Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 12:10 pm BST

PDB ID	:	3C07
Title	:	Crystal structure of a TetR family transcriptional regulator from Streptomyces coelicolor A3(2)
Authors	:	Tan, K.; Xu, X.; Zheng, H.; Savchenko, A.; Edwards, A.M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2008-01-18
Resolution	:	2.70 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:

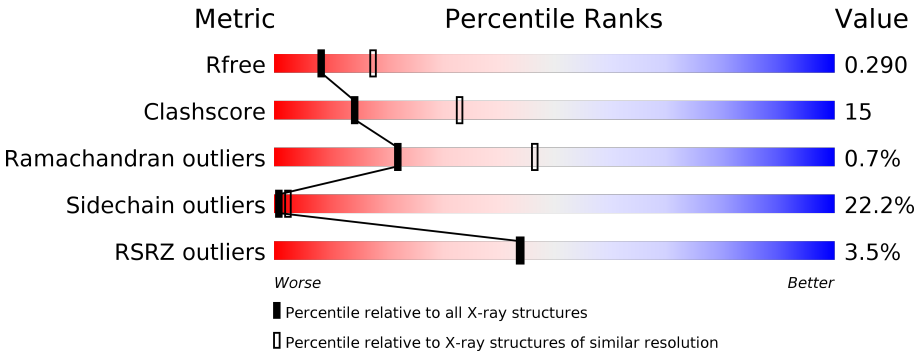
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	273	3% 52% 21% 8% 19%
1	B	273	3% 44% 26% 9% 22%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3529 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 Putative tetR-family transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	Se	0	0	0
			1781	1136	323	317	5			
1	B	214	Total	C	N	O	Se	0	0	0
			1733	1106	315	308	4			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MSE	-	EXPRESSION TAG	UNP Q9KZ96
A	-20	GLY	-	EXPRESSION TAG	UNP Q9KZ96
A	-19	SER	-	EXPRESSION TAG	UNP Q9KZ96
A	-18	SER	-	EXPRESSION TAG	UNP Q9KZ96
A	-17	HIS	-	EXPRESSION TAG	UNP Q9KZ96
A	-16	HIS	-	EXPRESSION TAG	UNP Q9KZ96
A	-15	HIS	-	EXPRESSION TAG	UNP Q9KZ96
A	-14	HIS	-	EXPRESSION TAG	UNP Q9KZ96
A	-13	HIS	-	EXPRESSION TAG	UNP Q9KZ96
A	-12	HIS	-	EXPRESSION TAG	UNP Q9KZ96
A	-11	SER	-	EXPRESSION TAG	UNP Q9KZ96
A	-10	SER	-	EXPRESSION TAG	UNP Q9KZ96
A	-9	GLY	-	EXPRESSION TAG	UNP Q9KZ96
A	-8	ARG	-	EXPRESSION TAG	UNP Q9KZ96
A	-7	GLU	-	EXPRESSION TAG	UNP Q9KZ96
A	-6	ASN	-	EXPRESSION TAG	UNP Q9KZ96
A	-5	LEU	-	EXPRESSION TAG	UNP Q9KZ96
A	-4	TYR	-	EXPRESSION TAG	UNP Q9KZ96
A	-3	PHE	-	EXPRESSION TAG	UNP Q9KZ96
A	-2	GLN	-	EXPRESSION TAG	UNP Q9KZ96
A	-1	GLY	-	EXPRESSION TAG	UNP Q9KZ96
A	0	HIS	-	EXPRESSION TAG	UNP Q9KZ96
B	-21	MSE	-	EXPRESSION TAG	UNP Q9KZ96
B	-20	GLY	-	EXPRESSION TAG	UNP Q9KZ96
B	-19	SER	-	EXPRESSION TAG	UNP Q9KZ96

