



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:57 PM UTC

PDB ID : 6FWB / pdb_00006fwb
Title : Crystal structure of Mat2A at 1.79 Angstrom resolution
Authors : Zhou, A.; Wei, Z.; Bai, J.; Wang, H.
Deposited on : 2018-03-06
Resolution : 1.79 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

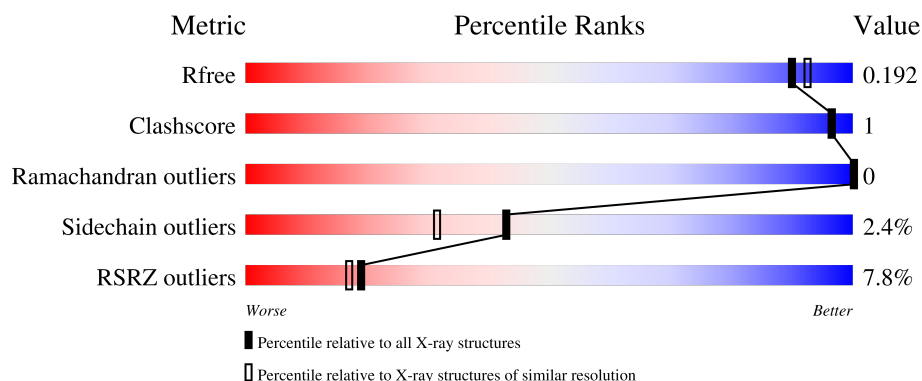
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	A	410	3% 86% 10%
1	B	410	5% 88% 9%
1	C	410	15% 85% 11%
1	D	410	5% 83% 6% 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12195 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 S-adenosylmethionine synthase isoform type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	373	Total	C	N	O	S	0	4	0
			2917	1843	506	555	13			
1	A	368	Total	C	N	O	S	0	2	0
			2862	1813	498	539	12			
1	C	364	Total	C	N	O	S	0	2	0
			2841	1797	499	534	11			
1	D	367	Total	C	N	O	S	0	1	0
			2855	1808	497	539	11			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP P31153
B	-14	ALA	-	expression tag	UNP P31153
B	-13	HIS	-	expression tag	UNP P31153
B	-12	HIS	-	expression tag	UNP P31153
B	-11	HIS	-	expression tag	UNP P31153
B	-10	HIS	-	expression tag	UNP P31153
B	-9	HIS	-	expression tag	UNP P31153
B	-8	HIS	-	expression tag	UNP P31153
B	-7	GLU	-	expression tag	UNP P31153
B	-6	ASN	-	expression tag	UNP P31153
B	-5	LEU	-	expression tag	UNP P31153
B	-4	TYR	-	expression tag	UNP P31153
B	-3	PHE	-	expression tag	UNP P31153
B	-2	GLN	-	expression tag	UNP P31153
B	-1	GLY	-	expression tag	UNP P31153
B	0	SER	-	expression tag	UNP P31153
A	-15	MET	-	initiating methionine	UNP P31153
A	-14	ALA	-	expression tag	UNP P31153
A	-13	HIS	-	expression tag	UNP P31153
A	-12	HIS	-	expression tag	UNP P31153
A	-11	HIS	-	expression tag	UNP P31153

