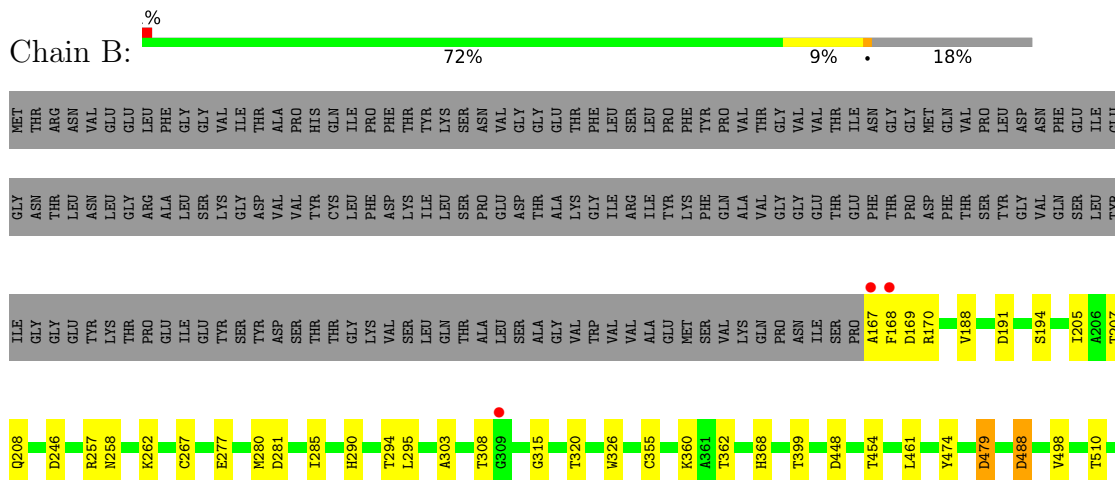
3 Residue-property plots [i](#)

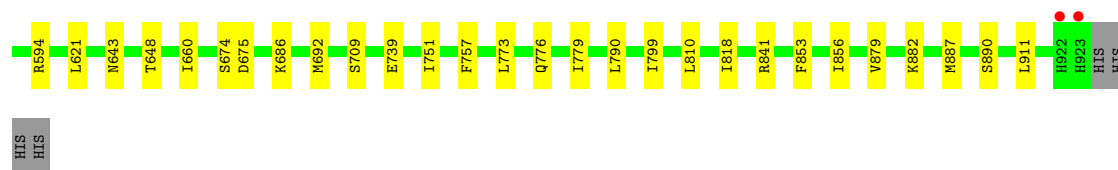
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

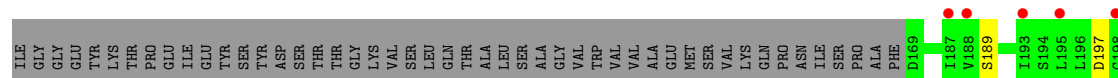
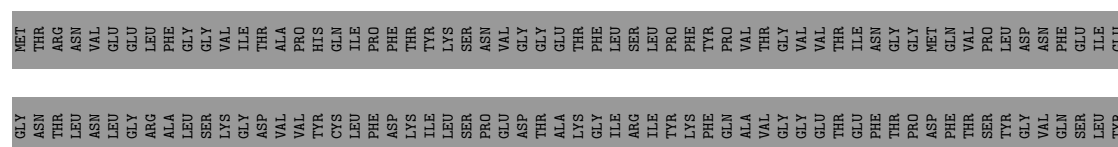


• Molecule 1: Tail fiber

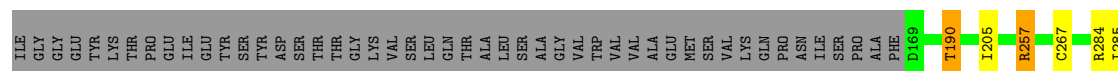
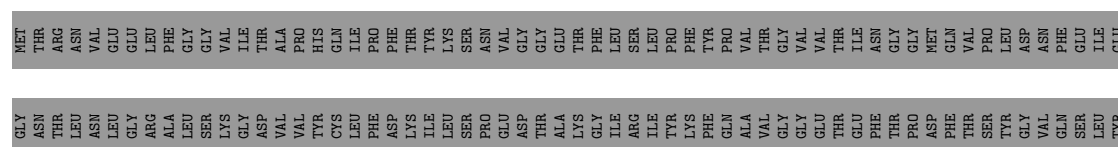




• Molecule 1: Tail fiber



• Molecule 1: Tail fiber



4 Data and refinement statistics

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) 99.7 (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)	Xtriage
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 (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,l,k	Xtriage
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

Xtriage'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: EDO, CO3, SO4, CL, 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	0.78	2/5848 (0.0%)	1.15	9/7962 (0.1%)
1	B	0.78	2/5833 (0.0%)	1.22	20/7940 (0.3%)
1	C	0.78	1/5822 (0.0%)	1.24	25/7927 (0.3%)
1	D	0.74	0/5814	1.11	7/7915 (0.1%)
1	E	0.75	1/5783 (0.0%)	1.12	6/7872 (0.1%)
1	F	0.71	0/5753	1.13	14/7831 (0.2%)
All	All	0.76	6/34853 (0.0%)	1.16	81/47447 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	368	HIS	CE1-NE2	5.71	1.38	1.32
1	A	452	HIS	CE1-NE2	5.53	1.38	1.32
1	C	452	HIS	CE1-NE2	5.52	1.38	1.32
1	E	497	GLN	CA-C	5.42	1.55	1.52
1	B	290	HIS	CE1-NE2	5.40	1.38	1.32
1	A	290	HIS	CE1-NE2	5.10	1.37	1.32

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	493	ASN	CB-CA-C	-9.22	89.10	109.56
1	F	257	ARG	CB-CG-CD	8.78	131.49	111.30
1	C	739	GLU	CB-CG-CD	8.16	126.47	112.60
1	C	786	THR	CA-CB-OG1	-7.33	98.60	109.60
1	B	258	ASN	CB-CA-C	-6.96	98.85	110.68
1	F	510	THR	CA-CB-OG1	-6.96	99.16	109.60
1	F	758	ASN	CB-CA-C	-6.94	99.65	111.31
1	A	258	ASN	CB-CA-C	-6.39	100.13	110.74
1	C	168	PHE	CB-CA-C	-6.35	99.49	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	883	VAL	N-CA-CB	-6.34	103.62	110.53
1	F	674	SER	N-CA-CB	6.33	119.05	110.38
1	B	294	THR	N-CA-C	-6.29	107.45	114.62
1	B	281	ASP	CB-CA-C	6.21	120.03	109.53
1	F	697	THR	CA-CB-OG1	-6.17	100.34	109.60
1	A	215	THR	CB-CA-C	6.12	119.68	109.89
1	F	488	ASP	CB-CA-C	6.06	119.08	110.24
1	B	921	ILE	CA-C-N	5.95	132.40	121.70
1	B	921	ILE	C-N-CA	5.95	132.40	121.70
1	B	168	PHE	N-CA-C	-5.91	104.46	112.26
1	F	566	GLY	CA-C-N	-5.91	115.80	122.48
1	F	566	GLY	C-N-CA	-5.91	115.80	122.48
1	B	454	THR	CA-C-N	5.90	129.22	120.90
1	B	454	THR	C-N-CA	5.90	129.22	120.90
1	E	215	THR	CA-CB-OG1	-5.90	100.75	109.60
1	A	703	THR	CA-CB-OG1	-5.88	100.79	109.60
1	F	190	THR	CA-CB-OG1	-5.87	100.80	109.60
1	B	820	ILE	CA-C-N	-5.86	118.05	122.33
1	B	820	ILE	C-N-CA	-5.86	118.05	122.33
1	A	550	GLN	CB-CG-CD	5.84	122.53	112.60
1	F	872	GLY	CA-C-N	5.81	125.50	119.92
1	F	872	GLY	C-N-CA	5.81	125.50	119.92
1	C	835	GLN	CB-CG-CD	5.80	122.47	112.60
1	A	258	ASN	CA-CB-CG	-5.74	106.86	112.60
1	D	335	ASN	CB-CA-C	5.74	117.94	109.22
1	F	704	THR	CB-CA-C	-5.73	103.56	110.15
1	C	281	ASP	CB-CA-C	5.70	119.16	109.53
1	B	752	SER	CA-C-N	-5.67	112.63	123.29
1	B	752	SER	C-N-CA	-5.67	112.63	123.29
1	B	583	TYR	CB-CA-C	-5.62	100.53	109.80
1	C	735	THR	CA-CB-OG1	-5.57	101.25	109.60
1	C	192	THR	CA-CB-OG1	-5.54	101.29	109.60
1	A	267	CYS	CB-CA-C	5.51	118.84	109.53
1	B	922	HIS	CA-CB-CG	5.49	119.29	113.80
1	E	205	ILE	CA-C-N	5.48	127.56	120.44
1	E	205	ILE	C-N-CA	5.48	127.56	120.44
1	D	550	GLN	CB-CG-CD	5.45	121.87	112.60
1	B	479	ASP	CA-CB-CG	-5.44	107.16	112.60
1	A	673	ASN	CB-CA-C	-5.42	101.41	110.56
1	D	488	ASP	CA-CB-CG	-5.41	107.19	112.60
1	C	547	THR	CA-C-N	-5.41	115.61	122.37
1	C	547	THR	C-N-CA	-5.41	115.61	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	836	THR	CA-CB-OG1	-5.40	101.50	109.60
1	B	488	ASP	CB-CA-C	5.38	118.10	110.24
1	E	267	CYS	CB-CA-C	-5.38	99.63	109.54
1	C	742	THR	CA-CB-OG1	-5.38	101.53	109.60
1	C	750	THR	CA-CB-OG1	-5.35	101.57	109.60
1	A	335	ASN	CB-CA-C	5.34	117.34	109.22
1	A	667	ASN	CA-CB-CG	-5.33	107.27	112.60
1	C	791	LEU	CA-C-N	-5.33	118.03	121.65
1	C	791	LEU	C-N-CA	-5.33	118.03	121.65
1	F	694	GLU	CB-CG-CD	5.31	121.62	112.60
1	C	223	SER	N-CA-C	-5.28	106.90	113.55
1	C	601	ASN	CB-CA-C	-5.22	104.31	111.73
1	D	591	ASN	CA-C-N	-5.21	115.43	122.77
1	D	591	ASN	C-N-CA	-5.21	115.43	122.77
1	C	704	THR	CA-CB-OG1	-5.16	101.86	109.60
1	B	686	LYS	CA-C-N	-5.16	114.56	122.87
1	B	686	LYS	C-N-CA	-5.16	114.56	122.87
1	F	583	TYR	CB-CA-C	-5.12	100.49	109.71
1	E	258	ASN	CB-CA-C	-5.11	102.64	110.81
1	C	493	ASN	CA-CB-CG	5.09	117.69	112.60
1	C	428	THR	CA-CB-OG1	-5.09	101.97	109.60
1	D	247	SER	CA-C-N	5.06	127.02	120.44
1	D	247	SER	C-N-CA	5.06	127.02	120.44
1	C	796	THR	CA-CB-OG1	-5.05	102.03	109.60
1	C	166	PRO	CB-CA-C	-5.04	103.25	111.56
1	B	320	THR	CA-CB-OG1	-5.03	102.05	109.60
1	C	295	LEU	CA-C-N	-5.01	114.80	122.87
1	C	295	LEU	C-N-CA	-5.01	114.80	122.87
1	C	905	PRO	N-CA-CB	-5.01	99.11	103.32
1	E	272	ASP	CA-CB-CG	5.01	117.61	112.60