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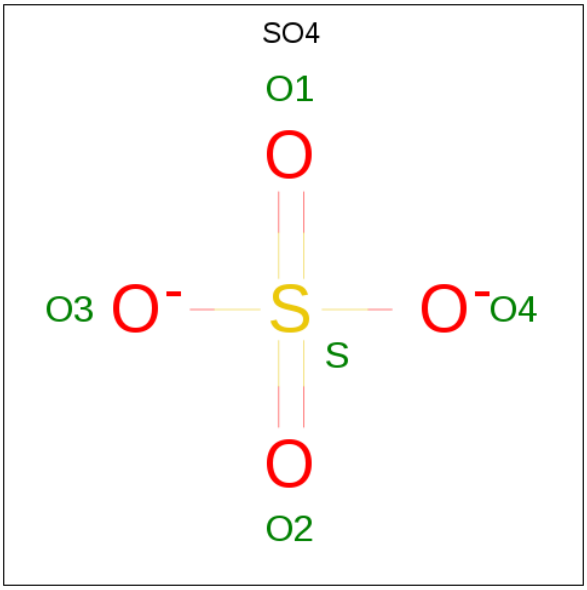
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	SER	-	EXPRESSION TAG	UNP Q9KZ96
B	-17	HIS	-	EXPRESSION TAG	UNP Q9KZ96
B	-16	HIS	-	EXPRESSION TAG	UNP Q9KZ96
B	-15	HIS	-	EXPRESSION TAG	UNP Q9KZ96
B	-14	HIS	-	EXPRESSION TAG	UNP Q9KZ96
B	-13	HIS	-	EXPRESSION TAG	UNP Q9KZ96
B	-12	HIS	-	EXPRESSION TAG	UNP Q9KZ96
B	-11	SER	-	EXPRESSION TAG	UNP Q9KZ96
B	-10	SER	-	EXPRESSION TAG	UNP Q9KZ96
B	-9	GLY	-	EXPRESSION TAG	UNP Q9KZ96
B	-8	ARG	-	EXPRESSION TAG	UNP Q9KZ96
B	-7	GLU	-	EXPRESSION TAG	UNP Q9KZ96
B	-6	ASN	-	EXPRESSION TAG	UNP Q9KZ96
B	-5	LEU	-	EXPRESSION TAG	UNP Q9KZ96
B	-4	TYR	-	EXPRESSION TAG	UNP Q9KZ96
B	-3	PHE	-	EXPRESSION TAG	UNP Q9KZ96
B	-2	GLN	-	EXPRESSION TAG	UNP Q9KZ96
B	-1	GLY	-	EXPRESSION TAG	UNP Q9KZ96
B	0	HIS	-	EXPRESSION TAG	UNP Q9KZ96

- 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

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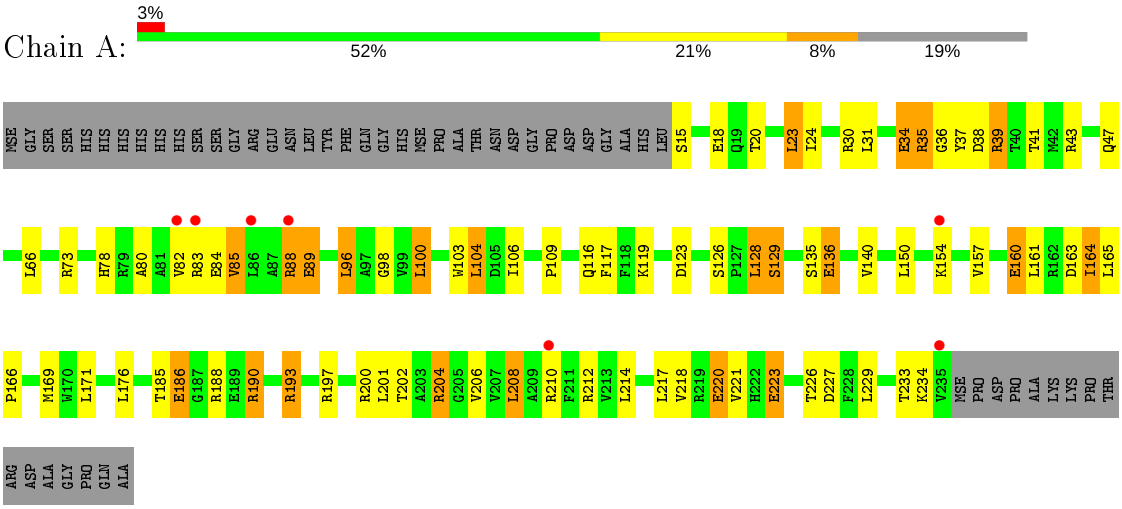
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

