



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2021 – 02:21 PM EST

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 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 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 : 2.16
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) : 2.16

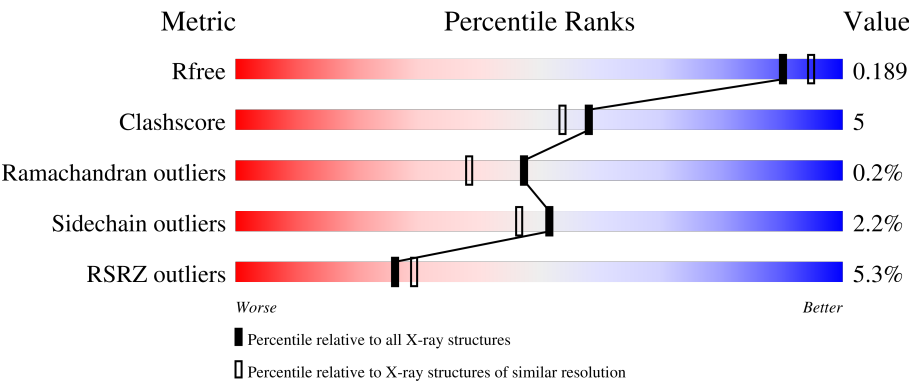
1 Overall quality at a glance i

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

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Mol	Chain	Length	Quality of chain
1	F	927	 % 72% 8% 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:

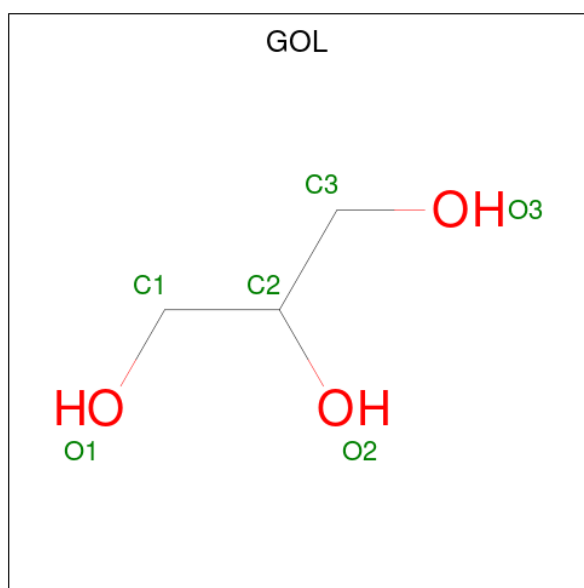
Chain	Residue	Modelled	Actual	Comment	Reference
A	922	HIS	-	expression tag	UNP G3M190
A	923	HIS	-	expression tag	UNP G3M190
A	924	HIS	-	expression tag	UNP G3M190
A	925	HIS	-	expression tag	UNP G3M190
A	926	HIS	-	expression tag	UNP G3M190
A	927	HIS	-	expression tag	UNP G3M190
B	922	HIS	-	expression tag	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 (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		
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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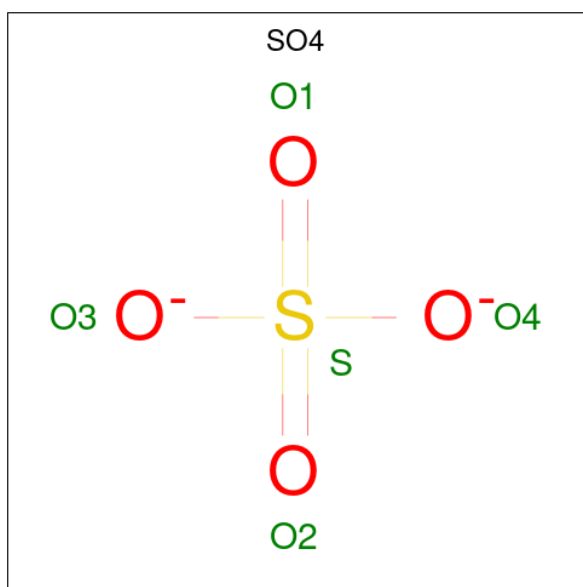
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	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 (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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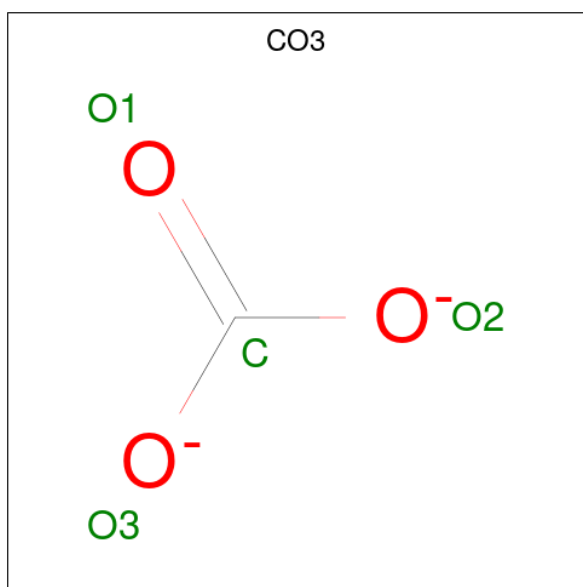
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			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	B	1	Total	Cl	0	0
			1	1		
4	A	3	Total	Cl	0	0
			3	3		
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: 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 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

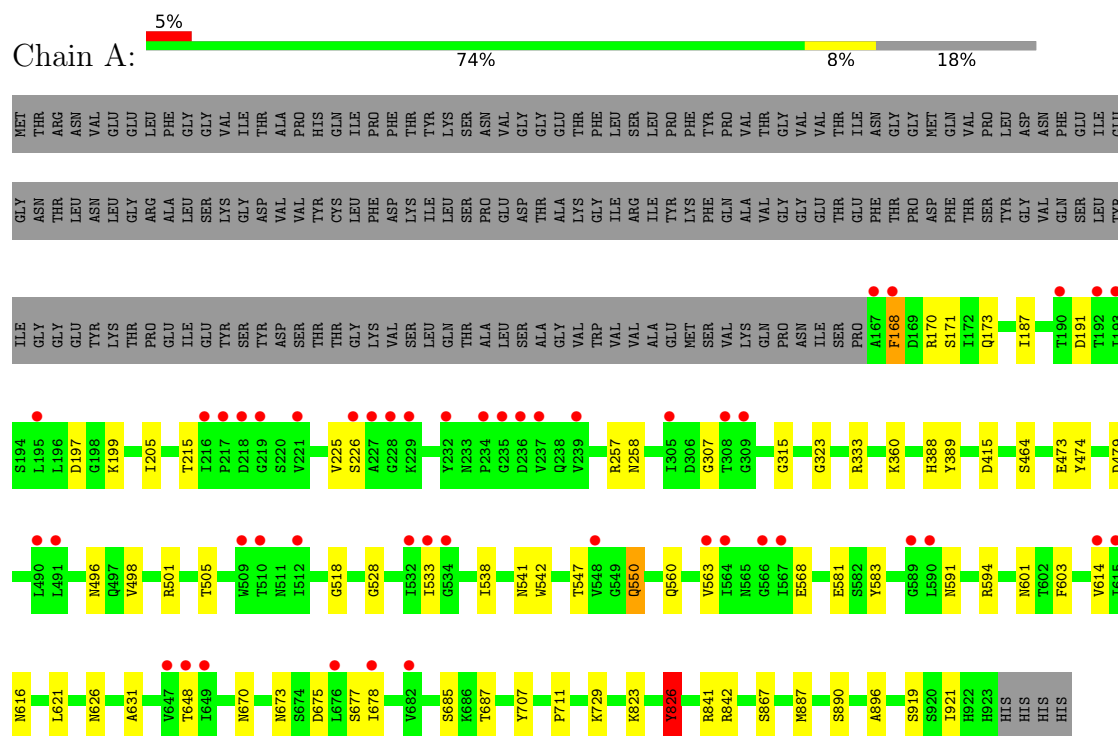
- Molecule 7 is water.

