Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 02:45 AM EDT

PDB ID	:	4KTT
Title	:	Structural insights of MAT enzymes: MATa2b complexed with SAM
Authors	:	Murray, B.; Antonyuk, S.V.; Marina, A.; Lu, S.C.; Mato, J.M.; Hasnain, S.S.; Rojas, A.L.
Deposited on	:	2013-05-21
Resolution	:	2.59 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 (i) 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 (i)) were used in the production of this report:

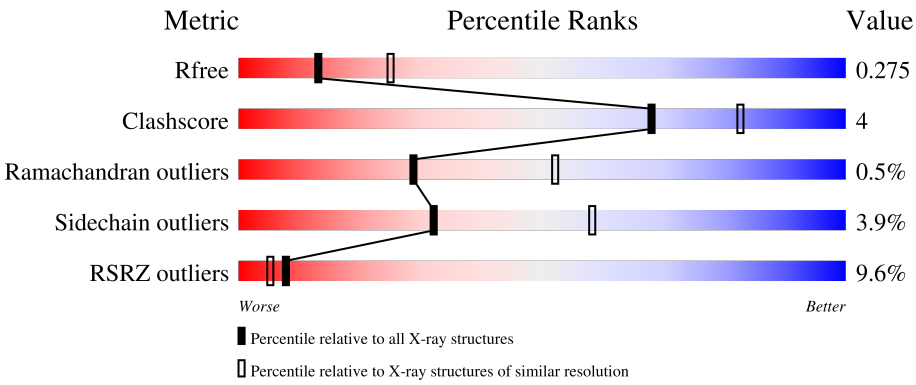
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	396	4% 83% 7% 9%
1	B	396	9% 84% 12% • •
1	C	396	11% 77% 13% • 9%
1	D	396	6% 85% 11% • •
2	E	327	3% 80% 13% • 6%

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Mol	Chain	Length	Quality of chain
2	F	327	22% 73% 11% • 14%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	401	-	-	-	X
5	PO4	A	406	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16501 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
			Total	C	N	O	S			
1	A	360	2811	1783	490	527	11	0	0	0
1	B	382	2972	1877	519	565	11	0	0	0
1	C	360	2813	1784	490	528	11	0	0	0
1	D	380	2954	1867	517	559	11	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Methionine adenosyltransferase 2 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	306	2429	1533	443	443	10	0	0	0
2	F	280	2237	1418	406	403	10	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP Q9NZL9
E	-2	SER	-	expression tag	UNP Q9NZL9
E	-1	HIS	-	expression tag	UNP Q9NZL9
E	0	MET	-	expression tag	UNP Q9NZL9

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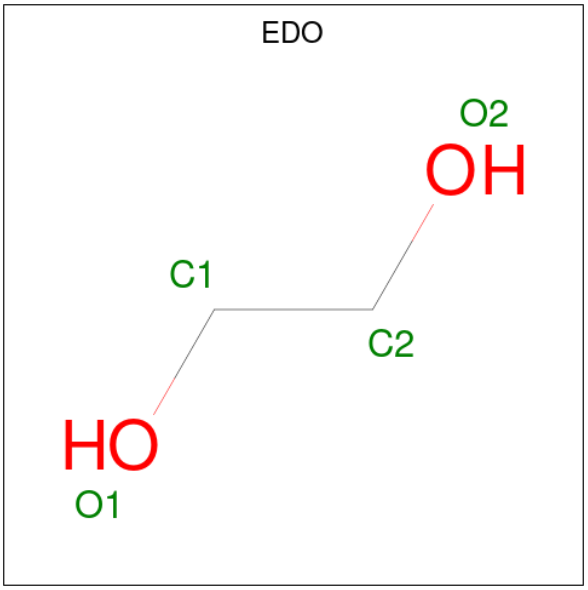
Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	GLY	-	expression tag	UNP Q9NZL9
F	-2	SER	-	expression tag	UNP Q9NZL9
F	-1	HIS	-	expression tag	UNP Q9NZL9
F	0	MET	-	expression tag	UNP Q9NZL9

