



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 10:59 AM UTC

PDB ID : 1JMK / pdb_00001jmk
Title : Structural Basis for the Cyclization of the Lipopeptide Antibiotic Surfactin by the Thioesterase Domain SrfTE
Authors : Bruner, S.D.; Weber, T.; Kohli, R.M.; Schwarzer, D.; Marahiel, M.A.; Walsh, C.T.; Stubbs, M.T.
Deposited on : 2001-07-18
Resolution : 1.71 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

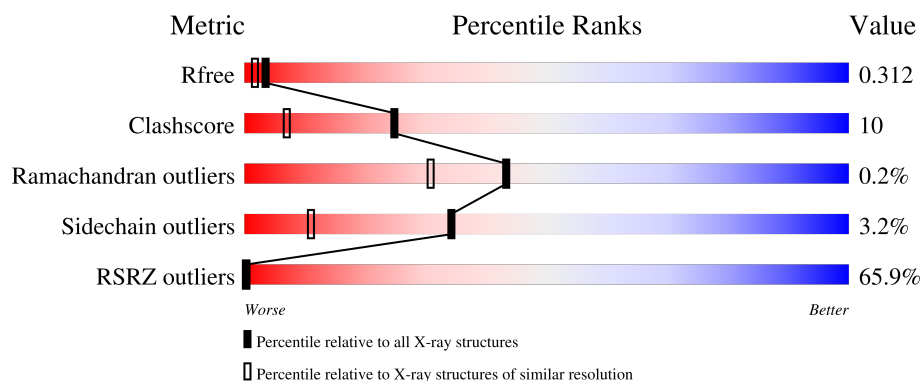
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	C	230	55% 76% 20% ••
1	O	230	75% 78% 19% •

2 Entry composition [i](#)

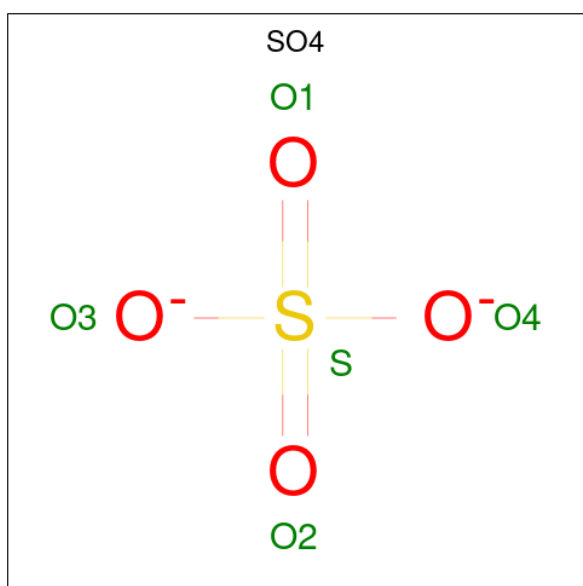
There are 3 unique types of molecules in this entry. The entry contains 3779 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Surfactin Synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	222	Total	C	N	O	S	0	0	0
			1733	1098	289	338	8			
1	O	230	Total	C	N	O	S	0	0	0
			1798	1134	301	355	8			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