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

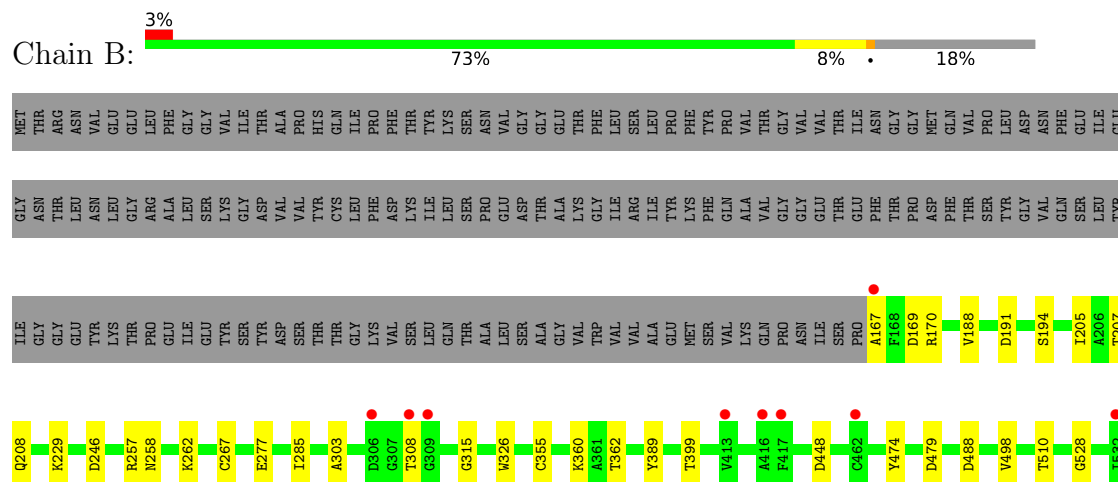
3 Residue-property plots [i](#)

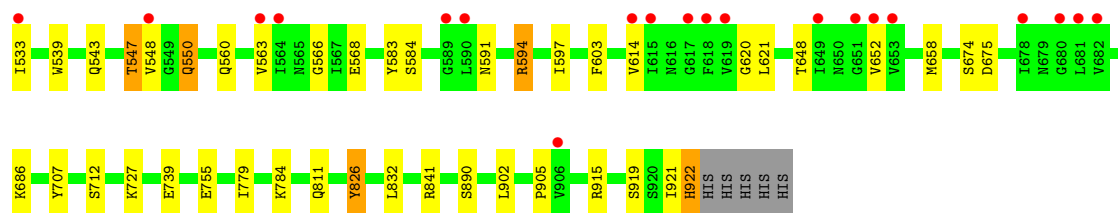
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

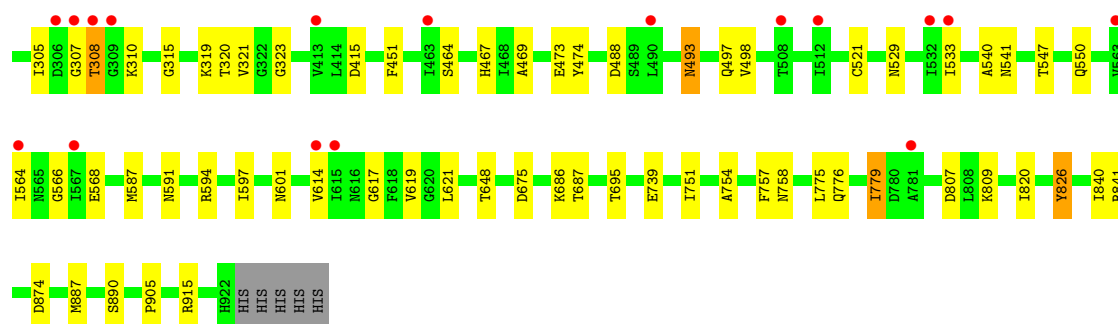
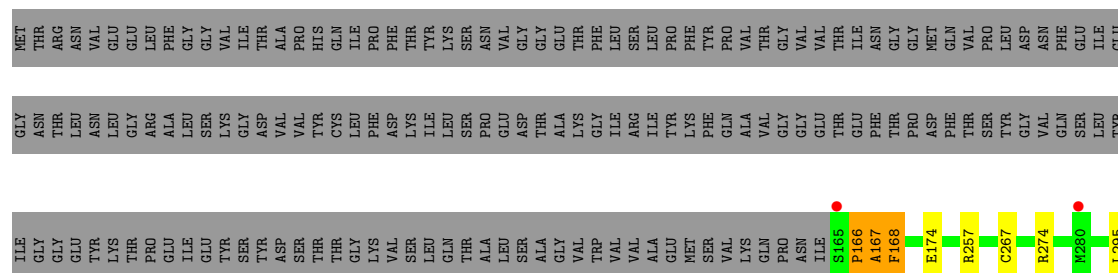


• Molecule 1: Tail fiber

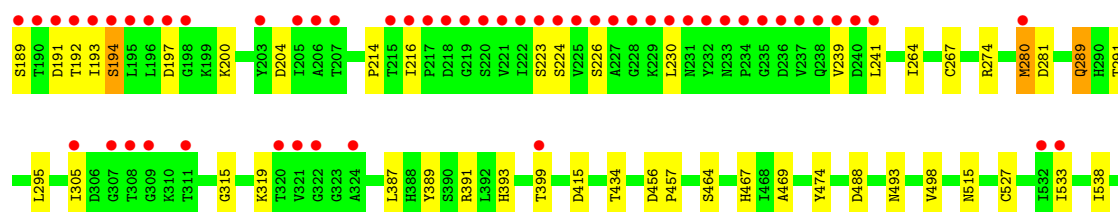
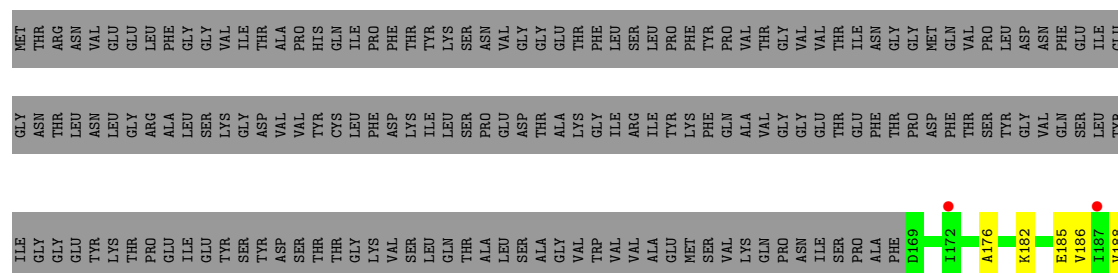


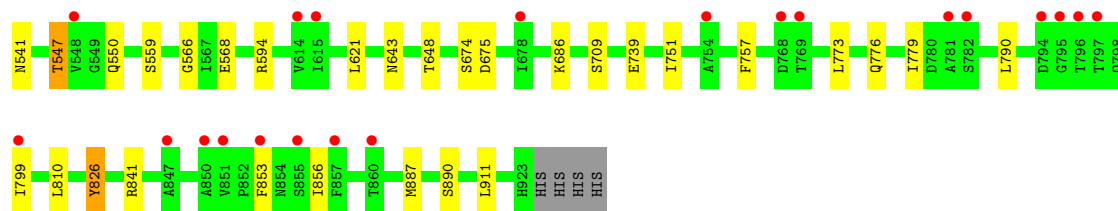


• Molecule 1: Tail fiber

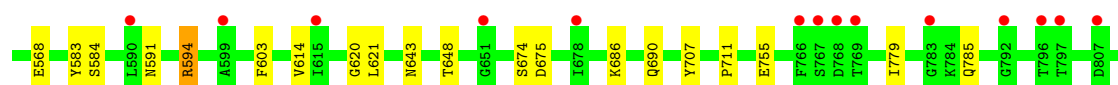
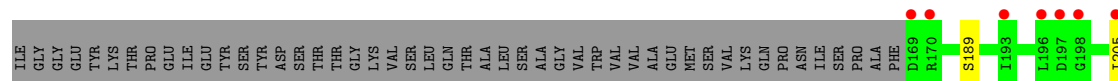
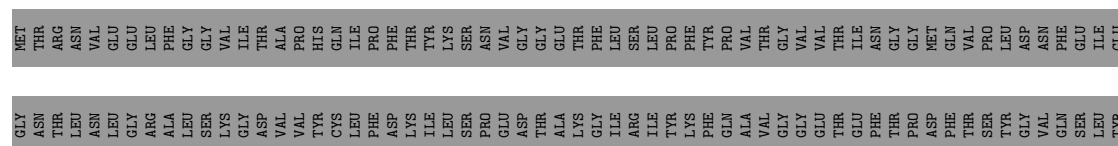


