Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 07:33 PM BST

PDB ID	:	6I9G
Title	:	Crystal structure of encapsulin from Mycolicibacterium hassiacum
Authors	:	Rozeboom, H.J.; Fraaije, M.W.
Deposited on	:	2018-11-23
Resolution	:	2.50 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:

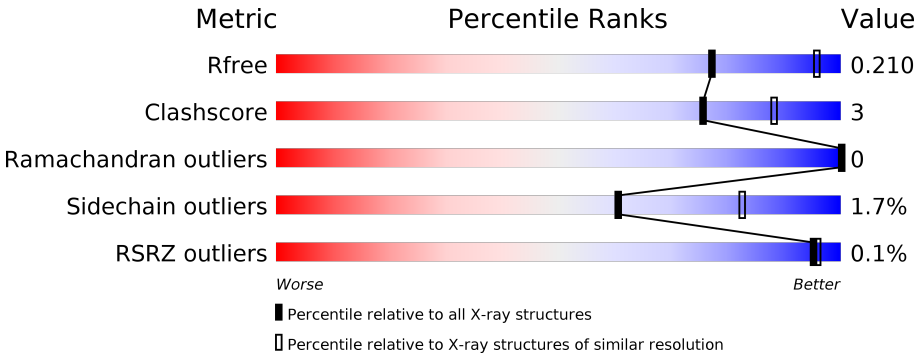
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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 <=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	265	94% 6%
1	B	265	92% 8%
1	C	265	90% 10%
1	D	265	95% 5%
1	E	265	89% 11%
1	F	265	92% 8%

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Mol	Chain	Length	Quality of chain
1	G	265	89% 11%
1	H	265	92% 8%
1	I	265	93% 6%
1	J	265	92% 7%
1	K	265	93% 6%
1	L	265	89% 11%
1	M	265	90% 10%
1	N	265	92% 8%
1	O	265	90% 10%

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	SO4	H	302	-	-	X	-

2 Entry composition

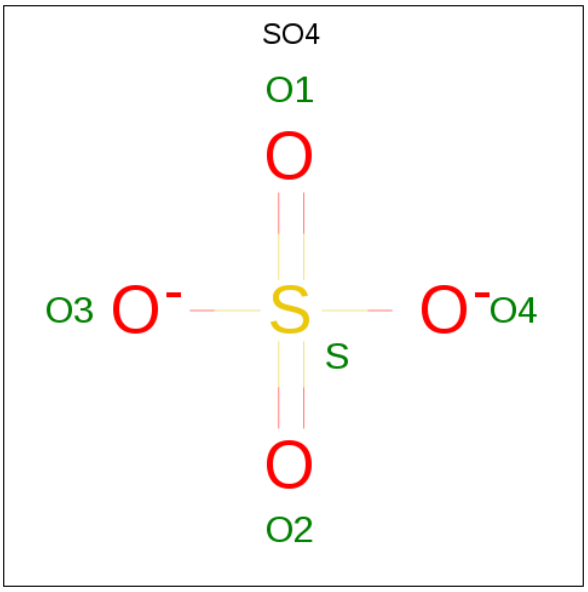
There are 4 unique types of molecules in this entry. The entry contains 34092 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Linocin-M18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	1	0
			2056	1290	359	404	3			
1	B	265	Total	C	N	O	S	0	0	0
			2045	1284	355	403	3			
1	C	265	Total	C	N	O	S	0	0	0
			2045	1284	355	403	3			
1	D	265	Total	C	N	O	S	0	0	0
			2045	1284	355	403	3			
1	E	265	Total	C	N	O	S	0	0	0
			2045	1284	355	403	3			
1	F	265	Total	C	N	O	S	0	0	0
			2045	1284	355	403	3			
1	G	265	Total	C	N	O	S	0	0	0
			2045	1284	355	403	3			
1	H	265	Total	C	N	O	S	0	0	0
			2045	1284	355	403	3			
1	I	265	Total	C	N	O	S	0	0	0
			2045	1284	355	403	3			
1	J	265	Total	C	N	O	S	0	0	0
			2045	1284	355	403	3			
1	K	265	Total	C	N	O	S	0	0	0
			2045	1284	355	403	3			
1	L	265	Total	C	N	O	S	0	0	0
			2045	1284	355	403	3			
1	M	265	Total	C	N	O	S	0	0	0
			2045	1284	355	403	3			
1	N	265	Total	C	N	O	S	0	0	0
			2045	1284	355	403	3			
1	O	265	Total	C	N	O	S	0	0	0
			2045	1284	355	403	3			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	J	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0

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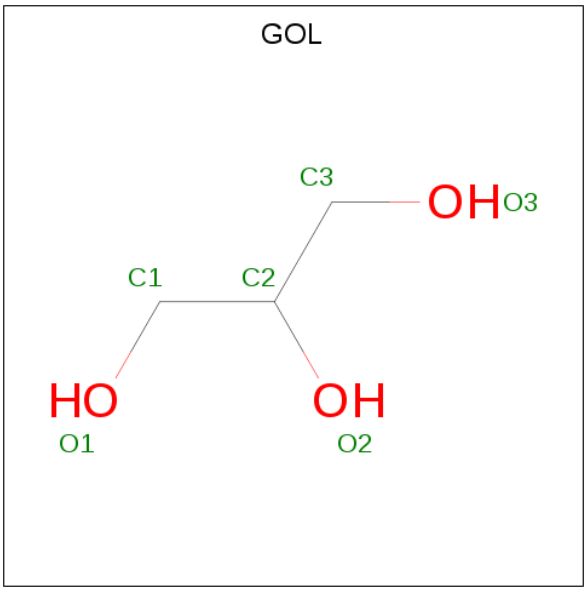
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	M	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0
2	O	1	Total O S 5 4 1	0	0
2	O	1	Total O S 5 4 1	0	0
2	O	1	Total O S 5 4 1	0	0
2	O	1	Total O S 5 4 1	0	0
2	O	1	Total O S 5 4 1	0	0
2	O	1	Total O S 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	L	1	Total C O 6 3 3	0	0
3	N	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	188	Total O 188 188	0	0
4	B	177	Total O 177 177	0	0
4	C	196	Total O 196 196	0	0
4	D	193	Total O 193 193	0	0
4	E	178	Total O 178 178	0	0
4	F	206	Total O 206 206	0	0
4	G	178	Total O 178 178	0	0
4	H	189	Total O 189 189	0	0

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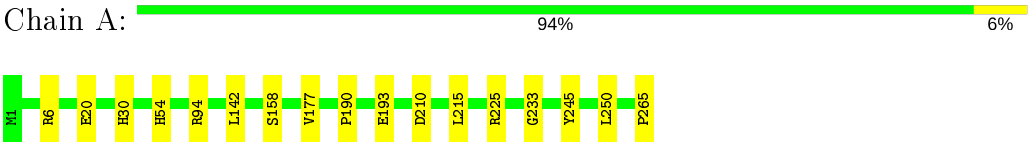
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	198	Total O 198 198	0	0
4	J	189	Total O 189 189	0	0
4	K	179	Total O 179 179	0	0
4	L	171	Total O 171 171	0	0
4	M	171	Total O 171 171	0	0
4	N	193	Total O 193 193	0	0
4	O	191	Total O 191 191	0	0

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.

