Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 12:17 AM JST

PDB ID	:	5YL5
Title	:	Crystal structure of dodecameric Dehydroquinate dehydratase from Acinetobacter baumannii at 1.9A resolution
Authors	:	Iqbal, N.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on	:	2017-10-17
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

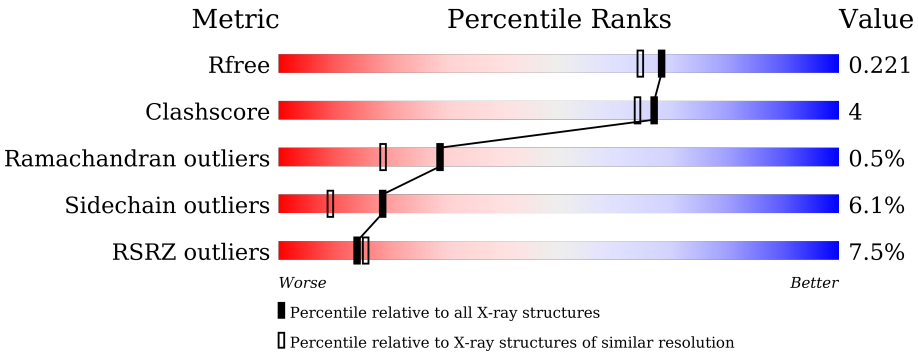
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 <=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	151	11% 83% 9%
1	B	151	5% 88% 7%
1	C	151	9% 81% 11%
1	D	151	8% 79% 12%
1	E	151	% 85% 8%
1	F	151	6% 83% 11%

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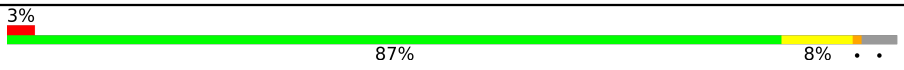
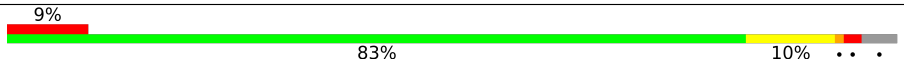
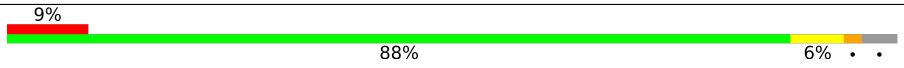
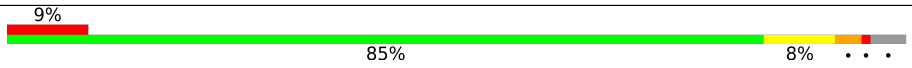
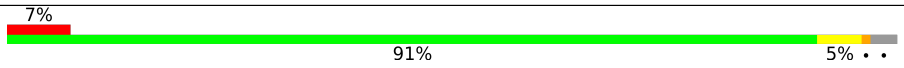
Mol	Chain	Length	Quality of chain
1	G	151	
1	H	151	
1	I	151	
1	J	151	
1	K	151	
1	L	151	

2 Entry composition (i)

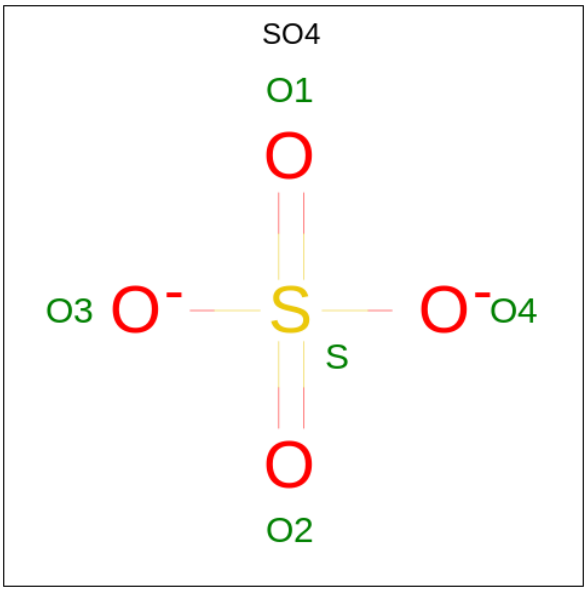
There are 5 unique types of molecules in this entry. The entry contains 14153 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-dehydroquinate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	0	0
			1121	715	199	206	1			
1	B	145	Total	C	N	O	S	0	0	0
			1121	715	199	206	1			
1	C	145	Total	C	N	O	S	0	0	0
			1121	715	199	206	1			
1	D	145	Total	C	N	O	S	0	0	0
			1121	715	199	206	1			
1	E	145	Total	C	N	O	S	0	0	0
			1121	715	199	206	1			
1	F	145	Total	C	N	O	S	0	0	0
			1121	715	199	206	1			
1	G	145	Total	C	N	O	S	0	0	0
			1121	715	199	206	1			
1	H	145	Total	C	N	O	S	0	0	0
			1121	715	199	206	1			
1	I	145	Total	C	N	O	S	0	0	0
			1121	715	199	206	1			
1	J	145	Total	C	N	O	S	0	0	0
			1121	715	199	206	1			
1	K	147	Total	C	N	O	S	0	0	0
			1135	723	201	209	2			
1	L	145	Total	C	N	O	S	0	0	0
			1121	715	199	206	1			

- 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	B	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	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	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	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