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	61	0
1	B	5697	0	5584	65	0
1	C	5697	0	5569	63	0
1	D	5687	0	5559	62	0
1	E	5663	0	5532	48	0
1	F	5643	0	5506	61	0
2	A	150	0	200	27	0
2	B	96	0	128	13	0
2	C	126	0	168	23	0
2	D	30	0	40	3	0
2	E	42	0	56	7	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	18	1
7	B	793	0	0	18	1
7	C	759	0	0	18	0
7	D	502	0	0	7	0
7	E	504	0	0	9	0
7	F	527	0	0	6	0
All	All	38610	0	33996	356	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.

All (356) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:1020:GOL:H31	7:C:1641:HOH:O	1.71	0.88
1:A:168:PHE:HD1	1:A:168:PHE:H	1.19	0.86
2:C:1022:GOL:H11	7:C:1486:HOH:O	1.78	0.81
1:B:915:ARG:NH1	1:B:922:HIS:HB3	1.95	0.81
1:B:399[B]:THR:HG21	7:B:1342:HOH:O	1.82	0.78
1:F:391:ARG:HH22	2:F:1004:GOL:H12	1.47	0.78
1:A:170:ARG:HH21	1:A:173:GLN:HG2	1.48	0.78
3:C:1025:SO4:O4	7:C:1101:HOH:O	2.01	0.76
2:C:1018:GOL:H12	7:C:1491:HOH:O	1.86	0.75
1:A:168:PHE:HD1	1:A:168:PHE:N	1.84	0.75
7:E:1213:HOH:O	2:F:1004:GOL:H32	1.87	0.75
2:B:1012:GOL:H32	7:B:1619:HOH:O	1.85	0.74
1:A:711:PRO:HA	6:A:1035:EDO:H21	1.70	0.72
1:D:493:ASN:OD1	1:D:515[A]:ASN:ND2	2.24	0.71
1:C:307:GLY:HA3	1:C:323:GLY:O	1.90	0.71
1:B:594:ARG:HH22	2:B:1008:GOL:H32	1.55	0.71
1:C:305:ILE:O	7:C:1102:HOH:O	2.08	0.71
3:D:1012:SO4:O3	1:F:583:TYR:OH	2.10	0.69
1:D:391:ARG:HH12	2:D:1010:GOL:C1	2.05	0.68
1:A:168:PHE:N	1:A:168:PHE:CD1	2.55	0.68
1:C:467:HIS:NE2	1:C:493:ASN:OD1	2.24	0.68
2:A:1008:GOL:H31	7:A:1490:HOH:O	1.94	0.68
1:D:751:ILE:HG23	1:D:779:ILE:HD13	1.75	0.67
1:F:190:THR:HG23	1:F:205:ILE:HG12	1.75	0.67
1:C:257:ARG:HD2	2:C:1009:GOL:C3	2.22	0.67
2:E:1007:GOL:H31	7:E:1398:HOH:O	1.94	0.67
1:B:597:ILE:HD12	2:B:1008:GOL:H31	1.77	0.65
1:B:727[A]:LYS:HE2	7:B:1130:HOH:O	1.96	0.65
1:C:274:ARG:HD2	7:C:1228:HOH:O	1.97	0.65
2:A:1009:GOL:H31	7:A:1236:HOH:O	1.97	0.65
1:C:751:ILE:HG23	1:C:779:ILE:HD12	1.79	0.65
1:A:687:THR:O	2:A:1024:GOL:H31	1.95	0.65
1:C:597:ILE:HD12	2:C:1018:GOL:H32	1.79	0.64
1:B:167:ALA:HA	7:B:1224:HOH:O	1.96	0.64
1:A:583:TYR:OH	3:B:1001:SO4:O4	2.17	0.63
1:B:188:VAL:HG22	7:B:1485:HOH:O	1.99	0.63
1:B:547:THR:HB	7:B:1268:HOH:O	1.97	0.62
1:A:614[B]:VAL:CG2	1:B:652:VAL:HG23	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:621:LEU:HD23	1:B:621:LEU:C	2.24	0.62
1:C:308:THR:N	7:C:1105:HOH:O	2.33	0.62
1:E:214:PRO:O	1:E:216:ILE:HG13	1.99	0.62
1:E:189:SER:OG	1:E:205:ILE:HG22	2.00	0.62
1:F:493:ASN:OD1	1:F:515[B]:ASN:ND2	2.32	0.61
1:D:751:ILE:HG23	1:D:779:ILE:CD1	2.30	0.61
1:B:399[B]:THR:CG2	7:B:1342:HOH:O	2.46	0.61
1:F:376:LYS:HE2	7:F:1217:HOH:O	2.00	0.61
1:C:497:GLN:OE1	2:C:1021:GOL:C1	2.44	0.60
1:D:515[A]:ASN:HB2	1:D:538:ILE:HG13	1.83	0.60
1:C:758:ASN:HD21	2:C:1008:GOL:H12	1.66	0.60
1:E:307:GLY:O	1:E:310:LYS:HB2	2.01	0.60
1:B:303:ALA:HB2	1:B:326:TRP:CZ3	2.36	0.60
1:D:391:ARG:HH12	2:D:1010:GOL:H12	1.66	0.60
1:D:643:ASN:HA	1:D:674:SER:HB3	1.83	0.60
1:F:376:LYS:CE	7:F:1217:HOH:O	2.49	0.59
1:C:308:THR:HA	7:C:1145:HOH:O	2.01	0.59
1:B:277:GLU:OE1	7:B:1101:HOH:O	2.16	0.59
1:A:631:ALA:HB1	2:A:1011:GOL:H2	1.84	0.58
1:B:712:SER:H	2:B:1007:GOL:H2	1.69	0.58
1:E:530:GLY:HA3	1:E:562:MET:HE1	1.84	0.58
1:A:887:MET:HE3	7:A:1295:HOH:O	2.02	0.58
1:D:176:ALA:HB2	1:D:186:VAL:HG21	1.85	0.58
1:E:648[A]:THR:HG22	7:E:1179:HOH:O	2.03	0.58
1:A:533:ILE:HG21	1:B:533:ILE:HG22	1.85	0.57
1:D:887:MET:HG3	1:F:686:LYS:HA	1.87	0.57
1:F:267[A]:CYS:SG	1:F:285:ILE:HD11	2.45	0.57
1:F:779:ILE:CD1	1:F:785:GLN:HG2	2.33	0.57
1:E:621:LEU:C	1:E:621:LEU:HD23	2.30	0.57
1:A:187:ILE:HB	1:A:199:LYS:HE3	1.86	0.56
1:A:542:TRP:CH2	2:A:1016:GOL:H11	2.40	0.56
1:D:853:PHE:HB3	1:D:856:ILE:HD12	1.85	0.56
1:E:675:ASP:OD2	1:F:890:SER:HB3	2.06	0.56
1:D:182:LYS:HE2	1:E:207:THR:O	2.05	0.56
2:A:1021:GOL:H2	7:A:1445:HOH:O	2.06	0.56
1:D:790:LEU:HD22	1:D:799:ILE:HG12	1.86	0.56
1:D:648[A]:THR:HG22	7:D:1124:HOH:O	2.05	0.56
1:D:289:GLN:HG3	1:D:291:THR:O	2.06	0.55
1:D:191:ASP:OD1	1:D:191:ASP:C	2.48	0.55
1:D:686:LYS:HA	1:E:887:MET:HG3	1.88	0.55
1:C:695:THR:HB	6:C:1026:EDO:H22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1003:GOL:H2	7:C:1255:HOH:O	2.05	0.55
2:A:1011:GOL:O2	7:A:1101:HOH:O	2.18	0.55
1:D:890:SER:HB3	1:F:675:ASP:OD2	2.06	0.55
1:B:543:GLN:HG2	7:B:1136:HOH:O	2.07	0.55
2:B:1004:GOL:C1	7:B:1655:HOH:O	2.54	0.54
1:B:811:GLN:HG3	7:B:1841:HOH:O	2.06	0.54
1:F:739[A]:GLU:CD	1:F:739[A]:GLU:H	2.15	0.54
1:C:621:LEU:C	1:C:621:LEU:HD23	2.33	0.54
1:C:166:PRO:O	1:C:168:PHE:N	2.33	0.54
1:D:621:LEU:HD23	1:D:621:LEU:C	2.33	0.54
1:B:548:VAL:HG23	1:B:548:VAL:O	2.06	0.54
1:D:393:HIS:CD2	7:D:1472:HOH:O	2.60	0.54
1:A:673:ASN:ND2	1:B:739[A]:GLU:OE1	2.41	0.54
1:C:751:ILE:HG23	1:C:779:ILE:CD1	2.38	0.53
1:F:621:LEU:C	1:F:621:LEU:HD23	2.33	0.53
1:A:583:TYR:CE1	2:A:1013:GOL:H32	2.44	0.53
1:E:560:GLN:HA	1:E:583:TYR:O	2.09	0.53
1:A:550:GLN:H	2:A:1021:GOL:H31	1.74	0.53
1:A:621:LEU:C	1:A:621:LEU:HD23	2.34	0.53
1:D:675:ASP:OD2	1:E:890:SER:HB3	2.09	0.53
1:F:461:LEU:C	1:F:461:LEU:HD12	2.33	0.53
1:B:887:MET:HE3	7:B:1181:HOH:O	2.08	0.53
2:B:1004:GOL:H12	7:B:1655:HOH:O	2.09	0.52
1:D:192:THR:HG23	1:D:193:ILE:HG23	1.92	0.52
1:D:739[B]:GLU:OE2	1:F:673:ASN:ND2	2.40	0.52
1:B:675:ASP:OD2	1:C:890:SER:HB3	2.09	0.52
1:E:274:ARG:HG2	1:E:319:LYS:O	2.09	0.52
1:E:594:ARG:HH22	2:E:1004:GOL:H2	1.73	0.52
2:B:1009:GOL:H11	7:C:1391:HOH:O	2.09	0.52