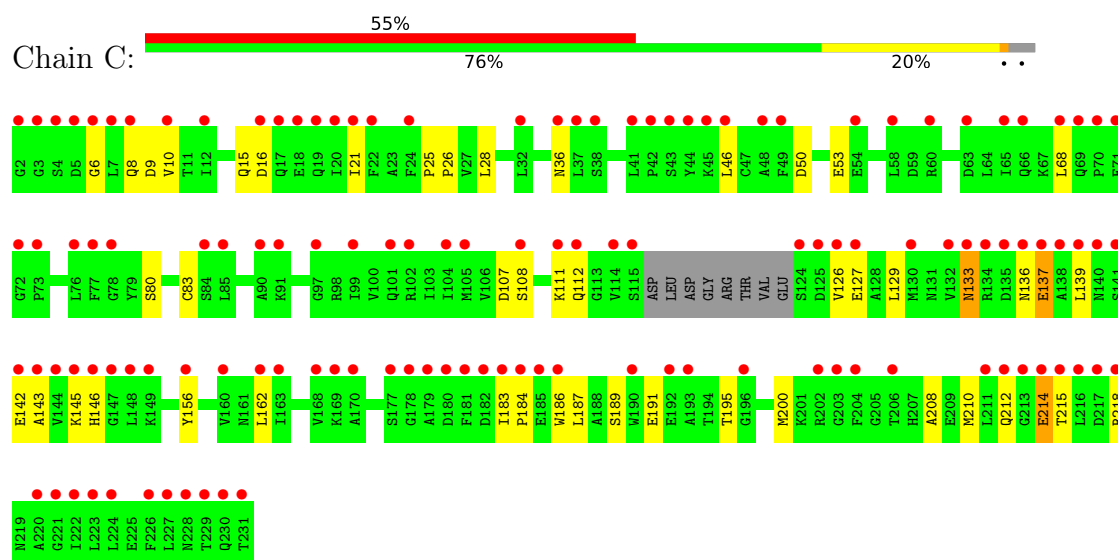
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	141	Total 141	O 141	0	0
3	O	97	Total 97	O 97	0	0