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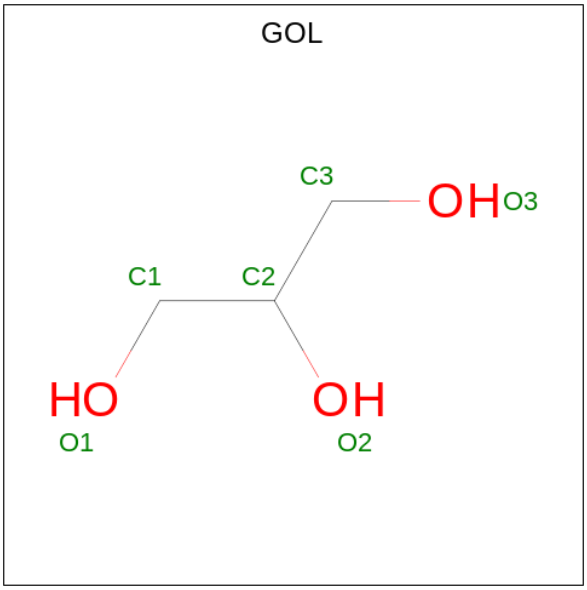
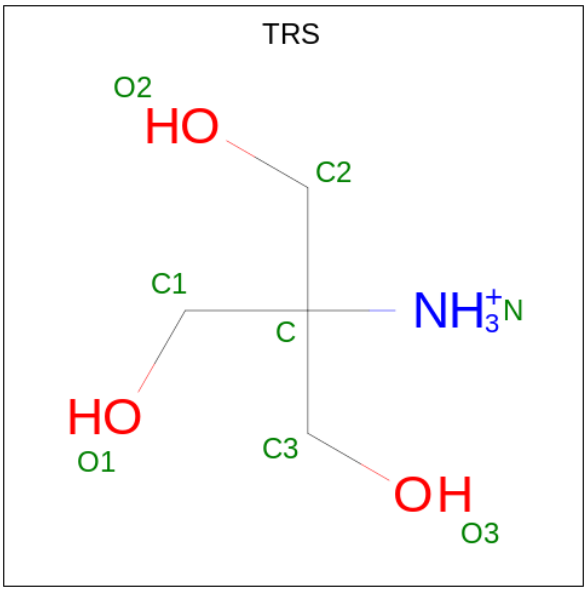
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0

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



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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C N O 8 4 1 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	54	Total O 54 54	0	0
5	B	47	Total O 47 47	0	0
5	C	35	Total O 35 35	0	0
5	D	48	Total O 48 48	0	0
5	E	57	Total O 57 57	0	0
5	F	56	Total O 56 56	0	0
5	G	62	Total O 62 62	0	0
5	H	46	Total O 46 46	0	0
5	I	47	Total O 47 47	0	0
5	J	35	Total O 35 35	0	0
5	K	45	Total O 45 45	0	0

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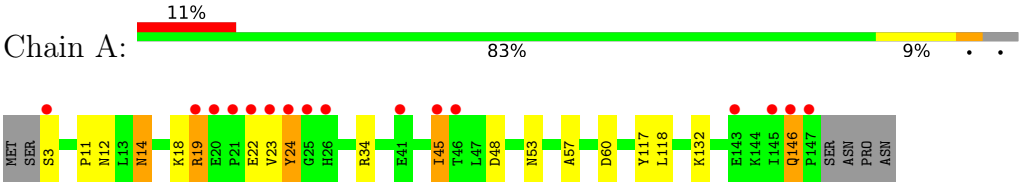
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	43	Total	O	0	0
			43	43		

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.

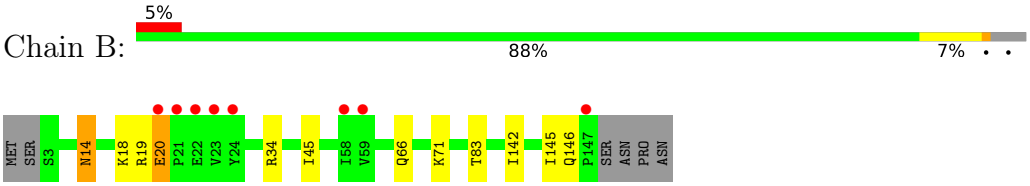
• Molecule 1: 3-dehydroquinate dehydratase

Chain A:



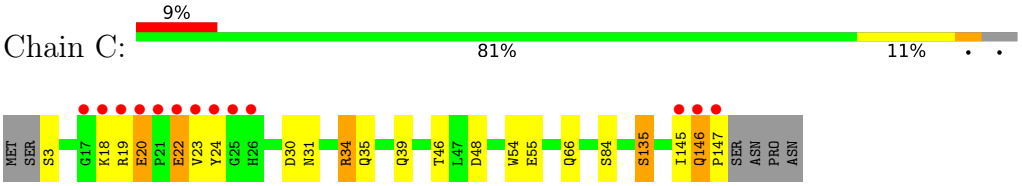
• Molecule 1: 3-dehydroquinate dehydratase

Chain B:



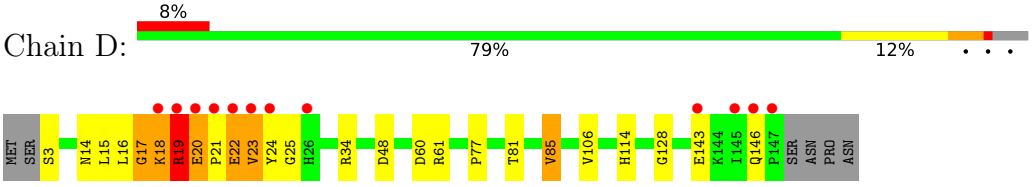
• Molecule 1: 3-dehydroquinate dehydratase

Chain C:



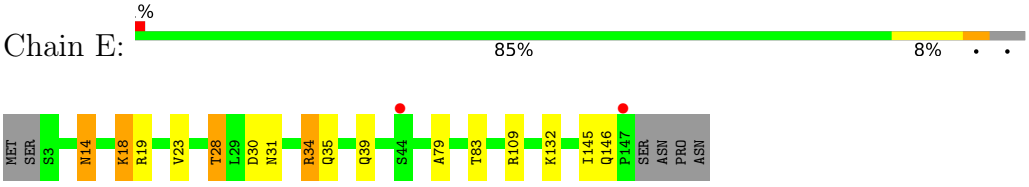
• Molecule 1: 3-dehydroquinate dehydratase

