



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:02 am GMT

PDB ID : 5ICR
Title : 2.25 Angstrom Resolution Crystal Structure of Fatty-Acid-CoA Ligase (FadD32) from Mycobacterium smegmatis in complex with Inhibitor 5'-O-[(11-phenoxyundecanoyl)sulfamoyl]adenosine.
Authors : Minasov, G.; Shuvalova, L.; Hung, D.; Fisher, S.L.; Edelstein, J.; Kiryukhina, O.; Dubrovskaya, I.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2016-02-23
Resolution : 2.25 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

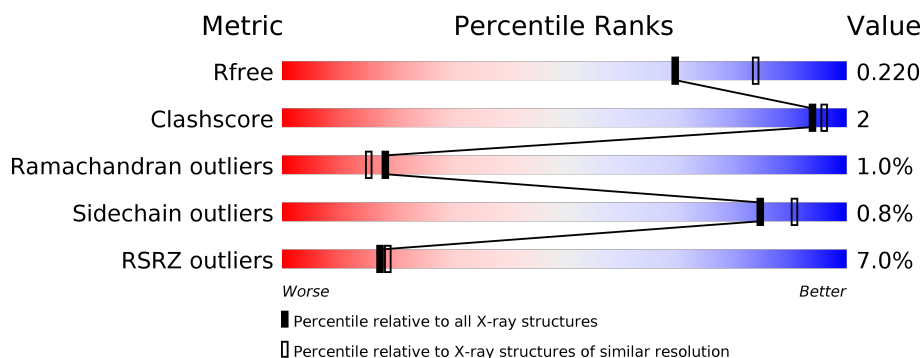
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	100719	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	650	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>• • 7%</div> </div> </div>
1	B	650	<div> <div>7%</div> <div> <div></div> <div>90%</div> <div>• 6%</div> </div> </div>
1	C	650	<div> <div>6%</div> <div> <div></div> <div>91%</div> <div>• 5%</div> </div> </div>
1	D	650	<div> <div>9%</div> <div> <div></div> <div>86%</div> <div>7% 6%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	702	-	-	-	X
3	SO4	A	703	-	-	-	X
3	SO4	B	703	-	-	-	X
3	SO4	C	702	-	-	-	X
3	SO4	D	702	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20342 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 Acyl-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	14	0
			4782	3012	851	911	8			
1	B	609	Total	C	N	O	S	0	1	0
			4680	2957	829	887	7			
1	C	618	Total	C	N	O	S	0	4	0
			4768	3003	849	908	8			
1	D	609	Total	C	N	O	S	0	8	0
			4732	2989	839	897	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0R618
A	-18	GLY	-	expression tag	UNP A0R618
A	-17	SER	-	expression tag	UNP A0R618
A	-16	SER	-	expression tag	UNP A0R618
A	-15	HIS	-	expression tag	UNP A0R618
A	-14	HIS	-	expression tag	UNP A0R618
A	-13	HIS	-	expression tag	UNP A0R618
A	-12	HIS	-	expression tag	UNP A0R618
A	-11	HIS	-	expression tag	UNP A0R618
A	-10	HIS	-	expression tag	UNP A0R618
A	-9	SER	-	expression tag	UNP A0R618
A	-8	SER	-	expression tag	UNP A0R618
A	-7	GLY	-	expression tag	UNP A0R618
A	-6	LEU	-	expression tag	UNP A0R618
A	-5	VAL	-	expression tag	UNP A0R618
A	-4	PRO	-	expression tag	UNP A0R618
A	-3	ARG	-	expression tag	UNP A0R618
A	-2	GLY	-	expression tag	UNP A0R618
A	-1	SER	-	expression tag	UNP A0R618
A	0	HIS	-	expression tag	UNP A0R618
B	-19	MET	-	initiating methionine	UNP A0R618