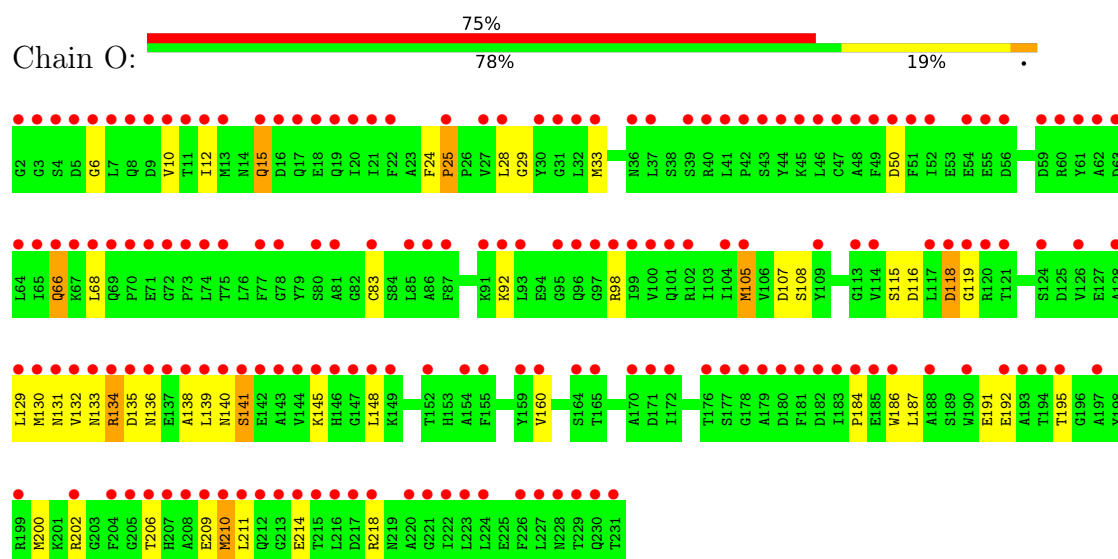
3 Residue-property plots

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: Surfactin Synthetase



• Molecule 1: Surfactin Synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.01Å 76.37Å 119.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.71 25.00 – 1.71	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-1.71) 96.1 (25.00-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.70Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.230 , 0.245 0.306 , 0.312	Depositor DCC
R_{free} test set	6162 reflections (9.85%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3779	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	C	0.39	0/1764	0.94	8/2380 (0.3%)
1	O	0.35	0/1830	0.91	9/2471 (0.4%)
All	All	0.37	0/3594	0.92	17/4851 (0.4%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	25	PRO	N-CA-C	8.69	121.30	110.70
1	C	25	PRO	N-CA-C	8.51	121.08	110.70
1	C	210	MET	N-CA-C	7.06	119.83	111.71
1	C	107	ASP	N-CA-C	6.84	120.84	111.54
1	O	50	ASP	N-CA-C	-6.26	101.19	110.46
1	C	50	ASP	N-CA-C	-6.20	100.81	110.42
1	C	15	GLN	N-CA-C	5.98	119.68	112.38
1	O	15	GLN	N-CA-C	5.85	119.52	112.38
1	O	29	GLY	N-CA-C	5.47	122.87	115.32
1	O	107	ASP	N-CA-C	5.46	118.87	111.17
1	O	210	MET	N-CA-C	5.46	117.23	111.28
1	O	195	THR	N-CA-C	-5.38	106.39	113.17
1	C	208	ALA	N-CA-C	5.37	119.46	113.01
1	C	195	THR	N-CA-C	-5.28	106.61	113.16
1	C	53	GLU	N-CA-C	5.12	117.76	111.82
1	O	24	PHE	CA-C-N	5.00	125.53	120.38
1	O	24	PHE	C-N-CA	5.00	125.53	120.38

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	C	1733	0	1683	34	4
1	O	1798	0	1746	36	4
2	C	5	0	0	0	0
2	O	5	0	0	0	0
3	C	141	0	0	2	1
3	O	97	0	0	1	1
All	All	3779	0	3429	68	5

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 10.