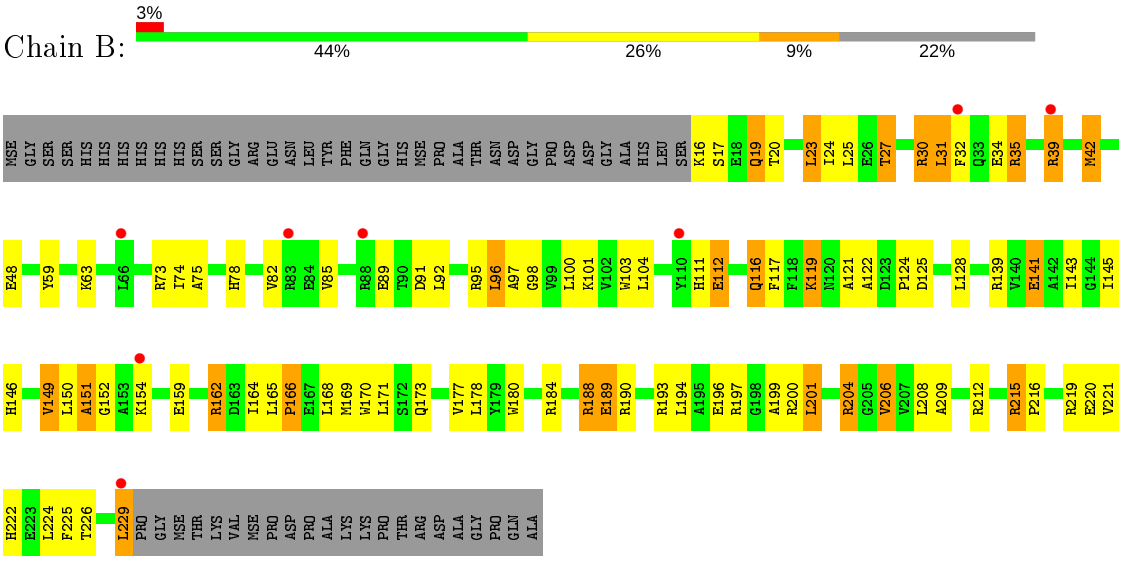
- Molecule 1: Putative tetR-family transcriptional regulator

Chain A:



- Molecule 1: Putative tetR-family transcriptional regulator

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	74.95Å 74.95Å 208.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.25 – 2.70 47.22 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.25-2.70) 99.4 (47.22-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.218 , 0.289 0.215 , 0.290	Depositor DCC
R_{free} test set	854 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	77.6	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 78.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3529	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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: 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	0.95	3/1815 (0.2%)	0.94	2/2446 (0.1%)
1	B	0.83	0/1767	0.93	3/2383 (0.1%)
All	All	0.89	3/3582 (0.1%)	0.93	5/4829 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	GLU	CG-CD	5.61	1.60	1.51
1	A	223	GLU	CD-OE2	5.15	1.31	1.25
1	A	117	PHE	CE2-CZ	5.04	1.47	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	229	LEU	CA-CB-CG	5.83	128.71	115.30
1	B	215	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	23	LEU	CA-CB-CG	5.21	127.28	115.30
1	B	215	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	188	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1781	0	1787	53	0
1	B	1733	0	1734	66	0
2	A	10	0	0	0	0
2	B	5	0	0	1	0
All	All	3529	0	3521	109	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 15.