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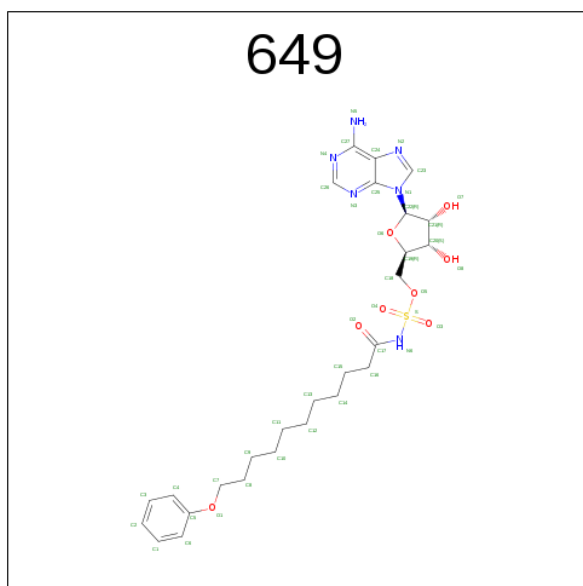
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A0R618
B	-17	SER	-	expression tag	UNP A0R618
B	-16	SER	-	expression tag	UNP A0R618
B	-15	HIS	-	expression tag	UNP A0R618
B	-14	HIS	-	expression tag	UNP A0R618
B	-13	HIS	-	expression tag	UNP A0R618
B	-12	HIS	-	expression tag	UNP A0R618
B	-11	HIS	-	expression tag	UNP A0R618
B	-10	HIS	-	expression tag	UNP A0R618
B	-9	SER	-	expression tag	UNP A0R618
B	-8	SER	-	expression tag	UNP A0R618
B	-7	GLY	-	expression tag	UNP A0R618
B	-6	LEU	-	expression tag	UNP A0R618
B	-5	VAL	-	expression tag	UNP A0R618
B	-4	PRO	-	expression tag	UNP A0R618
B	-3	ARG	-	expression tag	UNP A0R618
B	-2	GLY	-	expression tag	UNP A0R618
B	-1	SER	-	expression tag	UNP A0R618
B	0	HIS	-	expression tag	UNP A0R618
C	-19	MET	-	initiating methionine	UNP A0R618
C	-18	GLY	-	expression tag	UNP A0R618
C	-17	SER	-	expression tag	UNP A0R618
C	-16	SER	-	expression tag	UNP A0R618
C	-15	HIS	-	expression tag	UNP A0R618
C	-14	HIS	-	expression tag	UNP A0R618
C	-13	HIS	-	expression tag	UNP A0R618
C	-12	HIS	-	expression tag	UNP A0R618
C	-11	HIS	-	expression tag	UNP A0R618
C	-10	HIS	-	expression tag	UNP A0R618
C	-9	SER	-	expression tag	UNP A0R618
C	-8	SER	-	expression tag	UNP A0R618
C	-7	GLY	-	expression tag	UNP A0R618
C	-6	LEU	-	expression tag	UNP A0R618
C	-5	VAL	-	expression tag	UNP A0R618
C	-4	PRO	-	expression tag	UNP A0R618
C	-3	ARG	-	expression tag	UNP A0R618
C	-2	GLY	-	expression tag	UNP A0R618
C	-1	SER	-	expression tag	UNP A0R618
C	0	HIS	-	expression tag	UNP A0R618
D	-19	MET	-	initiating methionine	UNP A0R618
D	-18	GLY	-	expression tag	UNP A0R618
D	-17	SER	-	expression tag	UNP A0R618

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A0R618
D	-15	HIS	-	expression tag	UNP A0R618
D	-14	HIS	-	expression tag	UNP A0R618
D	-13	HIS	-	expression tag	UNP A0R618
D	-12	HIS	-	expression tag	UNP A0R618
D	-11	HIS	-	expression tag	UNP A0R618
D	-10	HIS	-	expression tag	UNP A0R618
D	-9	SER	-	expression tag	UNP A0R618
D	-8	SER	-	expression tag	UNP A0R618
D	-7	GLY	-	expression tag	UNP A0R618
D	-6	LEU	-	expression tag	UNP A0R618
D	-5	VAL	-	expression tag	UNP A0R618
D	-4	PRO	-	expression tag	UNP A0R618
D	-3	ARG	-	expression tag	UNP A0R618
D	-2	GLY	-	expression tag	UNP A0R618
D	-1	SER	-	expression tag	UNP A0R618
D	0	HIS	-	expression tag	UNP A0R618

- Molecule 2 is 5'-O-[(11-phenoxyundecanoyl)sulfamoyl]adenosine (three-letter code: 649) (formula: C₂₇H₃₈N₆O₈S).