All (68) 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:O:134:ARG:HE	1:O:135:ASP:H	1.03	0.97
1:C:36:ASN:HD22	1:C:212:GLN:NE2	1.69	0.90
1:C:36:ASN:HD22	1:C:212:GLN:HE22	1.23	0.86
1:O:134:ARG:HE	1:O:135:ASP:N	1.72	0.85
1:O:83:CYS:SG	1:O:105:MET:HG3	2.19	0.83
1:C:28:LEU:HD11	1:C:133:ASN:HD21	1.46	0.80
1:O:134:ARG:NE	1:O:135:ASP:H	1.84	0.73
1:C:28:LEU:HD11	1:C:133:ASN:ND2	2.06	0.71
1:C:215:THR:HG22	1:C:218:ARG:NH1	2.08	0.68
1:O:130:MET:HE3	1:O:148:LEU:HG	1.75	0.67
1:C:21:ILE:HB	1:C:46:LEU:HD23	1.76	0.65
1:O:66:GLN:NE2	1:O:98:ARG:HH11	1.94	0.64
1:C:184:PRO:HD2	1:C:187:LEU:HD12	1.80	0.64
1:C:36:ASN:ND2	1:C:212:GLN:NE2	2.43	0.63
1:O:214:GLU:HG3	1:O:218:ARG:NH1	2.13	0.63
1:O:214:GLU:HG3	1:O:218:ARG:HH12	1.68	0.59
1:C:215:THR:HG22	1:C:218:ARG:HH11	1.69	0.58
1:O:140:ASN:HA	1:O:145:LYS:HE3	1.85	0.57
1:O:134:ARG:HA	3:O:592:HOH:O	2.05	0.56
1:O:184:PRO:HD2	1:O:187:LEU:HD12	1.88	0.55
1:C:36:ASN:ND2	1:C:212:GLN:HE22	1.99	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:ILE:HD11	1:C:187:LEU:HB3	1.88	0.55
1:O:28:LEU:HD12	1:O:33:MET:CE	2.37	0.54
1:O:131:ASN:O	1:O:134:ARG:HD3	2.07	0.54
1:C:112:GLN:HG3	3:C:581:HOH:O	2.09	0.53
1:O:134:ARG:NE	1:O:134:ARG:N	2.56	0.53
1:O:28:LEU:HD12	1:O:33:MET:HE1	1.91	0.53
1:O:136:ASN:ND2	1:O:138:ALA:HB3	2.24	0.52
1:O:83:CYS:SG	1:O:108:SER:HB3	2.50	0.52
1:C:142:GLU:HG2	1:C:143:ALA:N	2.27	0.49
1:C:191:GLU:HG3	1:O:200:MET:SD	2.53	0.49
1:C:111:LYS:HG2	1:C:162:LEU:O	2.12	0.49
1:C:28:LEU:CD1	1:C:133:ASN:ND2	2.73	0.49
1:O:12:ILE:HG22	1:O:15:GLN:HG2	1.95	0.49
1:O:66:GLN:HA	1:O:66:GLN:HE21	1.77	0.49
1:C:26:PRO:HA	1:C:80:SER:HB3	1.95	0.48
1:C:136:ASN:HD22	1:C:137:GLU:N	2.12	0.48
1:O:130:MET:HE3	1:O:148:LEU:CG	2.45	0.47
1:C:145:LYS:HG3	1:C:146:HIS:N	2.29	0.47
1:O:115:SER:HB2	1:O:160:VAL:HG13	1.97	0.47
1:C:129:LEU:O	1:C:133:ASN:ND2	2.48	0.47
1:C:126:VAL:HG11	1:C:156:TYR:CD1	2.50	0.47
1:C:139:LEU:HD12	1:C:139:LEU:N	2.30	0.46
1:C:183:ILE:O	1:C:183:ILE:HG23	2.15	0.46
1:C:8:GLN:O	1:C:9:ASP:HB2	2.16	0.46
1:O:134:ARG:HE	1:O:134:ARG:N	2.13	0.45
1:O:66:GLN:NE2	1:O:98:ARG:NH1	2.62	0.45
1:O:206:THR:O	1:O:210:MET:HG3	2.17	0.45
1:C:83:CYS:SG	1:C:108:SER:HB3	2.57	0.45
1:O:134:ARG:NE	1:O:134:ARG:H	2.14	0.45
1:C:126:VAL:HG23	1:C:127:GLU:N	2.32	0.44
1:C:183:ILE:HD11	1:C:187:LEU:CB	2.48	0.44
1:O:83:CYS:CB	1:O:105:MET:HG3	2.47	0.44
1:O:116:ASP:HB3	1:O:186:TRP:CZ3	2.53	0.43
1:C:111:LYS:CG	1:C:162:LEU:O	2.66	0.43
1:C:214:GLU:N	1:C:214:GLU:OE1	2.51	0.43
1:O:83:CYS:HB3	1:O:105:MET:HG3	2.00	0.42
1:O:129:LEU:O	1:O:132:VAL:HG22	2.19	0.42
1:O:133:ASN:O	1:O:139:LEU:HD12	2.20	0.42
1:O:206:THR:OG1	1:O:209:GLU:HG2	2.20	0.41
1:C:36:ASN:HB2	1:C:212:GLN:HE22	1.84	0.41
1:O:206:THR:H	1:O:209:GLU:CG	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:MET:SD	1:O:191:GLU:HG3	2.61	0.41
1:O:134:ARG:NE	1:O:135:ASP:N	2.54	0.41
1:C:186:TRP:CD1	1:C:186:TRP:H	2.39	0.41
1:C:136:ASN:HD22	1:C:136:ASN:C	2.28	0.40
1:O:118:ASP:HB3	1:O:119:GLY:H	1.55	0.40
1:C:189:SER:HB2	3:C:633:HOH:O	2.22	0.40

All (5) 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)
1:C:68:LEU:O	1:O:6:GLY:N[2_664]	1.93	0.27
1:C:16:ASP:OD2	1:O:141:SER:OG[2_664]	1.97	0.23
1:C:10:VAL:O	3:O:503:HOH:O[2_664]	2.11	0.09
1:O:10:VAL:O	3:C:538:HOH:O[2_665]	2.11	0.09
1:C:6:GLY:N	1:O:68:LEU:O[2_664]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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	C	218/230 (95%)	210 (96%)	8 (4%)	0	100	100
1	O	228/230 (99%)	221 (97%)	6 (3%)	1 (0%)	30	16
All	All	446/460 (97%)	431 (97%)	14 (3%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	141	SER