1:B:658:MET:HE3	7:B:1335:HOH:O	2.09	0.52
1:F:779:ILE:HD13	1:F:785:GLN:HG2	1.89	0.52
1:F:840:ILE:HG23	2:F:1002:GOL:H12	1.92	0.52
7:B:1620:HOH:O	1:C:739:GLU:HB3	2.10	0.52
2:E:1006:GOL:H12	7:E:1485:HOH:O	2.10	0.52
1:B:686:LYS:HA	1:C:887:MET:HG3	1.90	0.52
2:C:1010:GOL:C3	3:C:1024:SO4:O4	2.58	0.52
1:A:225:VAL:O	1:A:226:SER:HB3	2.10	0.51
2:A:1014:GOL:H11	7:A:1451:HOH:O	2.09	0.51
1:A:533:ILE:HG22	1:C:533:ILE:HG21	1.92	0.51
1:C:307:GLY:CA	1:C:323:GLY:O	2.59	0.51
1:E:474:TYR:HA	1:E:498:VAL:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267[A]:CYS:SG	1:B:285:ILE:HD11	2.51	0.51
1:C:547:THR:HA	2:C:1017:GOL:H31	1.93	0.51
1:D:280:MET:O	1:D:305:ILE:HD11	2.11	0.51
1:B:707:TYR:HB2	2:B:1015:GOL:H2	1.92	0.51
1:F:391:ARG:HH22	2:F:1004:GOL:C1	2.20	0.51
1:A:648[B]:THR:HG22	1:A:677:SER:HB3	1.93	0.50
1:B:563:VAL:HG11	1:C:566:GLY:HA2	1.92	0.50
2:A:1005:GOL:H11	1:C:451:PHE:HD1	1.76	0.50
1:A:707:TYR:CG	1:A:919:SER:HA	2.46	0.50
1:C:274:ARG:HG2	1:C:319:LYS:O	2.11	0.50
1:B:755:GLU:OE1	2:B:1010:GOL:H31	2.12	0.50
1:C:687:THR:O	2:C:1013:GOL:H2	2.12	0.50
1:A:191:ASP:OD1	1:A:191:ASP:C	2.55	0.50
1:E:533:ILE:HG21	1:F:533:ILE:CG2	2.42	0.50
1:B:191:ASP:OD2	1:B:194:SER:OG	2.16	0.49
1:B:510[B]:THR:HG22	1:B:533:ILE:HB	1.94	0.49
1:D:533:ILE:HG22	1:F:533:ILE:HG21	1.94	0.49
1:E:711:PRO:HD3	7:E:1505:HOH:O	2.12	0.49
2:A:1022:GOL:O1	7:A:1103:HOH:O	2.20	0.49
1:B:915:ARG:HH11	1:B:922:HIS:HB3	1.74	0.49
1:A:415:ASP:HA	1:A:464:SER:O	2.12	0.49
1:C:809:LYS:HE3	7:C:1219:HOH:O	2.11	0.49
1:B:207:THR:O	1:B:208:GLN:HB2	2.13	0.49
1:B:832:LEU:HD21	1:B:902:LEU:HD22	1.94	0.49
1:A:170:ARG:HH12	1:B:170:ARG:H	1.61	0.49
1:E:686:LYS:HA	1:F:887:MET:HG3	1.95	0.49
1:E:755:GLU:OE2	1:E:877:SER:OG	2.30	0.49
1:F:763:GLY:HA2	7:F:1270:HOH:O	2.12	0.48
1:F:528:GLY:HA2	1:F:560:GLN:O	2.12	0.48
1:B:257:ARG:HH22	1:B:262:LYS:NZ	2.12	0.48
1:F:751:ILE:H	1:F:812:SER:HG	1.55	0.48
1:E:643:ASN:HA	1:E:674:SER:HB3	1.94	0.48
1:C:775:LEU:HD22	1:C:820:ILE:CG2	2.44	0.48
1:C:840:ILE:HG23	2:C:1005:GOL:H12	1.94	0.48
1:D:547:THR:HB	7:D:1228:HOH:O	2.13	0.48
1:E:568:GLU:HA	1:E:591:ASN:O	2.14	0.47
1:F:332:ASP:O	1:F:360:LYS:HD2	2.15	0.47
2:A:1005:GOL:H2	7:C:1296:HOH:O	2.13	0.47
1:B:533:ILE:HG21	1:C:533:ILE:HG22	1.96	0.47
2:A:1022:GOL:H31	7:A:1485:HOH:O	2.14	0.47
1:F:550:GLN:HG3	1:F:603:PHE:CE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:740:GLY:HA3	1:F:823:LYS:HB3	1.97	0.47
1:B:594:ARG:NH2	2:B:1008:GOL:H32	2.25	0.47
1:A:614[B]:VAL:HG21	1:B:652:VAL:HG23	1.96	0.47
1:C:874:ASP:OD2	2:C:1008:GOL:H11	2.15	0.47
1:D:568:GLU:OE2	1:F:529:ASN:HB3	2.15	0.47
1:E:779:ILE:HD13	1:E:785:GLN:HG2	1.97	0.47
1:F:568:GLU:HA	1:F:591:ASN:O	2.15	0.47
1:D:391:ARG:HH22	2:D:1010:GOL:H12	1.79	0.47
1:E:278:PRO:HG2	1:E:305:ILE:HD13	1.96	0.47
1:D:274:ARG:HG2	1:D:319:LYS:O	2.15	0.47
1:F:449:TYR:CD1	1:F:449:TYR:C	2.93	0.47
1:F:456:ASP:CG	1:F:457:PRO:HD2	2.40	0.47
1:F:751:ILE:N	1:F:812:SER:OG	2.30	0.47
1:A:170:ARG:NH1	1:B:170:ARG:H	2.13	0.47
1:B:474:TYR:HA	1:B:498:VAL:O	2.15	0.47
1:A:601:ASN:HD22	2:A:1020:GOL:H11	1.81	0.46
1:B:568:GLU:HA	1:B:591:ASN:O	2.15	0.46
1:C:473:GLU:HG2	2:C:1021:GOL:H2	1.96	0.46
1:D:230:LEU:HB2	1:D:241:LEU:HD21	1.97	0.46
1:E:369:TYR:HA	1:E:393:HIS:O	2.15	0.46
1:F:510:THR:HG23	7:F:1418:HOH:O	2.15	0.46
2:C:1015:GOL:H12	7:C:1538:HOH:O	2.15	0.46
1:D:264:ILE:HB	1:F:284:ARG:HH21	1.80	0.46
1:E:707:TYR:CG	1:E:919:SER:HA	2.50	0.46
1:A:533:ILE:HG21	1:B:533:ILE:CG2	2.44	0.46
2:A:1020:GOL:H31	7:A:1482:HOH:O	2.14	0.46
1:D:533:ILE:HG21	1:E:533:ILE:CG2	2.45	0.46
1:E:319:LYS:NZ	7:E:1113:HOH:O	2.48	0.46
1:E:510:THR:HG23	7:E:1473:HOH:O	2.15	0.46
1:E:283:GLN:O	1:E:302:ARG:HA	2.15	0.46
1:D:911:LEU:C	1:D:911:LEU:HD23	2.41	0.46
1:F:564:ILE:O	1:F:587:MET:HA	2.15	0.46
1:D:456:ASP:CG	1:D:457:PRO:HD2	2.41	0.46
1:C:887:MET:HE3	7:C:1327:HOH:O	2.15	0.46
1:D:773:LEU:C	1:D:773:LEU:HD23	2.41	0.46
1:F:547:THR:HB	7:F:1239:HOH:O	2.15	0.46
1:A:823:LYS:HG2	1:A:826:TYR:HB3	1.99	0.45
1:B:399[B]:THR:HG22	7:B:1461:HOH:O	2.16	0.45
1:A:890:SER:HB3	1:C:675:ASP:OD2	2.16	0.45
1:C:564:ILE:O	1:C:587:MET:HA	2.16	0.45
1:C:648[A]:THR:HG22	7:C:1333:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:614:VAL:HG23	1:E:648[B]:THR:OG1	2.15	0.45
1:E:840:ILE:HG23	2:E:1005:GOL:H2	1.98	0.45
1:C:469:ALA:HA	1:C:493:ASN:O	2.17	0.45
1:B:584:SER:HB2	1:C:619:VAL:HB	1.97	0.45
1:F:714:VAL:O	1:F:882:LYS:NZ	2.50	0.45
1:A:550:GLN:HG3	1:A:603:PHE:CE1	2.51	0.45
1:A:568:GLU:OE1	1:C:529:ASN:HB3	2.16	0.45
1:B:915:ARG:NH1	1:B:922:HIS:CB	2.75	0.45
1:D:191:ASP:OD1	1:D:194:SER:HB2	2.16	0.45
1:B:539:TRP:CE2	2:B:1004:GOL:H31	2.52	0.45
1:E:413:VAL:HG12	1:E:415:ASP:HB2	1.98	0.45
1:A:550:GLN:N	2:A:1021:GOL:H31	2.30	0.45
1:B:461:LEU:HD12	1:B:461:LEU:C	2.42	0.45
1:B:308:THR:HA	7:B:1581:HOH:O	2.16	0.45
1:B:448:ASP:HB2	2:C:1001:GOL:H2	1.99	0.45
1:A:773:LEU:C	1:A:773:LEU:HD23	2.42	0.44
1:E:388:HIS:NE2	2:E:1003:GOL:H12	2.32	0.44
2:E:1007:GOL:C3	7:E:1398:HOH:O	2.60	0.44
1:F:474:TYR:HA	1:F:498:VAL:O	2.17	0.44
2:A:1033:GOL:H32	7:A:1490:HOH:O	2.17	0.44
1:D:280:MET:H	1:D:280:MET:HG2	1.40	0.44
1:E:512:ILE:O	1:E:535:GLY:HA2	2.17	0.44
1:D:195:LEU:C	1:D:197:ASP:H	2.26	0.44
1:B:921:ILE:C	2:B:1016:GOL:H32	2.42	0.44
1:C:415:ASP:HA	1:C:464:SER:O	2.16	0.44
1:E:245:GLU:HB2	2:E:1008:GOL:H2	2.00	0.44