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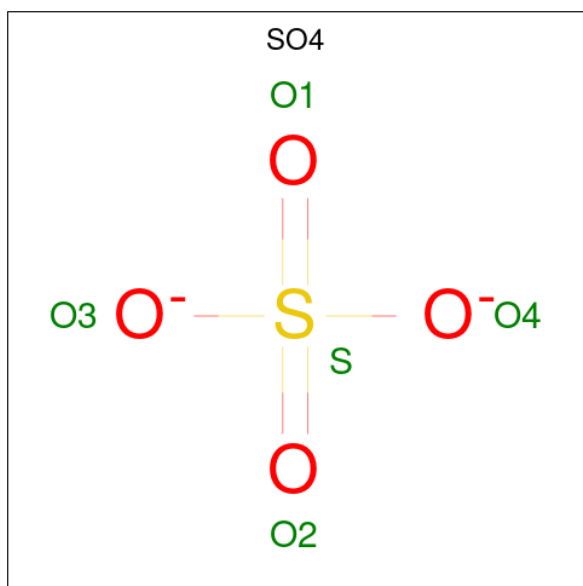
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	HIS	-	expression tag	UNP P31153
A	-9	HIS	-	expression tag	UNP P31153
A	-8	HIS	-	expression tag	UNP P31153
A	-7	GLU	-	expression tag	UNP P31153
A	-6	ASN	-	expression tag	UNP P31153
A	-5	LEU	-	expression tag	UNP P31153
A	-4	TYR	-	expression tag	UNP P31153
A	-3	PHE	-	expression tag	UNP P31153
A	-2	GLN	-	expression tag	UNP P31153
A	-1	GLY	-	expression tag	UNP P31153
A	0	SER	-	expression tag	UNP P31153
C	-15	MET	-	initiating methionine	UNP P31153
C	-14	ALA	-	expression tag	UNP P31153
C	-13	HIS	-	expression tag	UNP P31153
C	-12	HIS	-	expression tag	UNP P31153
C	-11	HIS	-	expression tag	UNP P31153
C	-10	HIS	-	expression tag	UNP P31153
C	-9	HIS	-	expression tag	UNP P31153
C	-8	HIS	-	expression tag	UNP P31153
C	-7	GLU	-	expression tag	UNP P31153
C	-6	ASN	-	expression tag	UNP P31153
C	-5	LEU	-	expression tag	UNP P31153
C	-4	TYR	-	expression tag	UNP P31153
C	-3	PHE	-	expression tag	UNP P31153
C	-2	GLN	-	expression tag	UNP P31153
C	-1	GLY	-	expression tag	UNP P31153
C	0	SER	-	expression tag	UNP P31153
D	-15	MET	-	initiating methionine	UNP P31153
D	-14	ALA	-	expression tag	UNP P31153
D	-13	HIS	-	expression tag	UNP P31153
D	-12	HIS	-	expression tag	UNP P31153
D	-11	HIS	-	expression tag	UNP P31153
D	-10	HIS	-	expression tag	UNP P31153
D	-9	HIS	-	expression tag	UNP P31153
D	-8	HIS	-	expression tag	UNP P31153
D	-7	GLU	-	expression tag	UNP P31153
D	-6	ASN	-	expression tag	UNP P31153
D	-5	LEU	-	expression tag	UNP P31153
D	-4	TYR	-	expression tag	UNP P31153
D	-3	PHE	-	expression tag	UNP P31153
D	-2	GLN	-	expression tag	UNP P31153
D	-1	GLY	-	expression tag	UNP P31153

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP P31153

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



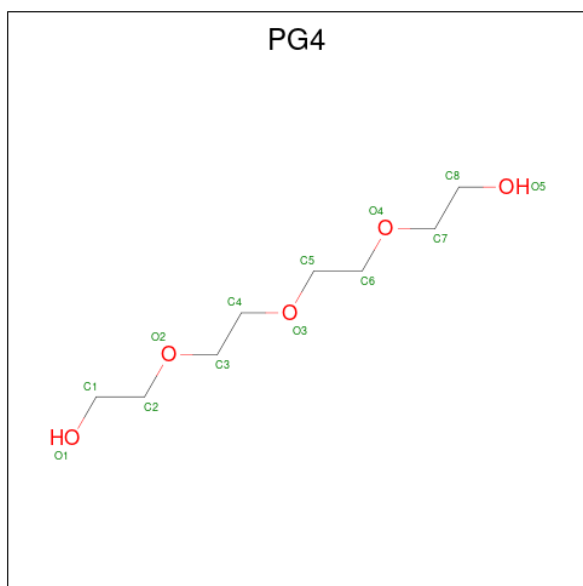
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	B	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	B	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	A	1	Total	O	S	0	0
			5	4	1		
			Total	O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