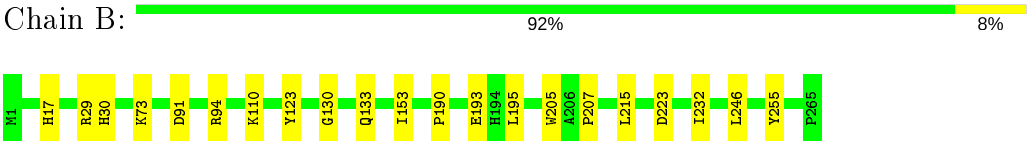
- Molecule 1: Linocin-M18

Chain A:



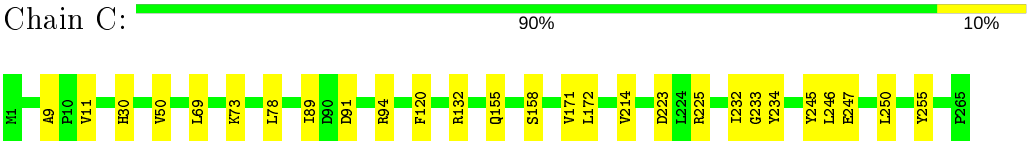
- Molecule 1: Linocin-M18

Chain B:



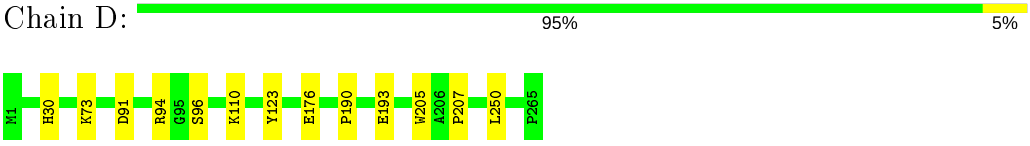
- Molecule 1: Linocin-M18

Chain C:



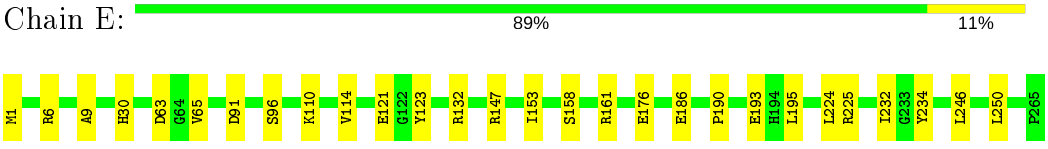
- Molecule 1: Linocin-M18

Chain D:



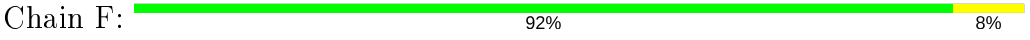
- Molecule 1: Linocin-M18

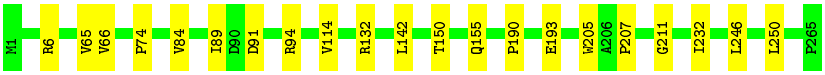
Chain E:



- Molecule 1: Linocin-M18

Chain F:



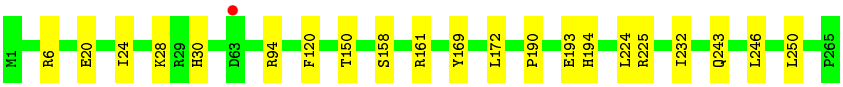


• Molecule 1: Linocin-M18

Chain G:

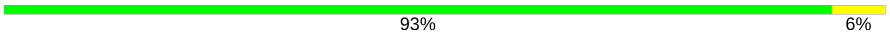
• Molecule 1: Linocin-M18

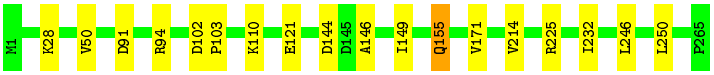
Chain H:



• Molecule 1: Linocin-M18

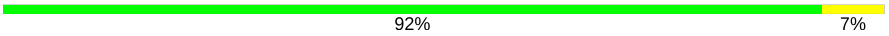
Chain I:

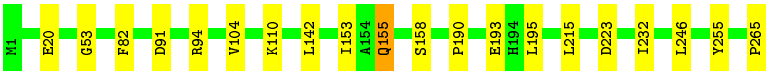




• Molecule 1: Linocin-M18

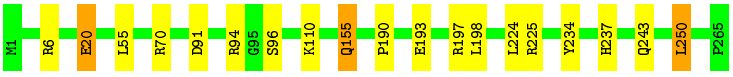
Chain J:





• Molecule 1: Linocin-M18

Chain K:

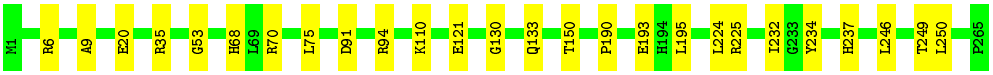


• Molecule 1: Linocin-M18

Chain L:

• Molecule 1: Linocin-M18

Chain M:

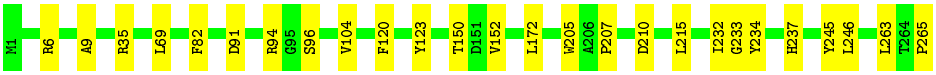


• Molecule 1: Linocin-M18

Chain N:

• Molecule 1: Linocin-M18

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	231.27Å 242.15Å 271.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.80 – 2.50 47.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (47.80-2.50) 98.0 (47.77-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.172 , 0.210 0.173 , 0.210	Depositor DCC
R_{free} test set	12567 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 35.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	34092	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	0.49	0/2098	0.65	1/2862 (0.0%)
1	B	0.47	0/2087	0.65	0/2848
1	C	0.48	0/2087	0.63	0/2848
1	D	0.45	0/2087	0.64	0/2848
1	E	0.47	0/2087	0.65	1/2848 (0.0%)
1	F	0.47	0/2087	0.65	0/2848
1	G	0.45	0/2087	0.64	0/2848
1	H	0.48	0/2087	0.64	1/2848 (0.0%)
1	I	0.50	0/2087	0.65	0/2848
1	J	0.47	0/2087	0.66	0/2848
1	K	0.45	0/2087	0.65	1/2848 (0.0%)
1	L	0.46	0/2087	0.66	0/2848
1	M	0.46	0/2087	0.65	1/2848 (0.0%)
1	N	0.47	0/2087	0.65	0/2848
1	O	0.47	0/2087	0.65	0/2848
All	All	0.47	0/31316	0.65	5/42734 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	225	ARG	CG-CD-NE	-5.72	99.78	111.80
1	E	225	ARG	CG-CD-NE	-5.66	99.91	111.80
1	A	225	ARG	CG-CD-NE	-5.49	100.27	111.80
1	H	225	ARG	CG-CD-NE	-5.49	100.27	111.80
1	M	225	ARG	CG-CD-NE	-5.05	101.19	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2056	0	2021	9	0
1	B	2045	0	2009	12	0
1	C	2045	0	2009	16	0
1	D	2045	0	2009	5	0
1	E	2045	0	2009	16	0
1	F	2045	0	2009	11	0
1	G	2045	0	2009	17	0
1	H	2045	0	2009	14	0
1	I	2045	0	2009	10	0
1	J	2045	0	2009	12	0
1	K	2045	0	2009	12	0
1	L	2045	0	2009	15	0
1	M	2045	0	2009	18	0
1	N	2045	0	2009	17	0
1	O	2045	0	2009	18	0
2	A	40	0	0	2	0
2	B	40	0	0	0	0
2	C	50	0	0	0	0
2	D	35	0	0	0	0
2	E	40	0	0	2	0
2	F	40	0	0	2	0
2	G	55	0	0	0	0
2	H	50	0	0	2	0
2	I	25	0	0	0	0
2	J	35	0	0	0	0
2	K	35	0	0	0	0
2	L	35	0	0	1	0
2	M	35	0	0	0	0
2	N	35	0	0	0	0
2	O	35	0	0	1	0
3	C	6	0	8	0	0
3	F	6	0	8	0	0
3	L	6	0	8	0	0
3	N	6	0	8	0	0
4	A	188	0	0	2	0
4	B	177	0	0	3	0
4	C	196	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	193	0	0	0	0
4	E	178	0	0	3	0
4	F	206	0	0	2	0
4	G	178	0	0	4	0
4	H	189	0	0	5	0
4	I	198	0	0	2	0
4	J	189	0	0	3	0
4	K	179	0	0	1	0
4	L	171	0	0	0	0
4	M	171	0	0	3	0
4	N	193	0	0	4	0
4	O	191	0	0	2	0
All	All	34092	0	30179	192	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (192) 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:M:121:GLU:HG2	4:M:551:HOH:O	1.83	0.78
1:N:91:ASP:OD1	1:N:94:ARG:NH2	2.17	0.78
1:B:91:ASP:OD1	1:B:94:ARG:NH1	2.20	0.75
1:B:17:HIS:HB2	4:B:542:HOH:O	1.88	0.72
1:H:150:THR:HG21	1:H:194:HIS:CE1	2.24	0.72
1:M:6:ARG:NH2	1:M:20:GLU:OE2	2.23	0.71
1:N:234:TYR:OH	1:N:237:HIS:HD2	1.74	0.70
1:H:6:ARG:NH2	1:H:20:GLU:OE2	2.25	0.70
1:K:234:TYR:OH	1:K:237:HIS:HD2	1.75	0.69
1:L:1:MET:HE3	1:L:7:GLU:HB2	1.74	0.69
1:L:234:TYR:OH	1:L:237:HIS:HD2	1.75	0.69
1:O:152:VAL:CG1	1:O:263:LEU:HD23	2.22	0.68
1:M:234:TYR:OH	1:M:237:HIS:HD2	1.75	0.68
1:L:232:ILE:HG12	1:L:246:LEU:HD23	1.76	0.66
1:M:91:ASP:OD1	1:M:94:ARG:NH2	2.30	0.65
1:L:1:MET:HE2	1:L:7:GLU:OE1	1.97	0.65
1:N:6:ARG:NH2	1:N:20:GLU:OE2	2.22	0.64
1:G:35:ARG:HD2	4:G:484:HOH:O	1.97	0.64
1:O:152:VAL:HG12	1:O:263:LEU:CD2	2.28	0.64
1:F:132:ARG:HD3	4:F:569:HOH:O	1.98	0.63
1:K:91:ASP:OD1	1:K:94:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:120:PHE:CZ	1:L:172:LEU:HD22	2.36	0.61
1:J:91:ASP:OD1	1:J:94:ARG:NH2	2.34	0.61
1:E:63:ASP:O	1:N:110:LYS:HE2	1.99	0.61
1:A:6:ARG:NH2	1:A:20:GLU:OE2	2.32	0.60
1:E:132:ARG:HD3	4:E:518:HOH:O	2.02	0.60
1:O:210:ASP:HB3	1:O:265:PRO:HG3	1.84	0.59
1:E:9:ALA:HB2	1:E:234:TYR:CD1	2.37	0.59
1:C:232:ILE:HG12	1:C:246:LEU:HD23	1.84	0.59
1:L:232:ILE:HG12	1:L:246:LEU:CD2	2.33	0.58
1:M:232:ILE:HG12	1:M:246:LEU:CD2	2.33	0.58
1:B:94:ARG:NH2	4:B:402:HOH:O	2.35	0.58
1:L:6:ARG:NH2	1:L:20:GLU:OE2	2.34	0.57
1:O:233:GLY:HA3	1:O:245:TYR:CZ	2.39	0.57
1:C:91:ASP:OD1	1:C:94:ARG:NH1	2.38	0.57
1:L:130:GLY:N	1:L:133:GLN:OE1	2.33	0.57
1:G:232:ILE:HG12	1:G:246:LEU:HD23	1.88	0.56
1:H:169:TYR:HE2	2:H:302:SO4:O4	1.89	0.55
1:B:232:ILE:HG12	1:B:246:LEU:HD23	1.89	0.55