1:B:550:GLN:HG3	1:B:603:PHE:CE1	2.53	0.44
1:A:538:ILE:HD12	2:A:1008:GOL:H2	2.00	0.44
1:D:216:ILE:O	1:D:216:ILE:HD12	2.18	0.44
1:C:169:ASP:OD1	1:C:169:ASP:C	2.60	0.44
1:D:474:TYR:HA	1:D:498:VAL:O	2.18	0.44
1:C:568:GLU:HA	1:C:591:ASN:O	2.18	0.43
1:C:754:ALA:HA	1:C:779:ILE:O	2.18	0.43
1:D:464:SER:HA	1:D:488:ASP:O	2.18	0.43
1:D:515[A]:ASN:HA	1:D:538:ILE:O	2.18	0.43
1:E:533:ILE:HG21	1:F:533:ILE:HG22	2.01	0.43
1:F:413:VAL:HG12	1:F:415:ASP:HB2	2.00	0.43
1:B:921:ILE:O	1:B:922:HIS:HB3	2.18	0.43
1:D:566:GLY:HA2	1:F:563:VAL:HG11	2.00	0.43
1:A:921:ILE:HG22	1:A:921:ILE:O	2.19	0.43
6:A:1035:EDO:H22	7:D:1530:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:THR:C	1:C:322:GLY:H	2.26	0.43
1:C:757:PHE:O	1:C:776:GLN:HA	2.19	0.43
1:F:911:LEU:C	1:F:911:LEU:HD23	2.43	0.43
2:A:1018:GOL:O1	1:B:246:ASP:HA	2.18	0.43
1:D:185:GLU:OE2	1:D:200:LYS:HD2	2.18	0.43
1:A:204:ASP:OD1	1:A:204:ASP:C	2.62	0.43
1:E:515[A]:ASN:HB2	1:E:538:ILE:HG13	2.01	0.43
1:A:496:ASN:O	1:A:518:GLY:HA3	2.18	0.43
1:B:188:VAL:HB	1:B:205:ILE:HD11	2.00	0.43
2:B:1004:GOL:H11	7:B:1655:HOH:O	2.18	0.43
1:A:678:ILE:HG12	1:A:896:ALA:HB1	2.01	0.43
1:C:915:ARG:HA	1:C:915:ARG:HD3	1.91	0.43
1:C:807:ASP:OD1	1:C:807:ASP:N	2.52	0.43
1:E:493:ASN:HA	1:E:515[B]:ASN:O	2.18	0.43
1:F:415:ASP:HA	1:F:464:SER:O	2.19	0.43
1:A:307:GLY:HA3	1:A:323:GLY:O	2.19	0.42
1:F:315:GLY:HA3	1:F:339:PHE:CD2	2.53	0.42
2:A:1022:GOL:C3	7:A:1485:HOH:O	2.67	0.42
1:D:295:LEU:O	1:D:295:LEU:HG	2.19	0.42
1:C:274:ARG:O	1:C:320:THR:HA	2.19	0.42
1:E:302:ARG:HD2	1:F:295:LEU:HD11	2.00	0.42
1:E:773:LEU:HD23	1:E:773:LEU:C	2.44	0.42
1:C:310:LYS:HB2	1:C:319:LYS:HE3	2.01	0.42
1:D:773:LEU:HA	1:D:790:LEU:O	2.19	0.42
1:A:560:GLN:HA	1:A:583:TYR:O	2.19	0.42
1:A:759:PHE:HB3	1:A:760:MET:HE3	2.01	0.42
1:C:521:CYS:SG	1:C:540:ALA:HB2	2.60	0.42
1:D:223:SER:O	1:D:224:SER:HB3	2.18	0.42
1:E:280:MET:O	1:E:283:GLN:HB2	2.20	0.42
1:E:376:LYS:CE	7:E:1131:HOH:O	2.68	0.42
1:B:528:GLY:HA2	1:B:560:GLN:O	2.19	0.42
1:F:469:ALA:HA	1:F:493:ASN:O	2.20	0.42
1:F:547:THR:HG21	1:F:551:PHE:CE2	2.55	0.42
1:A:601:ASN:HD22	2:A:1020:GOL:C1	2.33	0.42
1:B:707:TYR:CG	1:B:919:SER:HA	2.55	0.42
1:B:779:ILE:HA	1:B:784:LYS:O	2.20	0.42
2:C:1014:GOL:H2	7:C:1669:HOH:O	2.19	0.42
1:D:882:LYS:NZ	7:D:1128:HOH:O	2.53	0.42
1:A:670:ASN:ND2	7:A:1142:HOH:O	2.53	0.42
1:B:648:THR:HG22	2:C:1003:GOL:H11	2.02	0.42
1:E:415:ASP:HA	1:E:464:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HD23	1:A:230:LEU:C	2.45	0.41
1:A:528:GLY:HA2	1:A:560:GLN:O	2.20	0.41
1:A:568:GLU:HA	1:A:591:ASN:O	2.20	0.41
1:F:621:LEU:HD12	1:F:655:THR:HG21	2.01	0.41
2:A:1005:GOL:H11	1:C:451:PHE:CD1	2.55	0.41
1:D:399:THR:HA	1:D:434:THR:HG22	2.01	0.41
1:C:307:GLY:O	1:C:308:THR:C	2.63	0.41
1:F:355:CYS:HB3	1:F:362:THR:OG1	2.20	0.41
1:A:711:PRO:HD3	7:A:1683:HOH:O	2.20	0.41
1:A:729:LYS:HE2	1:A:867:SER:CB	2.51	0.41
1:A:887:MET:HG3	1:C:686:LYS:HA	2.02	0.41
1:C:597:ILE:HB	2:C:1018:GOL:H11	2.02	0.41
1:D:393:HIS:HD2	7:D:1472:HOH:O	2.02	0.41
1:F:521:CYS:SG	1:F:540:ALA:HB2	2.60	0.41
1:F:890:SER:OG	1:F:892:ASN:HB3	2.21	0.41
2:A:1012:GOL:H31	7:A:1166:HOH:O	2.19	0.41
1:A:360:LYS:CE	7:A:1576:HOH:O	2.69	0.41
1:B:560:GLN:HA	1:B:583:TYR:O	2.21	0.41
1:D:387:LEU:HD23	1:D:467:HIS:HB2	2.02	0.41
1:F:823:LYS:HB2	1:F:823:LYS:HE2	1.86	0.41
1:D:189:SER:HB3	1:D:204:ASP:HA	2.02	0.41
1:E:449:TYR:OH	1:E:460:ASP:OD2	2.29	0.41
1:F:832:LEU:HD21	1:F:902:LEU:HD22	2.02	0.41
1:A:182:LYS:O	1:A:183:ASP:C	2.63	0.41
1:C:295:LEU:HD12	1:C:295:LEU:HA	1.91	0.41
1:D:527:CYS:O	1:D:559:SER:HA	2.20	0.41
1:F:720:LEU:HD12	1:F:720:LEU:HA	1.87	0.41
1:A:505:THR:HA	1:A:528:GLY:O	2.21	0.41
1:A:675:ASP:OD2	1:B:890:SER:HB3	2.20	0.41
1:A:685:SER:HA	2:A:1007:GOL:H32	2.03	0.41
1:B:614[B]:VAL:HG11	1:C:617:GLY:HA2	2.03	0.41
1:C:347:ASP:OD1	1:C:347:ASP:C	2.62	0.41
1:D:214:PRO:HG2	1:D:239:VAL:HG21	2.02	0.41
1:D:709[A]:SER:HB2	7:D:1103:HOH:O	2.21	0.41
1:D:810:LEU:HD12	1:D:810:LEU:N	2.36	0.41
1:F:459:ARG:HA	1:F:459:ARG:NE	2.35	0.41
1:F:709:SER:HB2	7:F:1174:HOH:O	2.21	0.41
1:C:166:PRO:HB2	1:C:167:ALA:H	1.76	0.41
1:C:191:ASP:OD1	1:C:191:ASP:C	2.63	0.41
1:C:614[B]:VAL:HG13	7:C:1385:HOH:O	2.21	0.41
1:E:550:GLN:HG3	1:E:603:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:ARG:NH1	7:A:1109:HOH:O	2.33	0.40
1:B:915:ARG:HH12	1:B:922:HIS:CG	2.39	0.40
1:D:176:ALA:HB2	1:D:186:VAL:CG2	2.50	0.40
1:D:515[A]:ASN:OD1	1:D:515[A]:ASN:C	2.64	0.40
1:A:233:ASN:HA	1:A:234:PRO:C	2.46	0.40
1:A:616:ASN:HB3	7:A:1105:HOH:O	2.21	0.40
1:B:548:VAL:O	1:B:548:VAL:CG2	2.70	0.40
1:C:474:TYR:HA	1:C:498:VAL:O	2.22	0.40
1:E:469:ALA:HA	1:E:493:ASN:O	2.21	0.40
1:F:775:LEU:HD22	1:F:820:ILE:CG2	2.51	0.40
1:B:355:CYS:HB3	1:B:362:THR:OG1	2.21	0.40
1:D:469:ALA:HA	1:D:493:ASN:O	2.21	0.40
1:D:692:MET:HE2	1:D:692:MET:HB3	1.83	0.40
1:E:355:CYS:HB3	1:E:362:THR:OG1	2.21	0.40
1:F:515[B]:ASN:CB	1:F:538:ILE:HG13	2.52	0.40
1:F:758:ASN:OD1	1:F:774:HIS:HD2	2.04	0.40
1:A:474:TYR:HA	1:A:498:VAL:O	2.21	0.40
1:A:563:VAL:HG11	1:B:566:GLY:HA2	2.02	0.40
1:B:533:ILE:HG21	1:C:533:ILE:CG2	2.50	0.40
1:D:281:ASP:HA	1:D:305:ILE:HD13	2.04	0.40
1:D:757:PHE:O	1:D:776:GLN:HA	2.21	0.40
1:E:584:SER:HB2	1:F:619:VAL:HB	2.04	0.40
1:F:773:LEU:HD23	1:F:773:LEU:C	2.47	0.40
2:C:1010:GOL:H32	3:C:1024:SO4:O4	2.21	0.40
1:D:415:ASP:HA	1:D:464:SER:O	2.21	0.40
1:E:505:THR:HA	1:E:528:GLY:O	2.21	0.40