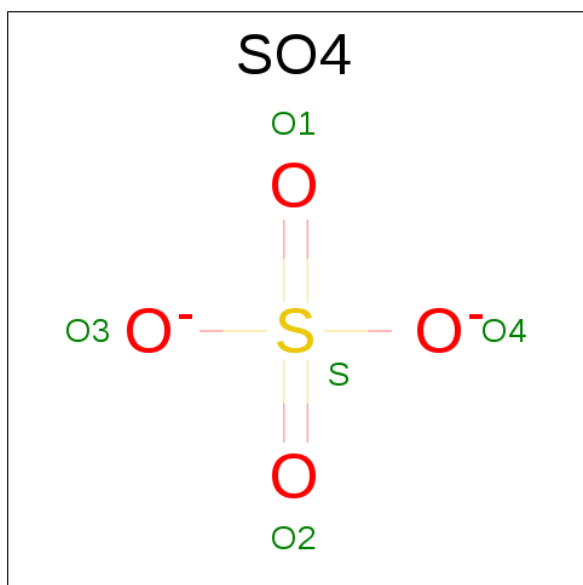
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			42	27	6	8	1		
2	B	1	Total	C	N	O	S	0	0
			42	27	6	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			42	27	6	8	1		
2	D	1	Total	C	N	O	S	0	0
			42	27	6	8	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



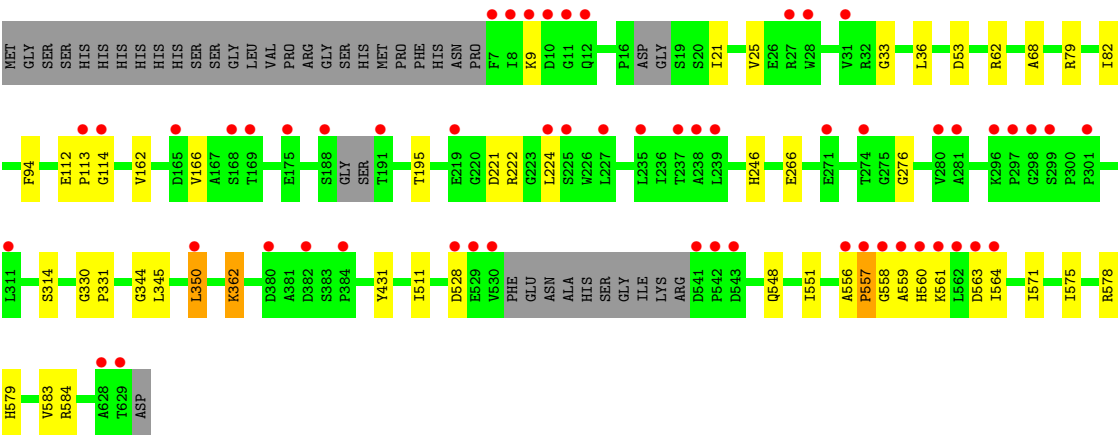
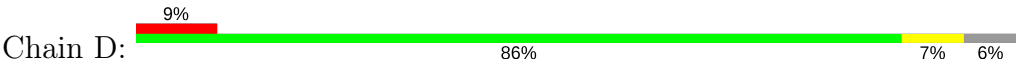
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	369	Total	O	0	22
			388	388		
6	B	241	Total	O	0	13
			252	252		
6	C	283	Total	O	0	12
			294	294		
6	D	232	Total	O	0	15
			246	246		