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

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			13	8	5		
3	A	1	Total	C	O	0	0
			13	8	5		

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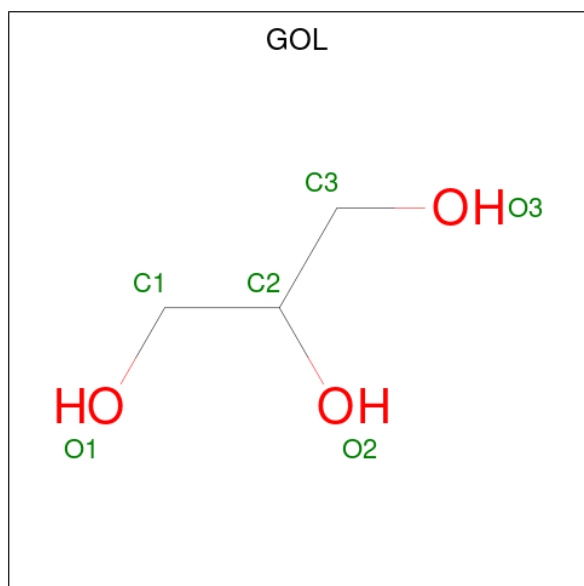
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	C	1	Total	C	O	0	0
			13	8	5		
3	D	1	Total	C	O	0	0
			13	8	5		
3	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is water.

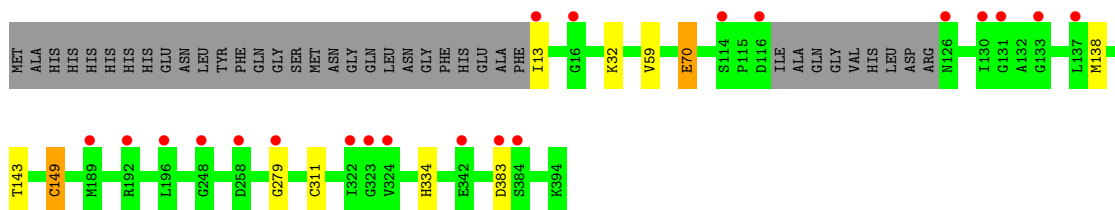
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	168	Total 168	O 168	0	0
6	A	168	Total 168	O 168	0	0
6	C	75	Total 75	O 75	0	0
6	D	110	Total 110	O 110	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

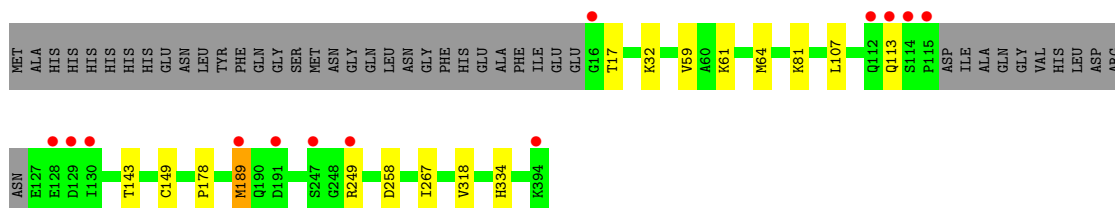
- Molecule 1: S-adenosylmethionine synthase isoform type-2

Chain B: 