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	A	1	4	2	2		0	0
3	A	1	4	2	2		0	0
3	A	1	4	2	2		0	0
3	A	1	4	2	2		0	0
3	B	1	4	2	2		0	0
3	B	1	4	2	2		0	0
3	B	1	4	2	2		0	0
3	B	1	4	2	2		0	0
3	B	1	4	2	2		0	0

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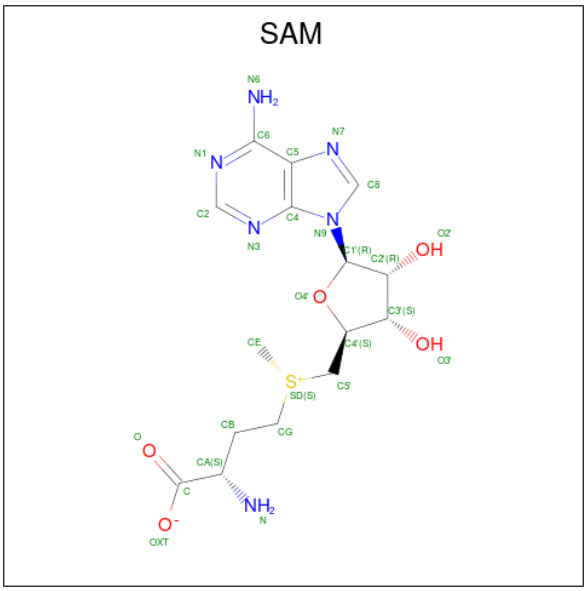
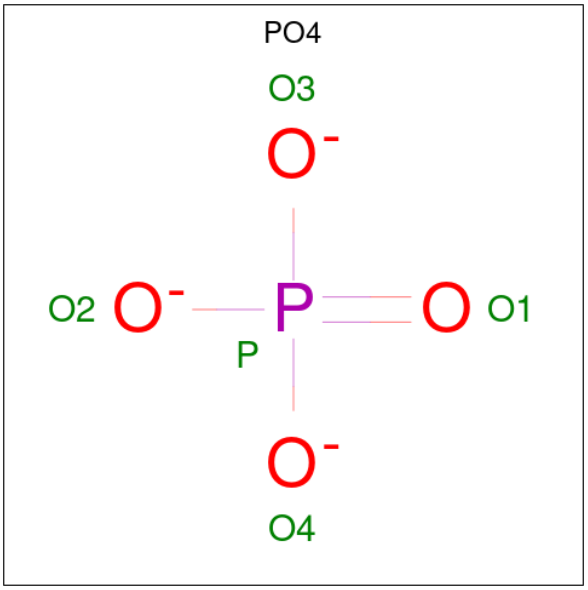
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	C	1	4	2	2	0	0
			Total	C	O		
3	C	1	4	2	2	0	0
			Total	C	O		
3	C	1	4	2	2	0	0
			Total	C	O		
3	D	1	4	2	2	0	0
			Total	C	O		
3	D	1	4	2	2	0	0
			Total	C	O		
3	D	1	4	2	2	0	0
			Total	C	O		
3	D	1	4	2	2	0	0
			Total	C	O		
3	D	1	4	2	2	0	0
			Total	C	O		
3	D	1	4	2	2	0	0
			Total	C	O		
3	D	1	4	2	2	0	0
			Total	C	O		
3	E	1	4	2	2	0	0
			Total	C	O		
3	E	1	4	2	2	0	0
			Total	C	O		
3	E	1	4	2	2	0	0
			Total	C	O		
3	E	1	4	2	2	0	0
			Total	C	O		
3	F	1	4	2	2	0	0

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	27	15	6	5	1	0	0
			Total	C	N	O	S		
4	C	1	27	15	6	5	1	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
5	A	1	5	4	1	0	0
			Total	O	P		
5	C	1	5	4	1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	B	1	1	1	0	0

- Molecule 7 is water.