● Molecule 1: Acyl-CoA synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.29Å 153.56Å 201.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 2.25 29.86 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.86-2.25) 100.0 (29.86-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.47 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.173 , 0.219 0.178 , 0.220	Depositor DCC
R_{free} test set	6648 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20342	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.87% 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: 649, GOL, SO4, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.58	0/4894	0.79	2/6665 (0.0%)
1	B	0.55	0/4790	0.79	4/6529 (0.1%)
1	C	0.54	0/4877	0.76	2/6642 (0.0%)
1	D	0.54	0/4844	0.75	0/6601
All	All	0.55	0/19405	0.77	8/26437 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	605	ARG	NE-CZ-NH1	9.59	125.10	120.30
1	B	605	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	B	605	ARG	CG-CD-NE	6.99	126.48	111.80
1	C	192	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	B	605	ARG	CD-NE-CZ	5.26	130.96	123.60
1	A	405	ASP	N-CA-C	-5.23	96.88	111.00
1	A	18	GLY	N-CA-C	5.22	126.15	113.10
1	C	405	ASP	N-CA-C	-5.16	97.07	111.00

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	4782	0	4662	14	0
1	B	4680	0	4593	11	0
1	C	4768	0	4668	12	0
1	D	4732	0	4637	25	0
2	A	42	0	0	0	0
2	B	42	0	0	0	0
2	C	42	0	0	0	0
2	D	42	0	0	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	B	1	0	0	0	0
5	C	6	0	8	0	0
6	A	388	0	0	0	0
6	B	252	0	0	1	0
6	C	294	0	0	3	0
6	D	246	0	0	0	0
All	All	20342	0	18568	62	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 2.