Chain D:



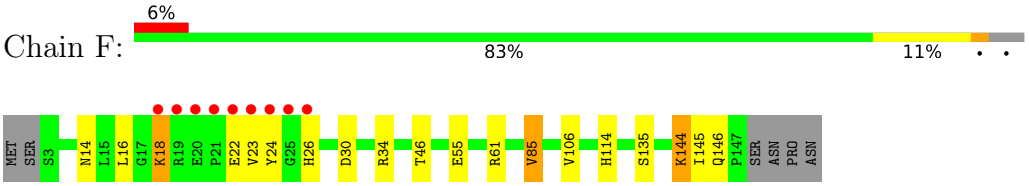
• Molecule 1: 3-dehydroquinate dehydratase

Chain E:



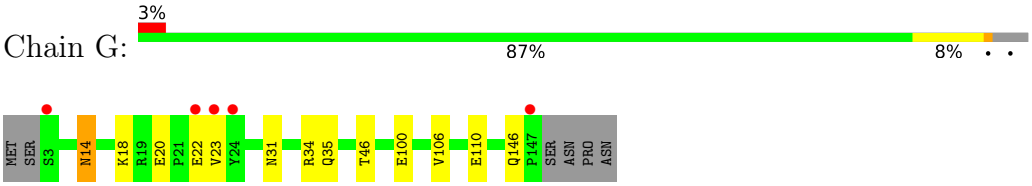
• Molecule 1: 3-dehydroquinate dehydratase

Chain F:



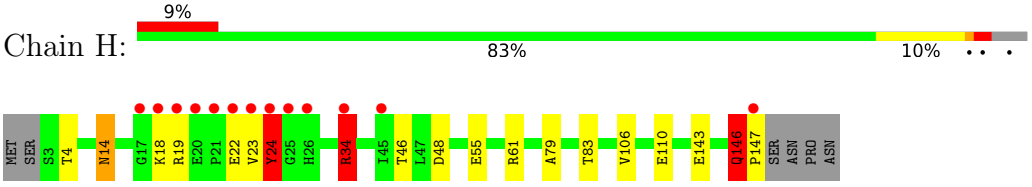
• Molecule 1: 3-dehydroquinate dehydratase

Chain G:



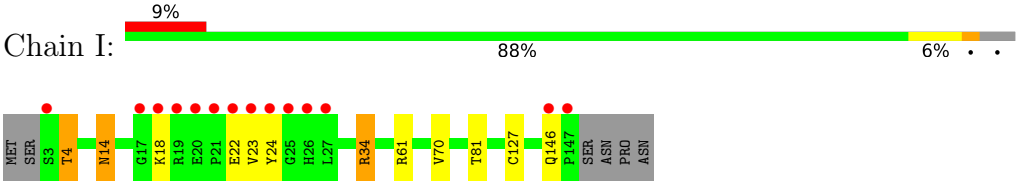
• Molecule 1: 3-dehydroquinate dehydratase

Chain H:



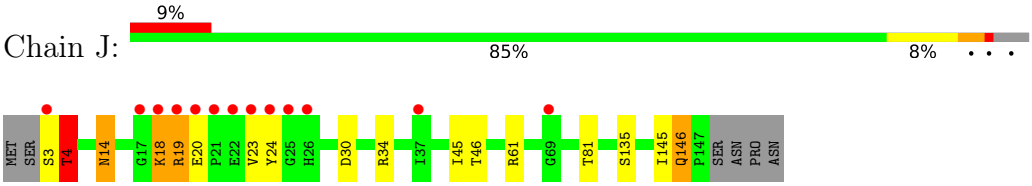
• Molecule 1: 3-dehydroquinate dehydratase

Chain I:



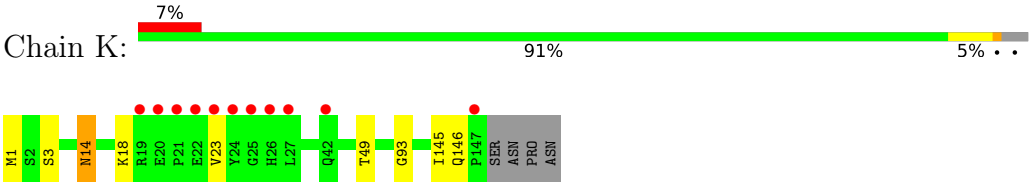
• Molecule 1: 3-dehydroquinate dehydratase

Chain J:



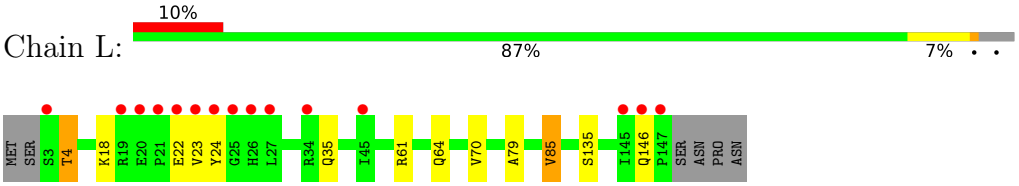
• Molecule 1: 3-dehydroquinate dehydratase

Chain K:



• Molecule 1: 3-dehydroquinate dehydratase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.80Å 155.13Å 155.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 1.90 49.15 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.15-1.90) 93.4 (49.15-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.181 , 0.218 0.191 , 0.221	Depositor DCC
R_{free} test set	1538 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14153	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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 (i)