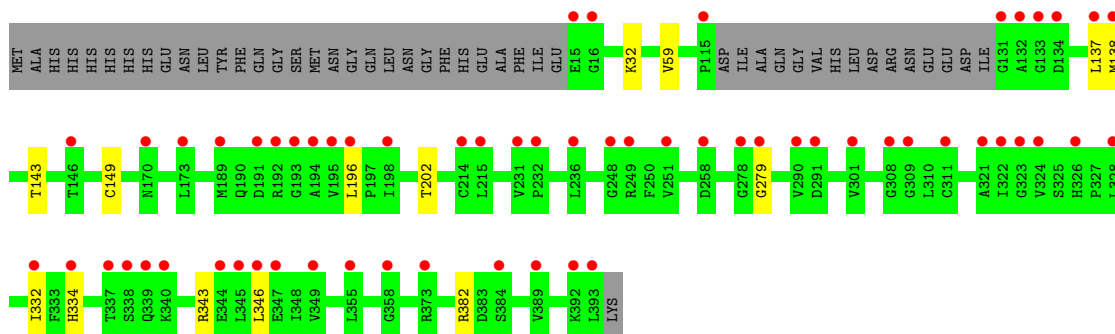
- Molecule 1: S-adenosylmethionine synthase isoform type-2

Chain A: 

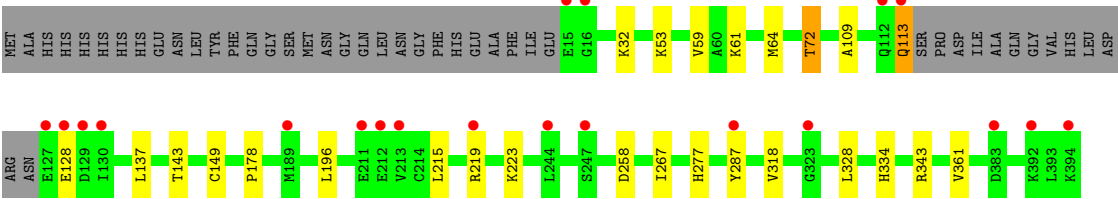
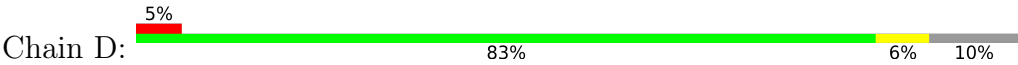


- Molecule 1: S-adenosylmethionine synthase isoform type-2

Chain C: 



- Molecule 1: S-adenosylmethionine synthase isoform type-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.43Å 103.03Å 114.47Å 90.00° 93.36° 90.00°	Depositor
Resolution (Å)	57.13 – 1.79 57.13 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.4 (57.13-1.79) 98.4 (57.13-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.172 , 0.183 0.182 , 0.192	Depositor DCC
R_{free} test set	7223 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12195	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, GOL, NA, 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	0.76	1/2924 (0.0%)	0.87	1/3955 (0.0%)
1	B	0.78	0/2979	0.88	2/4028 (0.0%)
1	C	0.71	0/2897	0.83	0/3919
1	D	0.75	1/2913 (0.0%)	0.87	1/3939 (0.0%)
All	All	0.75	2/11713 (0.0%)	0.86	4/15841 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	ASP	C-O	5.21	1.30	1.23
1	D	258	ASP	C-O	5.16	1.30	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	GLU	CB-CG-CD	6.18	123.10	112.60
1	D	178	PRO	N-CA-C	6.07	121.53	113.57
1	A	178	PRO	N-CA-C	5.48	120.75	113.57
1	B	383	ASP	N-CA-C	5.29	118.84	112.38

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	2862	0	2873	8	0
1	B	2917	0	2914	6	0
1	C	2841	0	2845	6	0
1	D	2855	0	2862	10	0
2	A	40	0	0	1	0
2	B	35	0	0	0	0
2	D	20	0	0	1	0
3	A	26	0	36	0	0
3	B	26	0	36	0	0
3	C	13	0	18	0	0
3	D	26	0	36	0	0
4	B	1	0	0	0	0
5	A	6	0	8	0	0
5	D	6	0	8	0	0
6	A	168	0	0	0	0
6	B	168	0	0	0	0
6	C	75	0	0	0	0
6	D	110	0	0	0	0
All	All	12195	0	11636	23	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 1.