All (62) 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:D:511:ILE:HD11	1:D:571:ILE:HD11	1.63	0.80
1:D:362[A]:LYS:HB2	1:D:362[A]:LYS:NZ	2.00	0.75
1:D:362[A]:LYS:HB2	1:D:362[A]:LYS:HZ3	1.55	0.69
1:C:317:ILE:HD13	1:C:341:PRO:HB3	1.76	0.68
1:A:555:ARG:NH1	1:A:562:LEU:O	2.27	0.66
1:D:36:LEU:HD11	1:D:53:ASP:HB3	1.80	0.63
1:D:564:ILE:HD12	1:D:564:ILE:H	1.64	0.63
1:C:555:ARG:NH1	1:C:562:LEU:O	2.33	0.61
1:C:31:VAL:HG23	1:C:32:ARG:HG3	1.86	0.56
1:B:28[A]:TRP:NE1	6:B:801[A]:HOH:O	1.98	0.55
1:A:15:PHE:O	1:A:16:PRO:C	2.46	0.54
1:D:68:ALA:HB3	1:D:166:VAL:HG12	1.90	0.54
1:B:375:ARG:NE	1:B:416:GLN:OE1	2.41	0.53
1:C:483:ARG:NH2	6:C:801:HOH:O	2.39	0.53
1:B:165:ASP:OD1	1:B:165:ASP:N	2.36	0.53
1:A:444:ASN:ND2	1:A:466[B]:ARG:HG3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ILE:HD13	1:B:341:PRO:HB3	1.92	0.51
1:A:240:LEU:C	1:A:240:LEU:HD12	2.31	0.50
1:D:564:ILE:HD12	1:D:564:ILE:N	2.26	0.50
1:C:222:ARG:NH2	1:C:270:LYS:HD3	2.28	0.49
1:D:578:ARG:HG3	1:D:579:HIS:CD2	2.48	0.48
1:A:452[B]:PRO:O	1:A:453[B]:SER:HB3	2.13	0.48
1:A:16:PRO:HA	1:A:18:GLY:N	2.28	0.48
1:D:557:PRO:HA	1:D:559:ALA:N	2.29	0.48
1:D:551:ILE:HD11	1:D:575:ILE:CD1	2.43	0.48
1:D:222:ARG:HB3	1:D:246:HIS:CD2	2.50	0.46
1:A:466[A]:ARG:O	1:A:466[A]:ARG:HG3	2.15	0.46
1:C:344:GLY:HA3	1:C:350:LEU:O	2.16	0.46
1:B:344:GLY:HA3	1:B:350:LEU:O	2.16	0.45
1:B:524:ASN:OD1	1:B:545:THR:HG22	2.16	0.45
1:C:375[B]:ARG:NE	1:C:416:GLN:HG2	2.32	0.45
1:D:221:ASP:HA	1:D:276:GLY:O	2.16	0.45
1:B:70:LEU:HD11	1:B:132:LEU:HD11	1.99	0.45
1:B:311:LEU:N	1:B:311:LEU:HD12	2.31	0.45
1:C:192:ARG:HH21	1:C:192:ARG:HG3	1.81	0.45
1:D:224:LEU:HD22	1:D:266:GLU:HB3	1.98	0.45
1:D:330:GLY:N	1:D:331:PRO:CD	2.80	0.44
1:C:224:LEU:HA	1:C:249:THR:O	2.17	0.44
1:D:62:ARG:NH1	1:D:162:VAL:O	2.50	0.44
1:A:450:THR:O	1:A:453[B]:SER:HB2	2.16	0.44
1:B:568:THR:HG23	1:B:586:VAL:HB	2.00	0.44
1:C:142:ARG:NH2	6:C:806:HOH:O	2.51	0.44
1:B:236:ILE:HB	1:B:350:LEU:HD22	2.00	0.44
1:A:330:GLY:N	1:A:331:PRO:CD	2.81	0.43
1:A:36:LEU:HD11	1:A:53:ASP:HB3	2.01	0.43
1:D:556:ALA:O	1:D:558:GLY:HA3	2.20	0.42
1:B:330:GLY:N	1:B:331:PRO:CD	2.83	0.42
1:D:82:ILE:HD11	1:D:94:PHE:HA	2.00	0.42
1:A:441:THR:O	1:A:465:VAL:HA	2.19	0.42
1:D:548:GLN:HB3	1:D:584:ARG:HG3	2.02	0.42
1:A:224:LEU:HA	1:A:249:THR:O	2.20	0.42
1:C:112:GLU:O	1:C:112:GLU:HG3	2.20	0.41
1:D:345:LEU:N	1:D:345:LEU:HD23	2.35	0.41
1:C:375[B]:ARG:NH2	6:C:803:HOH:O	2.46	0.41
1:D:564:ILE:CD1	1:D:564:ILE:H	2.33	0.41
1:D:195:THR:HB	1:D:431:TYR:CD1	2.56	0.41
1:D:21:ILE:O	1:D:25:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:GLY:HA3	1:D:350:LEU:O	2.21	0.41
1:A:578:ARG:HG3	1:A:579:HIS:CD2	2.56	0.40
1:D:112:GLU:HB3	1:D:113:PRO:HD2	2.04	0.40
1:A:344:GLY:HA3	1:A:350:LEU:O	2.21	0.40
1:D:551:ILE:HD12	1:D:583:VAL:HG21	2.02	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	613/650 (94%)	593 (97%)	10 (2%)	10 (2%)	11	7
1	B	602/650 (93%)	580 (96%)	18 (3%)	4 (1%)	25	25
1	C	614/650 (94%)	598 (97%)	13 (2%)	3 (0%)	32	33
1	D	609/650 (94%)	582 (96%)	19 (3%)	8 (1%)	14	9
All	All	2438/2600 (94%)	2353 (96%)	60 (2%)	25 (1%)	18	15

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLY
1	A	16	PRO
1	A	17	ASP
1	B	33	GLY
1	D	33	GLY
1	A	15	PHE
1	C	9	LYS
1	D	314	SER
1	D	561	LYS
1	D	563	ASP

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Mol	Chain	Res	Type
1	A	314	SER
1	B	45	THR
1	B	314	SER
1	C	314	SER
1	D	114	GLY
1	D	560	HIS
1	A	350	LEU
1	A	453[A]	SER
1	A	453[B]	SER
1	B	9	LYS
1	D	350	LEU
1	C	8	ILE
1	D	557	PRO
1	A	452[A]	PRO
1	A	452[B]	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	497/518 (96%)	494 (99%)	3 (1%)	89	93
1	B	486/518 (94%)	481 (99%)	5 (1%)	80	87
1	C	495/518 (96%)	492 (99%)	3 (1%)	89	93
1	D	491/518 (95%)	486 (99%)	5 (1%)	80	87
All	All	1969/2072 (95%)	1953 (99%)	16 (1%)	85	91

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ARG
1	A	451	ASN
1	A	524	ASN
1	B	79	ARG
1	B	165	ASP
1	B	416	GLN