5.1 Standard geometry (i)

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

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	1.08	0/1143	0.99	1/1555 (0.1%)
1	B	1.06	0/1143	0.94	0/1555
1	C	1.12	0/1143	1.09	2/1555 (0.1%)
1	D	1.12	3/1143 (0.3%)	1.11	5/1555 (0.3%)
1	E	1.13	0/1143	0.98	2/1555 (0.1%)
1	F	1.21	2/1143 (0.2%)	1.16	6/1555 (0.4%)
1	G	1.18	3/1143 (0.3%)	1.04	1/1555 (0.1%)
1	H	1.12	2/1143 (0.2%)	1.03	5/1555 (0.3%)
1	I	1.00	2/1143 (0.2%)	0.96	2/1555 (0.1%)
1	J	1.16	3/1143 (0.3%)	1.08	6/1555 (0.4%)
1	K	1.02	0/1157	0.97	2/1573 (0.1%)
1	L	1.02	0/1143	1.00	1/1555 (0.1%)
All	All	1.10	15/13730 (0.1%)	1.03	33/18678 (0.2%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	20	GLU	CD-OE2	-6.25	1.18	1.25
1	H	146	GLN	C-O	-5.66	1.12	1.23
1	H	55	GLU	CG-CD	5.58	1.60	1.51
1	D	128	GLY	N-CA	5.55	1.54	1.46
1	D	17	GLY	CA-C	-5.51	1.43	1.51
1	G	110	GLU	CD-OE2	-5.50	1.19	1.25
1	F	55	GLU	CD-OE1	5.35	1.31	1.25
1	D	24	TYR	CA-CB	5.33	1.65	1.53
1	J	81	THR	CB-CG2	-5.21	1.35	1.52
1	J	146	GLN	CD-OE1	-5.19	1.12	1.24
1	I	81	THR	CB-CG2	-5.16	1.35	1.52
1	J	135	SER	CB-OG	-5.11	1.35	1.42
1	I	127	CYS	CB-SG	-5.11	1.73	1.81
1	G	100	GLU	CG-CD	5.06	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	135	SER	CB-OG	-5.00	1.35	1.42

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	34	ARG	NE-CZ-NH1	14.22	127.41	120.30
1	C	24	TYR	CB-CG-CD2	-12.51	113.49	121.00
1	C	24	TYR	CB-CG-CD1	10.41	127.25	121.00
1	D	18	LYS	N-CA-C	-8.53	87.96	111.00
1	F	34	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	E	19	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	H	34	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	K	3	SER	N-CA-C	-6.20	94.26	111.00
1	F	34	ARG	CD-NE-CZ	6.13	132.19	123.60
1	E	18	LYS	CA-CB-CG	6.07	126.74	113.40
1	I	18	LYS	CA-CB-CG	6.05	126.70	113.40
1	F	18	LYS	CA-CB-CG	6.02	126.64	113.40
1	I	61	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	F	61	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	J	3	SER	CA-C-N	-5.69	104.69	117.20
1	H	61	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	18	LYS	CG-CD-CE	5.47	128.30	111.90
1	J	18	LYS	CA-CB-CG	5.41	125.30	113.40
1	H	34	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	H	24	TYR	CB-CG-CD1	5.39	124.23	121.00
1	K	23	VAL	CB-CA-C	5.38	121.63	111.40
1	H	110	GLU	OE1-CD-OE2	-5.36	116.87	123.30
1	G	20	GLU	CA-CB-CG	5.34	125.14	113.40
1	F	18	LYS	CG-CD-CE	5.30	127.80	111.90
1	J	3	SER	CB-CA-C	5.18	119.93	110.10
1	D	24	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	D	61	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	J	18	LYS	C-N-CA	5.07	134.37	121.70
1	L	61	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	D	60	ASP	CB-CG-OD1	5.03	122.83	118.30
1	J	61	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	60	ASP	CB-CG-OD1	5.01	122.81	118.30
1	J	30	ASP	CB-CG-OD2	5.01	122.81	118.30