• Molecule 1: Tail fiber

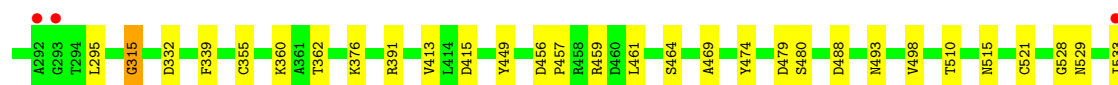
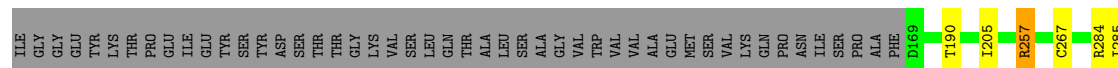
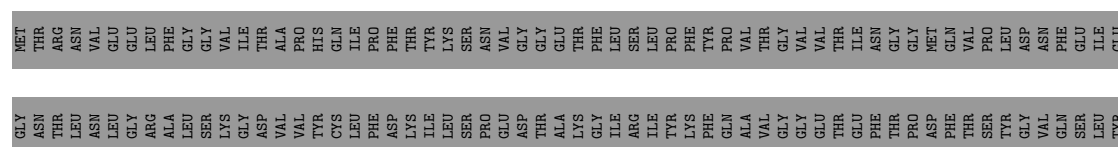


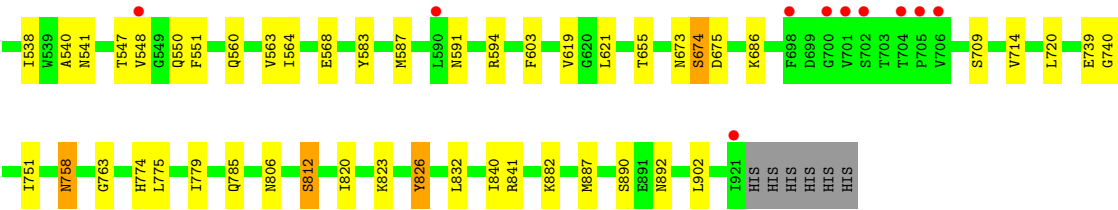


● Molecule 1: Tail fiber



● 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) 99.8 (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)	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 (5.07%)	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 , 54.5	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: SO4, GOL, CO3, EDO, CL

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

All (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
1	E	826	TYR	CB-CG-CD2	-6.10	117.34	121.00
1	A	501	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	B	258	ASN	CB-CA-C	-5.78	98.85	110.40
1	F	674	SER	N-CA-CB	5.70	119.05	110.50
1	C	826	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	D	826	TYR	CB-CG-CD1	5.67	124.40	121.00
1	F	826	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	C	826	TYR	CB-CG-CD1	5.46	124.28	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	168	PHE	CB-CA-C	-5.46	99.49	110.40
1	E	267	CYS	CB-CA-C	-5.38	99.63	110.40
1	F	758	ASN	CB-CA-C	-5.38	99.65	110.40
1	B	826	TYR	CB-CG-CD1	5.31	124.19	121.00
1	E	501	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	257	ARG	CG-CD-NE	-5.14	101.00	111.80
1	A	258	ASN	CB-CA-C	-5.13	100.13	110.40

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
2:C:1020:GOL:H31	7:C:1641:HOH:O	1.71	0.88
1:A:168:PHE:H	1:A:168:PHE:HD1	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:N	1:A:168:PHE:HD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:ILE:HG21	1:B:533:ILE:HG22	1.85	0.57
1:B:621:LEU:HD23	1:B:621:LEU:C	2.24	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:A:542:TRP:CH2	2:A:1016:GOL:H11	2.40	0.56
1:A:187:ILE:HB	1:A:199:LYS:HE3	1.86	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:686:LYS:HA	1:E:887:MET:HG3	1.88	0.55
2:C:1003:GOL:H2	7:C:1255:HOH:O	2.05	0.55
1:C:695:THR:HB	6:C:1026:EDO:H22	1.89	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:C:166:PRO:O	1:C:168:PHE:N	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:B:658:MET:HE3	7:B:1335:HOH:O	2.07	0.54
1:C:751:ILE:HG23	1:C:779:ILE:CD1	2.38	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:D:675:ASP:OD2	1:E:890:SER:HB3	2.09	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:621:LEU:HD23	1:E:621:LEU:C	2.30	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:D:191:ASP:OD1	1:D:191:ASP:C	2.48	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
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:E:388:HIS:HE2	2:E:1003:GOL:H12	1.77	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:E:533:ILE:HG21	1:F:533:ILE:CG2	2.42	0.50
1:F:739[A]:GLU:CD	1:F:739[A]:GLU:H	2.15	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:C:621:LEU:C	1:C:621:LEU:HD23	2.33	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:D:621:LEU:C	1:D:621:LEU:HD23	2.33	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:F:461:LEU:C	1:F:461:LEU:HD12	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:621:LEU:C	1:F:621:LEU:HD23	2.33	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:A:621:LEU:C	1:A:621:LEU:HD23	2.34	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
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:E:779:ILE:HD13	1:E:785:GLN:HG2	1.97	0.47
1:D:568:GLU:OE2	1:F:529:ASN:HB3	2.15	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: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:E:707:TYR:CG	1:E:919:SER:HA	2.50	0.46
1:D:264:ILE:HB	1:F:284:ARG:HH21	1.80	0.46
2:A:1020:GOL:H31	7:A:1482:HOH:O	2.14	0.46
1:A:533:ILE:HG21	1:B:533:ILE:CG2	2.44	0.46
1:E:510:THR:HG23	7:E:1473:HOH:O	2.15	0.46
1:D:533:ILE:HG21	1:E:533:ILE:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:751:ILE:H	1:F:812:SER:HG	1.57	0.46
1:E:283:GLN:O	1:E:302:ARG:HA	2.15	0.46
1:E:755:GLU:OE2	1:E:877:SER:OG	2.30	0.46
1:F:564:ILE:O	1:F:587:MET:HA	2.15	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
1:E:840:ILE:HG23	2:E:1005:GOL:H2	1.98	0.45
1:E:614:VAL:HG23	1:E:648[B]:THR:OG1	2.15	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:A:191:ASP:OD1	1:A:191:ASP:C	2.55	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:B:915:ARG:NH1	1:B:922:HIS:CB	2.75	0.45
1:A:568:GLU:OE1	1:C:529:ASN:HB3	2.16	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: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: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: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:HD12	1:D:216:ILE:O	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:413:VAL:HG12	1:F:415:ASP:HB2	2.00	0.43
1:E:533:ILE:HG21	1:F:533:ILE:HG22	2.01	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
6:A:1035:EDO:H22	7:D:1530:HOH:O	2.18	0.43
1:A:921:ILE:O	1:A:921:ILE:HG22	2.19	0.43
1:C:757:PHE:O	1:C:776:GLN:HA	2.19	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: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
2:B:1004:GOL:H11	7:B:1655:HOH:O	2.18	0.43
1:B:188:VAL:HB	1:B:205:ILE:HD11	2.00	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:N	1:C:807:ASP:OD1	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: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: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:449:TYR:C	1:F:449:TYR:CD1	2.93	0.42
1:F:456:ASP:CG	1:F:457:PRO:HD2	2.40	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:A:670:ASN:ND2	7:A:1142:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:D:911:LEU:HD23	1:D:911:LEU:C	2.41	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:HE2	1:F:823:LYS:HB2	1.86	0.41
1:D:189:SER:HB3	1:D:204:ASP:HA	2.02	0.41
1:D:456:ASP:CG	1:D:457:PRO:HD2	2.41	0.41
1:D:773:LEU:HD23	1:D:773:LEU:C	2.41	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:C:295:LEU:HA	1:C:295:LEU:HD12	1.91	0.41
1:D:527:CYS:O	1:D:559:SER:HA	2.20	0.41
1:F:720:LEU:HA	1:F:720:LEU:HD12	1.87	0.41
1:F:709:SER:HB2	7:F:1174:HOH:O	2.21	0.41
1:A:505:THR:HA	1:A:528:GLY:O	2.21	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:A:675:ASP:OD2	1:B:890:SER:HB3	2.20	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:N	1:D:810:LEU:HD12	2.36	0.41
1:F:459:ARG:NE	1:F:459:ARG:HA	2.35	0.41
1:C:166:PRO:HB2	1:C:167:ALA:H	1.76	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:A:616:ASN:HB3	7:A:1105:HOH:O	2.21	0.40
1:B:548:VAL:CG2	1:B:548:VAL:O	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: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
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%)	51	43
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	43
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	43
All	All	4566/5562 (82%)	4346 (95%)	209 (5%)	11 (0%)	47	38