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	C	181/192 (94%)	178 (98%)	3 (2%)	53	31
1	O	190/192 (99%)	181 (95%)	9 (5%)	23	4
All	All	371/384 (97%)	359 (97%)	12 (3%)	34	11

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	133	ASN
1	C	137	GLU
1	C	214	GLU
1	O	25	PRO
1	O	66	GLN
1	O	92	LYS
1	O	105	MET
1	O	118	ASP
1	O	134	ARG
1	O	192	GLU
1	O	202	ARG
1	O	211	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	8	GLN
1	C	14	ASN
1	C	35	GLN
1	C	96	GLN
1	C	112	GLN
1	C	133	ASN
1	C	136	ASN
1	C	167	GLN
1	C	212	GLN
1	C	228	ASN

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Mol	Chain	Res	Type
1	O	8	GLN
1	O	14	ASN
1	O	35	GLN
1	O	36	ASN
1	O	66	GLN
1	O	96	GLN
1	O	101	GLN
1	O	112	GLN
1	O	131	ASN
1	O	133	ASN
1	O	136	ASN
1	O	140	ASN
1	O	228	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	O	501	-	4,4,4	0.59	0	6,6,6	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	502	-	4,4,4	0.59	0	6,6,6	0.97	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	C	222/230 (96%)	2.56	126 (56%) 0 0	15, 24, 55, 68	0
1	O	230/230 (100%)	2.91	172 (74%) 0 0	18, 30, 57, 64	0
All	All	452/460 (98%)	2.74	298 (65%) 0 0	15, 27, 57, 68	0

All (298) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	4	SER	9.6
1	O	2	GLY	9.4
1	O	3	GLY	8.9
1	C	115	SER	7.4
1	C	146	HIS	7.3
1	O	138	ALA	7.0
1	C	4	SER	6.6
1	C	142	GLU	6.5
1	O	132	VAL	6.5
1	O	6	GLY	6.4
1	C	5	ASP	6.3
1	C	231	THR	6.2
1	O	139	LEU	6.2
1	C	138	ALA	6.1
1	O	143	ALA	6.1
1	O	231	THR	6.0
1	C	147	GLY	6.0
1	C	3	GLY	6.0
1	C	2	GLY	5.9
1	O	146	HIS	5.9
1	O	70	PRO	5.8
1	C	183	ILE	5.6
1	C	137	GLU	5.6
1	C	133	ASN	5.6