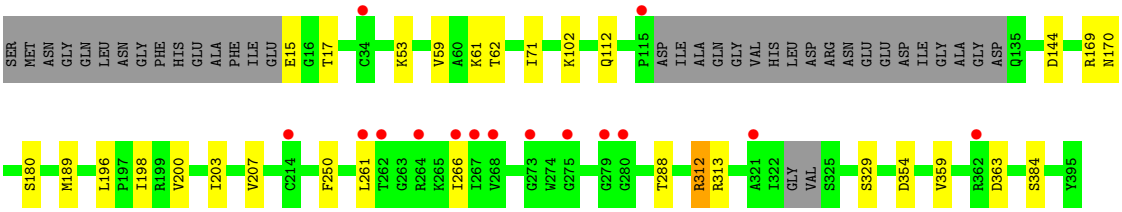
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	23	23	23	0	0
			Total	O		
7	B	21	21	21	0	0
			Total	O		
7	C	15	15	15	0	0
			Total	O		
7	D	35	35	35	0	0
			Total	O		
7	E	11	11	11	0	0
			Total	O		
7	F	3	3	3	0	0

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.

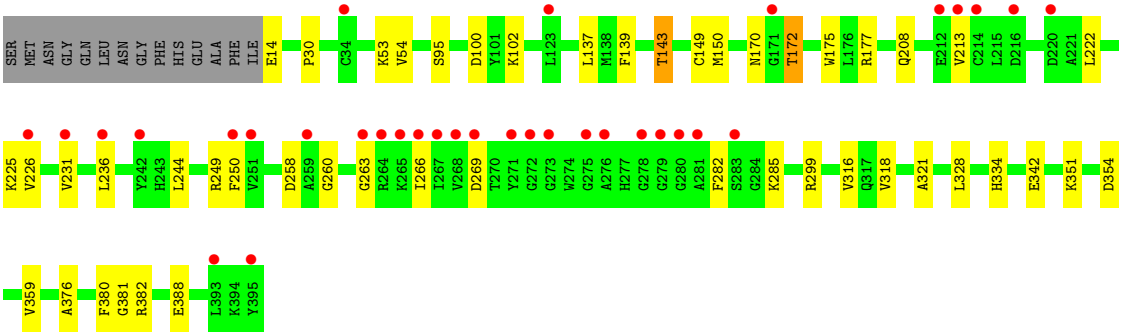
• Molecule 1: S-adenosylmethionine synthase isoform type-2

Chain A:



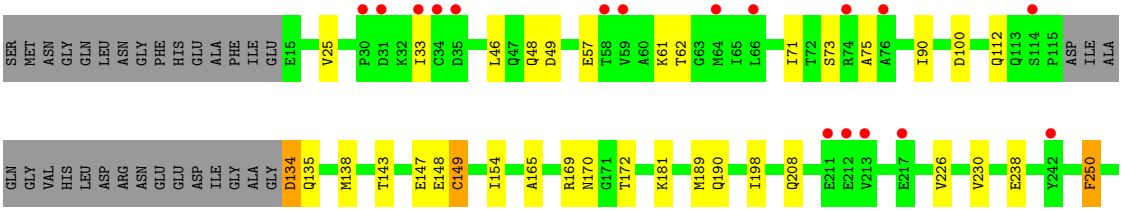
• Molecule 1: S-adenosylmethionine synthase isoform type-2

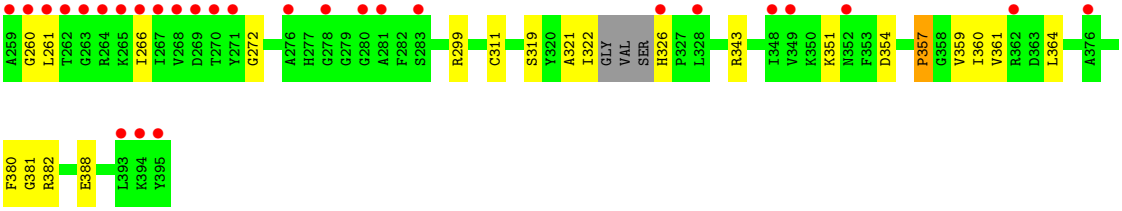
Chain B:



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

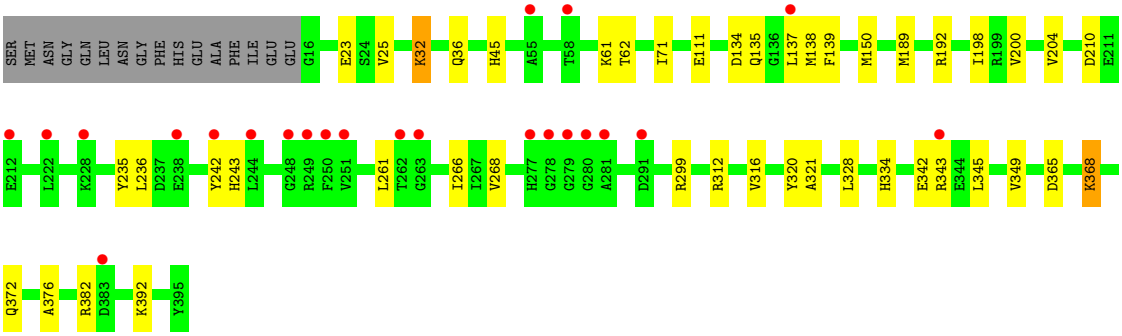
Chain C:





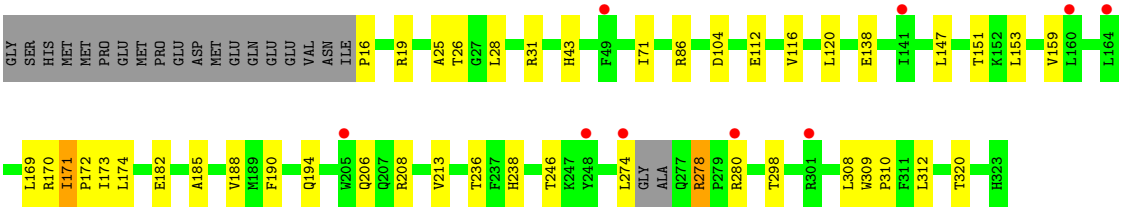
• Molecule 1: S-adenosylmethionine synthase isoform type-2

Chain D:



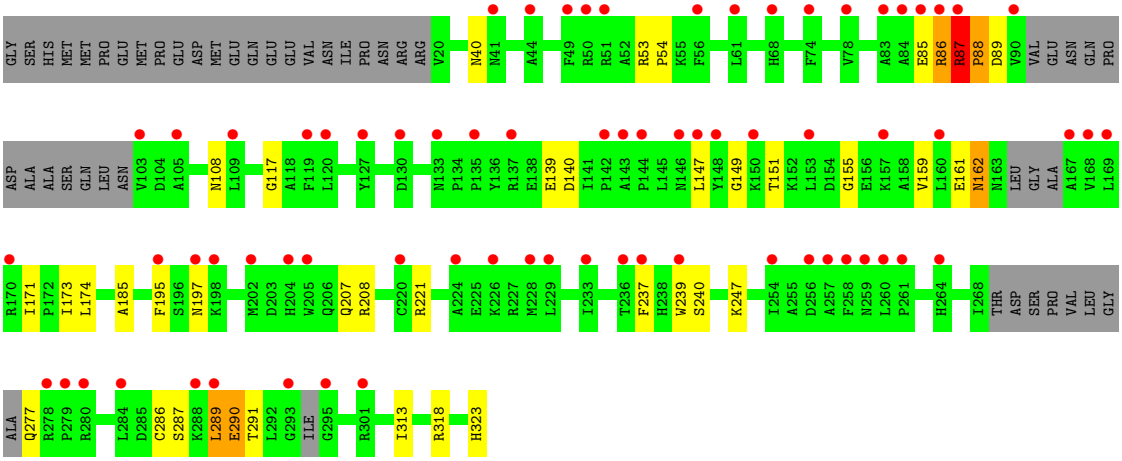
• Molecule 2: Methionine adenosyltransferase 2 subunit beta

Chain E:



• Molecule 2: Methionine adenosyltransferase 2 subunit beta

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.44Å 115.72Å 298.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.41 – 2.59 47.41 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.8 (47.41-2.59) 96.8 (47.41-2.59)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.10 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.7.0029, PHENIX	Depositor
R, R_{free}	0.218 , 0.279 0.217 , 0.275	Depositor DCC
R_{free} test set	3847 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	65.9	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16501	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EDO, PO4, SAM