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%)	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3789/4620 (82%)	3705 (98%)	84 (2%)	52 47

All (84) 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	389	TYR
1	A	479	ASP
1	A	541	ASN
1	A	547	THR
1	A	550	GLN
1	A	581	GLU
1	A	594	ARG
1	A	626	ASN
1	A	826	TYR
1	A	841	ARG
1	B	169	ASP
1	B	229	LYS
1	B	360	LYS
1	B	389	TYR
1	B	479	ASP
1	B	488	ASP
1	B	547	THR
1	B	550	GLN
1	B	594	ARG
1	B	674	SER
1	B	826	TYR
1	B	841	ARG
1	B	905	PRO
1	B	922	HIS
1	C	267	CYS
1	C	321	VAL
1	C	488	ASP
1	C	541	ASN
1	C	550	GLN
1	C	594	ARG
1	C	601	ASN
1	C	779	ILE

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Mol	Chain	Res	Type
1	C	826	TYR
1	C	841	ARG
1	C	905	PRO
1	D	188	VAL
1	D	194	SER
1	D	197	ASP
1	D	226	SER
1	D	267	CYS
1	D	280	MET
1	D	289	GLN
1	D	389	TYR
1	D	541	ASN
1	D	547	THR
1	D	550	GLN
1	D	594	ARG
1	D	826	TYR
1	D	841	ARG
1	E	216	ILE
1	E	236	ASP
1	E	267	CYS
1	E	272	ASP
1	E	279	THR
1	E	280	MET
1	E	389	TYR
1	E	399	THR
1	E	479	ASP
1	E	488	ASP
1	E	493	ASN
1	E	547	THR
1	E	550	GLN
1	E	594	ARG
1	E	690	GLN
1	E	826	TYR
1	E	841	ARG
1	E	915	ARG
1	F	257	ARG
1	F	479	ASP
1	F	480	SER
1	F	488	ASP
1	F	541	ASN
1	F	548	VAL
1	F	594	ARG

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Mol	Chain	Res	Type
1	F	674	SER
1	F	806	ASN
1	F	812	SER
1	F	826	TYR
1	F	841	ARG