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	1121	0	1133	15	0
1	B	1121	0	1133	9	0
1	C	1121	0	1133	13	0
1	D	1121	0	1133	14	0
1	E	1121	0	1133	19	0
1	F	1121	0	1133	7	0
1	G	1121	0	1133	3	0
1	H	1121	0	1133	12	0
1	I	1121	0	1133	6	0
1	J	1121	0	1133	11	0
1	K	1135	0	1150	3	0
1	L	1121	0	1133	10	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	10	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	10	0	0	0	0
2	I	10	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
3	A	6	0	8	1	0
3	E	18	0	24	0	0
4	D	8	0	12	0	0
5	A	54	0	0	0	0
5	B	47	0	0	1	0
5	C	35	0	0	0	0
5	D	48	0	0	0	0
5	E	57	0	0	2	0
5	F	56	0	0	0	0
5	G	62	0	0	0	0
5	H	46	0	0	0	0
5	I	47	0	0	0	0
5	J	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	45	0	0	0	0
5	L	43	0	0	2	0
All	All	14153	0	13657	105	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (105) 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:E:28:THR:HG22	1:E:31:ASN:H	1.44	0.82
1:J:19:ARG:HD3	1:K:93:GLY:O	1.80	0.82
1:E:79:ALA:HB1	1:F:85:VAL:HG22	1.59	0.82
1:L:4:THR:HG23	1:L:70:VAL:HG22	1.63	0.80
1:C:20:GLU:HB3	1:C:22:GLU:OE1	1.83	0.78
1:I:4:THR:HG23	1:I:70:VAL:HG22	1.67	0.76
1:H:146:GLN:HB3	1:H:147:PRO:CD	2.16	0.76
1:E:28:THR:HG21	5:E:351:HOH:O	1.85	0.76
1:L:4:THR:HG22	1:L:70:VAL:HA	1.70	0.74
1:A:19:ARG:HG3	1:B:66:GLN:HE22	1.56	0.70
1:L:64:GLN:NE2	5:L:301:HOH:O	2.23	0.70
1:C:145:ILE:C	1:C:147:PRO:HD3	2.11	0.70
1:G:22:GLU:HG3	1:G:22:GLU:O	1.93	0.68
1:J:19:ARG:HG2	1:J:19:ARG:O	1.92	0.68
1:C:3:SER:OG	1:C:48:ASP:HB2	1.94	0.68
1:I:4:THR:HG22	1:I:70:VAL:HA	1.76	0.66
1:D:23:VAL:HG13	1:D:25:GLY:H	1.61	0.66
1:A:19:ARG:CG	1:B:66:GLN:HE22	2.09	0.66
1:D:85:VAL:HG22	1:L:79:ALA:HB1	1.79	0.65
1:H:79:ALA:HB1	1:L:85:VAL:HG22	1.79	0.65
1:J:4:THR:HG22	1:J:46:THR:OG1	1.98	0.64
1:J:4:THR:CG2	1:J:45:ILE:HG23	2.28	0.63
1:J:4:THR:HG23	1:J:45:ILE:HG23	1.81	0.63
1:J:4:THR:HG22	1:J:46:THR:O	2.02	0.60
1:L:4:THR:CG2	1:L:70:VAL:HA	2.30	0.60
1:D:3:SER:OG	1:D:48:ASP:HB2	2.03	0.59
1:H:19:ARG:HB2	5:L:332:HOH:O	2.02	0.59
1:A:14:ASN:HD22	1:A:14:ASN:H	1.51	0.59
1:A:12:ASN:H	1:A:53:ASN:ND2	2.01	0.58
1:E:34:ARG:HH11	1:E:34:ARG:CB	2.17	0.58
1:A:3:SER:OG	1:A:48:ASP:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ARG:HD2	1:C:20:GLU:OE2	2.05	0.56
1:C:31:ASN:O	1:C:35:GLN:HG3	2.06	0.56
1:L:35:GLN:NE2	1:L:135:SER:HB2	2.21	0.56
1:E:34:ARG:HH11	1:E:34:ARG:CG	2.19	0.56
1:H:146:GLN:HB3	1:H:147:PRO:HD3	1.86	0.56
1:I:4:THR:CG2	1:I:70:VAL:HA	2.36	0.56
1:D:21:PRO:O	1:D:22:GLU:HG2	2.06	0.55
1:L:35:GLN:HE22	1:L:135:SER:HB2	1.69	0.55
1:F:14:ASN:HD22	1:F:14:ASN:H	1.55	0.54
1:B:19:ARG:O	1:B:20:GLU:C	2.46	0.53
1:E:132:LYS:HE3	1:H:143:GLU:HG3	1.91	0.53
1:H:23:VAL:HG12	1:H:24:TYR:N	2.23	0.53
1:E:79:ALA:CB	1:F:85:VAL:HG22	2.37	0.52
1:A:19:ARG:HE	1:A:19:ARG:H	1.57	0.52
1:E:14:ASN:HD22	1:E:14:ASN:H	1.58	0.52
1:E:83:THR:CG2	1:F:85:VAL:HG13	2.40	0.51
1:J:23:VAL:HG12	1:J:24:TYR:N	2.26	0.51
1:A:23:VAL:HG12	1:A:24:TYR:N	2.26	0.51
1:F:23:VAL:HG12	1:F:24:TYR:N	2.26	0.50
1:J:14:ASN:HD22	1:J:14:ASN:H	1.59	0.50
1:B:14:ASN:HD22	1:B:14:ASN:H	1.60	0.50
1:I:23:VAL:HG12	1:I:24:TYR:N	2.27	0.49
1:E:28:THR:HG23	1:E:30:ASP:H	1.77	0.49
1:A:45:ILE:HD11	1:A:146:GLN:CD	2.33	0.49
1:A:117:TYR:C	1:A:118:LEU:HD12	2.33	0.49
1:D:19:ARG:HA	1:D:19:ARG:HH11	1.78	0.48
1:A:11:PRO:HA	1:A:53:ASN:HD22	1.78	0.48
1:L:23:VAL:HG12	1:L:24:TYR:N	2.28	0.48
1:I:14:ASN:HD22	1:I:14:ASN:H	1.60	0.48
1:E:34:ARG:HH11	1:E:34:ARG:CA	2.27	0.48
1:E:34:ARG:HH11	1:E:34:ARG:HA	1.78	0.48
3:A:203:GOL:H32	1:B:83:THR:HB	1.96	0.47
1:F:144:LYS:HA	1:F:144:LYS:HD2	1.51	0.47
1:C:34:ARG:HD3	1:C:34:ARG:HA	1.56	0.46
1:D:17:GLY:O	1:D:20:GLU:N	2.48	0.46
1:D:23:VAL:HG13	1:D:25:GLY:N	2.28	0.46
1:H:34:ARG:CG	1:H:34:ARG:HH11	2.28	0.46
1:B:19:ARG:HG3	1:C:66:GLN:NE2	2.31	0.46
1:C:3:SER:HA	1:C:46:THR:CG2	2.46	0.45
1:E:34:ARG:N	1:E:34:ARG:HD2	2.25	0.45
1:C:146:GLN:N	1:C:147:PRO:HD3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ARG:HG3	1:B:66:GLN:NE2	2.29	0.45
1:D:15:LEU:O	1:D:21:PRO:HD3	2.17	0.45
1:E:132:LYS:CE	1:H:143:GLU:HG3	2.47	0.45
1:D:23:VAL:C	1:D:25:GLY:H	2.20	0.44
1:J:19:ARG:CD	1:K:93:GLY:O	2.57	0.44
1:A:118:LEU:HD12	1:A:118:LEU:N	2.33	0.44
1:E:34:ARG:CG	1:E:34:ARG:NH1	2.77	0.44
1:K:14:ASN:H	1:K:14:ASN:HD22	1.66	0.44
1:A:132:LYS:HE3	1:D:143:GLU:HG3	2.00	0.44
1:B:71:LYS:HE3	5:B:339:HOH:O	2.17	0.43
1:D:20:GLU:C	1:D:22:GLU:H	2.22	0.43
1:H:14:ASN:H	1:H:14:ASN:HD22	1.65	0.43
1:H:83:THR:CG2	1:L:85:VAL:HG13	2.49	0.42
1:D:23:VAL:HG13	1:D:25:GLY:CA	2.50	0.42
1:E:109:ARG:CZ	5:E:315:HOH:O	2.67	0.42
1:G:31:ASN:O	1:G:35:GLN:HG3	2.19	0.42
1:H:146:GLN:CB	1:H:147:PRO:CD	2.93	0.42
1:E:35:GLN:HE22	1:E:39:GLN:NE2	2.17	0.42
1:B:45:ILE:HD13	1:B:142:ILE:HG12	2.02	0.42
1:E:34:ARG:NH1	1:E:34:ARG:HG3	2.35	0.42
1:F:14:ASN:H	1:F:14:ASN:ND2	2.17	0.42
1:A:132:LYS:CE	1:D:143:GLU:HG3	2.49	0.41
1:C:39:GLN:HE22	1:C:135:SER:HB3	1.85	0.41
1:A:57:ALA:HB2	1:C:54:TRP:CH2	2.54	0.41
1:H:34:ARG:HH11	1:H:34:ARG:CB	2.33	0.41
1:I:34:ARG:HA	1:I:34:ARG:HD2	1.71	0.41
1:J:19:ARG:O	1:J:19:ARG:CG	2.63	0.41
1:C:30:ASP:OD1	1:C:34:ARG:NH1	2.54	0.41
1:C:55:GLU:OE2	1:C:84:SER:OG	2.36	0.41
1:J:4:THR:HG21	1:J:45:ILE:HG23	2.03	0.41
1:G:14:ASN:H	1:G:14:ASN:HD22	1.68	0.40
1:D:77:PRO:HG2	1:D:81:THR:HB	2.04	0.40
1:E:35:GLN:HE22	1:E:39:GLN:HE21	1.70	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	143/151 (95%)	137 (96%)	6 (4%)	0	100 100
1	B	143/151 (95%)	139 (97%)	4 (3%)	0	100 100
1	C	143/151 (95%)	137 (96%)	4 (3%)	2 (1%)	11 3
1	D	143/151 (95%)	137 (96%)	3 (2%)	3 (2%)	7 1
1	E	143/151 (95%)	141 (99%)	2 (1%)	0	100 100
1	F	143/151 (95%)	136 (95%)	7 (5%)	0	100 100
1	G	143/151 (95%)	139 (97%)	4 (3%)	0	100 100
1	H	143/151 (95%)	137 (96%)	5 (4%)	1 (1%)	22 12
1	I	143/151 (95%)	139 (97%)	4 (3%)	0	100 100
1	J	143/151 (95%)	136 (95%)	5 (4%)	2 (1%)	11 3
1	K	145/151 (96%)	140 (97%)	5 (3%)	0	100 100
1	L	143/151 (95%)	138 (96%)	5 (4%)	0	100 100
All	All	1718/1812 (95%)	1656 (96%)	54 (3%)	8 (0%)	29 18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	23	VAL
1	D	22	GLU
1	H	146	GLN
1	D	19	ARG
1	D	20	GLU
1	J	4	THR
1	J	20	GLU
1	C	20	GLU