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%)	48	40
1	B	764/927 (82%)	730 (96%)	32 (4%)	2 (0%)	36	29
1	C	763/927 (82%)	727 (95%)	32 (4%)	4 (0%)	24	16
1	D	761/927 (82%)	724 (95%)	36 (5%)	1 (0%)	48	40
1	E	758/927 (82%)	721 (95%)	35 (5%)	2 (0%)	36	29
1	F	754/927 (81%)	718 (95%)	35 (5%)	1 (0%)	48	40
All	All	4566/5562 (82%)	4346 (95%)	209 (5%)	11 (0%)	43	36

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	167	ALA
1	F	315	GLY
1	B	315	GLY
1	C	308	THR
1	C	315	GLY
1	D	315	GLY
1	E	315	GLY
1	A	315	GLY
1	C	166	PRO
1	B	620	GLY
1	E	620	GLY

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	636/770 (83%)	624 (98%)	12 (2%)	50	47
1	B	634/770 (82%)	622 (98%)	12 (2%)	50	47
1	C	633/770 (82%)	621 (98%)	12 (2%)	50	47
1	D	632/770 (82%)	615 (97%)	17 (3%)	39	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	629/770 (82%)	611 (97%)	18 (3%)	37	31
1	F	625/770 (81%)	607 (97%)	18 (3%)	37	31
All	All	3789/4620 (82%)	3700 (98%)	89 (2%)	43	40

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	PHE
1	A	171	SER
1	A	197	ASP
1	A	205	ILE
1	A	215	THR
1	A	304	LEU
1	A	547	THR
1	A	581	GLU
1	A	594	ARG
1	A	841	ARG
1	A	879	VAL
1	A	883	VAL
1	B	169	ASP
1	B	280	MET
1	B	295	LEU
1	B	360	LYS
1	B	479	ASP
1	B	488	ASP
1	B	547	THR
1	B	594	ARG
1	B	674	SER
1	B	841	ARG
1	B	905	PRO
1	B	922	HIS
1	C	205	ILE
1	C	280	MET
1	C	321	VAL
1	C	488	ASP
1	C	533	ILE
1	C	541	ASN
1	C	547	THR
1	C	594	ARG
1	C	779	ILE
1	C	841	ARG

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Mol	Chain	Res	Type
1	C	883	VAL
1	C	905	PRO
1	D	182	LYS
1	D	188	VAL
1	D	194	SER
1	D	197	ASP
1	D	226	SER
1	D	237	VAL
1	D	267	CYS
1	D	280	MET
1	D	304	LEU
1	D	429	SER
1	D	541	ASN
1	D	547	THR
1	D	594	ARG
1	D	660	ILE
1	D	818	ILE
1	D	841	ARG
1	D	879	VAL
1	E	197	ASP
1	E	205	ILE
1	E	216	ILE
1	E	230	LEU
1	E	236	ASP
1	E	267	CYS
1	E	272	ASP
1	E	279	THR
1	E	280	MET
1	E	399	THR
1	E	479	ASP
1	E	488	ASP
1	E	493	ASN
1	E	547	THR
1	E	594	ARG
1	E	690	GLN
1	E	841	ARG
1	E	883	VAL
1	F	257	ARG
1	F	304	LEU
1	F	465	LYS
1	F	480	SER
1	F	488	ASP

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Mol	Chain	Res	Type
1	F	541	ASN
1	F	547	THR
1	F	548	VAL
1	F	594	ARG
1	F	674	SER
1	F	708	VAL
1	F	806	ASN
1	F	812	SER
1	F	818	ILE
1	F	841	ARG
1	F	883	VAL
1	F	903	ILE
1	F	916	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	372	ASN
1	A	393	HIS
1	A	515	ASN
1	A	588	ASN
1	A	601	ASN
1	A	616	ASN
1	A	626	ASN
1	A	639	GLN
1	A	670	ASN
1	A	758	ASN
1	B	425	GLN
1	B	493	ASN
1	B	639	GLN
1	B	670	ASN
1	B	835	GLN
1	C	268	HIS
1	C	393	HIS
1	C	639	GLN
1	C	690	GLN
1	C	758	ASN
1	C	776	GLN
1	D	372	ASN
1	D	425	GLN
1	D	560	GLN
1	D	565	ASN