All (23) 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:59:VAL:HG21	1:A:59:VAL:HG21	1.73	0.70
1:C:59:VAL:HG21	1:D:59:VAL:HG21	1.73	0.70
1:A:17:THR:HG22	1:A:189:MET:HG2	1.78	0.65
1:D:53:LYS:HB2	1:D:72:THR:HG23	1.82	0.59
1:B:279:GLY:HA2	1:A:267:ILE:HG13	1.89	0.54
1:D:277:HIS:CE1	2:D:405:SO4:O3	2.61	0.53
1:D:72:THR:HB	1:D:113:GLN:O	2.12	0.49
1:D:61:LYS:HG2	1:D:64:MET:HE2	1.95	0.48
1:D:287:TYR:CD2	1:D:361:VAL:HB	2.49	0.48
1:C:279:GLY:HA2	1:D:267:ILE:HG13	1.99	0.45
1:A:61:LYS:HG2	1:A:64:MET:HE2	1.99	0.44
1:C:137:LEU:O	1:C:138:MET:SD	2.75	0.43
1:C:332:ILE:HD12	1:C:346:LEU:HA	2.00	0.43
1:C:202:THR:HG21	1:D:328:LEU:HD13	1.99	0.42
1:A:249:ARG:NH2	2:A:408:SO4:O3	2.52	0.42
1:B:279:GLY:HA2	1:A:267:ILE:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:THR:O	1:D:149:CYS:HA	2.19	0.42
1:A:143:THR:O	1:A:149:CYS:HA	2.19	0.42
1:B:138:MET:HE2	1:B:138:MET:HB2	1.76	0.41
1:C:143:THR:O	1:C:149:CYS:HA	2.20	0.41
1:B:143:THR:O	1:B:149[B]:CYS:HA	2.20	0.41
1:B:143:THR:O	1:B:149[A]:CYS:HA	2.20	0.41
1:A:107:LEU:HD23	1:D:109:ALA:HB2	2.03	0.41

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	366/410 (89%)	359 (98%)	7 (2%)	0	100	100
1	B	373/410 (91%)	367 (98%)	6 (2%)	0	100	100
1	C	362/410 (88%)	355 (98%)	7 (2%)	0	100	100
1	D	364/410 (89%)	356 (98%)	8 (2%)	0	100	100
All	All	1465/1640 (89%)	1437 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/340 (90%)	300 (98%)	7 (2%)	44	33
1	B	314/340 (92%)	306 (98%)	8 (2%)	42	30
1	C	303/340 (89%)	298 (98%)	5 (2%)	53	45
1	D	305/340 (90%)	292 (96%)	13 (4%)	26	13
All	All	1229/1360 (90%)	1196 (97%)	33 (3%)	43	27

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	13	ILE
1	B	32	LYS
1	B	70	GLU
1	B	149[A]	CYS
1	B	149[B]	CYS
1	B	311[A]	CYS
1	B	311[B]	CYS
1	B	334	HIS
1	A	32	LYS
1	A	81	LYS
1	A	113	GLN
1	A	189	MET
1	A	318[A]	VAL
1	A	318[B]	VAL
1	A	334	HIS
1	C	32	LYS
1	C	196	LEU
1	C	334	HIS
1	C	343	ARG
1	C	382	ARG
1	D	32	LYS
1	D	72	THR
1	D	113	GLN
1	D	128	GLU
1	D	137	LEU
1	D	196	LEU
1	D	215	LEU
1	D	219	ARG
1	D	223	LYS
1	D	318[A]	VAL
1	D	318[B]	VAL
1	D	334	HIS
1	D	343	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	256	GLN
1	A	243	HIS
1	A	326	HIS
1	C	243	HIS
1	C	317	GLN
1	D	113	GLN
1	D	243	HIS
1	D	326	HIS

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](#)