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	0.36	0/2867	0.57	0/3875
1	B	0.34	0/3031	0.55	0/4100
1	C	0.33	0/2869	0.55	0/3878
1	D	0.37	0/3013	0.59	0/4076
2	E	0.33	0/2486	0.54	1/3370 (0.0%)
2	F	0.32	0/2289	0.52	0/3095
All	All	0.34	0/16555	0.55	1/22394 (0.0%)

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	E	16	PRO	N-CA-CB	6.07	110.59	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2811	0	2819	17	0
1	B	2972	0	2962	22	0
1	C	2813	0	2818	28	0
1	D	2954	0	2950	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2429	0	2393	21	0
2	F	2237	0	2203	19	0
3	A	16	0	24	1	0
3	B	36	0	54	3	0
3	C	12	0	18	0	0
3	D	28	0	42	1	0
3	E	16	0	24	0	0
3	F	4	0	6	0	0
4	A	27	0	22	0	0
4	C	27	0	22	0	0
5	A	5	0	0	0	0
5	C	5	0	0	0	0
6	B	1	0	0	0	0
7	A	23	0	0	0	0
7	B	21	0	0	0	0
7	C	15	0	0	0	0
7	D	35	0	0	0	0
7	E	11	0	0	0	0
7	F	3	0	0	0	0
All	All	16501	0	16357	124	0