All (109) 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:B:162:ARG:HH11	1:B:162:ARG:HG2	1.20	1.05
1:A:164:ILE:HD11	1:A:218:VAL:HG12	1.50	0.92
1:A:36:GLY:HA3	1:A:39:ARG:HH12	1.36	0.89
1:B:139:ARG:O	1:B:143:ILE:HG12	1.74	0.88
1:A:96:LEU:CD2	1:A:100:LEU:HD22	2.11	0.80
1:A:165:LEU:HB3	1:A:169:MSE:HE3	1.62	0.80
1:B:122:ALA:O	1:B:124:PRO:HD3	1.84	0.77
1:A:150:LEU:HD11	1:A:169:MSE:HE1	1.66	0.77
1:A:119:LYS:HD2	1:B:119:LYS:HB2	1.67	0.76
1:A:104:LEU:HD21	1:A:176:LEU:HD21	1.68	0.75
1:A:89:GLU:OE2	1:A:89:GLU:HA	1.86	0.75
1:B:30:ARG:O	1:B:34:GLU:HG2	1.86	0.75
1:B:39:ARG:HH11	1:B:39:ARG:HB3	1.54	0.73
1:B:162:ARG:HH11	1:B:162:ARG:CG	2.00	0.73
1:A:96:LEU:HD22	1:A:100:LEU:HD22	1.71	0.71
1:A:35:ARG:O	1:A:39:ARG:NH1	2.23	0.71
1:B:193:ARG:NH2	2:B:252:SO4:O3	2.24	0.71
1:A:165:LEU:HB3	1:A:169:MSE:CE	2.22	0.70
1:A:85:VAL:HG11	1:A:98:GLY:HA3	1.74	0.69
1:B:146:HIS:HA	1:B:149:VAL:CG1	2.23	0.68
1:B:92:LEU:HD11	1:B:169:MSE:HE1	1.74	0.68
1:B:145:ILE:O	1:B:149:VAL:HG12	1.95	0.66
1:B:215:ARG:N	1:B:216:PRO:HD2	2.10	0.66
1:B:164:ILE:HD13	1:B:222:HIS:HA	1.76	0.66
1:A:223:GLU:HA	1:A:226:THR:HG22	1.79	0.65
1:B:146:HIS:HA	1:B:149:VAL:HG13	1.79	0.65
1:A:227:ASP:OD2	1:B:197:ARG:NH2	2.29	0.65
1:B:89:GLU:O	1:B:95:ARG:HD3	1.98	0.64
1:B:117:PHE:CE1	1:B:121:ALA:HB2	2.33	0.63
1:A:150:LEU:HD22	1:A:157:VAL:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LYS:HE3	1:B:196:GLU:HG3	1.81	0.63
1:B:97:ALA:O	1:B:101:LYS:HG2	1.99	0.63
1:B:35:ARG:NE	1:B:35:ARG:HA	2.14	0.62
1:B:150:LEU:HD12	1:B:151:ALA:H	1.68	0.58
1:B:150:LEU:HD12	1:B:151:ALA:N	2.17	0.58
1:B:111:HIS:HE1	1:B:180:TRP:O	1.86	0.56
1:B:162:ARG:NH1	1:B:162:ARG:HG2	2.01	0.56
1:A:100:LEU:O	1:A:103:TRP:HB3	2.06	0.56
1:A:104:LEU:CD2	1:A:176:LEU:HD21	2.36	0.55
1:B:23:LEU:O	1:B:27:THR:HG22	2.07	0.55
1:A:123:ASP:OD1	1:B:184:ARG:NH2	2.40	0.54
1:B:35:ARG:HE	1:B:35:ARG:HA	1.72	0.54
1:A:217:LEU:O	1:A:221:VAL:HG23	2.09	0.53
1:B:42:MSE:HA	1:B:42:MSE:HE3	1.89	0.53
1:A:201:LEU:HD12	1:B:221:VAL:HG12	1.89	0.53
1:B:139:ARG:HH11	1:B:139:ARG:HG3	1.74	0.53
1:A:20:THR:O	1:A:24:ILE:HG12	2.09	0.52
1:A:220:GLU:HG2	1:B:201:LEU:HD23	1.91	0.52
1:A:78:HIS:O	1:A:82:VAL:HG13	2.09	0.52
1:B:85:VAL:HG11	1:B:98:GLY:HA3	1.91	0.52
1:B:96:LEU:HG	1:B:169:MSE:HE2	1.91	0.51
1:A:37:TYR:CZ	1:A:128:LEU:HD21	2.45	0.51
1:B:206:VAL:O	1:B:209:ALA:HB3	2.11	0.51
1:A:136:GLU:O	1:A:140:VAL:HG23	2.11	0.51
1:A:80:ALA:O	1:A:83:ARG:HG3	2.10	0.50
1:A:135:SER:O	1:A:136:GLU:C	2.47	0.50
1:A:126:SER:OG	1:A:128:LEU:HB2	2.11	0.50