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	119/125 (95%)	111 (93%)	8 (7%)	16 7
1	B	119/125 (95%)	113 (95%)	6 (5%)	24 15
1	C	119/125 (95%)	114 (96%)	5 (4%)	30 20
1	D	119/125 (95%)	109 (92%)	10 (8%)	11 4
1	E	119/125 (95%)	112 (94%)	7 (6%)	19 10
1	F	119/125 (95%)	107 (90%)	12 (10%)	7 2
1	G	119/125 (95%)	112 (94%)	7 (6%)	19 10
1	H	119/125 (95%)	110 (92%)	9 (8%)	13 5
1	I	119/125 (95%)	114 (96%)	5 (4%)	30 20
1	J	119/125 (95%)	112 (94%)	7 (6%)	19 10
1	K	121/125 (97%)	115 (95%)	6 (5%)	24 15
1	L	119/125 (95%)	114 (96%)	5 (4%)	30 20
All	All	1430/1500 (95%)	1343 (94%)	87 (6%)	18 9

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	18	LYS
1	A	19	ARG
1	A	22	GLU
1	A	24	TYR
1	A	34	ARG
1	A	45	ILE
1	A	146	GLN
1	B	14	ASN
1	B	18	LYS
1	B	20	GLU
1	B	34	ARG
1	B	145	ILE
1	B	146	GLN

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Mol	Chain	Res	Type
1	C	18	LYS
1	C	22	GLU
1	C	34	ARG
1	C	135	SER
1	C	146	GLN
1	D	14	ASN
1	D	16	LEU
1	D	18	LYS
1	D	19	ARG
1	D	23	VAL
1	D	34	ARG
1	D	85	VAL
1	D	106	VAL
1	D	114	HIS
1	D	146	GLN
1	E	14	ASN
1	E	18	LYS
1	E	23	VAL
1	E	28	THR
1	E	34	ARG
1	E	145	ILE
1	E	146	GLN
1	F	16	LEU
1	F	18	LYS
1	F	22	GLU
1	F	26	HIS
1	F	30	ASP
1	F	46	THR
1	F	85	VAL
1	F	106	VAL
1	F	114	HIS
1	F	144	LYS
1	F	145	ILE
1	F	146	GLN
1	G	14	ASN
1	G	18	LYS
1	G	23	VAL
1	G	34	ARG
1	G	46	THR
1	G	106	VAL
1	G	146	GLN
1	H	4	THR