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	$\# Z > 2$
3	SO4	B	1019	-	4,4,4	0.40	0	6,6,6	0.21	0
2	GOL	A	1010	-	5,5,5	0.13	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	F	1006	-	4,4,4	0.29	0	6,6,6	0.17	0
2	GOL	C	1004	-	5,5,5	0.16	0	5,5,5	0.58	0
2	GOL	A	1021	-	5,5,5	0.13	0	5,5,5	0.43	0
2	GOL	D	1011	-	5,5,5	0.17	0	5,5,5	0.31	0
3	SO4	A	1034	-	4,4,4	0.47	0	6,6,6	0.43	0
2	GOL	B	1016	-	5,5,5	0.22	0	5,5,5	0.65	0
3	SO4	C	1002	-	4,4,4	0.35	0	6,6,6	0.30	0
2	GOL	D	1010	-	5,5,5	0.39	0	5,5,5	0.72	0
2	GOL	E	1008	-	5,5,5	0.24	0	5,5,5	0.59	0
2	GOL	B	1011	-	5,5,5	0.24	0	5,5,5	0.70	0
2	GOL	C	1006	-	5,5,5	0.31	0	5,5,5	0.98	0
2	GOL	C	1022	-	5,5,5	0.45	0	5,5,5	0.86	0
2	GOL	A	1003	-	5,5,5	0.23	0	5,5,5	1.64	1 (20%)
2	GOL	A	1014	-	5,5,5	0.15	0	5,5,5	0.52	0
2	GOL	E	1004	-	5,5,5	0.21	0	5,5,5	0.42	0
3	SO4	E	1010	-	4,4,4	0.27	0	6,6,6	0.19	0
2	GOL	A	1024	-	5,5,5	0.18	0	5,5,5	0.59	0
3	SO4	B	1018	-	4,4,4	0.30	0	6,6,6	0.45	0
2	GOL	B	1012	-	5,5,5	0.16	0	5,5,5	0.49	0
2	GOL	C	1003	-	5,5,5	0.46	0	5,5,5	1.36	0
2	GOL	A	1013	-	5,5,5	0.24	0	5,5,5	1.28	1 (20%)
3	SO4	C	1024	-	4,4,4	0.29	0	6,6,6	0.36	0
3	SO4	E	1001	-	4,4,4	0.29	0	6,6,6	0.45	0
6	EDO	A	1035	-	3,3,3	0.34	0	2,2,2	0.50	0
2	GOL	A	1033	-	5,5,5	0.15	0	5,5,5	0.26	0
2	GOL	B	1002	-	5,5,5	0.26	0	5,5,5	1.22	1 (20%)
2	GOL	A	1019	-	5,5,5	0.15	0	5,5,5	0.34	0
2	GOL	B	1015	-	5,5,5	0.22	0	5,5,5	0.54	0
2	GOL	F	1001	-	5,5,5	0.20	0	5,5,5	0.39	0
2	GOL	F	1004	-	5,5,5	0.17	0	5,5,5	0.50	0
2	GOL	C	1016	-	5,5,5	0.12	0	5,5,5	0.32	0
2	GOL	C	1019	-	5,5,5	0.14	0	5,5,5	0.44	0
2	GOL	B	1008	-	5,5,5	0.44	0	5,5,5	1.69	1 (20%)
2	GOL	B	1014	-	5,5,5	0.45	0	5,5,5	0.94	0
5	CO3	A	1031	-	0,3,3	0.00	-	0,3,3	0.00	-
2	GOL	A	1018	-	5,5,5	0.21	0	5,5,5	0.23	0
2	GOL	A	1011	-	5,5,5	0.61	0	5,5,5	1.03	0
2	GOL	A	1016	-	5,5,5	0.10	0	5,5,5	0.44	0
2	GOL	E	1002	-	5,5,5	0.24	0	5,5,5	0.57	0
2	GOL	D	1009	-	5,5,5	0.37	0	5,5,5	0.62	0
2	GOL	D	1002	-	5,5,5	0.35	0	5,5,5	0.66	0
3	SO4	D	1003	-	4,4,4	0.33	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	C	1018	-	5,5,5	0.39	0	5,5,5	1.01	0
2	GOL	A	1017	-	5,5,5	0.19	0	5,5,5	0.23	0
3	SO4	B	1020	-	4,4,4	0.21	0	6,6,6	0.46	0
2	GOL	B	1010	-	5,5,5	0.10	0	5,5,5	0.28	0
2	GOL	B	1007	-	5,5,5	0.24	0	5,5,5	0.39	0
2	GOL	B	1009	-	5,5,5	0.16	0	5,5,5	0.45	0
2	GOL	A	1015	-	5,5,5	0.11	0	5,5,5	0.53	0
2	GOL	C	1015	-	5,5,5	0.15	0	5,5,5	0.31	0
6	EDO	B	1022	-	3,3,3	0.29	0	2,2,2	0.67	0
3	SO4	A	1027	-	4,4,4	0.41	0	6,6,6	0.38	0
3	SO4	A	1026	-	4,4,4	0.31	0	6,6,6	0.64	0
2	GOL	B	1004	-	5,5,5	0.08	0	5,5,5	0.40	0
2	GOL	A	1012	-	5,5,5	0.55	0	5,5,5	0.88	0
2	GOL	F	1003	-	5,5,5	0.19	0	5,5,5	0.71	0
2	GOL	A	1002	-	5,5,5	0.42	0	5,5,5	0.60	0
2	GOL	A	1005	-	5,5,5	0.43	0	5,5,5	0.86	0
2	GOL	A	1009	-	5,5,5	0.17	0	5,5,5	0.80	0
2	GOL	C	1010	-	5,5,5	0.17	0	5,5,5	0.39	0
2	GOL	C	1014	-	5,5,5	0.09	0	5,5,5	0.34	0
2	GOL	A	1004	-	5,5,5	0.21	0	5,5,5	0.67	0
2	GOL	B	1003	-	5,5,5	0.22	0	5,5,5	0.32	0
2	GOL	E	1006	-	5,5,5	0.13	0	5,5,5	0.24	0
2	GOL	C	1011	-	5,5,5	0.08	0	5,5,5	0.42	0
2	GOL	A	1006	-	5,5,5	0.08	0	5,5,5	0.42	0
2	GOL	C	1008	-	5,5,5	0.11	0	5,5,5	0.43	0
2	GOL	A	1008	-	5,5,5	0.40	0	5,5,5	0.76	0
2	GOL	A	1001	-	5,5,5	0.49	0	5,5,5	0.84	0
2	GOL	F	1002	-	5,5,5	0.10	0	5,5,5	0.69	0
2	GOL	A	1022	-	5,5,5	0.15	0	5,5,5	0.35	0
2	GOL	B	1005	-	5,5,5	0.25	0	5,5,5	1.07	0
3	SO4	F	1007	-	4,4,4	0.27	0	6,6,6	0.18	0
2	GOL	C	1007	-	5,5,5	0.11	0	5,5,5	0.52	0
5	CO3	D	1007	-	0,3,3	0.00	-	0,3,3	0.00	-
2	GOL	E	1005	-	5,5,5	0.11	0	5,5,5	0.60	0
2	GOL	D	1001	-	5,5,5	0.10	0	5,5,5	0.79	0
2	GOL	A	1007	-	5,5,5	0.11	0	5,5,5	0.41	0
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	C	1009	-	5,5,5	0.24	0	5,5,5	0.50	0
2	GOL	C	1021	-	5,5,5	0.50	0	5,5,5	0.97	0
2	GOL	E	1003	-	5,5,5	0.15	0	5,5,5	0.32	0
2	GOL	C	1013	-	5,5,5	0.12	0	5,5,5	0.94	0
2	GOL	B	1013	-	5,5,5	0.11	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	1023	-	5,5,5	0.27	0	5,5,5	1.10	0
3	SO4	D	1012	-	4,4,4	0.37	0	6,6,6	0.37	0
3	SO4	A	1032	-	4,4,4	0.43	0	6,6,6	0.32	0
3	SO4	B	1001	-	4,4,4	0.36	0	6,6,6	0.63	0
6	EDO	C	1028	-	3,3,3	0.13	0	2,2,2	0.68	0
6	EDO	C	1026	-	3,3,3	0.30	0	2,2,2	1.42	0
2	GOL	B	1006	-	5,5,5	0.23	0	5,5,5	0.47	0
3	SO4	E	1011	-	4,4,4	0.29	0	6,6,6	0.29	0
2	GOL	C	1017	-	5,5,5	0.25	0	5,5,5	0.86	0
2	GOL	B	1017	-	5,5,5	0.10	0	5,5,5	0.32	0
2	GOL	A	1020	-	5,5,5	0.32	0	5,5,5	0.84	0
2	GOL	C	1020	-	5,5,5	0.10	0	5,5,5	0.33	0
2	GOL	C	1001	-	5,5,5	0.16	0	5,5,5	0.50	0
3	SO4	F	1005	-	4,4,4	0.18	0	6,6,6	0.44	0
3	SO4	C	1025	-	4,4,4	0.35	0	6,6,6	0.47	0
2	GOL	C	1005	-	5,5,5	0.31	0	5,5,5	1.33	1 (20%)
3	SO4	C	1023	-	4,4,4	0.42	0	6,6,6	0.56	0
2	GOL	E	1007	-	5,5,5	0.11	0	5,5,5	0.42	0
3	SO4	D	1013	-	4,4,4	0.40	0	6,6,6	0.30	0
3	SO4	A	1025	-	4,4,4	0.40	0	6,6,6	0.42	0
6	EDO	C	1027	-	3,3,3	0.24	0	2,2,2	1.74	0
3	SO4	F	1008	-	4,4,4	0.31	0	6,6,6	0.16	0
3	SO4	E	1009	-	4,4,4	0.40	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	A	1033	-	-	4/4/4/4	-
2	GOL	B	1002	-	-	4/4/4/4	-
2	GOL	C	1015	-	-	4/4/4/4	-
6	EDO	B	1022	-	-	1/1/1/1	-
2	GOL	A	1019	-	-	4/4/4/4	-
2	GOL	B	1015	-	-	2/4/4/4	-
2	GOL	A	1010	-	-	4/4/4/4	-
2	GOL	F	1001	-	-	2/4/4/4	-
2	GOL	D	1001	-	-	3/4/4/4	-
2	GOL	A	1015	-	-	1/4/4/4	-
6	EDO	A	1035	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	F	1004	-	-	2/4/4/4	-
2	GOL	C	1004	-	-	0/4/4/4	-
2	GOL	B	1004	-	-	0/4/4/4	-
2	GOL	C	1012	-	-	4/4/4/4	-
2	GOL	A	1012	-	-	2/4/4/4	-
2	GOL	F	1003	-	-	3/4/4/4	-
2	GOL	C	1016	-	-	0/4/4/4	-
2	GOL	A	1002	-	-	0/4/4/4	-
2	GOL	A	1005	-	-	3/4/4/4	-
2	GOL	A	1008	-	-	4/4/4/4	-
2	GOL	A	1021	-	-	0/4/4/4	-
2	GOL	C	1008	-	-	2/4/4/4	-
2	GOL	A	1009	-	-	2/4/4/4	-
2	GOL	D	1011	-	-	4/4/4/4	-
2	GOL	C	1019	-	-	2/4/4/4	-
2	GOL	B	1008	-	-	0/4/4/4	-
2	GOL	B	1016	-	-	1/4/4/4	-
2	GOL	C	1010	-	-	2/4/4/4	-
2	GOL	E	1003	-	-	3/4/4/4	-
2	GOL	C	1013	-	-	2/4/4/4	-
2	GOL	C	1014	-	-	1/4/4/4	-
2	GOL	B	1013	-	-	0/4/4/4	-
2	GOL	A	1023	-	-	4/4/4/4	-
2	GOL	A	1004	-	-	0/4/4/4	-
2	GOL	B	1003	-	-	0/4/4/4	-
2	GOL	D	1010	-	-	0/4/4/4	-
2	GOL	E	1008	-	-	0/4/4/4	-
2	GOL	E	1006	-	-	2/4/4/4	-
2	GOL	C	1011	-	-	0/4/4/4	-
2	GOL	A	1006	-	-	3/4/4/4	-
2	GOL	B	1011	-	-	0/4/4/4	-
2	GOL	C	1006	-	-	3/4/4/4	-
2	GOL	C	1022	-	-	4/4/4/4	-
2	GOL	C	1009	-	-	1/4/4/4	-
2	GOL	A	1003	-	-	3/4/4/4	-
2	GOL	B	1006	-	-	0/4/4/4	-
2	GOL	A	1014	-	-	2/4/4/4	-
2	GOL	A	1007	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	E	1004	-	-	2/4/4/4	-
2	GOL	A	1018	-	-	2/4/4/4	-
2	GOL	C	1017	-	-	2/4/4/4	-
2	GOL	C	1021	-	-	2/4/4/4	-
2	GOL	B	1017	-	-	4/4/4/4	-
2	GOL	A	1020	-	-	4/4/4/4	-
2	GOL	C	1020	-	-	3/4/4/4	-
2	GOL	C	1001	-	-	1/4/4/4	-
2	GOL	A	1024	-	-	3/4/4/4	-
2	GOL	A	1001	-	-	0/4/4/4	-
2	GOL	C	1005	-	-	2/4/4/4	-
2	GOL	A	1011	-	-	2/4/4/4	-
2	GOL	A	1016	-	-	4/4/4/4	-
2	GOL	E	1002	-	-	0/4/4/4	-
2	GOL	E	1005	-	-	2/4/4/4	-
2	GOL	D	1009	-	-	0/4/4/4	-
2	GOL	D	1002	-	-	0/4/4/4	-
2	GOL	B	1012	-	-	2/4/4/4	-
2	GOL	F	1002	-	-	2/4/4/4	-
2	GOL	A	1022	-	-	2/4/4/4	-
2	GOL	B	1014	-	-	2/4/4/4	-
2	GOL	B	1005	-	-	2/4/4/4	-
2	GOL	C	1003	-	-	4/4/4/4	-
6	EDO	C	1028	-	-	1/1/1/1	-
2	GOL	C	1007	-	-	2/4/4/4	-
2	GOL	A	1013	-	-	2/4/4/4	-
2	GOL	C	1018	-	-	2/4/4/4	-
2	GOL	A	1017	-	-	0/4/4/4	-
6	EDO	C	1026	-	-	1/1/1/1	-
6	EDO	C	1027	-	-	1/1/1/1	-
2	GOL	B	1010	-	-	3/4/4/4	-
2	GOL	E	1007	-	-	2/4/4/4	-
2	GOL	B	1007	-	-	0/4/4/4	-
2	GOL	B	1009	-	-	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.