1:A:193:ARG:HG2	1:A:197:ARG:HH21	1.76	0.50
1:B:78:HIS:CD2	1:B:103:TRP:HD1	2.30	0.49
1:B:75:ALA:O	1:B:78:HIS:HB3	2.12	0.49
1:B:139:ARG:HG3	1:B:139:ARG:NH1	2.27	0.49
1:A:39:ARG:HH11	1:A:39:ARG:HG2	1.77	0.48
1:A:88:ARG:HB3	1:A:88:ARG:NH2	2.29	0.48
1:B:78:HIS:O	1:B:82:VAL:HG13	2.12	0.48
1:A:150:LEU:HD11	1:A:169:MSE:CE	2.42	0.48
1:A:201:LEU:CD1	1:B:221:VAL:HG12	2.44	0.47
1:B:91:ASP:O	1:B:95:ARG:HG2	2.14	0.47
1:A:128:LEU:HD12	1:A:128:LEU:HA	1.70	0.47
1:A:185:THR:HG21	1:A:190:ARG:HB2	1.96	0.47
1:A:202:THR:O	1:A:206:VAL:HG13	2.15	0.47
1:A:106:ILE:O	1:A:109:PRO:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HD12	1:A:166:PRO:HG3	1.96	0.47
1:B:200:ARG:HD2	1:B:204:ARG:CZ	2.45	0.47
1:B:116:GLN:O	1:B:119:LYS:HD3	2.15	0.47
1:B:222:HIS:O	1:B:226:THR:HG23	2.15	0.47
1:B:204:ARG:O	1:B:208:LEU:HD12	2.15	0.46
1:B:39:ARG:NH1	1:B:39:ARG:HB3	2.26	0.46
1:B:17:SER:HB3	1:B:59:TYR:HE2	1.80	0.46
1:B:24:ILE:HA	1:B:27:THR:HG23	1.97	0.46
1:A:39:ARG:NH1	1:A:39:ARG:HG2	2.31	0.46
1:B:180:TRP:CD1	1:B:188:ARG:HG2	2.51	0.46
1:B:150:LEU:O	1:B:152:GLY:N	2.49	0.45
1:B:165:LEU:O	1:B:166:PRO:C	2.55	0.45
1:B:16:LYS:O	1:B:19:GLN:N	2.46	0.45
1:A:123:ASP:CG	1:B:184:ARG:HH22	2.20	0.45
1:B:112:GLU:H	1:B:112:GLU:HG2	1.53	0.44
1:A:119:LYS:HD2	1:B:119:LYS:CB	2.45	0.44
1:B:96:LEU:HD13	1:B:199:ALA:HA	2.00	0.44
1:A:204:ARG:O	1:A:208:LEU:HB2	2.17	0.43
1:A:212:ARG:HB3	1:A:212:ARG:NH1	2.33	0.43
1:B:27:THR:O	1:B:31:LEU:HB2	2.19	0.43
1:A:15:SER:HA	1:A:18:GLU:OE1	2.18	0.43
1:B:200:ARG:HD2	1:B:204:ARG:NH2	2.34	0.43
1:B:173:GLN:O	1:B:177:VAL:HG23	2.18	0.43
1:A:37:TYR:CE2	1:A:128:LEU:HD21	2.54	0.43
1:B:188:ARG:O	1:B:189:GLU:C	2.56	0.43
1:A:126:SER:O	1:A:129:SER:HB3	2.20	0.42
1:A:30:ARG:O	1:A:34:GLU:HG3	2.19	0.42
1:B:141:GLU:HA	1:B:141:GLU:OE2	2.18	0.42
1:A:88:ARG:NH2	1:A:89:GLU:OE1	2.53	0.42
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.75	0.42
1:B:215:ARG:N	1:B:216:PRO:CD	2.81	0.42
1:A:96:LEU:HD22	1:A:100:LEU:CD2	2.46	0.42
1:B:178:LEU:HD12	1:B:178:LEU:HA	1.82	0.41
1:B:143:ILE:HD13	1:B:170:TRP:CG	2.56	0.41
1:B:171:LEU:HD23	1:B:171:LEU:HA	1.88	0.41
1:A:204:ARG:NH2	1:B:220:GLU:OE1	2.54	0.40
1:A:217:LEU:HB2	1:B:208:LEU:HD13	2.03	0.40
1:A:37:TYR:O	1:A:38:ASP:C	2.57	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	219/273 (80%)	208 (95%)	10 (5%)	1 (0%)	29 54
1	B	212/273 (78%)	189 (89%)	21 (10%)	2 (1%)	17 40
All	All	431/546 (79%)	397 (92%)	31 (7%)	3 (1%)	22 46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLU
1	B	151	ALA
1	B	166	PRO