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Mol	Chain	Res	Type
1	H	14	ASN
1	H	18	LYS
1	H	22	GLU
1	H	24	TYR
1	H	34	ARG
1	H	46	THR
1	H	48	ASP
1	H	106	VAL
1	I	4	THR
1	I	14	ASN
1	I	22	GLU
1	I	34	ARG
1	I	146	GLN
1	J	4	THR
1	J	14	ASN
1	J	18	LYS
1	J	19	ARG
1	J	34	ARG
1	J	145	ILE
1	J	146	GLN
1	K	1	MET
1	K	14	ASN
1	K	18	LYS
1	K	49	THR
1	K	145	ILE
1	K	146	GLN
1	L	4	THR
1	L	18	LYS
1	L	22	GLU
1	L	85	VAL
1	L	146	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	53	ASN
1	B	14	ASN
1	B	31	ASN
1	B	66	GLN
1	C	39	GLN
1	C	64	GLN

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Mol	Chain	Res	Type
1	C	66	GLN
1	D	14	ASN
1	D	35	GLN
1	D	39	GLN
1	D	115	HIS
1	E	14	ASN
1	E	26	HIS
1	E	39	GLN
1	E	115	HIS
1	F	14	ASN
1	F	26	HIS
1	F	35	GLN
1	F	39	GLN
1	G	14	ASN
1	G	31	ASN
1	H	14	ASN
1	H	31	ASN
1	H	35	GLN
1	H	39	GLN
1	I	14	ASN
1	J	14	ASN
1	K	14	ASN
1	K	115	HIS
1	L	35	GLN
1	L	39	GLN
1	L	64	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

21 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	G	201	-	4,4,4	1.08	0	6,6,6	0.58	0
2	SO4	D	201	-	4,4,4	0.33	0	6,6,6	1.00	0
2	SO4	L	201	-	4,4,4	0.37	0	6,6,6	0.63	0
3	GOL	E	205	-	5,5,5	0.36	0	5,5,5	0.60	0
2	SO4	B	201	-	4,4,4	0.71	0	6,6,6	0.81	0
2	SO4	A	202	-	4,4,4	0.54	0	6,6,6	0.85	0
2	SO4	H	201	-	4,4,4	1.10	0	6,6,6	0.51	0
2	SO4	A	201	-	4,4,4	0.60	0	6,6,6	1.02	1 (16%)
3	GOL	E	204	-	5,5,5	0.62	0	5,5,5	0.68	0
3	GOL	E	203	-	5,5,5	0.68	0	5,5,5	1.36	1 (20%)
2	SO4	C	201	-	4,4,4	0.37	0	6,6,6	0.51	0
2	SO4	H	202	-	4,4,4	0.37	0	6,6,6	1.43	1 (16%)
2	SO4	K	201	-	4,4,4	0.59	0	6,6,6	0.42	0
2	SO4	I	201	-	4,4,4	0.74	0	6,6,6	0.71	0
2	SO4	I	202	-	4,4,4	0.49	0	6,6,6	0.84	0
2	SO4	E	202	-	4,4,4	0.59	0	6,6,6	0.97	0
2	SO4	J	201	-	4,4,4	0.73	0	6,6,6	0.84	0
2	SO4	E	201	-	4,4,4	0.55	0	6,6,6	0.95	0
3	GOL	A	203	-	5,5,5	1.92	1 (20%)	5,5,5	2.15	2 (40%)
2	SO4	F	201	-	4,4,4	0.77	0	6,6,6	0.51	0
4	TRS	D	202	-	7,7,7	1.26	1 (14%)	9,9,9	1.16	1 (11%)

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	E	204	-	-	0/4/4/4	-
3	GOL	E	205	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	203	-	-	0/4/4/4	-
3	GOL	A	203	-	-	2/4/4/4	-
4	TRS	D	202	-	-	0/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	203	GOL	O2-C2	3.23	1.53	1.43
4	D	202	TRS	O3-C3	2.17	1.49	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	203	GOL	O3-C3-C2	3.04	124.78	110.20
3	A	203	GOL	O2-C2-C3	2.56	120.42	109.12
3	E	203	GOL	C3-C2-C1	-2.51	101.94	111.70
2	H	202	SO4	O3-S-O1	-2.41	96.75	109.31
4	D	202	TRS	O2-C2-C	2.13	117.74	111.00
2	A	201	SO4	O4-S-O2	-2.05	98.62	109.31

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	203	GOL	C1-C2-C3-O3
3	A	203	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	203	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	145/151 (96%)	0.67	16 (11%) 5 6	30, 40, 89, 129	0
1	B	145/151 (96%)	0.56	8 (5%) 25 28	28, 38, 78, 111	0
1	C	145/151 (96%)	0.70	13 (8%) 9 10	28, 38, 119, 171	0
1	D	145/151 (96%)	0.49	12 (8%) 11 13	32, 40, 92, 137	0
1	E	145/151 (96%)	0.06	2 (1%) 75 77	27, 36, 62, 74	0
1	F	145/151 (96%)	0.47	9 (6%) 20 23	26, 33, 82, 156	0
1	G	145/151 (96%)	0.13	5 (3%) 45 48	26, 36, 65, 98	0
1	H	145/151 (96%)	0.48	13 (8%) 9 10	29, 39, 84, 126	0
1	I	145/151 (96%)	0.47	14 (9%) 7 9	31, 43, 98, 147	0
1	J	145/151 (96%)	0.60	13 (8%) 9 10	30, 40, 131, 169	0
1	K	147/151 (97%)	0.40	11 (7%) 14 15	31, 40, 85, 140	0
1	L	145/151 (96%)	0.59	15 (10%) 6 7	32, 43, 89, 150	0
All	All	1742/1812 (96%)	0.47	131 (7%) 14 15	26, 40, 87, 171	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	23	VAL	16.4
1	C	21	PRO	15.2
1	L	24	TYR	15.2
1	C	26	HIS	15.0
1	K	24	TYR	14.7
1	F	24	TYR	14.6
1	I	23	VAL	14.3
1	C	147	PRO	12.9
1	A	24	TYR	12.8
1	J	25	GLY	12.6
1	I	24	TYR	12.5