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Mol	Chain	Res	Type
1	B	596	ARG
1	B	605	ARG
1	C	79	ARG
1	C	192	ARG
1	C	274	THR
1	D	9	LYS
1	D	79	ARG
1	D	362[A]	LYS
1	D	362[B]	LYS
1	D	528	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	649	A	701	-	42,45,45	1.86	5 (11%)	46,61,61	2.26	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	702	-	4,4,4	0.44	0	6,6,6	0.07	0
3	SO4	A	703	-	4,4,4	0.55	0	6,6,6	0.08	0
2	649	B	701	-	42,45,45	2.07	6 (14%)	46,61,61	2.04	6 (13%)
3	SO4	B	703	-	4,4,4	0.44	0	6,6,6	0.09	0
2	649	C	701	-	42,45,45	1.98	6 (14%)	46,61,61	1.94	7 (15%)
3	SO4	C	702	-	4,4,4	0.44	0	6,6,6	0.11	0
5	GOL	C	703	-	5,5,5	0.28	0	5,5,5	0.14	0
2	649	D	701	-	42,45,45	1.76	5 (11%)	46,61,61	1.91	5 (10%)
3	SO4	D	702	-	4,4,4	0.42	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	649	A	701	-	-	0/24/45/45	0/4/4/4
3	SO4	A	702	-	-	0/0/0/0	0/0/0/0
3	SO4	A	703	-	-	0/0/0/0	0/0/0/0
2	649	B	701	-	-	0/24/45/45	0/4/4/4
3	SO4	B	703	-	-	0/0/0/0	0/0/0/0
2	649	C	701	-	-	0/24/45/45	0/4/4/4
3	SO4	C	702	-	-	0/0/0/0	0/0/0/0
5	GOL	C	703	-	-	0/4/4/4	0/0/0/0
2	649	D	701	-	-	0/24/45/45	0/4/4/4
3	SO4	D	702	-	-	0/0/0/0	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	649	S-N6	-7.50	1.51	1.59
2	D	701	649	S-N6	-5.93	1.53	1.59
2	C	701	649	S-N6	-5.48	1.53	1.59
2	A	701	649	S-N6	-5.38	1.53	1.59
2	B	701	649	O5-S	-4.05	1.53	1.59
2	C	701	649	O5-S	-3.70	1.53	1.59
2	A	701	649	O5-S	-3.26	1.54	1.59
2	D	701	649	O5-S	-3.17	1.54	1.59
2	B	701	649	C17-N6	-2.67	1.33	1.38
2	C	701	649	C17-N6	-2.34	1.33	1.38
2	D	701	649	C17-N6	-2.23	1.34	1.38
2	A	701	649	C17-N6	-2.11	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	649	C26-N3	2.02	1.35	1.32
2	B	701	649	C26-N3	2.24	1.35	1.32
2	A	701	649	O4-S	5.39	1.46	1.42
2	D	701	649	O3-S	5.71	1.47	1.42
2	D	701	649	O4-S	5.73	1.47	1.42
2	B	701	649	O3-S	6.13	1.47	1.42
2	C	701	649	O4-S	6.14	1.47	1.42
2	B	701	649	O4-S	6.55	1.47	1.42
2	A	701	649	O3-S	7.58	1.48	1.42
2	C	701	649	O3-S	7.81	1.48	1.42