1:I:91:ASP:OD1	1:I:94:ARG:NH2	2.40	0.55
1:N:6:ARG:HD3	4:N:509:HOH:O	2.07	0.55
1:A:94:ARG:NH1	2:A:304:SO4:O1	2.39	0.54
1:K:91:ASP:HB3	1:K:96:SER:HB2	1.88	0.54
1:I:232:ILE:HG12	1:I:246:LEU:CD2	2.37	0.53
1:I:232:ILE:HG12	1:I:246:LEU:HD23	1.90	0.53
1:K:6:ARG:NH2	1:K:20:GLU:OE2	2.33	0.53
1:G:150:THR:HG22	1:G:195:LEU:HD13	1.90	0.53
1:O:234:TYR:OH	1:O:237:HIS:HD2	1.90	0.53
1:H:30:HIS:HD2	4:H:478:HOH:O	1.92	0.53
1:F:6:ARG:HD2	4:F:574:HOH:O	2.09	0.53
1:F:190:PRO:HB2	1:F:193:GLU:HG2	1.89	0.53
1:G:30:HIS:HE1	4:G:554:HOH:O	1.92	0.53
4:H:417:HOH:O	1:M:68:HIS:HD2	1.91	0.53
1:F:232:ILE:HG12	1:F:246:LEU:HD23	1.92	0.52
1:N:190:PRO:HB2	1:N:193:GLU:HG2	1.92	0.52
1:B:29:ARG:NH1	2:F:302:SO4:O2	2.37	0.52
1:M:9:ALA:HB2	1:M:234:TYR:CD1	2.45	0.52
1:K:193:GLU:HB3	1:K:197:ARG:HH12	1.75	0.51
1:N:155:GLN:HG2	4:N:582:HOH:O	2.10	0.51
1:L:205:TRP:CD1	1:L:207:PRO:HD3	2.46	0.51
1:O:120:PHE:CZ	1:O:172:LEU:HD22	2.46	0.51
1:K:190:PRO:HB2	1:K:193:GLU:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:58:ILE:HG21	1:L:69:LEU:HG	1.93	0.51
1:M:70:ARG:NH2	1:N:94:ARG:HB3	2.26	0.51
1:O:152:VAL:CG1	1:O:263:LEU:CD2	2.85	0.50
1:A:210:ASP:HB3	1:A:265:PRO:HG3	1.94	0.50
1:G:120:PHE:CZ	1:G:172:LEU:HD22	2.47	0.50
1:D:91:ASP:OD1	1:D:94:ARG:NH1	2.45	0.49
1:C:171:VAL:HG22	1:C:214:VAL:HG22	1.94	0.49
1:B:130:GLY:N	1:B:133:GLN:OE1	2.40	0.49
1:H:232:ILE:HG12	1:H:246:LEU:HD23	1.94	0.49
1:N:9:ALA:HB2	1:N:234:TYR:CD1	2.47	0.49
1:G:30:HIS:HD2	4:G:456:HOH:O	1.96	0.49
1:N:210:ASP:HB3	1:N:265:PRO:HG3	1.95	0.49
1:J:142:LEU:HD12	1:J:265:PRO:HA	1.95	0.49
1:J:232:ILE:HG12	1:J:246:LEU:HD23	1.94	0.49
1:L:233:GLY:HA3	1:L:245:TYR:CZ	2.48	0.48
1:E:91:ASP:HB3	1:E:96:SER:HB2	1.95	0.48
2:E:303:SO4:O2	1:O:94:ARG:HD3	2.12	0.48
1:B:153:ILE:HG13	1:B:195:LEU:HD11	1.95	0.48
2:F:301:SO4:O2	1:H:94:ARG:NH1	2.40	0.48
1:K:155:GLN:HG2	4:K:535:HOH:O	2.14	0.48
1:C:120:PHE:CZ	1:C:172:LEU:HD22	2.48	0.48
1:I:110:LYS:HE2	4:I:474:HOH:O	2.14	0.48
1:G:91:ASP:HB3	1:G:96:SER:HB2	1.94	0.47
1:C:11:VAL:HG22	1:C:89:ILE:HD13	1.97	0.47
1:E:161:ARG:HD3	2:E:306:SO4:O1	2.14	0.47
1:M:35:ARG:HD2	4:M:483:HOH:O	2.14	0.47
1:C:9:ALA:HB2	1:C:234:TYR:CD1	2.49	0.47
1:H:6:ARG:HD3	4:H:542:HOH:O	2.15	0.47
1:C:233:GLY:HA3	1:C:245:TYR:CZ	2.50	0.47
1:E:232:ILE:HG12	1:E:246:LEU:HD23	1.95	0.47
1:O:152:VAL:HG11	1:O:263:LEU:HD23	1.93	0.47
1:E:1:MET:HB2	4:O:402:HOH:O	2.14	0.46
1:K:55:LEU:HD23	1:K:70:ARG:HD2	1.98	0.46
1:N:232:ILE:HG12	1:N:246:LEU:HD23	1.97	0.46
1:O:35:ARG:NH1	2:O:302:SO4:O4	2.39	0.46
1:F:114:VAL:HG21	1:G:65:VAL:HG21	1.97	0.46
1:G:50:VAL:HG21	1:G:225:ARG:HG3	1.98	0.46
1:E:91:ASP:HB3	1:E:96:SER:CB	2.45	0.46
1:C:132:ARG:HD3	4:C:511:HOH:O	2.16	0.46
1:M:224:LEU:HD11	1:M:250:LEU:HD22	1.98	0.46
1:E:65:VAL:HG22	1:N:80:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:GLY:O	1:G:37:VAL:HG22	2.16	0.46
1:L:73:LYS:HD2	1:L:73:LYS:HA	1.77	0.46
1:I:171:VAL:HG22	1:I:214:VAL:HG22	1.97	0.46
1:M:232:ILE:HG12	1:M:246:LEU:HD23	1.98	0.46
1:B:205:TRP:CD1	1:B:207:PRO:HD3	2.51	0.45
1:G:232:ILE:HG12	1:G:246:LEU:CD2	2.46	0.45
1:N:155:GLN:HB3	4:N:506:HOH:O	2.15	0.45
1:H:24:ILE:O	1:H:28:LYS:HB2	2.16	0.45
1:M:190:PRO:HB2	1:M:193:GLU:HG2	1.99	0.45
1:J:110:LYS:HE3	4:J:647:HOH:O	2.17	0.45
1:C:78:LEU:O	1:C:247:GLU:HA	2.17	0.45
1:H:30:HIS:CD2	4:H:478:HOH:O	2.67	0.44
1:I:146:ALA:O	1:I:149:ILE:HG13	2.17	0.44
1:E:190:PRO:HB2	1:E:193:GLU:HG2	2.00	0.44
1:G:205:TRP:CD1	1:G:207:PRO:HD3	2.52	0.44
1:C:50:VAL:HG21	1:C:225:ARG:HG3	1.99	0.44
1:O:82:PHE:CE2	1:O:104:VAL:HG22	2.53	0.44
1:C:30:HIS:HD2	4:C:449:HOH:O	1.99	0.44
1:C:73:LYS:HG3	4:C:527:HOH:O	2.17	0.44
4:C:432:HOH:O	1:D:30:HIS:CD2	2.70	0.44
1:O:91:ASP:HB3	1:O:96:SER:HB2	1.99	0.44
1:M:250:LEU:HD12	1:M:250:LEU:C	2.38	0.44
1:C:232:ILE:HG12	1:C:246:LEU:CD2	2.48	0.44
1:N:232:ILE:HG12	1:N:246:LEU:CD2	2.47	0.44
1:O:152:VAL:HG12	1:O:263:LEU:HD21	1.98	0.44
1:E:114:VAL:HG21	1:N:65:VAL:HG21	1.99	0.43
1:J:82:PHE:CE2	1:J:104:VAL:HG22	2.52	0.43
1:E:147:ARG:HD2	1:E:186:GLU:HG3	2.00	0.43
1:E:153:ILE:HG13	1:E:195:LEU:HD11	1.99	0.43
1:D:91:ASP:HB3	1:D:96:SER:CB	2.48	0.43
1:A:233:GLY:HA3	1:A:245:TYR:CZ	2.53	0.43