Of 29 ligands modelled in this entry, 1 is monoatomic - leaving 28 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	SO4	D	403	-	4,4,4	0.41	0	6,6,6	0.11	0
5	GOL	A	401	-	5,5,5	0.56	0	5,5,5	0.69	0
3	PG4	D	406	-	12,12,12	0.58	0	11,11,11	0.36	0
2	SO4	D	402	-	4,4,4	0.42	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	403	-	4,4,4	0.44	0	6,6,6	0.09	0
2	SO4	B	405	-	4,4,4	0.48	0	6,6,6	0.08	0
2	SO4	A	406	-	4,4,4	0.46	0	6,6,6	0.07	0
2	SO4	B	407	-	4,4,4	0.46	0	6,6,6	0.18	0
2	SO4	B	401	-	4,4,4	0.43	0	6,6,6	0.18	0
3	PG4	A	410	-	12,12,12	0.36	0	11,11,11	0.48	0
2	SO4	A	408	-	4,4,4	0.48	0	6,6,6	0.19	0
2	SO4	D	404	-	4,4,4	0.35	0	6,6,6	0.17	0
2	SO4	A	405	-	4,4,4	0.43	0	6,6,6	0.18	0
2	SO4	A	404	-	4,4,4	0.43	0	6,6,6	0.05	0
3	PG4	B	409	-	12,12,12	0.52	0	11,11,11	0.33	0
2	SO4	A	409	-	4,4,4	0.37	0	6,6,6	0.27	0
2	SO4	D	405	-	4,4,4	0.51	0	6,6,6	0.33	0
2	SO4	A	403	-	4,4,4	0.44	0	6,6,6	0.16	0
3	PG4	B	408	-	12,12,12	0.49	0	11,11,11	0.33	0
2	SO4	B	404	-	4,4,4	0.44	0	6,6,6	0.21	0
2	SO4	B	402	-	4,4,4	0.43	0	6,6,6	0.12	0
3	PG4	A	411	-	12,12,12	0.51	0	11,11,11	0.25	0
3	PG4	C	401	-	12,12,12	0.50	0	11,11,11	0.24	0
3	PG4	D	407	-	12,12,12	0.50	0	11,11,11	0.32	0
2	SO4	A	407	-	4,4,4	0.44	0	6,6,6	0.09	0
5	GOL	D	401	-	5,5,5	0.46	0	5,5,5	0.71	0
2	SO4	A	402	-	4,4,4	0.47	0	6,6,6	0.30	0
2	SO4	B	406	-	4,4,4	0.46	0	6,6,6	0.42	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
5	GOL	A	401	-	-	0/4/4/4	-
3	PG4	A	410	-	-	3/10/10/10	-
3	PG4	D	406	-	-	6/10/10/10	-
3	PG4	B	409	-	-	6/10/10/10	-
3	PG4	B	408	-	-	7/10/10/10	-
3	PG4	A	411	-	-	5/10/10/10	-
3	PG4	C	401	-	-	5/10/10/10	-
3	PG4	D	407	-	-	7/10/10/10	-
5	GOL	D	401	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	401	PG4	O3-C5-C6-O4
3	B	408	PG4	O2-C3-C4-O3
3	C	401	PG4	O2-C3-C4-O3
3	D	407	PG4	O3-C5-C6-O4
3	A	411	PG4	O3-C5-C6-O4
3	B	409	PG4	O2-C3-C4-O3
3	B	409	PG4	O3-C5-C6-O4
3	A	411	PG4	O1-C1-C2-O2
3	B	408	PG4	O1-C1-C2-O2
3	B	408	PG4	O4-C7-C8-O5
3	B	409	PG4	O1-C1-C2-O2
3	D	406	PG4	O4-C7-C8-O5
3	D	407	PG4	O1-C1-C2-O2
3	D	406	PG4	O3-C5-C6-O4
3	D	407	PG4	O4-C7-C8-O5
3	B	408	PG4	O3-C5-C6-O4
3	A	410	PG4	O2-C3-C4-O3
3	C	401	PG4	O1-C1-C2-O2
3	C	401	PG4	O4-C7-C8-O5
3	A	410	PG4	O1-C1-C2-O2