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

All (124) 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)
2:F:162:ASN:C	2:F:162:ASN:HD22	1.87	0.78
2:F:173:ILE:HD11	2:F:185:ALA:HB3	1.72	0.72
2:F:237:PHE:HB3	2:F:289:LEU:HD21	1.74	0.70
1:D:376:ALA:O	1:D:382:ARG:NH2	2.31	0.64
1:C:57:GLU:HB3	1:D:261:LEU:HD11	1.80	0.64
1:C:134:ASP:OD1	1:C:134:ASP:N	2.33	0.60
1:C:354:ASP:HB3	1:C:359:VAL:HG11	1.83	0.59
1:B:354:ASP:OD2	1:B:359:VAL:HG21	2.03	0.58
1:A:59:VAL:HG22	1:A:261:LEU:HD22	1.86	0.58
1:B:334:HIS:CD2	1:B:342:GLU:HG3	2.38	0.58
1:A:266:ILE:HD11	1:B:266:ILE:HD11	1.86	0.57
1:A:53:LYS:HE3	1:A:288:THR:HG21	1.86	0.57
2:E:169:LEU:HG	2:E:171:ILE:HD13	1.87	0.57
1:C:165:ALA:HB1	1:C:169:ARG:NH2	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ALA:O	1:B:382:ARG:NH2	2.39	0.56
2:E:71:ILE:HG22	2:E:116:VAL:HG21	1.88	0.56
1:D:36:GLN:HE21	1:D:372:GLN:HE21	1.54	0.55
1:B:231:VAL:HG11	1:B:236:LEU:HD21	1.88	0.55
1:A:71:ILE:O	1:A:112:GLN:HA	2.08	0.54
1:C:25:VAL:HG12	1:C:181:LYS:HG2	1.90	0.54
1:B:30:PRO:HB2	1:B:260:GLY:HA3	1.91	0.53
2:F:162:ASN:C	2:F:162:ASN:ND2	2.61	0.52
1:C:299:ARG:HG2	1:C:380:PHE:CD1	2.45	0.52
1:B:177:ARG:HB2	1:B:208:GLN:HB3	1.91	0.51
2:E:190:PHE:O	2:E:194:GLN:HG3	2.10	0.51
1:C:266:ILE:HD11	1:D:266:ILE:HD11	1.93	0.51
2:F:88:PRO:HA	2:F:89:ASP:HB2	1.93	0.51
2:E:116:VAL:HG12	2:E:116:VAL:O	2.10	0.51
1:B:222:LEU:O	1:B:226:VAL:HB	2.11	0.51
1:C:189:MET:HB2	1:C:198:ILE:HD11	1.91	0.51
2:E:182:GLU:HA	2:E:188:VAL:CG1	2.42	0.50
1:B:321:ALA:HB2	1:B:328:LEU:HD21	1.93	0.50
2:E:173:ILE:HD11	2:E:185:ALA:HB3	1.92	0.50
1:D:189:MET:HB2	1:D:198:ILE:HD11	1.94	0.50
1:D:345:LEU:O	1:D:349:VAL:HG23	2.12	0.50
1:A:15:GLU:HB3	1:A:17:THR:HG23	1.93	0.49
2:E:190:PHE:CD1	2:E:308:LEU:HD13	2.48	0.49
2:E:170:ARG:O	2:E:171:ILE:HD12	2.13	0.49
1:C:357:PRO:O	1:C:361:VAL:HG13	2.13	0.49
2:F:171:ILE:HD12	2:F:174:LEU:HD11	1.95	0.49
1:A:15:GLU:CB	1:A:17:THR:HG23	2.43	0.48
1:A:180:SER:HB3	1:A:207:VAL:HG23	1.95	0.48
2:E:171:ILE:HG23	2:E:174:LEU:HD21	1.94	0.48
2:E:309:TRP:CG	2:E:310:PRO:HD3	2.49	0.48
1:B:139:PHE:HA	1:B:316:VAL:O	2.14	0.47
1:C:154:ILE:HD12	1:C:272:GLY:CA	2.45	0.47
2:E:182:GLU:HA	2:E:188:VAL:HG12	1.96	0.47
1:C:208:GLN:HA	1:C:250:PHE:O	2.15	0.47
1:B:175:TRP:CG	1:B:213:VAL:HG21	2.48	0.47
1:C:62:THR:OG1	1:D:111:GLU:OE2	2.33	0.47
1:D:204:VAL:HG22	1:D:243:HIS:HB2	1.97	0.47
2:F:173:ILE:HD11	2:F:185:ALA:CB	2.42	0.47
1:A:144:ASP:OD2	1:A:312:ARG:CG	2.63	0.47
1:C:226:VAL:O	1:C:230:VAL:HG23	2.15	0.47
2:F:161:GLU:O	2:F:162:ASN:CG	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:VAL:HG22	1:A:261:LEU:CD2	2.44	0.46
1:B:299:ARG:HG2	1:B:380:PHE:CD1	2.50	0.46
1:D:365:ASP:OD2	1:D:368:LYS:HD3	2.15	0.46
2:F:173:ILE:HD12	2:F:208:ARG:NH1	2.30	0.46
1:A:189:MET:HB2	1:A:198:ILE:HD11	1.98	0.46
1:D:23:GLU:O	1:D:268:VAL:HG22	2.16	0.46
1:C:33:ILE:HG12	1:C:90:ILE:HD13	1.97	0.46
1:D:139:PHE:HA	1:D:316:VAL:O	2.16	0.46
2:E:274:LEU:HD22	2:E:278:ARG:HD2	1.98	0.46