All (150) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1010	GOL	O1-C1-C2-C3
2	A	1010	GOL	C1-C2-C3-O3
2	C	1006	GOL	O1-C1-C2-C3
2	C	1022	GOL	O1-C1-C2-C3
2	C	1022	GOL	C1-C2-C3-O3
2	B	1012	GOL	C1-C2-C3-O3
2	C	1003	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	1002	GOL	C1-C2-C3-O3
2	A	1019	GOL	O1-C1-C2-C3
2	B	1015	GOL	O1-C1-C2-O2
2	F	1001	GOL	C1-C2-C3-O3
2	F	1004	GOL	C1-C2-C3-O3
2	B	1014	GOL	O1-C1-C2-C3
2	A	1018	GOL	O1-C1-C2-O2
2	A	1018	GOL	O1-C1-C2-C3
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	C	1018	GOL	C1-C2-C3-O3
2	C	1015	GOL	C1-C2-C3-O3
2	F	1003	GOL	C1-C2-C3-O3
2	A	1005	GOL	O1-C1-C2-C3
2	A	1009	GOL	C1-C2-C3-O3
2	C	1010	GOL	O1-C1-C2-C3
2	E	1006	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

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Mol	Chain	Res	Type	Atoms
2	F	1002	GOL	C1-C2-C3-O3
2	F	1002	GOL	O2-C2-C3-O3
2	C	1007	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	C	1013	GOL	O1-C1-C2-C3
2	A	1023	GOL	O1-C1-C2-C3
2	A	1023	GOL	C1-C2-C3-O3
2	C	1017	GOL	C1-C2-C3-O3
2	B	1017	GOL	C1-C2-C3-O3
2	A	1020	GOL	C1-C2-C3-O3
2	E	1007	GOL	C1-C2-C3-O3
2	A	1010	GOL	O2-C2-C3-O3
2	A	1003	GOL	O2-C2-C3-O3
2	A	1014	GOL	O2-C2-C3-O3
2	B	1012	GOL	O2-C2-C3-O3
2	F	1004	GOL	O2-C2-C3-O3
2	A	1006	GOL	O2-C2-C3-O3
2	A	1023	GOL	O1-C1-C2-O2
2	C	1017	GOL	O2-C2-C3-O3
2	E	1007	GOL	O2-C2-C3-O3
2	D	1011	GOL	O1-C1-C2-C3
2	D	1011	GOL	C1-C2-C3-O3
2	C	1006	GOL	C1-C2-C3-O3
2	A	1003	GOL	C1-C2-C3-O3
2	A	1014	GOL	C1-C2-C3-O3
2	E	1004	GOL	O1-C1-C2-C3
2	A	1024	GOL	C1-C2-C3-O3
2	A	1013	GOL	O1-C1-C2-C3
2	A	1019	GOL	C1-C2-C3-O3
2	B	1015	GOL	O1-C1-C2-C3
2	C	1019	GOL	C1-C2-C3-O3
2	B	1014	GOL	C1-C2-C3-O3
2	C	1015	GOL	O1-C1-C2-C3
2	A	1012	GOL	C1-C2-C3-O3
2	A	1005	GOL	C1-C2-C3-O3
2	C	1008	GOL	C1-C2-C3-O3
2	E	1005	GOL	C1-C2-C3-O3
2	C	1021	GOL	C1-C2-C3-O3
2	B	1017	GOL	O1-C1-C2-C3
2	A	1020	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	C	1020	GOL	O1-C1-C2-C3
2	C	1005	GOL	C1-C2-C3-O3
2	D	1011	GOL	O2-C2-C3-O3
2	C	1006	GOL	O2-C2-C3-O3
2	C	1022	GOL	O1-C1-C2-O2
2	C	1022	GOL	O2-C2-C3-O3
2	C	1003	GOL	O2-C2-C3-O3
2	A	1013	GOL	O1-C1-C2-O2
2	A	1033	GOL	O2-C2-C3-O3
2	B	1002	GOL	O2-C2-C3-O3
2	C	1019	GOL	O2-C2-C3-O3
2	C	1015	GOL	O2-C2-C3-O3
2	A	1012	GOL	O2-C2-C3-O3
2	F	1003	GOL	O2-C2-C3-O3
2	A	1005	GOL	O1-C1-C2-O2
2	A	1009	GOL	O2-C2-C3-O3
2	E	1006	GOL	O1-C1-C2-O2
2	C	1008	GOL	O2-C2-C3-O3
2	E	1005	GOL	O2-C2-C3-O3
2	D	1001	GOL	O1-C1-C2-O2
2	C	1021	GOL	O2-C2-C3-O3
2	A	1023	GOL	O2-C2-C3-O3
2	B	1017	GOL	O1-C1-C2-O2
2	B	1017	GOL	O2-C2-C3-O3
2	A	1020	GOL	O1-C1-C2-O2
2	C	1005	GOL	O2-C2-C3-O3
6	A	1035	EDO	O1-C1-C2-O2
6	C	1027	EDO	O1-C1-C2-O2
2	A	1010	GOL	O1-C1-C2-O2
2	E	1004	GOL	O1-C1-C2-O2
2	C	1003	GOL	O1-C1-C2-O2
2	A	1019	GOL	O1-C1-C2-O2
2	C	1018	GOL	O2-C2-C3-O3
2	C	1010	GOL	O1-C1-C2-O2
2	C	1007	GOL	O1-C1-C2-O2
2	A	1020	GOL	O2-C2-C3-O3
2	C	1020	GOL	O1-C1-C2-O2
6	B	1022	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
6	C	1028	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	1033	GOL	O1-C1-C2-O2
2	A	1011	GOL	O2-C2-C3-O3
2	A	1016	GOL	O1-C1-C2-O2
2	C	1015	GOL	O1-C1-C2-O2
2	B	1005	GOL	O1-C1-C2-O2
2	D	1001	GOL	O2-C2-C3-O3
2	C	1012	GOL	O1-C1-C2-O2
2	C	1001	GOL	O1-C1-C2-O2
2	C	1003	GOL	O1-C1-C2-C3
2	B	1010	GOL	C1-C2-C3-O3
2	C	1014	GOL	C1-C2-C3-O3
2	A	1022	GOL	C1-C2-C3-O3
2	D	1011	GOL	O1-C1-C2-O2
6	C	1026	EDO	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	C	1012	GOL	C1-C2-C3-O3
2	F	1001	GOL	O2-C2-C3-O3
2	B	1016	GOL	O2-C2-C3-O3
2	C	1013	GOL	O1-C1-C2-O2
2	A	1024	GOL	O1-C1-C2-C3
2	A	1033	GOL	O1-C1-C2-C3
2	B	1010	GOL	O1-C1-C2-C3
2	A	1006	GOL	O1-C1-C2-C3
2	B	1005	GOL	O1-C1-C2-C3
2	C	1012	GOL	O1-C1-C2-C3
2	C	1020	GOL	C1-C2-C3-O3
2	F	1003	GOL	O1-C1-C2-O2
2	A	1022	GOL	O2-C2-C3-O3
2	C	1012	GOL	O2-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	1021	GOL	3	0
2	D	1010	GOL	3	0
2	E	1008	GOL	1	0
2	C	1022	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1014	GOL	1	0
2	E	1004	GOL	1	0
2	A	1024	GOL	1	0
2	B	1012	GOL	1	0
2	C	1003	GOL	2	0
2	A	1013	GOL	1	0
3	C	1024	SO4	2	0
6	A	1035	EDO	2	0
2	A	1033	GOL	1	0
2	B	1015	GOL	1	0
2	F	1004	GOL	3	0
2	B	1008	GOL	3	0
2	A	1018	GOL	1	0
2	A	1011	GOL	2	0
2	A	1016	GOL	1	0
2	C	1018	GOL	4	0
2	B	1010	GOL	1	0
2	B	1007	GOL	1	0
2	B	1009	GOL	1	0
2	C	1015	GOL	1	0
2	B	1004	GOL	4	0
2	A	1012	GOL	1	0
2	A	1005	GOL	4	0
2	A	1009	GOL	1	0
2	C	1010	GOL	2	0
2	C	1014	GOL	1	0
2	E	1006	GOL	1	0
2	C	1008	GOL	2	0
2	A	1008	GOL	2	0
2	F	1002	GOL	1	0
2	A	1022	GOL	3	0
2	E	1005	GOL	1	0
2	A	1007	GOL	1	0
2	C	1009	GOL	2	0
2	C	1021	GOL	3	0
2	E	1003	GOL	2	0
2	C	1013	GOL	1	0
3	D	1012	SO4	1	0
3	B	1001	SO4	1	0
6	C	1026	EDO	1	0
2	C	1017	GOL	1	0
2	A	1020	GOL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1020	GOL	1	0
2	C	1001	GOL	1	0
3	C	1025	SO4	1	0
2	C	1005	GOL	1	0
2	E	1007	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	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%)