3	D	406	PG4	O1-C1-C2-O2
3	D	407	PG4	C4-C3-O2-C2
3	A	411	PG4	C5-C6-O4-C7
3	B	408	PG4	C4-C3-O2-C2
3	B	409	PG4	O4-C7-C8-O5
3	D	406	PG4	C6-C5-O3-C4
3	C	401	PG4	C5-C6-O4-C7
3	B	409	PG4	C6-C5-O3-C4
3	D	407	PG4	C8-C7-O4-C6
3	A	411	PG4	O4-C7-C8-O5
3	A	410	PG4	O4-C7-C8-O5
3	B	408	PG4	C6-C5-O3-C4
3	B	409	PG4	C1-C2-O2-C3
3	A	411	PG4	C6-C5-O3-C4
3	D	406	PG4	O2-C3-C4-O3
3	D	406	PG4	C5-C6-O4-C7
3	D	407	PG4	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
3	B	408	PG4	C3-C4-O3-C5
3	D	407	PG4	C6-C5-O3-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	408	SO4	1	0
2	D	405	SO4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	368/410 (89%)	0.03	13 (3%)	47	47	14, 26, 43, 69	2 (0%)
1	B	373/410 (90%)	0.19	21 (5%)	30	29	13, 26, 45, 67	4 (1%)
1	C	364/410 (88%)	0.87	61 (16%)	4	3	12, 43, 68, 92	2 (0%)
1	D	367/410 (89%)	0.31	20 (5%)	31	30	18, 32, 51, 76	1 (0%)
All	All	1472/1640 (89%)	0.35	115 (7%)	19	17	12, 30, 60, 92	9 (0%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	ILE	8.4
1	A	115	PRO	4.8
1	A	114	SER	4.6
1	C	324	VAL	4.6
1	C	132	ALA	4.6
1	C	393	LEU	4.4
1	D	130	ILE	4.3
1	D	16	GLY	4.1
1	C	339	GLN	4.1
1	C	346	LEU	3.7
1	D	247	SER	3.7
1	C	322	ILE	3.6
1	C	137	LEU	3.6
1	B	116	ASP	3.6
1	B	279	GLY	3.5
1	D	113	GLN	3.5
1	A	113	GLN	3.4
1	C	248	GLY	3.4
1	B	137	LEU	3.3
1	C	358	GLY	3.3
1	D	128	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	131	GLY	3.2
1	B	323	GLY	3.2
1	B	322	ILE	3.2
1	B	384	SER	3.2
1	C	308	GLY	3.2
1	A	394	LYS	3.1
1	C	192	ARG	3.1
1	C	215	LEU	3.1
1	A	112	GLN	3.1
1	C	138	MET	3.0
1	A	16	GLY	3.0
1	C	337	THR	2.9
1	C	214	CYS	2.9
1	C	133	GLY	2.9
1	C	249	ARG	2.8
1	C	195	VAL	2.8
1	D	112	GLN	2.8
1	C	278	GLY	2.8
1	C	323	GLY	2.8
1	B	383	ASP	2.8
1	C	321	ALA	2.7
1	C	345	LEU	2.7
1	B	248	GLY	2.7
1	C	196	LEU	2.7
1	C	311	CYS	2.7
1	C	193	GLY	2.7
1	C	191	ASP	2.7
1	D	15	GLU	2.7
1	C	349	VAL	2.7
1	C	189	MET	2.7
1	A	129	ASP	2.6
1	A	189	MET	2.6
1	D	219	ARG	2.6
1	C	232	PRO	2.5
1	C	338	SER	2.5
1	C	170	ASN	2.5
1	C	355	LEU	2.5
1	C	134	ASP	2.5
1	C	115	PRO	2.5
1	C	279	GLY	2.5
1	B	192	ARG	2.5
1	B	114	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	258	ASP	2.4
1	C	344	GLU	2.4
1	C	334	HIS	2.4
1	D	189	MET	2.4