1:L:9:ALA:HB2	1:L:234:TYR:CD1	2.53	0.43
1:O:205:TRP:CD1	1:O:207:PRO:HD3	2.54	0.43
1:O:232:ILE:HG12	1:O:246:LEU:HD23	2.01	0.43
1:K:224:LEU:HD11	1:K:250:LEU:HD22	2.00	0.43
1:A:54:HIS:ND1	1:L:91:ASP:OD2	2.38	0.43
1:J:232:ILE:HG12	1:J:246:LEU:CD2	2.49	0.43
1:E:6:ARG:HD2	4:E:553:HOH:O	2.18	0.43
1:C:223:ASP:HB2	1:C:255:TYR:CE2	2.52	0.43
1:F:74:PRO:HB2	1:G:69:LEU:HD22	1.99	0.43
1:J:190:PRO:HB2	1:J:193:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:PHE:CE2	1:G:104:VAL:HG22	2.54	0.42
1:C:30:HIS:CD2	4:C:449:HOH:O	2.71	0.42
1:I:28:LYS:HE3	1:I:28:LYS:HB2	1.37	0.42
1:G:182:SER:HB2	1:K:198:LEU:HD11	2.01	0.42
1:O:6:ARG:HD3	4:O:520:HOH:O	2.19	0.42
1:A:30:HIS:HE1	4:A:553:HOH:O	2.02	0.42
1:D:205:TRP:CD1	1:D:207:PRO:HD3	2.54	0.42
1:F:142:LEU:CD1	1:F:211:GLY:HA2	2.49	0.42
1:H:30:HIS:HE1	4:H:546:HOH:O	2.02	0.42
1:O:9:ALA:HB2	1:O:234:TYR:CD1	2.55	0.42
2:A:305:SO4:O2	2:L:304:SO4:O3	2.37	0.42
1:J:155:GLN:HG2	4:J:639:HOH:O	2.20	0.42
1:K:234:TYR:OH	1:K:237:HIS:CD2	2.64	0.42
1:L:1:MET:CE	1:L:5:TYR:HA	2.50	0.42
1:I:102:ASP:N	1:I:103:PRO:CD	2.83	0.41
1:M:75:LEU:HD23	1:M:249:THR:HG22	2.02	0.41
1:B:30:HIS:CD2	4:B:461:HOH:O	2.74	0.41
1:D:190:PRO:HB2	1:D:193:GLU:HG2	2.02	0.41
1:F:84:VAL:HG23	1:F:89:ILE:HD11	2.02	0.41
1:M:53:GLY:O	1:N:94:ARG:HD2	2.20	0.41
1:A:158:SER:HB2	4:A:426:HOH:O	2.19	0.41
1:I:50:VAL:HG21	1:I:225:ARG:HG3	2.02	0.41
1:J:110:LYS:CE	4:J:647:HOH:O	2.67	0.41
1:M:6:ARG:HD3	4:M:535:HOH:O	2.20	0.41
1:A:190:PRO:HB2	1:A:193:GLU:HG2	2.03	0.41
1:F:205:TRP:CD1	1:F:207:PRO:HD3	2.56	0.41
1:B:232:ILE:HG12	1:B:246:LEU:CD2	2.49	0.41
1:M:130:GLY:N	1:M:133:GLN:OE1	2.49	0.41
1:E:30:HIS:CD2	4:E:450:HOH:O	2.73	0.41
1:C:69:LEU:HD23	1:C:69:LEU:HA	1.96	0.41
1:J:53:GLY:O	1:K:94:ARG:HD2	2.20	0.41
1:A:142:LEU:HD13	1:A:177:VAL:HG21	2.02	0.41
1:B:190:PRO:HB2	1:B:193:GLU:HG2	2.03	0.41
1:H:120:PHE:CZ	1:H:172:LEU:HD22	2.56	0.41
1:H:161:ARG:NE	2:H:302:SO4:O2	2.45	0.41
1:J:153:ILE:HG13	1:J:195:LEU:HD11	2.03	0.41
1:F:65:VAL:HG21	1:G:114:VAL:HG21	2.03	0.41
1:G:30:HIS:CD2	4:G:456:HOH:O	2.71	0.41
1:H:224:LEU:HD11	1:H:250:LEU:HD22	2.03	0.41
1:B:223:ASP:HB2	1:B:255:TYR:CE2	2.57	0.40
1:E:224:LEU:HD11	1:E:250:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:190:PRO:HB2	1:H:193:GLU:HG2	2.03	0.40
1:N:35:ARG:HD2	4:N:460:HOH:O	2.21	0.40
1:F:91:ASP:OD1	1:F:94:ARG:NH2	2.42	0.40
1:J:223:ASP:HB2	1:J:255:TYR:CE2	2.56	0.40
1:I:155:GLN:HG3	4:I:589:HOH:O	2.21	0.40
1:M:150:THR:HG22	1:M:195:LEU:HD13	2.03	0.40
1:O:69:LEU:HA	1:O:69:LEU:HD23	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	264/265 (100%)	260 (98%)	4 (2%)	0	100	100
1	B	263/265 (99%)	258 (98%)	5 (2%)	0	100	100
1	C	263/265 (99%)	258 (98%)	5 (2%)	0	100	100
1	D	263/265 (99%)	257 (98%)	6 (2%)	0	100	100
1	E	263/265 (99%)	258 (98%)	5 (2%)	0	100	100
1	F	263/265 (99%)	255 (97%)	8 (3%)	0	100	100
1	G	263/265 (99%)	256 (97%)	7 (3%)	0	100	100
1	H	263/265 (99%)	258 (98%)	5 (2%)	0	100	100
1	I	263/265 (99%)	258 (98%)	5 (2%)	0	100	100
1	J	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	K	263/265 (99%)	258 (98%)	5 (2%)	0	100	100
1	L	263/265 (99%)	256 (97%)	7 (3%)	0	100	100
1	M	263/265 (99%)	257 (98%)	6 (2%)	0	100	100
1	N	263/265 (99%)	257 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	263/265 (99%)	260 (99%)	3 (1%)	0	100	100
All	All	3946/3975 (99%)	3865 (98%)	81 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	222/221 (100%)	220 (99%)	2 (1%)	78	92
1	B	221/221 (100%)	217 (98%)	4 (2%)	59	81
1	C	221/221 (100%)	218 (99%)	3 (1%)	67	86
1	D	221/221 (100%)	216 (98%)	5 (2%)	50	76
1	E	221/221 (100%)	216 (98%)	5 (2%)	50	76
1	F	221/221 (100%)	217 (98%)	4 (2%)	59	81
1	G	221/221 (100%)	215 (97%)	6 (3%)	44	71
1	H	221/221 (100%)	219 (99%)	2 (1%)	78	92
1	I	221/221 (100%)	217 (98%)	4 (2%)	59	81
1	J	221/221 (100%)	217 (98%)	4 (2%)	59	81
1	K	221/221 (100%)	216 (98%)	5 (2%)	50	76
1	L	221/221 (100%)	215 (97%)	6 (3%)	44	71
1	M	221/221 (100%)	220 (100%)	1 (0%)	88	96
1	N	221/221 (100%)	217 (98%)	4 (2%)	59	81
1	O	221/221 (100%)	218 (99%)	3 (1%)	67	86
All	All	3316/3315 (100%)	3258 (98%)	58 (2%)	60	82