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Mol	Chain	Res	Type
1	D	588	ASN
1	D	616	ASN
1	D	670	ASN
1	D	806	ASN
1	E	173	GLN
1	E	233	ASN
1	E	493	ASN
1	E	593	ASN
1	E	670	ASN
1	E	758	ASN
1	E	776	GLN
1	F	372	ASN
1	F	511	ASN
1	F	588	ASN
1	F	616	ASN
1	F	626	ASN
1	F	639	GLN
1	F	718	ASN
1	F	835	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	C	1019	-	5,5,5	0.14	0	5,5,5	0.44	0
6	EDO	B	1022	-	3,3,3	0.29	0	2,2,2	0.62	0
2	GOL	A	1011	-	5,5,5	0.63	0	5,5,5	1.07	0
3	SO4	D	1013	-	4,4,4	0.30	0	6,6,6	0.31	0
2	GOL	F	1004	-	5,5,5	0.17	0	5,5,5	0.52	0
2	GOL	F	1001	-	5,5,5	0.20	0	5,5,5	0.39	0
2	GOL	B	1011	-	5,5,5	0.25	0	5,5,5	0.73	0
2	GOL	E	1005	-	5,5,5	0.11	0	5,5,5	0.62	0
2	GOL	C	1017	-	5,5,5	0.25	0	5,5,5	0.90	0
3	SO4	E	1010	-	4,4,4	0.31	0	6,6,6	0.22	0
2	GOL	A	1001	-	5,5,5	0.51	0	5,5,5	0.87	0
2	GOL	E	1008	-	5,5,5	0.24	0	5,5,5	0.60	0
2	GOL	A	1023	-	5,5,5	0.28	0	5,5,5	1.15	0
3	SO4	A	1034	-	4,4,4	0.35	0	6,6,6	0.46	0
2	GOL	C	1006	-	5,5,5	0.32	0	5,5,5	1.03	0
5	CO3	D	1007	-	3,3,3	0.66	0	2,3,3	0.21	0
3	SO4	A	1025	-	4,4,4	0.38	0	6,6,6	0.35	0
2	GOL	D	1010	-	5,5,5	0.40	0	5,5,5	0.75	0
2	GOL	B	1008	-	5,5,5	0.46	0	5,5,5	1.80	1 (20%)
2	GOL	C	1010	-	5,5,5	0.17	0	5,5,5	0.41	0
2	GOL	B	1009	-	5,5,5	0.17	0	5,5,5	0.48	0
2	GOL	B	1017	-	5,5,5	0.10	0	5,5,5	0.33	0
2	GOL	A	1003	-	5,5,5	0.25	0	5,5,5	1.75	2 (40%)
2	GOL	C	1013	-	5,5,5	0.12	0	5,5,5	1.00	0
3	SO4	B	1018	-	4,4,4	0.17	0	6,6,6	0.45	0
2	GOL	B	1005	-	5,5,5	0.27	0	5,5,5	1.15	0
2	GOL	F	1003	-	5,5,5	0.19	0	5,5,5	0.74	0
2	GOL	C	1014	-	5,5,5	0.10	0	5,5,5	0.35	0
2	GOL	C	1012	-	5,5,5	0.22	0	5,5,5	0.42	0
3	SO4	E	1001	-	4,4,4	0.20	0	6,6,6	0.45	0
2	GOL	A	1024	-	5,5,5	0.18	0	5,5,5	0.61	0
3	SO4	A	1027	-	4,4,4	0.43	0	6,6,6	0.38	0
2	GOL	A	1019	-	5,5,5	0.14	0	5,5,5	0.34	0
2	GOL	A	1018	-	5,5,5	0.23	0	5,5,5	0.26	0
2	GOL	C	1004	-	5,5,5	0.16	0	5,5,5	0.61	0
2	GOL	A	1013	-	5,5,5	0.25	0	5,5,5	1.36	1 (20%)
2	GOL	B	1004	-	5,5,5	0.08	0	5,5,5	0.40	0
2	GOL	B	1013	-	5,5,5	0.11	0	5,5,5	0.39	0
2	GOL	A	1006	-	5,5,5	0.09	0	5,5,5	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	1002	-	5,5,5	0.28	0	5,5,5	1.30	1 (20%)
3	SO4	E	1011	-	4,4,4	0.29	0	6,6,6	0.26	0
2	GOL	C	1020	-	5,5,5	0.10	0	5,5,5	0.34	0
3	SO4	B	1019	-	4,4,4	0.36	0	6,6,6	0.21	0
2	GOL	C	1021	-	5,5,5	0.52	0	5,5,5	1.03	0
6	EDO	C	1028	-	3,3,3	0.13	0	2,2,2	0.71	0
2	GOL	B	1016	-	5,5,5	0.23	0	5,5,5	0.67	0
2	GOL	A	1007	-	5,5,5	0.12	0	5,5,5	0.42	0
3	SO4	D	1012	-	4,4,4	0.30	0	6,6,6	0.35	0
2	GOL	A	1033	-	5,5,5	0.15	0	5,5,5	0.28	0
2	GOL	C	1018	-	5,5,5	0.40	0	5,5,5	1.06	0
3	SO4	A	1026	-	4,4,4	0.26	0	6,6,6	0.59	0
2	GOL	B	1007	-	5,5,5	0.25	0	5,5,5	0.40	0
3	SO4	F	1007	-	4,4,4	0.30	0	6,6,6	0.20	0
2	GOL	C	1005	-	5,5,5	0.33	0	5,5,5	1.43	1 (20%)
2	GOL	C	1011	-	5,5,5	0.09	0	5,5,5	0.44	0
6	EDO	A	1035	-	3,3,3	0.32	0	2,2,2	0.51	0
2	GOL	E	1002	-	5,5,5	0.24	0	5,5,5	0.58	0
2	GOL	A	1012	-	5,5,5	0.56	0	5,5,5	0.92	0
2	GOL	A	1008	-	5,5,5	0.41	0	5,5,5	0.79	0
2	GOL	B	1003	-	5,5,5	0.21	0	5,5,5	0.31	0
3	SO4	F	1006	-	4,4,4	0.28	0	6,6,6	0.17	0
2	GOL	C	1008	-	5,5,5	0.11	0	5,5,5	0.44	0
2	GOL	A	1016	-	5,5,5	0.11	0	5,5,5	0.46	0
2	GOL	B	1012	-	5,5,5	0.16	0	5,5,5	0.49	0
2	GOL	C	1022	-	5,5,5	0.49	0	5,5,5	0.92	0
2	GOL	B	1010	-	5,5,5	0.09	0	5,5,5	0.28	0
3	SO4	C	1023	-	4,4,4	0.36	0	6,6,6	0.58	0
6	EDO	C	1026	-	3,3,3	0.28	0	2,2,2	1.40	0
2	GOL	A	1005	-	5,5,5	0.45	0	5,5,5	0.91	0
3	SO4	B	1020	-	4,4,4	0.15	0	6,6,6	0.47	0
2	GOL	D	1011	-	5,5,5	0.17	0	5,5,5	0.31	0
3	SO4	A	1032	-	4,4,4	0.39	0	6,6,6	0.28	0
2	GOL	A	1004	-	5,5,5	0.21	0	5,5,5	0.69	0
3	SO4	C	1024	-	4,4,4	0.35	0	6,6,6	0.35	0
2	GOL	F	1002	-	5,5,5	0.10	0	5,5,5	0.73	0
3	SO4	E	1009	-	4,4,4	0.34	0	6,6,6	0.18	0
2	GOL	A	1015	-	5,5,5	0.11	0	5,5,5	0.56	0
2	GOL	E	1007	-	5,5,5	0.11	0	5,5,5	0.44	0
3	SO4	F	1008	-	4,4,4	0.32	0	6,6,6	0.18	0
2	GOL	C	1015	-	5,5,5	0.15	0	5,5,5	0.33	0
2	GOL	A	1020	-	5,5,5	0.32	0	5,5,5	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	1015	-	5,5,5	0.22	0	5,5,5	0.56	0
5	CO3	A	1031	-	3,3,3	1.18	0	2,3,3	0.39	0
2	GOL	A	1021	-	5,5,5	0.12	0	5,5,5	0.44	0
3	SO4	D	1003	-	4,4,4	0.40	0	6,6,6	0.14	0
6	EDO	C	1027	-	3,3,3	0.22	0	2,2,2	1.71	0
2	GOL	A	1009	-	5,5,5	0.18	0	5,5,5	0.86	0
2	GOL	A	1014	-	5,5,5	0.15	0	5,5,5	0.53	0
2	GOL	B	1006	-	5,5,5	0.23	0	5,5,5	0.47	0
2	GOL	A	1017	-	5,5,5	0.19	0	5,5,5	0.24	0
3	SO4	D	1004	-	4,4,4	0.17	0	6,6,6	0.38	0
2	GOL	E	1003	-	5,5,5	0.15	0	5,5,5	0.33	0
2	GOL	D	1001	-	5,5,5	0.10	0	5,5,5	0.82	0
2	GOL	C	1001	-	5,5,5	0.16	0	5,5,5	0.51	0
3	SO4	C	1002	-	4,4,4	0.38	0	6,6,6	0.31	0
2	GOL	E	1004	-	5,5,5	0.22	0	5,5,5	0.42	0
2	GOL	C	1003	-	5,5,5	0.47	0	5,5,5	1.42	0
2	GOL	A	1022	-	5,5,5	0.16	0	5,5,5	0.36	0
2	GOL	D	1009	-	5,5,5	0.38	0	5,5,5	0.64	0
3	SO4	C	1025	-	4,4,4	0.34	0	6,6,6	0.46	0
2	GOL	A	1010	-	5,5,5	0.13	0	5,5,5	0.31	0
3	SO4	F	1005	-	4,4,4	0.20	0	6,6,6	0.35	0
2	GOL	C	1007	-	5,5,5	0.11	0	5,5,5	0.56	0
2	GOL	A	1002	-	5,5,5	0.43	0	5,5,5	0.63	0
2	GOL	C	1009	-	5,5,5	0.24	0	5,5,5	0.51	0
2	GOL	B	1014	-	5,5,5	0.46	0	5,5,5	0.97	0
3	SO4	B	1001	-	4,4,4	0.40	0	6,6,6	0.65	0
2	GOL	C	1016	-	5,5,5	0.12	0	5,5,5	0.32	0
2	GOL	D	1002	-	5,5,5	0.36	0	5,5,5	0.67	0
2	GOL	E	1006	-	5,5,5	0.12	0	5,5,5	0.23	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	C	1019	-	-	2/4/4/4	-
6	EDO	B	1022	-	-	1/1/1/1	-
2	GOL	A	1011	-	-	2/4/4/4	-
2	GOL	F	1004	-	-	2/4/4/4	-
2	GOL	F	1001	-	-	2/4/4/4	-
2	GOL	B	1011	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	E	1005	-	-	2/4/4/4	-
2	GOL	C	1017	-	-	2/4/4/4	-
2	GOL	A	1001	-	-	0/4/4/4	-
2	GOL	E	1008	-	-	0/4/4/4	-
2	GOL	A	1023	-	-	4/4/4/4	-
2	GOL	C	1006	-	-	3/4/4/4	-
2	GOL	D	1010	-	-	0/4/4/4	-
2	GOL	B	1008	-	-	0/4/4/4	-
2	GOL	C	1010	-	-	2/4/4/4	-
2	GOL	B	1009	-	-	0/4/4/4	-
2	GOL	B	1017	-	-	4/4/4/4	-
2	GOL	A	1003	-	-	3/4/4/4	-
2	GOL	C	1013	-	-	2/4/4/4	-
2	GOL	B	1005	-	-	1/4/4/4	-
2	GOL	F	1003	-	-	3/4/4/4	-
2	GOL	C	1014	-	-	1/4/4/4	-
2	GOL	C	1012	-	-	2/4/4/4	-
2	GOL	A	1024	-	-	2/4/4/4	-
2	GOL	A	1019	-	-	4/4/4/4	-
2	GOL	A	1018	-	-	2/4/4/4	-
2	GOL	C	1004	-	-	0/4/4/4	-
2	GOL	A	1013	-	-	2/4/4/4	-
2	GOL	B	1004	-	-	0/4/4/4	-
2	GOL	B	1013	-	-	0/4/4/4	-
2	GOL	A	1006	-	-	2/4/4/4	-
2	GOL	B	1002	-	-	4/4/4/4	-
2	GOL	C	1020	-	-	2/4/4/4	-
2	GOL	C	1021	-	-	2/4/4/4	-
6	EDO	C	1028	-	-	1/1/1/1	-
2	GOL	B	1016	-	-	1/4/4/4	-
2	GOL	A	1007	-	-	0/4/4/4	-
2	GOL	A	1033	-	-	3/4/4/4	-
2	GOL	C	1018	-	-	2/4/4/4	-
2	GOL	B	1007	-	-	0/4/4/4	-
2	GOL	C	1005	-	-	2/4/4/4	-
2	GOL	C	1011	-	-	0/4/4/4	-
6	EDO	A	1035	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	E	1002	-	-	0/4/4/4	-
2	GOL	A	1012	-	-	2/4/4/4	-
2	GOL	A	1008	-	-	4/4/4/4	-
2	GOL	B	1003	-	-	0/4/4/4	-
2	GOL	C	1008	-	-	3/4/4/4	-
2	GOL	A	1016	-	-	4/4/4/4	-
2	GOL	B	1012	-	-	2/4/4/4	-
2	GOL	C	1022	-	-	4/4/4/4	-
2	GOL	B	1010	-	-	2/4/4/4	-
6	EDO	C	1026	-	-	1/1/1/1	-
2	GOL	A	1005	-	-	3/4/4/4	-
2	GOL	D	1011	-	-	4/4/4/4	-
2	GOL	A	1004	-	-	0/4/4/4	-
2	GOL	F	1002	-	-	2/4/4/4	-
2	GOL	A	1015	-	-	1/4/4/4	-
2	GOL	E	1007	-	-	2/4/4/4	-
2	GOL	C	1015	-	-	4/4/4/4	-
2	GOL	A	1020	-	-	4/4/4/4	-
2	GOL	B	1015	-	-	2/4/4/4	-
2	GOL	A	1021	-	-	0/4/4/4	-
6	EDO	C	1027	-	-	1/1/1/1	-
2	GOL	A	1009	-	-	2/4/4/4	-
2	GOL	A	1014	-	-	2/4/4/4	-
2	GOL	B	1006	-	-	0/4/4/4	-
2	GOL	A	1017	-	-	0/4/4/4	-
2	GOL	E	1003	-	-	3/4/4/4	-
2	GOL	D	1001	-	-	3/4/4/4	-
2	GOL	C	1001	-	-	1/4/4/4	-
2	GOL	E	1004	-	-	2/4/4/4	-
2	GOL	C	1003	-	-	4/4/4/4	-
2	GOL	A	1022	-	-	2/4/4/4	-
2	GOL	D	1009	-	-	0/4/4/4	-
2	GOL	A	1010	-	-	4/4/4/4	-
2	GOL	C	1007	-	-	2/4/4/4	-
2	GOL	A	1002	-	-	0/4/4/4	-
2	GOL	C	1009	-	-	1/4/4/4	-
2	GOL	B	1014	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	1016	-	-	0/4/4/4	-
2	GOL	D	1002	-	-	0/4/4/4	-
2	GOL	E	1006	-	-	2/4/4/4	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1008	GOL	O2-C2-C3	-3.07	96.49	109.18
2	A	1003	GOL	O2-C2-C1	2.87	121.08	109.18
2	C	1005	GOL	O3-C3-C2	-2.47	99.25	110.38
2	A	1013	GOL	O2-C2-C3	2.44	119.28	109.18
2	B	1002	GOL	O2-C2-C3	2.35	118.89	109.18
2	A	1003	GOL	O3-C3-C2	-2.14	100.73	110.38

There are no chirality outliers.