1	B	131	GLY	2.4
1	B	324	VAL	2.4
1	D	213	VAL	2.4
1	C	347	GLU	2.4
1	A	191	ASP	2.4
1	B	16	GLY	2.3
1	D	211	GLU	2.3
1	C	15	GLU	2.3
1	C	328	LEU	2.3
1	B	126	ASN	2.3
1	A	128	GLU	2.3
1	C	198	ILE	2.3
1	C	301	VAL	2.3
1	D	212	GLU	2.3
1	C	16	GLY	2.3
1	C	291	ASP	2.3
1	C	384	SER	2.2
1	C	392	LYS	2.2
1	C	258	ASP	2.2
1	B	130	ILE	2.2
1	A	130	ILE	2.2
1	C	290	VAL	2.2
1	D	383	ASP	2.2
1	B	196	LEU	2.2
1	B	133	GLY	2.2
1	B	342	GLU	2.2
1	D	127	GLU	2.2
1	C	332	ILE	2.2
1	B	189	MET	2.2
1	C	173	LEU	2.2
1	C	373	ARG	2.2
1	C	309	GLY	2.1
1	D	323	GLY	2.1
1	C	236	LEU	2.1
1	D	244	LEU	2.1
1	A	247	SER	2.1
1	C	146	THR	2.1
1	D	129	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	249	ARG	2.1
1	C	326	HIS	2.1
1	C	340	LYS	2.1
1	D	394	LYS	2.1
1	C	231	VAL	2.1
1	C	251	VAL	2.1
1	D	392	LYS	2.1
1	C	389	VAL	2.0
1	D	287	TYR	2.0
1	C	194	ALA	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	B	403	5/5	0.57	0.15	87,88,91,95	0
2	SO4	B	406	5/5	0.59	0.25	61,65,69,71	0
2	SO4	A	409	5/5	0.62	0.21	62,71,72,74	0
2	SO4	A	406	5/5	0.63	0.15	97,99,100,101	0
2	SO4	D	402	5/5	0.72	0.13	95,96,98,99	0
2	SO4	D	405	5/5	0.72	0.23	59,66,77,79	0
2	SO4	B	405	5/5	0.73	0.19	80,84,91,93	0
3	PG4	B	409	13/13	0.74	0.23	52,62,81,83	0
3	PG4	D	406	13/13	0.78	0.20	58,68,75,75	0
2	SO4	A	403	5/5	0.79	0.16	88,91,93,95	0
2	SO4	B	401	5/5	0.80	0.12	81,83,84,85	0
2	SO4	B	407	5/5	0.81	0.17	79,83,85,87	0
2	SO4	A	407	5/5	0.82	0.12	86,86,88,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	405	5/5	0.82	0.12	87,90,92,93	0
3	PG4	C	401	13/13	0.82	0.20	68,71,79,82	0
2	SO4	B	404	5/5	0.82	0.12	56,57,59,62	0
3	PG4	B	408	13/13	0.83	0.18	63,66,70,70	0
3	PG4	A	410	13/13	0.83	0.20	52,60,63,66	0
2	SO4	B	402	5/5	0.84	0.14	90,92,92,94	0
2	SO4	D	403	5/5	0.84	0.09	88,89,90,91	0
3	PG4	D	407	13/13	0.85	0.21	68,76,78,78	0
3	PG4	A	411	13/13	0.87	0.19	64,69,74,76	0
2	SO4	A	408	5/5	0.87	0.12	60,61,64,68	0
2	SO4	A	404	5/5	0.89	0.09	74,75,77,77	0
5	GOL	A	401	6/6	0.89	0.12	25,26,26,26	0
5	GOL	D	401	6/6	0.91	0.10	31,34,34,35	0
4	NA	B	410	1/1	0.93	0.09	33,33,33,33	0
2	SO4	D	404	5/5	0.94	0.08	39,43,46,46	0
2	SO4	A	402	5/5	0.98	0.07	30,32,36,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.