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Mol	Chain	Res	Type	RSRZ
1	O	144	VAL	5.5
1	C	124	SER	5.4
1	O	129	LEU	5.4
1	C	6	GLY	5.4
1	O	44	TYR	5.2
1	C	144	VAL	5.2
1	O	131	ASN	5.1
1	O	46	LEU	5.1
1	O	207	HIS	5.1
1	O	5	ASP	5.1
1	O	97	GLY	5.1
1	C	143	ALA	5.1
1	O	95	GLY	5.1
1	C	184	PRO	5.0
1	O	72	GLY	4.9
1	C	139	LEU	4.8
1	O	148	LEU	4.8
1	C	181	PHE	4.8
1	C	46	LEU	4.8
1	O	211	LEU	4.7
1	C	125	ASP	4.7
1	C	135	ASP	4.7
1	O	181	PHE	4.7
1	O	178	GLY	4.7
1	C	182	ASP	4.6
1	O	137	GLU	4.6
1	C	7	LEU	4.6
1	C	179	ALA	4.6
1	C	126	VAL	4.6
1	O	140	ASN	4.6
1	O	147	GLY	4.5
1	C	44	TYR	4.5
1	O	134	ARG	4.5
1	O	12	ILE	4.5
1	O	184	PRO	4.4
1	C	220	ALA	4.4
1	O	128	ALA	4.4
1	O	208	ALA	4.4
1	C	214	GLU	4.4
1	O	228	ASN	4.3
1	O	229	THR	4.3
1	O	119	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	O	99	ILE	4.2
1	O	67	LYS	4.2
1	C	114	VAL	4.2
1	O	118	ASP	4.2
1	O	212	GLN	4.2
1	C	70	PRO	4.1
1	O	179	ALA	4.1
1	O	7	LEU	4.1
1	C	178	GLY	4.0
1	C	230	GLN	4.0
1	O	48	ALA	4.0
1	O	192	GLU	4.0
1	O	68	LEU	4.0
1	O	117	LEU	4.0
1	C	145	LYS	4.0
1	C	215	THR	4.0
1	O	43	SER	4.0
1	C	228	ASN	3.9
1	O	227	LEU	3.9
1	O	182	ASP	3.9
1	C	213	GLY	3.9
1	O	10	VAL	3.8
1	O	183	ILE	3.8
1	C	149	LYS	3.8
1	O	177	SER	3.8
1	O	36	ASN	3.8
1	O	199	ARG	3.7
1	C	180	ASP	3.7
1	C	140	ASN	3.7
1	C	169	LYS	3.7
1	C	229	THR	3.7
1	O	74	LEU	3.7
1	O	130	MET	3.6
1	O	209	GLU	3.6
1	O	170	ALA	3.6
1	C	78	GLY	3.6
1	O	186	TRP	3.6
1	O	101	GLN	3.5
1	O	142	GLU	3.5
1	O	218	ARG	3.5
1	O	19	GLN	3.5
1	C	108	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	O	145	LYS	3.4
1	C	185	GLU	3.4
1	O	51	PHE	3.4
1	O	37	LEU	3.4
1	O	109	TYR	3.4
1	C	102	ARG	3.4
1	C	177	SER	3.4
1	C	202	ARG	3.4
1	C	18	GLU	3.4
1	C	68	LEU	3.4
1	O	220	ALA	3.3
1	O	213	GLY	3.3
1	O	126	VAL	3.3
1	C	17	GLN	3.3
1	C	19	GLN	3.3
1	C	186	TRP	3.3
1	O	17	GLN	3.3
1	O	49	PHE	3.3
1	O	62	ALA	3.3
1	O	133	ASN	3.3
1	O	20	ILE	3.3
1	C	211	LEU	3.3
1	O	230	GLN	3.3
1	C	54	GLU	3.2
1	C	204	PHE	3.2
1	C	91	LYS	3.2
1	O	42	PRO	3.2
1	C	227	LEU	3.2
1	O	141	SER	3.2
1	O	226	PHE	3.2
1	C	12	ILE	3.1
1	O	93	LEU	3.1
1	C	97	GLY	3.1
1	C	10	VAL	3.1
1	C	20	ILE	3.1
1	C	224	LEU	3.1
1	C	134	ARG	3.1
1	O	39	SER	3.1
1	C	32	LEU	3.0
1	O	28	LEU	3.0
1	C	112	GLN	3.0
1	O	18	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	O	202	ARG	3.0
1	O	135	ASP	3.0
1	C	99	ILE	3.0
1	O	45	LYS	3.0
1	C	192	GLU	3.0
1	C	136	ASN	3.0
1	O	98	ARG	2.9
1	O	120	ARG	2.9
1	O	136	ASN	2.9
1	O	21	ILE	2.9
1	O	47	CYS	2.9
1	O	73	PRO	2.9
1	O	105	MET	2.9
1	O	195	THR	2.9