All (143) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1005	GOL	O1-C1-C2-C3
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
2	A	1008	GOL	O2-C2-C3-O3
2	A	1009	GOL	C1-C2-C3-O3
2	A	1010	GOL	C1-C2-C3-O3
2	A	1016	GOL	O1-C1-C2-C3
2	A	1016	GOL	C1-C2-C3-O3
2	A	1016	GOL	O2-C2-C3-O3
2	A	1018	GOL	O1-C1-C2-O2
2	A	1018	GOL	O1-C1-C2-C3
2	A	1019	GOL	O1-C1-C2-C3
2	A	1020	GOL	C1-C2-C3-O3
2	A	1023	GOL	O1-C1-C2-C3
2	A	1023	GOL	C1-C2-C3-O3
2	A	1033	GOL	C1-C2-C3-O3
2	B	1002	GOL	O1-C1-C2-O2
2	B	1002	GOL	O1-C1-C2-C3
2	B	1012	GOL	C1-C2-C3-O3
2	B	1015	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	1017	GOL	C1-C2-C3-O3
2	C	1003	GOL	C1-C2-C3-O3
2	C	1006	GOL	O1-C1-C2-C3
2	C	1007	GOL	O1-C1-C2-C3
2	C	1010	GOL	O1-C1-C2-C3
2	C	1013	GOL	O1-C1-C2-C3
2	C	1015	GOL	C1-C2-C3-O3
2	C	1017	GOL	C1-C2-C3-O3
2	C	1018	GOL	C1-C2-C3-O3
2	C	1022	GOL	O1-C1-C2-C3
2	D	1001	GOL	O1-C1-C2-C3
2	E	1003	GOL	C1-C2-C3-O3
2	E	1003	GOL	O2-C2-C3-O3
2	E	1006	GOL	O1-C1-C2-C3
2	E	1007	GOL	C1-C2-C3-O3
2	F	1001	GOL	C1-C2-C3-O3
2	F	1002	GOL	C1-C2-C3-O3
2	F	1002	GOL	O2-C2-C3-O3
2	F	1003	GOL	C1-C2-C3-O3
2	F	1004	GOL	C1-C2-C3-O3
2	A	1003	GOL	O2-C2-C3-O3
2	A	1006	GOL	O2-C2-C3-O3
2	A	1010	GOL	O2-C2-C3-O3
2	A	1014	GOL	O2-C2-C3-O3
2	A	1023	GOL	O1-C1-C2-O2
2	B	1012	GOL	O2-C2-C3-O3
2	C	1017	GOL	O2-C2-C3-O3
2	E	1007	GOL	O2-C2-C3-O3
2	F	1004	GOL	O2-C2-C3-O3
2	A	1003	GOL	C1-C2-C3-O3
2	A	1005	GOL	C1-C2-C3-O3
2	A	1010	GOL	O1-C1-C2-C3
2	A	1012	GOL	C1-C2-C3-O3
2	A	1013	GOL	O1-C1-C2-C3
2	A	1014	GOL	C1-C2-C3-O3
2	A	1019	GOL	C1-C2-C3-O3
2	A	1020	GOL	O1-C1-C2-C3
2	A	1024	GOL	C1-C2-C3-O3
2	B	1002	GOL	C1-C2-C3-O3
2	B	1014	GOL	O1-C1-C2-C3
2	B	1014	GOL	C1-C2-C3-O3
2	B	1015	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	B	1017	GOL	O1-C1-C2-C3
2	C	1005	GOL	C1-C2-C3-O3
2	C	1006	GOL	C1-C2-C3-O3
2	C	1008	GOL	C1-C2-C3-O3
2	C	1015	GOL	O1-C1-C2-C3
2	C	1019	GOL	C1-C2-C3-O3
2	C	1021	GOL	C1-C2-C3-O3
2	C	1022	GOL	C1-C2-C3-O3
2	D	1011	GOL	O1-C1-C2-C3
2	D	1011	GOL	C1-C2-C3-O3
2	E	1005	GOL	C1-C2-C3-O3
2	A	1005	GOL	O1-C1-C2-O2
2	A	1009	GOL	O2-C2-C3-O3
2	A	1012	GOL	O2-C2-C3-O3
2	A	1013	GOL	O1-C1-C2-O2
2	A	1020	GOL	O1-C1-C2-O2
2	A	1023	GOL	O2-C2-C3-O3
2	A	1033	GOL	O2-C2-C3-O3
2	B	1002	GOL	O2-C2-C3-O3
2	B	1017	GOL	O1-C1-C2-O2
2	B	1017	GOL	O2-C2-C3-O3
2	C	1003	GOL	O2-C2-C3-O3
2	C	1005	GOL	O2-C2-C3-O3
2	C	1006	GOL	O2-C2-C3-O3
2	C	1008	GOL	O2-C2-C3-O3
2	C	1015	GOL	O2-C2-C3-O3
2	C	1019	GOL	O2-C2-C3-O3
2	C	1021	GOL	O2-C2-C3-O3
2	C	1022	GOL	O1-C1-C2-O2
2	C	1022	GOL	O2-C2-C3-O3
2	D	1001	GOL	O1-C1-C2-O2
2	D	1011	GOL	O2-C2-C3-O3
2	E	1005	GOL	O2-C2-C3-O3
2	E	1006	GOL	O1-C1-C2-O2
2	F	1003	GOL	O2-C2-C3-O3
6	A	1035	EDO	O1-C1-C2-O2
2	A	1010	GOL	O1-C1-C2-O2
2	A	1019	GOL	O1-C1-C2-O2
2	A	1020	GOL	O2-C2-C3-O3
2	C	1003	GOL	O1-C1-C2-O2
2	C	1007	GOL	O1-C1-C2-O2
2	C	1010	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	C	1018	GOL	O2-C2-C3-O3
2	C	1020	GOL	O1-C1-C2-O2
2	E	1004	GOL	O1-C1-C2-O2
6	B	1022	EDO	O1-C1-C2-O2
6	C	1027	EDO	O1-C1-C2-O2
2	A	1003	GOL	O1-C1-C2-O2
2	A	1024	GOL	O2-C2-C3-O3
2	B	1010	GOL	O2-C2-C3-O3
2	A	1011	GOL	O2-C2-C3-O3
2	A	1016	GOL	O1-C1-C2-O2
2	A	1033	GOL	O1-C1-C2-O2
2	B	1005	GOL	O1-C1-C2-O2
2	C	1001	GOL	O1-C1-C2-O2
2	C	1012	GOL	O1-C1-C2-O2
2	C	1015	GOL	O1-C1-C2-O2
2	D	1001	GOL	O2-C2-C3-O3
2	C	1020	GOL	O1-C1-C2-C3
2	E	1004	GOL	O1-C1-C2-C3
6	C	1028	EDO	O1-C1-C2-O2
2	D	1011	GOL	O1-C1-C2-O2
2	A	1019	GOL	O2-C2-C3-O3
2	E	1003	GOL	O1-C1-C2-O2
2	A	1011	GOL	O1-C1-C2-O2
2	A	1015	GOL	O2-C2-C3-O3
2	C	1009	GOL	O2-C2-C3-O3
2	A	1022	GOL	C1-C2-C3-O3
2	B	1010	GOL	C1-C2-C3-O3
2	C	1003	GOL	O1-C1-C2-C3
6	C	1026	EDO	O1-C1-C2-O2
2	F	1001	GOL	O2-C2-C3-O3
2	B	1016	GOL	O2-C2-C3-O3
2	C	1014	GOL	C1-C2-C3-O3
2	C	1013	GOL	O1-C1-C2-O2
2	F	1003	GOL	O1-C1-C2-O2
2	A	1022	GOL	O2-C2-C3-O3
2	C	1012	GOL	O2-C2-C3-O3
2	C	1008	GOL	O1-C1-C2-O2

There are no ring outliers.

52 monomers are involved in 83 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1011	GOL	2	0
2	F	1004	GOL	3	0
2	E	1005	GOL	1	0
2	C	1017	GOL	1	0
2	E	1008	GOL	1	0
2	D	1010	GOL	3	0
2	B	1008	GOL	3	0
2	C	1010	GOL	2	0
2	B	1009	GOL	1	0
2	C	1013	GOL	1	0
2	C	1014	GOL	1	0
2	A	1024	GOL	1	0
2	A	1018	GOL	1	0
2	A	1013	GOL	1	0
2	B	1004	GOL	4	0
2	C	1020	GOL	1	0
2	C	1021	GOL	3	0
2	B	1016	GOL	1	0
2	A	1007	GOL	1	0
3	D	1012	SO4	1	0
2	A	1033	GOL	1	0
2	C	1018	GOL	4	0
2	B	1007	GOL	1	0
2	C	1005	GOL	1	0
6	A	1035	EDO	2	0
2	A	1012	GOL	1	0
2	A	1008	GOL	2	0
2	C	1008	GOL	2	0
2	A	1016	GOL	1	0
2	B	1012	GOL	1	0
2	C	1022	GOL	1	0
2	B	1010	GOL	1	0
6	C	1026	EDO	1	0
2	A	1005	GOL	4	0
3	C	1024	SO4	2	0
2	F	1002	GOL	1	0
2	E	1007	GOL	2	0
2	C	1015	GOL	1	0
2	A	1020	GOL	4	0
2	B	1015	GOL	1	0
2	A	1021	GOL	3	0
2	A	1009	GOL	1	0
2	A	1014	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1003	GOL	1	0
2	C	1001	GOL	1	0
2	E	1004	GOL	1	0
2	C	1003	GOL	2	0
2	A	1022	GOL	3	0
3	C	1025	SO4	1	0
2	C	1009	GOL	2	0
3	B	1001	SO4	1	0
2	E	1006	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 ⓘ