All (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
1	D	236	ASP	6.2
1	E	548	VAL	6.2
1	D	234	PRO	5.7
1	E	216	ILE	5.6
1	D	239	VAL	5.5
1	D	754	ALA	5.5
1	D	192	THR	5.2
1	D	226	SER	5.1
1	D	230	LEU	5.1
1	F	701	VAL	5.1
1	D	221	VAL	5.0
1	D	195	LEU	4.9
1	E	232	TYR	4.9
1	D	206	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	548	VAL	4.7
1	D	231	ASN	4.6
1	E	236	ASP	4.6
1	B	167	ALA	4.6
1	D	190	THR	4.5
1	B	548	VAL	4.5
1	D	233	ASN	4.4
1	E	222	ILE	4.4
1	A	193	ILE	4.4
1	D	227	ALA	4.4
1	D	321	VAL	4.4
1	E	218	ASP	4.2
1	D	223	SER	4.2
1	A	237	VAL	4.2
1	F	548	VAL	4.2
1	D	795	GLY	4.1
1	D	193	ILE	4.1
1	D	224	SER	4.1
1	E	783	GLY	4.0
1	D	225	VAL	4.0
1	E	305	ILE	3.9
1	E	308	THR	3.8
1	D	196	LEU	3.8
1	D	219	GLY	3.8
1	D	217	PRO	3.8
1	D	198	GLY	3.8
1	D	205	ILE	3.8
1	D	781	ALA	3.8
1	E	237	VAL	3.7
1	B	649	ILE	3.7
1	B	308	THR	3.7
1	A	219	GLY	3.7
1	A	216	ILE	3.6
1	A	548	VAL	3.6
1	A	615	ILE	3.6
1	D	796	THR	3.6
1	A	195	LEU	3.5
1	E	766	PHE	3.5
1	A	227	ALA	3.5
1	D	197	ASP	3.5
1	D	218	ASP	3.4
1	E	227	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	203	TYR	3.4
1	A	614[A]	VAL	3.4
1	A	235	GLY	3.4
1	E	321	VAL	3.4
1	A	226	SER	3.3
1	D	782	SER	3.3
1	E	217	PRO	3.3
1	D	797	THR	3.3
1	C	533	ILE	3.3
1	B	615	ILE	3.3
1	A	239	VAL	3.3
1	D	768	ASP	3.3
1	E	235	GLY	3.2
1	A	533	ILE	3.2
1	D	189	SER	3.2
1	C	308	THR	3.2
1	E	234	PRO	3.2
1	F	921	ILE	3.2
1	B	681	LEU	3.1
1	D	305	ILE	3.2
1	D	307	GLY	3.1
1	A	649	ILE	3.1
1	B	309	GLY	3.1
1	D	228	GLY	3.1
1	D	851	VAL	3.1
1	F	702	SER	3.1
1	E	169	ASP	3.0
1	B	678	ILE	3.0
1	D	799	ILE	3.0
1	D	229	LYS	3.0
1	E	769	THR	3.0
1	A	236	ASP	3.0
1	D	238	GLN	2.9
1	E	873	GLY	2.9
1	C	309	GLY	2.9
1	F	704	THR	2.9
1	D	280	MET	2.9
1	D	769	THR	2.8
1	C	463	ILE	2.8
1	C	564	ILE	2.8
1	E	860	THR	2.8
1	B	614[A]	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	533	ILE	2.8
1	B	652	VAL	2.8
1	A	232	TYR	2.8
1	C	532	ILE	2.7
1	A	234	PRO	2.7
1	C	563	VAL	2.7
1	D	794	ASP	2.7
1	A	192	THR	2.7
1	E	599	ALA	2.7
1	D	311	THR	2.7
1	D	220	SER	2.7
1	B	653	VAL	2.7
1	E	858	GLY	2.7
1	A	510[A]	THR	2.7
1	A	532	ILE	2.6
1	E	307	GLY	2.6
1	E	196	LEU	2.6
1	E	230	LEU	2.6
1	A	648[A]	THR	2.6
1	F	292	ALA	2.6
1	D	309	GLY	2.6
1	E	219	GLY	2.6
1	E	233	ASN	2.6
1	D	308	THR	2.6
1	A	678	ILE	2.6
1	E	768	ASP	2.6
1	E	792	GLY	2.6
1	B	462	CYS	2.6
1	E	678	ILE	2.6
1	E	767	SER	2.6
1	E	322	GLY	2.6
1	C	280	MET	2.6
1	D	860	THR	2.6
1	D	187	ILE	2.5
1	E	193	ILE	2.5
1	D	322	GLY	2.5
1	D	207	THR	2.5
1	C	614[A]	VAL	2.5
1	A	676	LEU	2.5
1	E	306	ASP	2.5
1	A	218	ASP	2.4
1	E	238	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	304	LEU	2.4
1	E	615	ILE	2.4
1	A	309	GLY	2.4
1	A	490	LEU	2.4
1	B	618	PHE	2.4
1	A	512	ILE	2.4
1	D	532	ILE	2.4
1	D	615	ILE	2.4
1	D	853	PHE	2.4
1	E	549	GLY	2.4
1	F	293	GLY	2.4
1	A	567	ILE	2.4
1	B	563	VAL	2.4
1	E	205	ILE	2.4
1	D	847	ALA	2.3
1	F	698	PHE	2.3
1	E	275	ASN	2.3
1	E	214	PRO	2.3
1	C	512	ILE	2.3
1	E	239	VAL	2.3
1	C	781	ALA	2.3
1	A	228	GLY	2.3
1	A	168	PHE	2.3
1	D	240	ASP	2.3
1	E	861	SER	2.3
1	C	615	ILE	2.3
1	A	167	ALA	2.3
1	B	651	GLY	2.3
1	D	324	ALA	2.3
1	A	229	LYS	2.3
1	E	220	SER	2.3
1	B	619	VAL	2.3
1	B	680	GLY	2.3
1	E	309	GLY	2.3
1	E	215	THR	2.3
1	A	590	LEU	2.3
1	A	221	VAL	2.3
1	A	647	VAL	2.3
1	C	165	SER	2.3
1	F	705	PRO	2.2
1	B	416	ALA	2.2
1	D	614[A]	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	590	LEU	2.2
1	D	241	LEU	2.2
1	A	217	PRO	2.2
1	D	533	ILE	2.2
1	C	306	ASP	2.2
1	B	413	VAL	2.2
1	B	906	VAL	2.2
1	F	706	VAL	2.2
1	A	305	ILE	2.2
1	B	532	ILE	2.2
1	A	509	TRP	2.2
1	E	807	ASP	2.2
1	E	797	THR	2.2
1	E	197	ASP	2.2
1	A	564	ILE	2.2
1	F	533	ILE	2.2
1	D	855	SER	2.2
1	C	490	LEU	2.2
1	E	280	MET	2.2
1	A	566	GLY	2.2
1	C	307	GLY	2.2
1	F	700	GLY	2.2
1	A	563	VAL	2.2
1	A	534	GLY	2.1
1	E	223	SER	2.1
1	A	682	VAL	2.1
1	A	308	THR	2.1
1	D	172	ILE	2.1
1	E	231	ASN	2.1
1	E	651	GLY	2.1
1	E	590	LEU	2.1
1	B	682	VAL	2.1
1	B	589	GLY	2.1
1	A	190	THR	2.1
1	D	215	THR	2.1
1	E	796	THR	2.1
1	C	567	ILE	2.1
1	E	170	ARG	2.1
1	A	491	LEU	2.1
1	C	413	VAL	2.1
1	D	857	PHE	2.1
1	D	194	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	617	GLY	2.1
1	D	399	THR	2.0
1	B	306	ASP	2.0
1	D	850	ALA	2.0
1	E	198	GLY	2.0
1	B	564	ILE	2.0
1	D	678[A]	ILE	2.0
1	F	590	LEU	2.0
1	D	191	ASP	2.0
1	C	508	THR	2.0
1	A	589	GLY	2.0
1	B	417	PHE	2.0
1	D	320	THR	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 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(\AA^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	C	1021	6/6	0.73	0.31	29,53,56,56	0
2	GOL	C	1011	6/6	0.73	0.28	56,74,80,81	0