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	LEU

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Mol	Chain	Res	Type
1	A	250	LEU
1	B	73	LYS
1	B	110	LYS
1	B	123	TYR
1	B	215	LEU
1	C	155	GLN
1	C	158	SER
1	C	250	LEU
1	D	73	LYS
1	D	110	LYS
1	D	123	TYR
1	D	176	GLU
1	D	250	LEU
1	E	110	LYS
1	E	121	GLU
1	E	123	TYR
1	E	158	SER
1	E	176	GLU
1	F	66	VAL
1	F	150	THR
1	F	155	GLN
1	F	250	LEU
1	G	63	ASP
1	G	110	LYS
1	G	123	TYR
1	G	155	GLN
1	G	180	LYS
1	G	215	LEU
1	H	158	SER
1	H	243	GLN
1	I	121	GLU
1	I	144	ASP
1	I	155	GLN
1	I	250	LEU
1	J	20	GLU
1	J	155	GLN
1	J	158	SER
1	J	215	LEU
1	K	20	GLU
1	K	110	LYS
1	K	155	GLN
1	K	243	GLN

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Mol	Chain	Res	Type
1	K	250	LEU
1	L	123	TYR
1	L	155	GLN
1	L	158	SER
1	L	176	GLU
1	L	215	LEU
1	L	250	LEU
1	M	110	LYS
1	N	110	LYS
1	N	158	SER
1	N	176	GLU
1	N	215	LEU
1	O	123	TYR
1	O	150	THR
1	O	215	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	B	30	HIS
1	C	30	HIS
1	D	30	HIS
1	D	187	HIS
1	E	30	HIS
1	F	30	HIS
1	F	155	GLN
1	G	30	HIS
1	H	30	HIS
1	H	155	GLN
1	I	30	HIS
1	I	137	ASN
1	J	137	ASN
1	J	155	GLN
1	K	137	ASN
1	K	155	GLN
1	K	237	HIS
1	L	137	ASN
1	L	237	HIS
1	M	68	HIS
1	M	137	ASN
1	M	187	HIS

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Mol	Chain	Res	Type
1	M	237	HIS
1	N	137	ASN
1	N	237	HIS
1	O	137	ASN
1	O	237	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