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	757/927 (81%)	-0.50	6 (0%) 82 85	12, 25, 61, 89	11 (1%)
1	B	756/927 (81%)	-0.49	5 (0%) 84 86	13, 26, 46, 96	10 (1%)
1	C	758/927 (81%)	-0.48	9 (1%) 76 79	14, 27, 47, 88	7 (0%)
1	D	755/927 (81%)	-0.03	19 (2%) 58 62	17, 37, 77, 121	8 (1%)
1	E	754/927 (81%)	-0.06	20 (2%) 56 60	16, 37, 74, 114	7 (0%)
1	F	753/927 (81%)	-0.16	3 (0%) 88 90	21, 38, 56, 88	3 (0%)
All	All	4533/5562 (81%)	-0.29	62 (1%) 73 76	12, 33, 61, 121	46 (1%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	548	VAL	4.2
1	E	548	VAL	4.1
1	E	216	ILE	3.9
1	A	168	PHE	3.8
1	B	167	ALA	3.5
1	C	166	PRO	3.5
1	D	216	ILE	3.5
1	A	548	VAL	3.5
1	E	222	ILE	3.4
1	E	193	ILE	3.3
1	C	167	ALA	3.3
1	C	168	PHE	3.3
1	E	205	ILE	3.3
1	D	923	HIS	3.3
1	D	195	LEU	3.2
1	B	168	PHE	3.2
1	D	222	ILE	3.1
1	E	280	MET	3.1
1	E	922	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	922	HIS	3.0
1	B	548	VAL	2.9
1	D	548	VAL	2.9
1	E	228	GLY	2.9
1	F	921	ILE	2.9
1	B	922	HIS	2.8
1	E	781	ALA	2.8
1	D	193	ILE	2.7
1	A	167	ALA	2.6
1	E	195	LEU	2.6
1	C	922	HIS	2.6
1	E	227	ALA	2.6
1	D	234	PRO	2.6
1	D	237	VAL	2.6
1	E	237	VAL	2.5
1	E	187	ILE	2.5
1	A	237	VAL	2.5
1	D	280	MET	2.4
1	A	193	ILE	2.4
1	D	232	TYR	2.4
1	D	308	THR	2.4
1	D	169	ASP	2.3
1	E	230	LEU	2.3
1	C	292	ALA	2.3
1	E	213	LEU	2.3
1	E	239	VAL	2.3
1	D	221	VAL	2.2
1	C	165	SER	2.2
1	F	331	ALA	2.2
1	E	223	SER	2.2
1	C	280	MET	2.2
1	C	279	THR	2.2
1	B	309	GLY	2.2
1	D	230	LEU	2.2
1	D	331	ALA	2.1
1	A	923	HIS	2.1
1	E	188	VAL	2.1
1	D	196	LEU	2.1
1	C	308	THR	2.0
1	E	198	GLY	2.0
1	D	198	GLY	2.0
1	D	217	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	225	VAL	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($\text{\AA}^2$)	Q<0.9
2	GOL	A	1008	6/6	0.79	0.19	47,58,62,67	0
2	GOL	C	1021	6/6	0.79	0.15	29,53,56,56	0
2	GOL	D	1010	6/6	0.79	0.14	41,56,58,58	0
2	GOL	A	1012	6/6	0.80	0.16	45,49,56,57	0
2	GOL	B	1015	6/6	0.81	0.14	60,66,71,77	0
2	GOL	C	1017	6/6	0.81	0.18	46,62,75,79	0
3	SO4	E	1011	5/5	0.81	0.12	75,81,92,111	0
2	GOL	B	1013	6/6	0.82	0.18	82,84,96,96	0
2	GOL	C	1001	6/6	0.83	0.13	55,67,73,74	0
3	SO4	D	1004	5/5	0.83	0.11	67,78,85,118	0
3	SO4	E	1010	5/5	0.83	0.10	67,86,95,102	0
2	GOL	C	1011	6/6	0.83	0.13	56,74,80,81	0
6	EDO	C	1028	4/4	0.83	0.14	56,59,64,71	0
2	GOL	B	1007	6/6	0.84	0.14	48,61,67,78	0
2	GOL	A	1019	6/6	0.84	0.13	63,75,82,99	0
2	GOL	A	1021	6/6	0.84	0.12	54,70,80,83	0
3	SO4	A	1026	5/5	0.84	0.14	20,25,37,38	5
3	SO4	D	1003	5/5	0.84	0.15	36,37,39,48	5
2	GOL	A	1033	6/6	0.84	0.13	51,57,65,65	0
2	GOL	C	1005	6/6	0.84	0.17	38,40,41,45	6
2	GOL	C	1009	6/6	0.84	0.14	61,70,75,75	0
3	SO4	F	1008	5/5	0.84	0.11	70,88,95,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	1006	6/6	0.84	0.21	65,83,86,86	0
2	GOL	C	1006	6/6	0.85	0.12	41,51,54,58	0
2	GOL	B	1012	6/6	0.86	0.14	67,74,85,87	0
2	GOL	A	1022	6/6	0.86	0.12	64,68,74,83	0
2	GOL	E	1008	6/6	0.86	0.13	56,70,74,87	0
3	SO4	F	1007	5/5	0.86	0.10	55,55,58,66	5
2	GOL	C	1013	6/6	0.86	0.13	52,54,66,66	0
2	GOL	A	1005	6/6	0.86	0.13	40,40,49,49	0
2	GOL	E	1002	6/6	0.87	0.13	67,68,71,71	0
2	GOL	A	1023	6/6	0.87	0.14	60,63,65,68	0
2	GOL	C	1020	6/6	0.88	0.11	52,67,70,74	0
2	GOL	C	1008	6/6	0.88	0.14	59,71,75,80	0
2	GOL	B	1017	6/6	0.88	0.11	59,64,71,82	0
2	GOL	B	1014	6/6	0.88	0.13	49,60,61,62	0
2	GOL	E	1003	6/6	0.88	0.12	48,58,61,63	0
2	GOL	B	1011	6/6	0.88	0.13	45,50,59,62	0
6	EDO	B	1022	4/4	0.88	0.14	58,58,62,64	0
2	GOL	B	1016	6/6	0.88	0.11	38,45,58,63	0
2	GOL	F	1002	6/6	0.89	0.13	51,62,65,67	0
2	GOL	F	1004	6/6	0.89	0.12	48,56,64,65	0
2	GOL	C	1019	6/6	0.89	0.11	46,61,65,68	0
2	GOL	A	1009	6/6	0.89	0.13	57,61,70,71	0
2	GOL	A	1015	6/6	0.89	0.14	52,66,73,75	0
2	GOL	D	1002	6/6	0.89	0.13	43,53,56,60	0
2	GOL	B	1009	6/6	0.89	0.13	57,63,69,74	0
2	GOL	A	1017	6/6	0.89	0.14	48,66,68,78	0
2	GOL	A	1024	6/6	0.89	0.12	50,59,70,74	0
2	GOL	E	1004	6/6	0.89	0.12	50,55,66,68	0
6	EDO	C	1026	4/4	0.89	0.14	35,63,63,63	0
2	GOL	A	1010	6/6	0.89	0.12	59,62,70,80	0
2	GOL	C	1015	6/6	0.90	0.13	62,69,77,78	0
2	GOL	A	1007	6/6	0.90	0.12	51,59,64,69	0
2	GOL	F	1003	6/6	0.90	0.12	43,57,61,70	0
2	GOL	D	1011	6/6	0.90	0.14	55,65,73,85	0
2	GOL	B	1010	6/6	0.90	0.11	60,71,75,80	0
2	GOL	A	1020	6/6	0.90	0.11	50,64,67,81	0
2	GOL	A	1014	6/6	0.90	0.13	58,68,73,78	0
2	GOL	A	1003	6/6	0.91	0.10	33,37,43,43	0
3	SO4	F	1005	5/5	0.91	0.11	42,46,49,52	5
2	GOL	E	1007	6/6	0.91	0.10	40,58,61,73	0
2	GOL	B	1005	6/6	0.91	0.10	43,49,51,53	0
5	CO3	A	1031	4/4	0.91	0.10	55,59,62,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	C	1016	6/6	0.91	0.12	45,58,69,85	0
3	SO4	D	1013	5/5	0.91	0.10	61,73,80,92	0
6	EDO	C	1027	4/4	0.91	0.10	46,53,54,60	0
2	GOL	B	1008	6/6	0.91	0.14	32,43,48,55	0
3	SO4	C	1025	5/5	0.92	0.09	55,56,69,91	0
2	GOL	C	1010	6/6	0.92	0.11	62,66,69,76	0
2	GOL	A	1006	6/6	0.92	0.11	50,63,66,68	0
2	GOL	C	1012	6/6	0.92	0.10	47,54,61,66	0
3	SO4	E	1001	5/5	0.92	0.09	41,50,55,65	5
2	GOL	B	1002	6/6	0.92	0.09	40,42,50,51	0
2	GOL	C	1014	6/6	0.92	0.10	47,64,70,89	0
2	GOL	B	1004	6/6	0.92	0.09	47,59,62,63	0
2	GOL	A	1016	6/6	0.92	0.10	38,50,60,68	0
2	GOL	A	1013	6/6	0.92	0.10	36,39,44,48	0
4	CL	B	1021	1/1	0.92	0.11	71,71,71,71	0
2	GOL	C	1007	6/6	0.92	0.11	49,56,65,68	0
2	GOL	A	1018	6/6	0.92	0.13	48,51,58,71	0
2	GOL	A	1011	6/6	0.92	0.12	34,41,48,54	0
2	GOL	D	1001	6/6	0.92	0.10	50,58,61,64	0
3	SO4	B	1020	5/5	0.92	0.10	21,23,31,32	5
2	GOL	E	1006	6/6	0.93	0.10	42,58,64,71	0
2	GOL	C	1022	6/6	0.93	0.11	32,41,55,65	0
2	GOL	A	1004	6/6	0.93	0.12	30,59,66,68	0
2	GOL	F	1001	6/6	0.93	0.10	41,50,53,56	0
4	CL	D	1006	1/1	0.93	0.18	56,56,56,56	0
2	GOL	A	1001	6/6	0.94	0.09	34,37,38,42	0
3	SO4	F	1006	5/5	0.94	0.07	64,71,86,92	0
2	GOL	E	1005	6/6	0.94	0.09	52,55,61,65	0
2	GOL	A	1002	6/6	0.94	0.08	25,26,27,28	6
2	GOL	C	1018	6/6	0.94	0.11	41,45,57,60	0
3	SO4	D	1012	5/5	0.94	0.09	34,42,43,51	5
3	SO4	A	1025	5/5	0.94	0.08	45,54,65,70	0
5	CO3	D	1007	4/4	0.94	0.11	67,69,79,84	0
6	EDO	A	1035	4/4	0.94	0.09	44,47,56,60	0
2	GOL	D	1009	6/6	0.94	0.10	41,47,50,55	0
3	SO4	E	1009	5/5	0.94	0.07	50,53,57,65	5
3	SO4	A	1027	5/5	0.94	0.08	53,56,59,74	0
3	SO4	A	1032	5/5	0.94	0.09	52,63,77,78	0
3	SO4	B	1001	5/5	0.95	0.08	33,34,44,51	5
3	SO4	C	1024	5/5	0.95	0.08	35,37,44,49	5
3	SO4	B	1018	5/5	0.95	0.07	46,50,67,71	0
3	SO4	B	1019	5/5	0.95	0.07	58,59,65,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	1023	5/5	0.96	0.07	41,47,54,62	5
2	GOL	C	1004	6/6	0.96	0.07	29,38,43,50	0
2	GOL	B	1003	6/6	0.96	0.07	36,38,39,41	0
2	GOL	C	1003	6/6	0.96	0.07	32,34,40,41	0
3	SO4	A	1034	5/5	0.96	0.07	30,34,39,44	5
3	SO4	C	1002	5/5	0.96	0.06	44,45,49,55	0
4	CL	A	1030	1/1	0.98	0.06	61,61,61,61	0
4	CL	A	1029	1/1	0.98	0.09	40,40,40,40	0
4	CL	D	1008	1/1	0.99	0.06	41,41,41,41	0
4	CL	D	1005	1/1	1.00	0.03	30,30,30,30	0
4	CL	A	1028	1/1	1.00	0.01	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.