1:D:334:HIS:CD2	1:D:342:GLU:HG3	2.51	0.46
1:C:143:THR:O	1:C:149:CYS:HA	2.16	0.45
2:E:206:GLN:O	2:E:246:THR:HG22	2.16	0.45
1:C:48:GLN:HB2	1:C:75:ALA:HB2	1.98	0.45
1:A:200:VAL:HG11	1:A:203:ILE:HD11	1.99	0.45
2:F:195:PHE:CE1	2:F:313:ILE:HD11	2.51	0.45
1:D:321:ALA:HB2	1:D:328:LEU:HD11	1.99	0.45
2:F:286:CYS:O	2:F:290:GLU:HG2	2.17	0.44
1:B:143:THR:O	1:B:149:CYS:HA	2.16	0.44
2:E:147:LEU:O	2:E:151:THR:HG23	2.17	0.44
1:B:282:PHE:H	3:B:404:EDO:H21	1.82	0.44
1:A:144:ASP:OD2	1:A:312:ARG:HG2	2.16	0.44
1:C:154:ILE:HD12	1:C:272:GLY:HA3	1.99	0.44
1:C:170:ASN:HB3	1:C:172:THR:HG23	1.99	0.44
1:D:61:LYS:HG2	1:D:62:THR:H	1.82	0.44
1:C:71:ILE:O	1:C:112:GLN:HA	2.16	0.44
1:A:359:VAL:HG12	1:A:363:ASP:OD1	2.17	0.44
1:B:263:GLY:HA2	3:B:404:EDO:H22	1.99	0.43
1:C:62:THR:HG1	1:D:111:GLU:CD	2.21	0.43
2:E:19:ARG:HG2	2:E:43:HIS:HB3	2.01	0.43
1:A:169:ARG:NH2	3:A:403:EDO:O1	2.49	0.43
1:B:150:MET:HG3	1:B:381:GLY:HA3	2.01	0.43
2:F:40:ASN:HD22	2:F:221:ARG:NH2	2.17	0.43
2:F:239:TRP:CG	2:F:240:SER:N	2.86	0.43
1:A:313:ARG:NH2	2:F:323:HIS:O	2.49	0.43
2:E:138:GLU:OE2	2:E:238:HIS:N	2.49	0.43
1:D:45:HIS:NE2	1:D:71:ILE:HG21	2.34	0.43
1:A:61:LYS:O	1:A:62:THR:C	2.57	0.42
1:B:170:ASN:HB3	1:B:172:THR:HG22	2.01	0.42
1:C:360:ILE:CG2	1:C:364:LEU:HD12	2.49	0.42
1:C:46:LEU:HA	1:C:49:ASP:O	2.20	0.42
2:E:28:LEU:HG	2:E:213:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:MET:CE	1:D:299:ARG:NH1	2.82	0.42
1:D:25:VAL:HG23	1:D:32:LYS:HD2	2.00	0.42
2:F:53:ARG:HD2	2:F:54:PRO:HA	2.01	0.42
1:D:200:VAL:HG23	1:D:235:TYR:HB3	2.00	0.42
2:E:170:ARG:NH1	2:E:236:THR:HG21	2.35	0.42
1:C:61:LYS:HG3	1:C:62:THR:H	1.85	0.41
2:F:287:SER:O	2:F:291:THR:N	2.43	0.41
1:C:165:ALA:HB1	1:C:169:ARG:HH22	1.83	0.41
1:A:59:VAL:HG13	1:A:261:LEU:HD23	2.02	0.41
1:B:54:VAL:O	1:B:285:LYS:HA	2.20	0.41
1:C:321:ALA:O	1:C:322:ILE:HG12	2.21	0.41
1:D:312:ARG:HD3	3:D:405:EDO:C2	2.50	0.41
2:E:25:ALA:O	2:E:31:ARG:HG2	2.21	0.41
2:F:155:GLY:O	2:F:159:VAL:HG23	2.20	0.41
2:E:120:LEU:HD23	2:E:159:VAL:HG13	2.02	0.41
1:B:100:ASP:OD2	1:B:102:LYS:HB2	2.20	0.41
1:B:381:GLY:H	1:B:388:GLU:CD	2.25	0.41
1:C:381:GLY:H	1:C:388:GLU:CD	2.24	0.41
1:D:134:ASP:OD1	1:D:135:GLN:N	2.54	0.41
2:F:87:ARG:O	2:F:89:ASP:HB2	2.21	0.41
1:C:260:GLY:O	1:C:261:LEU:HD23	2.21	0.40
1:D:236:LEU:HD22	1:D:242:TYR:OH	2.21	0.40
2:E:309:TRP:N	2:E:310:PRO:CD	2.84	0.40
1:D:150:MET:HE2	1:D:299:ARG:NH1	2.37	0.40
1:B:95:SER:OG	1:C:100:ASP:OD2	2.26	0.40
1:B:269:ASP:OD2	3:B:404:EDO:H11	2.22	0.40
1:D:138:MET:HE3	1:D:320:TYR:CD1	2.57	0.40
2:F:86:ARG:O	2:F:87:ARG:HB2	2.21	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	354/396 (89%)	336 (95%)	18 (5%)	0	100	100
1	B	380/396 (96%)	363 (96%)	16 (4%)	1 (0%)	41	64
1	C	354/396 (89%)	335 (95%)	18 (5%)	1 (0%)	41	64
1	D	378/396 (96%)	362 (96%)	15 (4%)	1 (0%)	41	64
2	E	302/327 (92%)	287 (95%)	14 (5%)	1 (0%)	41	64
2	F	270/327 (83%)	237 (88%)	27 (10%)	6 (2%)	6	12
All	All	2038/2238 (91%)	1920 (94%)	108 (5%)	10 (0%)	29	52