2	GOL	A	1008	6/6	0.73	0.22	47,58,62,67	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	D	1010	6/6	0.80	0.18	41,56,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	B	1006	6/6	0.80	0.52	65,83,86,86	0
2	GOL	A	1022	6/6	0.81	0.27	64,68,74,83	0
2	GOL	C	1013	6/6	0.81	0.13	52,54,66,66	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
4	CL	B	1021	1/1	0.82	0.14	71,71,71,71	0
2	GOL	A	1019	6/6	0.83	0.20	63,75,82,99	0
2	GOL	B	1015	6/6	0.83	0.46	60,66,71,77	0
2	GOL	B	1014	6/6	0.83	0.15	49,60,61,62	0
2	GOL	C	1008	6/6	0.84	0.21	59,71,75,80	0
2	GOL	E	1003	6/6	0.84	0.17	48,58,61,63	0
2	GOL	E	1002	6/6	0.84	0.14	67,68,71,71	0
2	GOL	A	1024	6/6	0.85	0.18	50,59,70,74	0
2	GOL	E	1004	6/6	0.86	0.18	50,55,66,68	0
2	GOL	A	1007	6/6	0.86	0.15	51,59,64,69	0
2	GOL	E	1008	6/6	0.86	0.31	56,70,74,87	0
2	GOL	A	1014	6/6	0.86	0.22	58,68,73,78	0
2	GOL	A	1021	6/6	0.87	0.38	54,70,80,83	0
2	GOL	A	1010	6/6	0.87	0.17	59,62,70,80	0
2	GOL	F	1003	6/6	0.88	0.12	43,57,61,70	0
2	GOL	A	1005	6/6	0.88	0.13	40,40,49,49	0
5	CO3	A	1031	4/4	0.88	0.14	55,59,62,67	0
2	GOL	B	1010	6/6	0.88	0.18	60,71,75,80	0
2	GOL	B	1007	6/6	0.88	0.18	48,61,67,78	0
2	GOL	B	1012	6/6	0.88	0.19	67,74,85,87	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	B	1011	6/6	0.89	0.18	45,50,59,62	0
2	GOL	A	1020	6/6	0.89	0.31	50,64,67,81	0
2	GOL	A	1017	6/6	0.89	0.18	48,66,68,78	0
2	GOL	C	1005	6/6	0.89	0.15	38,40,41,45	6
2	GOL	C	1014	6/6	0.90	0.39	47,64,70,89	0
2	GOL	A	1011	6/6	0.90	0.18	34,41,48,54	0
2	GOL	A	1004	6/6	0.90	0.17	30,59,66,68	0
2	GOL	C	1015	6/6	0.90	0.21	62,69,77,78	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	C	1007	6/6	0.91	0.10	49,56,65,68	0
2	GOL	A	1033	6/6	0.91	0.10	51,57,65,65	0
2	GOL	A	1006	6/6	0.91	0.11	50,63,66,68	0
3	SO4	A	1026	5/5	0.91	0.15	20,25,37,38	5
2	GOL	F	1004	6/6	0.91	0.12	48,56,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	F	1002	6/6	0.91	0.13	51,62,65,67	0
2	GOL	C	1020	6/6	0.91	0.15	52,67,70,74	0
2	GOL	D	1011	6/6	0.91	0.13	55,65,73,85	0
2	GOL	B	1005	6/6	0.91	0.14	43,49,51,53	0
3	SO4	F	1008	5/5	0.91	0.14	70,88,95,111	0
6	EDO	C	1026	4/4	0.92	0.16	35,63,63,63	0
3	SO4	D	1004	5/5	0.92	0.14	67,78,85,118	0
2	GOL	A	1009	6/6	0.92	0.19	57,61,70,71	0
2	GOL	B	1008	6/6	0.92	0.17	32,43,48,55	0
2	GOL	A	1003	6/6	0.92	0.14	33,37,43,43	0
2	GOL	B	1016	6/6	0.92	0.24	38,45,58,63	0
2	GOL	C	1006	6/6	0.92	0.22	41,51,54,58	0
2	GOL	B	1009	6/6	0.92	0.12	57,63,69,74	0
2	GOL	C	1016	6/6	0.92	0.14	45,58,69,85	0
2	GOL	D	1001	6/6	0.93	0.13	50,58,61,64	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	A	1018	6/6	0.93	0.20	48,51,58,71	0
2	GOL	D	1002	6/6	0.94	0.24	43,53,56,60	0
3	SO4	E	1011	5/5	0.94	0.14	75,81,92,111	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
2	GOL	C	1019	6/6	0.94	0.29	46,61,65,68	0
2	GOL	A	1013	6/6	0.94	0.13	36,39,44,48	0
2	GOL	A	1016	6/6	0.94	0.18	38,50,60,68	0
2	GOL	B	1002	6/6	0.94	0.09	40,42,50,51	0
2	GOL	E	1007	6/6	0.94	0.17	40,58,61,73	0
6	EDO	C	1027	4/4	0.94	0.08	46,53,54,60	0
2	GOL	D	1009	6/6	0.94	0.14	41,47,50,55	0
3	SO4	D	1012	5/5	0.95	0.11	34,42,43,51	5
3	SO4	F	1007	5/5	0.95	0.11	55,55,58,66	5
2	GOL	E	1006	6/6	0.95	0.14	42,58,64,71	0
3	SO4	F	1005	5/5	0.95	0.12	42,46,49,52	5
2	GOL	A	1001	6/6	0.95	0.12	34,37,38,42	0
3	SO4	E	1010	5/5	0.95	0.15	67,86,95,102	0
3	SO4	B	1020	5/5	0.95	0.10	21,23,31,32	5
2	GOL	F	1001	6/6	0.95	0.15	41,50,53,56	0
4	CL	D	1006	1/1	0.96	0.18	56,56,56,56	0
2	GOL	C	1003	6/6	0.96	0.19	32,34,40,41	0
2	GOL	B	1003	6/6	0.96	0.08	36,38,39,41	0
2	GOL	C	1004	6/6	0.96	0.08	29,38,43,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CO3	D	1007	4/4	0.96	0.10	67,69,79,84	0
2	GOL	E	1005	6/6	0.96	0.18	52,55,61,65	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
3	SO4	C	1025	5/5	0.97	0.10	55,56,69,91	0
4	CL	A	1030	1/1	0.97	0.05	61,61,61,61	0
3	SO4	B	1001	5/5	0.97	0.08	33,34,44,51	5
3	SO4	E	1001	5/5	0.97	0.08	41,50,55,65	5
3	SO4	A	1027	5/5	0.97	0.07	53,56,59,74	0
3	SO4	E	1009	5/5	0.97	0.09	50,53,57,65	5
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	B	1018	5/5	0.98	0.06	46,50,67,71	0
3	SO4	C	1023	5/5	0.98	0.10	41,47,54,62	5
3	SO4	A	1032	5/5	0.98	0.18	52,63,77,78	0
3	SO4	D	1013	5/5	0.98	0.15	61,73,80,92	0
3	SO4	C	1002	5/5	0.98	0.09	44,45,49,55	0
4	CL	A	1029	1/1	0.98	0.13	40,40,40,40	0
3	SO4	B	1019	5/5	0.98	0.08	58,59,65,82	0
3	SO4	A	1025	5/5	0.99	0.08	45,54,65,70	0
4	CL	D	1008	1/1	0.99	0.12	41,41,41,41	0
4	CL	A	1028	1/1	1.00	0.16	22,22,22,22	0
4	CL	D	1005	1/1	1.00	0.14	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.