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Mol	Chain	Res	Type	RSRZ
1	D	24	TYR	12.4
1	B	24	TYR	11.5
1	J	22	GLU	11.5
1	J	24	TYR	11.4
1	B	23	VAL	11.0
1	K	23	VAL	11.0
1	H	24	TYR	10.8
1	H	23	VAL	10.6
1	L	23	VAL	9.8
1	J	20	GLU	9.0
1	J	26	HIS	8.8
1	J	21	PRO	8.8
1	C	24	TYR	8.1
1	A	23	VAL	8.0
1	J	23	VAL	8.0
1	F	22	GLU	7.8
1	C	19	ARG	7.6
1	F	25	GLY	7.1
1	J	18	LYS	7.0
1	A	147	PRO	6.8
1	I	20	GLU	6.7
1	C	20	GLU	6.4
1	C	22	GLU	6.4
1	K	147	PRO	6.0
1	A	20	GLU	6.0
1	L	26	HIS	5.9
1	I	3	SER	5.9
1	L	147	PRO	5.7
1	B	147	PRO	5.5
1	L	20	GLU	5.4
1	D	23	VAL	5.3
1	D	18	LYS	5.2
1	F	20	GLU	5.2
1	F	19	ARG	5.1
1	L	22	GLU	5.1
1	F	21	PRO	5.1
1	H	21	PRO	5.0
1	I	22	GLU	5.0
1	K	22	GLU	4.9
1	J	19	ARG	4.9
1	L	25	GLY	4.7
1	H	22	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	G	147	PRO	4.7
1	D	147	PRO	4.6
1	A	21	PRO	4.6
1	E	147	PRO	4.6
1	L	19	ARG	4.5
1	D	22	GLU	4.5
1	D	21	PRO	4.4
1	K	21	PRO	4.4
1	I	21	PRO	4.2
1	A	3	SER	4.1
1	A	19	ARG	4.1
1	I	26	HIS	4.1
1	B	20	GLU	4.0
1	C	25	GLY	4.0
1	L	21	PRO	4.0
1	A	22	GLU	4.0
1	D	20	GLU	3.9
1	K	25	GLY	3.9
1	A	145	ILE	3.7
1	K	26	HIS	3.7
1	G	23	VAL	3.7
1	H	147	PRO	3.7
1	C	18	LYS	3.7
1	H	20	GLU	3.6
1	A	26	HIS	3.6
1	C	23	VAL	3.6
1	C	17	GLY	3.6
1	H	25	GLY	3.5
1	A	45	ILE	3.4
1	F	26	HIS	3.4
1	G	24	TYR	3.4
1	C	146	GLN	3.4
1	I	27	LEU	3.3
1	E	44	SER	3.3
1	D	19	ARG	3.1
1	A	146	GLN	3.1
1	G	3	SER	3.1
1	D	145	ILE	3.0
1	I	19	ARG	3.0
1	L	34	ARG	2.9
1	C	145	ILE	2.8
1	K	42	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	46	THR	2.7
1	D	146	GLN	2.7
1	H	26	HIS	2.7
1	J	3	SER	2.7
1	K	19	ARG	2.7
1	B	22	GLU	2.7
1	D	143	GLU	2.6
1	K	20	GLU	2.6
1	J	37	ILE	2.6
1	B	21	PRO	2.6
1	I	147	PRO	2.6
1	J	17	GLY	2.6
1	I	17	GLY	2.6
1	H	19	ARG	2.5
1	L	27	LEU	2.5
1	H	18	LYS	2.5
1	K	27	LEU	2.5
1	D	26	HIS	2.4
1	B	58	ILE	2.4
1	H	17	GLY	2.4
1	H	45	ILE	2.3
1	A	143	GLU	2.3
1	B	59	VAL	2.3
1	G	22	GLU	2.2
1	A	25	GLY	2.2
1	H	34	ARG	2.2
1	I	18	LYS	2.2
1	F	18	LYS	2.1
1	I	146	GLN	2.1
1	I	25	GLY	2.1
1	L	145	ILE	2.1
1	L	146	GLN	2.1
1	L	3	SER	2.1
1	J	69	GLY	2.1
1	A	41	GLU	2.0
1	L	45	ILE	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, 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
3	GOL	A	203	6/6	0.78	0.18	43,50,54,56	0
3	GOL	E	204	6/6	0.89	0.13	38,50,56,57	0
3	GOL	E	203	6/6	0.90	0.14	38,45,46,65	0
3	GOL	E	205	6/6	0.91	0.13	53,57,59,60	0
4	TRS	D	202	8/8	0.92	0.16	42,49,57,58	0
2	SO4	H	202	5/5	0.96	0.21	36,36,59,64	5
2	SO4	E	202	5/5	0.96	0.12	47,48,69,87	0
2	SO4	I	202	5/5	0.97	0.11	47,54,73,91	0
2	SO4	J	201	5/5	0.98	0.09	36,39,47,49	0
2	SO4	K	201	5/5	0.98	0.09	37,41,45,49	0
2	SO4	L	201	5/5	0.98	0.12	44,44,46,50	0
2	SO4	A	201	5/5	0.98	0.10	40,42,44,45	0
2	SO4	H	201	5/5	0.98	0.11	39,41,45,48	0
2	SO4	A	202	5/5	0.98	0.14	48,51,53,84	0
2	SO4	I	201	5/5	0.98	0.11	42,48,54,58	0
2	SO4	C	201	5/5	0.98	0.09	35,41,45,46	0
2	SO4	B	201	5/5	0.99	0.10	34,38,41,46	0
2	SO4	F	201	5/5	0.99	0.09	33,34,38,42	0
2	SO4	G	201	5/5	0.99	0.09	36,38,45,46	0
2	SO4	D	201	5/5	0.99	0.10	42,45,47,51	0
2	SO4	E	201	5/5	0.99	0.10	32,33,38,40	0

6.5 Other polymers (i)

There are no such residues in this entry.