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	649	O4-S-O3	-9.94	111.14	121.30
2	B	701	649	O4-S-O3	-9.21	111.89	121.30
2	A	701	649	N3-C26-N4	-8.38	121.56	128.86
2	D	701	649	N3-C26-N4	-8.26	121.66	128.86
2	C	701	649	O4-S-O3	-8.04	113.09	121.30
2	B	701	649	N3-C26-N4	-7.19	122.60	128.86
2	C	701	649	N3-C26-N4	-7.05	122.72	128.86
2	D	701	649	O4-S-O3	-6.87	114.27	121.30
2	C	701	649	O3-S-N6	-2.38	105.14	108.47
2	B	701	649	C9-C8-C7	-2.03	104.34	113.48
2	A	701	649	O5-S-N6	2.01	110.61	106.34
2	C	701	649	C7-O1-C5	2.19	123.70	117.90
2	B	701	649	O5-S-N6	2.19	111.00	106.34
2	D	701	649	C7-O1-C5	2.30	123.98	117.90
2	C	701	649	O5-S-N6	2.51	111.67	106.34
2	D	701	649	O1-C7-C8	2.58	118.09	108.34
2	B	701	649	O1-C7-C8	2.65	118.33	108.34
2	A	701	649	O1-C7-C8	2.66	118.38	108.34
2	B	701	649	O2-C17-N6	2.88	123.44	121.56
2	C	701	649	O1-C7-C8	2.91	119.33	108.34
2	C	701	649	O2-C17-N6	2.94	123.48	121.56
2	A	701	649	C7-O1-C5	3.00	125.86	117.90
2	D	701	649	O2-C17-N6	3.50	123.85	121.56
2	A	701	649	O2-C17-N6	4.26	124.34	121.56