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	181/214 (85%)	143 (79%)	38 (21%)	1 3
1	B	175/214 (82%)	134 (77%)	41 (23%)	1 2
All	All	356/428 (83%)	277 (78%)	79 (22%)	1 2

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	34	GLU
1	A	35	ARG

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Mol	Chain	Res	Type
1	A	39	ARG
1	A	41	THR
1	A	43	ARG
1	A	47	GLN
1	A	66	LEU
1	A	73	ARG
1	A	84	GLU
1	A	85	VAL
1	A	88	ARG
1	A	89	GLU
1	A	96	LEU
1	A	100	LEU
1	A	104	LEU
1	A	116	GLN
1	A	128	LEU
1	A	129	SER
1	A	136	GLU
1	A	154	LYS
1	A	160	GLU
1	A	161	LEU
1	A	163	ASP
1	A	164	ILE
1	A	171	LEU
1	A	186	GLU
1	A	190	ARG
1	A	193	ARG
1	A	200	ARG
1	A	204	ARG
1	A	208	LEU
1	A	210	ARG
1	A	214	LEU
1	A	220	GLU
1	A	229	LEU
1	A	233	THR
1	A	234	LYS
1	B	19	GLN
1	B	20	THR
1	B	23	LEU
1	B	25	LEU
1	B	27	THR
1	B	30	ARG
1	B	31	LEU

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Mol	Chain	Res	Type
1	B	32	PHE
1	B	35	ARG
1	B	39	ARG
1	B	42	MSE
1	B	48	GLU
1	B	63	LYS
1	B	73	ARG
1	B	74	ILE
1	B	96	LEU
1	B	100	LEU
1	B	104	LEU
1	B	112	GLU
1	B	116	GLN
1	B	119	LYS
1	B	125	ASP
1	B	128	LEU
1	B	141	GLU
1	B	149	VAL
1	B	154	LYS
1	B	159	GLU
1	B	162	ARG
1	B	168	LEU
1	B	188	ARG
1	B	189	GLU
1	B	190	ARG
1	B	194	LEU
1	B	201	LEU
1	B	204	ARG
1	B	206	VAL
1	B	212	ARG
1	B	219	ARG
1	B	224	LEU
1	B	225	PHE
1	B	229	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	78	HIS
1	B	111	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 carbohydrates in this entry.

5.6 Ligand geometry

3 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	A	253	-	4,4,4	0.27	0	6,6,6	0.30	0
2	SO4	B	252	-	4,4,4	0.32	0	6,6,6	1.13	1 (16%)
2	SO4	A	252	-	4,4,4	0.17	0	6,6,6	0.18	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	252	SO4	O4-S-O3	2.06	117.86	109.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	252	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	216/273 (79%)	0.26	7 (3%) 47 48	59, 70, 82, 92	0
1	B	210/273 (76%)	0.31	8 (3%) 40 39	56, 72, 85, 93	0
All	All	426/546 (78%)	0.29	15 (3%) 44 44	56, 71, 84, 93	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	ARG	4.3
1	B	229	LEU	3.2
1	B	83	ARG	3.0
1	B	39	ARG	2.9
1	B	154	LYS	2.8
1	A	86	LEU	2.8
1	A	82	VAL	2.6
1	A	235	VAL	2.6
1	A	154	LYS	2.4
1	B	32	PHE	2.4
1	B	110	TYR	2.4
1	A	210	ARG	2.3
1	B	66	LEU	2.3
1	A	88	ARG	2.3
1	A	83	ARG	2.1

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

There are no carbohydrates in this entry.

6.4 Ligands

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	A	253	5/5	0.79	0.35	75,77,77,77	5
2	SO4	B	252	5/5	0.90	0.16	79,79,80,81	5
2	SO4	A	252	5/5	0.93	0.42	82,82,83,83	5

6.5 Other polymers

There are no such residues in this entry.