1	O	215	THR	2.9
1	O	71	GLU	2.9
1	C	43	SER	2.9
1	O	75	THR	2.8
1	O	59	ASP	2.8
1	C	218	ARG	2.8
1	C	206	THR	2.8
1	C	130	MET	2.8
1	O	180	ASP	2.8
1	C	42	PRO	2.8
1	O	25	PRO	2.8
1	O	224	LEU	2.8
1	O	96	GLN	2.8
1	O	56	ASP	2.8
1	C	73	PRO	2.8
1	O	216	LEU	2.8
1	O	206	THR	2.8
1	O	64	LEU	2.7
1	C	222	ILE	2.7
1	O	176	THR	2.7
1	O	32	LEU	2.7
1	C	127	GLU	2.7
1	O	205	GLY	2.7
1	O	190	TRP	2.7
1	C	156	TYR	2.7
1	C	71	GLU	2.6
1	O	185	GLU	2.6
1	O	214	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	196	GLY	2.6
1	O	8	GLN	2.6
1	O	154	ALA	2.6
1	C	221	GLY	2.6
1	O	172	ILE	2.6
1	O	222	ILE	2.6
1	O	11	THR	2.6
1	O	223	LEU	2.6
1	O	52	ILE	2.6
1	O	41	LEU	2.5
1	C	36	ASN	2.5
1	C	193	ALA	2.5
1	O	86	ALA	2.5
1	C	111	LYS	2.5
1	O	13	MET	2.5
1	O	80	SER	2.5
1	O	77	PHE	2.5
1	C	8	GLN	2.5
1	C	132	VAL	2.5
1	O	63	ASP	2.5
1	O	66	GLN	2.5
1	C	22	PHE	2.5
1	C	105	MET	2.5
1	C	38	SER	2.5
1	C	141	SER	2.5
1	C	66	GLN	2.4
1	O	69	GLN	2.4
1	O	55	GLU	2.4
1	O	87	PHE	2.4
1	O	81	ALA	2.4
1	O	188	ALA	2.4
1	O	65	ILE	2.4
1	C	37	LEU	2.4
1	C	77	PHE	2.4
1	C	101	GLN	2.4
1	O	149	LYS	2.4
1	O	31	GLY	2.4
1	C	41	LEU	2.4
1	C	223	LEU	2.4
1	O	54	GLU	2.4
1	O	102	ARG	2.4
1	O	83	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	171	ASP	2.3
1	O	197	ALA	2.3
1	C	49	PHE	2.3
1	O	204	PHE	2.3
1	C	21	ILE	2.3
1	O	104	ILE	2.3
1	C	168	VAL	2.3
1	C	16	ASP	2.3
1	O	50	ASP	2.3
1	O	91	LYS	2.3
1	O	92	LYS	2.3
1	O	165	THR	2.3
1	C	104	ILE	2.3
1	O	164	SER	2.3
1	O	60	ARG	2.3
1	C	90	ALA	2.3
1	O	193	ALA	2.3
1	C	216	LEU	2.3
1	C	24	PHE	2.3
1	O	40	ARG	2.3
1	C	163	ILE	2.3
1	O	114	VAL	2.3
1	C	76	LEU	2.2
1	O	16	ASP	2.2
1	O	22	PHE	2.2
1	O	78	GLY	2.2
1	O	113	GLY	2.2
1	O	217	ASP	2.2
1	C	148	LEU	2.2
1	C	212	GLN	2.2
1	O	121	THR	2.2
1	C	45	LYS	2.2
1	C	160	VAL	2.2
1	O	100	VAL	2.2
1	C	48	ALA	2.2
1	C	63	ASP	2.2
1	C	170	ALA	2.2
1	O	194	THR	2.2
1	C	84	SER	2.2
1	O	9	ASP	2.1
1	C	69	GLN	2.1
1	O	15	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	60	ARG	2.1
1	C	203	GLY	2.1
1	O	221	GLY	2.1
1	C	162	LEU	2.1
1	O	61	TYR	2.1
1	O	159	TYR	2.1
1	O	27	VAL	2.1
1	C	217	ASP	2.1
1	O	33	MET	2.1
1	O	124	SER	2.1
1	C	85	LEU	2.1
1	O	85	LEU	2.1
1	C	65	ILE	2.1
1	O	30	TYR	2.1
1	C	72	GLY	2.0
1	O	210	MET	2.0
1	C	58	LEU	2.0
1	O	152	THR	2.0
1	C	190	TRP	2.0
1	C	226	PHE	2.0
1	O	155	PHE	2.0
1	O	160	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	C	502	5/5	0.69	0.36	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	O	501	5/5	0.85	0.37	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.