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	A	607/650 (93%)	-0.10	32 (5%)	27	31	20, 36, 74, 122	0
1	B	609/650 (93%)	0.02	44 (7%)	16	18	26, 45, 92, 133	0
1	C	618/650 (95%)	-0.04	39 (6%)	21	23	24, 45, 92, 124	0
1	D	609/650 (93%)	0.18	56 (9%)	10	10	26, 49, 93, 144	0
All	All	2443/2600 (93%)	0.02	171 (6%)	17	19	20, 44, 91, 144	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	8	ILE	7.7
1	D	559	ALA	6.9
1	A	8	ILE	5.6
1	A	630	ASP	5.5
1	D	562	LEU	5.5
1	C	9	LYS	5.3
1	A	17	ASP	5.3
1	D	560	HIS	5.2
1	C	193	ILE	5.0
1	D	191	THR	4.8
1	B	9	LYS	4.8
1	C	18	GLY	4.5
1	D	542	PRO	4.5
1	D	271	GLU	4.4
1	A	10	ASP	4.4
1	C	10	ASP	4.3
1	A	11	GLY	4.3
1	A	16	PRO	4.3
1	B	274	THR	4.3
1	C	630	ASP	4.3
1	D	28[A]	TRP	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	31	VAL	4.2
1	D	561	LYS	4.1
1	B	219	GLU	4.1
1	D	543	ASP	4.1
1	A	543	ASP	4.0
1	C	17	ASP	4.0
1	B	628	ALA	3.9
1	D	27	ARG	3.9
1	C	165	ASP	3.9
1	C	235	LEU	3.8
1	A	561	LYS	3.8
1	A	562	LEU	3.8
1	B	31	VAL	3.8
1	D	7	PHE	3.7
1	D	563	ASP	3.7
1	C	7	PHE	3.7
1	B	10	ASP	3.7
1	B	193	ILE	3.7
1	D	188	SER	3.6
1	B	115	HIS	3.6
1	D	219	GLU	3.5
1	B	239	LEU	3.5
1	C	236	ILE	3.5
1	D	530	VAL	3.5
1	B	28[A]	TRP	3.4
1	C	629	THR	3.4
1	A	542	PRO	3.4
1	B	557	PRO	3.4
1	D	10	ASP	3.4
1	B	301	PRO	3.4
1	D	274	THR	3.3
1	B	47	ARG	3.3
1	C	561	LYS	3.3
1	C	237	THR	3.3
1	C	47	ARG	3.3
1	B	238	ALA	3.2
1	A	236	ILE	3.2
1	B	564	ILE	3.2
1	C	239	LEU	3.2
1	D	558	GLY	3.2
1	D	238	ALA	3.2
1	B	17	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	271	GLU	3.1
1	B	16	PRO	3.1
1	A	219	GLU	3.1
1	D	299	SER	3.1
1	C	46	GLU	3.1
1	D	380	ASP	3.1
1	D	239	LEU	3.1
1	D	12	GLN	3.1
1	D	557	PRO	3.1
1	A	274	THR	3.0
1	C	238	ALA	3.0
1	B	235	LEU	3.0
1	A	18	GLY	3.0
1	D	564	ILE	2.9
1	B	271	GLU	2.9
1	D	297[A]	PRO	2.9
1	A	237	THR	2.9
1	B	27	ARG	2.9
1	C	240	LEU	2.9
1	A	528	ASP	2.9
1	D	556	ALA	2.8
1	B	234	GLY	2.8
1	D	298[A]	GLY	2.8
1	C	563	ASP	2.8
1	B	237	THR	2.8
1	D	280	VAL	2.8
1	A	563	ASP	2.7
1	B	18	GLY	2.7
1	A	193	ILE	2.7
1	D	384	PRO	2.7
1	C	562	LEU	2.7
1	D	629	THR	2.7
1	C	272	GLY	2.7
1	B	19	SER	2.7
1	B	297	PRO	2.7
1	C	628	ALA	2.7
1	A	382	ASP	2.7
1	B	491	ASP	2.7
1	C	15	PHE	2.7
1	A	567	ILE	2.7
1	C	16	PRO	2.6
1	B	242	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	244	ILE	2.6
1	A	298	GLY	2.6
1	A	529	GLU	2.6
1	C	19	SER	2.6
1	D	235	LEU	2.6
1	D	528	ASP	2.6
1	B	298	GLY	2.6
1	D	168	SER	2.6
1	D	350	LEU	2.5
1	B	11	GLY	2.5
1	A	350	LEU	2.5
1	C	31	VAL	2.5
1	A	27	ARG	2.5
1	D	175	GLU	2.5
1	D	225	SER	2.5
1	D	301	PRO	2.5
1	A	12	GLN	2.5
1	C	358	ALA	2.5
1	B	240	LEU	2.5
1	B	20	SER	2.4
1	A	297	PRO	2.4
1	B	14	LYS	2.4
1	A	238	ALA	2.4
1	B	46	GLU	2.4
1	C	557	PRO	2.4
1	C	45	THR	2.4
1	C	274	THR	2.4
1	B	460	ASP	2.4
1	A	239	LEU	2.3
1	D	224	LEU	2.3
1	D	382	ASP	2.3
1	B	539	LYS	2.3
1	B	542	PRO	2.3
1	D	628	ALA	2.3
1	D	296	LYS	2.3
1	B	243	MET	2.3
1	C	113	PRO	2.3
1	A	564	ILE	2.3
1	C	174	ASP	2.2
1	D	165	ASP	2.2
1	B	236	ILE	2.2
1	D	169	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	311	LEU	2.2
1	D	114	GLY	2.2
1	A	32	ARG	2.2
1	B	407	GLU	2.1
1	A	91	LEU	2.1
1	C	75	GLN	2.1
1	B	248	PHE	2.1
1	B	34	ASP	2.1
1	B	91	LEU	2.1
1	D	9	LYS	2.1
1	D	529	GLU	2.1
1	C	243[A]	MET	2.1
1	C	12	GLN	2.1
1	A	245	GLY	2.1
1	B	227	LEU	2.1
1	D	541	ASP	2.1
1	C	30	LYS	2.1
1	D	281	ALA	2.1
1	D	113	PRO	2.1
1	D	227	LEU	2.0
1	C	219	GLU	2.0
1	D	11	GLY	2.0
1	C	280	VAL	2.0
1	D	237	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	C	702	5/5	0.87	0.15	5.91	85,92,99,105	0
3	SO4	A	703	5/5	0.68	0.24	4.89	73,82,83,109	0
3	SO4	D	702	5/5	0.79	0.18	2.81	99,100,115,117	0
3	SO4	A	702	5/5	0.88	0.13	2.51	97,99,107,111	0
3	SO4	B	703	5/5	0.84	0.15	2.08	89,97,107,109	0
2	649	A	701	42/42	0.96	0.18	0.17	22,25,46,49	0
2	649	C	701	42/42	0.97	0.16	-0.11	27,31,61,64	0
2	649	B	701	42/42	0.96	0.16	-0.21	27,31,52,55	0
4	CL	B	702	1/1	0.87	0.15	-0.49	79,79,79,79	0
2	649	D	701	42/42	0.97	0.15	-0.59	29,40,58,64	0
5	GOL	C	703	6/6	0.88	0.12	-0.69	67,74,75,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.