121 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	308	-	4,4,4	0.41	0	6,6,6	0.22	0
2	SO4	D	303	-	4,4,4	0.39	0	6,6,6	0.23	0
2	SO4	B	307	-	4,4,4	0.39	0	6,6,6	0.21	0
2	SO4	B	302	-	4,4,4	0.42	0	6,6,6	0.20	0
2	SO4	L	302	-	4,4,4	0.41	0	6,6,6	0.28	0
2	SO4	E	306	-	4,4,4	0.31	0	6,6,6	0.29	0
2	SO4	G	306	-	4,4,4	0.33	0	6,6,6	0.24	0
2	SO4	E	302	-	4,4,4	0.40	0	6,6,6	0.15	0
2	SO4	E	305	-	4,4,4	0.38	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	A	303	-	4,4,4	0.48	0	6,6,6	0.31	0
2	SO4	I	301	-	4,4,4	0.40	0	6,6,6	0.37	0
2	SO4	E	303	-	4,4,4	0.31	0	6,6,6	0.27	0
2	SO4	B	306	-	4,4,4	0.43	0	6,6,6	0.38	0
3	GOL	N	308	-	5,5,5	0.34	0	5,5,5	0.61	0
2	SO4	H	307	-	4,4,4	0.38	0	6,6,6	0.25	0
2	SO4	O	307	-	4,4,4	0.40	0	6,6,6	0.14	0
2	SO4	I	302	-	4,4,4	0.42	0	6,6,6	0.34	0
2	SO4	M	302	-	4,4,4	0.37	0	6,6,6	0.25	0
2	SO4	L	307	-	4,4,4	0.46	0	6,6,6	0.24	0
2	SO4	O	303	-	4,4,4	0.44	0	6,6,6	0.36	0
2	SO4	E	301	-	4,4,4	0.42	0	6,6,6	0.26	0
2	SO4	H	309	-	4,4,4	0.30	0	6,6,6	0.23	0
2	SO4	C	301	-	4,4,4	0.34	0	6,6,6	0.32	0
2	SO4	K	303	-	4,4,4	0.41	0	6,6,6	0.43	0
2	SO4	J	301	-	4,4,4	0.35	0	6,6,6	0.14	0
2	SO4	G	302	-	4,4,4	0.30	0	6,6,6	0.42	0
2	SO4	A	308	-	4,4,4	0.46	0	6,6,6	0.34	0
2	SO4	K	307	-	4,4,4	0.41	0	6,6,6	0.16	0
2	SO4	D	306	-	4,4,4	0.39	0	6,6,6	0.31	0
3	GOL	L	308	-	5,5,5	0.24	0	5,5,5	0.40	0
2	SO4	D	305	-	4,4,4	0.45	0	6,6,6	0.33	0
2	SO4	D	301	-	4,4,4	0.34	0	6,6,6	0.31	0
2	SO4	H	301	-	4,4,4	0.35	0	6,6,6	0.13	0
2	SO4	E	307	-	4,4,4	0.50	0	6,6,6	0.38	0
2	SO4	G	308	-	4,4,4	0.35	0	6,6,6	0.29	0
2	SO4	E	308	-	4,4,4	0.36	0	6,6,6	0.15	0
2	SO4	C	309	-	4,4,4	0.37	0	6,6,6	0.30	0
2	SO4	L	304	-	4,4,4	0.45	0	6,6,6	0.19	0
2	SO4	H	302	-	4,4,4	0.42	0	6,6,6	0.34	0
2	SO4	M	301	-	4,4,4	0.34	0	6,6,6	0.31	0
2	SO4	G	311	-	4,4,4	0.41	0	6,6,6	0.33	0
2	SO4	H	304	-	4,4,4	0.39	0	6,6,6	0.35	0
2	SO4	F	307	-	4,4,4	0.43	0	6,6,6	0.32	0
2	SO4	H	308	-	4,4,4	0.36	0	6,6,6	0.21	0
2	SO4	O	302	-	4,4,4	0.39	0	6,6,6	0.26	0
2	SO4	D	302	-	4,4,4	0.38	0	6,6,6	0.24	0
2	SO4	F	301	-	4,4,4	0.30	0	6,6,6	0.31	0
2	SO4	I	305	-	4,4,4	0.46	0	6,6,6	0.37	0
2	SO4	B	303	-	4,4,4	0.37	0	6,6,6	0.34	0
2	SO4	D	304	-	4,4,4	0.39	0	6,6,6	0.38	0
2	SO4	N	304	-	4,4,4	0.38	0	6,6,6	0.11	0
2	SO4	N	307	-	4,4,4	0.40	0	6,6,6	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	N	303	-	4,4,4	0.38	0	6,6,6	0.20	0
2	SO4	A	304	-	4,4,4	0.39	0	6,6,6	0.34	0
2	SO4	B	305	-	4,4,4	0.35	0	6,6,6	0.17	0
2	SO4	I	304	-	4,4,4	0.39	0	6,6,6	0.40	0
2	SO4	G	301	-	4,4,4	0.32	0	6,6,6	0.15	0
2	SO4	D	307	-	4,4,4	0.36	0	6,6,6	0.11	0
2	SO4	J	303	-	4,4,4	0.29	0	6,6,6	0.28	0
2	SO4	C	304	-	4,4,4	0.38	0	6,6,6	0.43	0
2	SO4	J	307	-	4,4,4	0.42	0	6,6,6	0.16	0
2	SO4	M	303	-	4,4,4	0.43	0	6,6,6	0.39	0
2	SO4	K	301	-	4,4,4	0.36	0	6,6,6	0.24	0
2	SO4	K	302	-	4,4,4	0.37	0	6,6,6	0.17	0
2	SO4	M	305	-	4,4,4	0.32	0	6,6,6	0.36	0
2	SO4	G	304	-	4,4,4	0.38	0	6,6,6	0.24	0
2	SO4	F	302	-	4,4,4	0.28	0	6,6,6	0.32	0
2	SO4	L	303	-	4,4,4	0.37	0	6,6,6	0.39	0
3	GOL	C	311	-	5,5,5	0.23	0	5,5,5	0.37	0
2	SO4	F	305	-	4,4,4	0.35	0	6,6,6	0.34	0
2	SO4	K	304	-	4,4,4	0.33	0	6,6,6	0.27	0
2	SO4	M	306	-	4,4,4	0.39	0	6,6,6	0.17	0
2	SO4	H	310	-	4,4,4	0.38	0	6,6,6	0.19	0
2	SO4	C	310	-	4,4,4	0.41	0	6,6,6	0.36	0
2	SO4	G	309	-	4,4,4	0.34	0	6,6,6	0.49	0
2	SO4	G	305	-	4,4,4	0.33	0	6,6,6	0.20	0
2	SO4	A	302	-	4,4,4	0.35	0	6,6,6	0.17	0
2	SO4	C	302	-	4,4,4	0.37	0	6,6,6	0.28	0
2	SO4	A	306	-	4,4,4	0.39	0	6,6,6	0.20	0
2	SO4	A	301	-	4,4,4	0.37	0	6,6,6	0.25	0
2	SO4	H	305	-	4,4,4	0.35	0	6,6,6	0.19	0
2	SO4	B	304	-	4,4,4	0.37	0	6,6,6	0.33	0
2	SO4	G	303	-	4,4,4	0.33	0	6,6,6	0.43	0
2	SO4	K	306	-	4,4,4	0.42	0	6,6,6	0.10	0
2	SO4	A	307	-	4,4,4	0.34	0	6,6,6	0.23	0
2	SO4	I	303	-	4,4,4	0.39	0	6,6,6	0.19	0
2	SO4	G	307	-	4,4,4	0.36	0	6,6,6	0.18	0
2	SO4	O	304	-	4,4,4	0.38	0	6,6,6	0.54	0
2	SO4	L	305	-	4,4,4	0.28	0	6,6,6	0.44	0
2	SO4	J	305	-	4,4,4	0.45	0	6,6,6	0.27	0
2	SO4	J	302	-	4,4,4	0.36	0	6,6,6	0.28	0
2	SO4	O	301	-	4,4,4	0.38	0	6,6,6	0.08	0
2	SO4	C	307	-	4,4,4	0.31	0	6,6,6	0.21	0
2	SO4	N	306	-	4,4,4	0.35	0	6,6,6	0.28	0
2	SO4	F	303	-	4,4,4	0.34	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	J	304	-	4,4,4	0.40	0	6,6,6	0.28	0
3	GOL	F	309	-	5,5,5	0.22	0	5,5,5	0.51	0
2	SO4	C	303	-	4,4,4	0.35	0	6,6,6	0.26	0
2	SO4	L	306	-	4,4,4	0.45	0	6,6,6	0.21	0
2	SO4	C	305	-	4,4,4	0.37	0	6,6,6	0.33	0
2	SO4	K	305	-	4,4,4	0.37	0	6,6,6	0.41	0
2	SO4	C	308	-	4,4,4	0.37	0	6,6,6	0.15	0
2	SO4	G	310	-	4,4,4	0.42	0	6,6,6	0.28	0
2	SO4	F	308	-	4,4,4	0.39	0	6,6,6	0.21	0
2	SO4	J	306	-	4,4,4	0.37	0	6,6,6	0.25	0
2	SO4	F	304	-	4,4,4	0.42	0	6,6,6	0.38	0
2	SO4	N	302	-	4,4,4	0.38	0	6,6,6	0.16	0
2	SO4	E	304	-	4,4,4	0.37	0	6,6,6	0.41	0
2	SO4	L	301	-	4,4,4	0.36	0	6,6,6	0.14	0
2	SO4	B	301	-	4,4,4	0.38	0	6,6,6	0.20	0
2	SO4	M	304	-	4,4,4	0.45	0	6,6,6	0.12	0
2	SO4	H	306	-	4,4,4	0.35	0	6,6,6	0.30	0
2	SO4	O	305	-	4,4,4	0.38	0	6,6,6	0.26	0
2	SO4	O	306	-	4,4,4	0.39	0	6,6,6	0.24	0
2	SO4	N	305	-	4,4,4	0.40	0	6,6,6	0.23	0
2	SO4	H	303	-	4,4,4	0.43	0	6,6,6	0.37	0
2	SO4	N	301	-	4,4,4	0.35	0	6,6,6	0.19	0
2	SO4	A	305	-	4,4,4	0.30	0	6,6,6	0.30	0
2	SO4	F	306	-	4,4,4	0.40	0	6,6,6	0.17	0
2	SO4	M	307	-	4,4,4	0.37	0	6,6,6	0.09	0
2	SO4	C	306	-	4,4,4	0.42	0	6,6,6	0.38	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
3	GOL	N	308	-	-	3/4/4/4	-
3	GOL	L	308	-	-	2/4/4/4	-
3	GOL	C	311	-	-	1/4/4/4	-
3	GOL	F	309	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	308	GOL	O1-C1-C2-C3
3	N	308	GOL	O1-C1-C2-O2
3	N	308	GOL	O1-C1-C2-C3
3	N	308	GOL	C1-C2-C3-O3
3	L	308	GOL	O1-C1-C2-O2
3	F	309	GOL	O1-C1-C2-O2
3	C	311	GOL	O1-C1-C2-C3
3	F	309	GOL	O1-C1-C2-C3

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	306	SO4	1	0
2	E	303	SO4	1	0
2	L	304	SO4	1	0
2	H	302	SO4	2	0
2	O	302	SO4	1	0
2	F	301	SO4	1	0
2	A	304	SO4	1	0
2	F	302	SO4	1	0
2	A	305	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	265/265 (100%)	-0.52	0 100 100	19, 25, 41, 55	0
1	B	265/265 (100%)	-0.63	0 100 100	17, 25, 41, 55	0
1	C	265/265 (100%)	-0.54	0 100 100	17, 24, 40, 60	0
1	D	265/265 (100%)	-0.54	0 100 100	18, 26, 40, 66	0
1	E	265/265 (100%)	-0.58	0 100 100	19, 25, 40, 57	0
1	F	265/265 (100%)	-0.59	0 100 100	18, 25, 40, 55	0
1	G	265/265 (100%)	-0.62	0 100 100	19, 26, 41, 55	0
1	H	265/265 (100%)	-0.56	1 (0%) 92 93	17, 24, 40, 56	0
1	I	265/265 (100%)	-0.59	0 100 100	19, 25, 40, 55	0
1	J	265/265 (100%)	-0.58	0 100 100	18, 25, 39, 52	0
1	K	265/265 (100%)	-0.55	0 100 100	18, 25, 41, 56	0
1	L	265/265 (100%)	-0.52	1 (0%) 92 93	20, 25, 41, 63	0
1	M	265/265 (100%)	-0.59	0 100 100	17, 25, 41, 56	0
1	N	265/265 (100%)	-0.57	0 100 100	18, 25, 42, 57	0
1	O	265/265 (100%)	-0.61	0 100 100	19, 26, 41, 57	0
All	All	3975/3975 (100%)	-0.57	2 (0%) 95 96	17, 25, 41, 66	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	63	ASP	2.1
1	L	134	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	K	306	5/5	0.70	0.37	93,103,118,122	0
2	SO4	H	308	5/5	0.71	0.37	106,118,128,132	0
2	SO4	G	308	5/5	0.72	0.31	89,102,113,116	0
2	SO4	A	308	5/5	0.74	0.34	75,85,100,106	0
2	SO4	B	303	5/5	0.76	0.28	80,90,96,100	0
2	SO4	H	310	5/5	0.77	0.33	111,117,125,135	0
2	SO4	E	307	5/5	0.78	0.32	67,80,93,99	0
2	SO4	B	308	5/5	0.79	0.36	105,113,123,142	0
2	SO4	J	307	5/5	0.79	0.23	89,95,108,118	0
2	SO4	D	306	5/5	0.80	0.28	90,97,109,127	0
2	SO4	B	306	5/5	0.80	0.28	80,94,106,115	0
2	SO4	H	307	5/5	0.81	0.23	88,90,106,112	0
2	SO4	A	303	5/5	0.81	0.27	70,85,88,90	0
2	SO4	A	302	5/5	0.82	0.21	91,94,102,111	0
2	SO4	L	307	5/5	0.83	0.27	79,83,91,94	0
2	SO4	N	307	5/5	0.83	0.30	77,95,101,108	0
2	SO4	I	305	5/5	0.83	0.26	78,78,90,95	0
2	SO4	O	306	5/5	0.83	0.34	82,90,100,106	0
2	SO4	O	307	5/5	0.84	0.25	84,87,95,95	0
2	SO4	O	303	5/5	0.84	0.21	79,80,100,101	0
2	SO4	F	307	5/5	0.84	0.29	78,89,94,101	0
2	SO4	H	303	5/5	0.84	0.22	78,92,97,98	0
2	SO4	M	307	5/5	0.84	0.28	100,106,112,113	0
2	SO4	G	311	5/5	0.85	0.22	80,85,94,97	0
2	SO4	M	305	5/5	0.85	0.26	79,100,101,103	0
2	SO4	L	303	5/5	0.85	0.21	77,84,99,105	0
2	SO4	C	310	5/5	0.86	0.28	88,91,102,113	0
2	SO4	M	303	5/5	0.86	0.22	69,71,81,89	0
2	SO4	L	302	5/5	0.86	0.22	76,81,89,90	0
2	SO4	G	307	5/5	0.86	0.24	84,92,96,100	0
2	SO4	C	303	5/5	0.86	0.34	87,93,97,106	0
2	SO4	E	304	5/5	0.86	0.24	81,93,102,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	I	304	5/5	0.86	0.27	87,89,98,112	0
2	SO4	M	306	5/5	0.86	0.24	89,106,112,117	0
2	SO4	B	307	5/5	0.86	0.24	75,85,89,89	0
2	SO4	K	305	5/5	0.87	0.22	78,92,100,107	0
2	SO4	M	301	5/5	0.87	0.30	88,92,97,103	0
2	SO4	H	306	5/5	0.87	0.25	81,89,96,97	0
2	SO4	G	309	5/5	0.87	0.19	81,83,88,93	0
2	SO4	F	305	5/5	0.87	0.21	83,97,103,104	0
2	SO4	L	306	5/5	0.87	0.27	73,84,94,102	0
2	SO4	G	310	5/5	0.88	0.27	77,97,102,106	0
2	SO4	D	307	5/5	0.88	0.29	103,104,111,112	0
2	SO4	N	304	5/5	0.88	0.29	96,103,105,109	0
2	SO4	E	303	5/5	0.88	0.27	79,89,91,92	0
2	SO4	F	301	5/5	0.88	0.23	77,80,89,90	0
2	SO4	C	308	5/5	0.88	0.21	96,100,107,108	0
2	SO4	C	306	5/5	0.88	0.28	78,90,95,103	0
2	SO4	O	301	5/5	0.89	0.30	81,91,92,97	0
2	SO4	L	301	5/5	0.89	0.27	85,92,98,106	0
2	SO4	H	301	5/5	0.89	0.33	78,86,93,98	0
2	SO4	H	304	5/5	0.89	0.17	86,89,94,94	0
2	SO4	A	307	5/5	0.89	0.26	93,94,99,104	0
2	SO4	A	305	5/5	0.89	0.21	79,82,88,93	0
2	SO4	C	309	5/5	0.89	0.19	79,83,87,92	0
2	SO4	F	304	5/5	0.89	0.16	82,83,89,90	0
2	SO4	E	306	5/5	0.90	0.21	63,67,80,83	0
2	SO4	F	303	5/5	0.90	0.39	94,95,99,104	0
2	SO4	F	308	5/5	0.90	0.15	79,82,90,93	0
2	SO4	N	303	5/5	0.90	0.33	76,88,90,97	0
2	SO4	F	306	5/5	0.90	0.27	87,94,102,107	0
2	SO4	O	302	5/5	0.90	0.21	65,78,82,83	0
2	SO4	D	305	5/5	0.90	0.18	67,85,86,88	0
2	SO4	G	305	5/5	0.91	0.33	92,94,99,103	0
3	GOL	N	308	6/6	0.91	0.33	54,62,67,70	0
2	SO4	O	305	5/5	0.91	0.16	63,73,80,83	0
2	SO4	B	304	5/5	0.91	0.17	71,84,91,93	0
2	SO4	A	304	5/5	0.91	0.30	68,81,85,86	0
2	SO4	K	302	5/5	0.91	0.20	86,88,93,94	0
2	SO4	E	301	5/5	0.91	0.15	75,75,85,91	0
2	SO4	J	305	5/5	0.91	0.16	68,72,79,83	0
2	SO4	J	301	5/5	0.91	0.27	89,93,94,97	0
2	SO4	K	304	5/5	0.92	0.23	81,85,88,91	0
2	SO4	D	304	5/5	0.92	0.17	72,77,85,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	305	5/5	0.92	0.32	84,86,93,101	0
2	SO4	N	302	5/5	0.92	0.26	87,88,102,103	0
2	SO4	O	304	5/5	0.92	0.25	65,73,77,78	0
2	SO4	L	305	5/5	0.92	0.18	73,77,81,88	0
2	SO4	M	302	5/5	0.92	0.16	86,90,92,94	0
2	SO4	J	302	5/5	0.92	0.20	76,94,96,101	0
2	SO4	G	304	5/5	0.92	0.25	73,80,85,85	0
2	SO4	K	303	5/5	0.92	0.18	71,78,81,84	0
3	GOL	C	311	6/6	0.92	0.18	50,56,57,58	0
2	SO4	C	305	5/5	0.92	0.20	67,77,80,83	0
2	SO4	C	302	5/5	0.92	0.19	65,75,81,83	0
2	SO4	K	307	5/5	0.92	0.26	84,86,94,95	0
2	SO4	M	304	5/5	0.93	0.22	77,79,84,88	0
2	SO4	D	301	5/5	0.93	0.32	85,92,100,100	0
2	SO4	C	307	5/5	0.93	0.33	81,87,97,105	0
2	SO4	I	301	5/5	0.93	0.17	77,78,84,87	0
2	SO4	J	306	5/5	0.93	0.24	73,79,85,89	0
2	SO4	J	303	5/5	0.93	0.24	77,79,83,87	0
2	SO4	G	302	5/5	0.93	0.22	67,68,77,84	0
2	SO4	A	306	5/5	0.93	0.15	77,77,81,85	0
2	SO4	D	303	5/5	0.93	0.19	73,75,81,82	0
2	SO4	E	302	5/5	0.94	0.31	75,82,87,89	0
2	SO4	E	308	5/5	0.94	0.29	84,85,89,93	0
2	SO4	C	301	5/5	0.94	0.21	78,79,84,86	0
2	SO4	L	304	5/5	0.94	0.16	73,73,78,81	0
2	SO4	A	301	5/5	0.94	0.15	56,60,64,66	0
2	SO4	H	305	5/5	0.94	0.27	76,85,86,88	0
2	SO4	H	302	5/5	0.94	0.19	69,77,81,85	0
2	SO4	G	303	5/5	0.94	0.19	76,81,87,88	0
2	SO4	J	304	5/5	0.94	0.17	83,84,92,94	0
2	SO4	G	306	5/5	0.94	0.26	88,91,94,95	0
2	SO4	K	301	5/5	0.95	0.34	90,91,95,96	0
2	SO4	D	302	5/5	0.95	0.27	70,72,80,85	0
3	GOL	L	308	6/6	0.95	0.17	46,48,54,55	0
2	SO4	I	302	5/5	0.95	0.20	63,73,75,77	0
2	SO4	F	302	5/5	0.95	0.27	72,78,81,86	0
2	SO4	N	305	5/5	0.95	0.27	86,92,95,96	0
2	SO4	N	306	5/5	0.95	0.10	77,80,85,86	0
2	SO4	C	304	5/5	0.95	0.19	73,74,79,79	0
2	SO4	B	302	5/5	0.95	0.17	68,73,77,78	0
3	GOL	F	309	6/6	0.95	0.20	44,48,49,53	0
2	SO4	E	305	5/5	0.95	0.26	77,82,86,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	I	303	5/5	0.96	0.18	70,73,76,77	0
2	SO4	N	301	5/5	0.97	0.20	67,72,79,82	0
2	SO4	H	309	5/5	0.98	0.14	50,52,53,61	0
2	SO4	B	301	5/5	0.98	0.14	57,57,60,62	0
2	SO4	G	301	5/5	0.99	0.13	57,60,60,60	0

6.5 Other polymers

There are no such residues in this entry.