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	87	ARG
1	D	210	ASP
2	F	197	ASN
1	B	249	ARG
2	F	88	PRO
2	E	172	PRO
2	F	85	GLU
2	F	149	GLY
1	C	357	PRO
2	F	117	GLY

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	301/328 (92%)	293 (97%)	8 (3%)	44	71
1	B	317/328 (97%)	306 (96%)	11 (4%)	36	62
1	C	301/328 (92%)	285 (95%)	16 (5%)	22	45
1	D	315/328 (96%)	309 (98%)	6 (2%)	57	79
2	E	260/279 (93%)	248 (95%)	12 (5%)	27	51
2	F	239/279 (86%)	225 (94%)	14 (6%)	19	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1733/1870 (93%)	1666 (96%)	67 (4%)	32 58

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LYS
1	A	170	ASN
1	A	196	LEU
1	A	250	PHE
1	A	312	ARG
1	A	329	SER
1	A	354	ASP
1	A	384	SER
1	B	14	GLU
1	B	53	LYS
1	B	137	LEU
1	B	143	THR
1	B	172	THR
1	B	225	LYS
1	B	244	LEU
1	B	250	PHE
1	B	258	ASP
1	B	318	VAL
1	B	351	LYS
1	C	73	SER
1	C	134	ASP
1	C	135	GLN
1	C	138	MET
1	C	147	GLU
1	C	148	GLU
1	C	149	CYS
1	C	190	GLN
1	C	238	GLU
1	C	250	PHE
1	C	311	CYS
1	C	319	SER
1	C	326	HIS
1	C	343	ARG
1	C	351	LYS
1	C	382	ARG
1	D	32	LYS
1	D	137	LEU

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Mol	Chain	Res	Type
1	D	192	ARG
1	D	343	ARG
1	D	368	LYS
1	D	392	LYS
2	E	26	THR
2	E	86	ARG
2	E	104	ASP
2	E	112	GLU
2	E	153	LEU
2	E	171	ILE
2	E	208	ARG
2	E	278	ARG
2	E	280	ARG
2	E	298	THR
2	E	312	LEU
2	E	320	THR
2	F	86	ARG
2	F	87	ARG
2	F	108	ASN
2	F	139	GLU
2	F	140	ASP
2	F	147	LEU
2	F	151	THR
2	F	162	ASN
2	F	207	GLN
2	F	247	LYS
2	F	277	GLN
2	F	289	LEU
2	F	290	GLU
2	F	318	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	161	ASN
1	C	135	GLN
1	D	112	GLN
1	D	135	GLN
1	D	183	GLN
1	D	372	GLN
2	E	40	ASN

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Mol	Chain	Res	Type
2	E	194	GLN
2	F	40	ASN
2	F	68	HIS
2	F	162	ASN
2	F	222	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 33 ligands modelled in this entry, 1 is monoatomic - leaving 32 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	$\#\|Z\| > 2$
3	EDO	E	404	-	3,3,3	0.49	0	2,2,2	0.15	0
3	EDO	B	402	-	3,3,3	0.42	0	2,2,2	0.38	0
4	SAM	C	404	-	24,29,29	1.13	1 (4%)	23,42,42	1.53	5 (21%)
3	EDO	C	403	-	3,3,3	0.49	0	2,2,2	0.07	0
3	EDO	D	401	-	3,3,3	0.49	0	2,2,2	0.23	0
3	EDO	E	403	-	3,3,3	0.40	0	2,2,2	0.34	0
3	EDO	D	407	-	3,3,3	0.43	0	2,2,2	0.29	0
3	EDO	F	401	-	3,3,3	0.52	0	2,2,2	0.22	0
3	EDO	C	402	-	3,3,3	0.48	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PO4	C	405	-	4,4,4	0.81	0	6,6,6	0.69	0
3	EDO	B	408	-	3,3,3	0.53	0	2,2,2	0.09	0
5	PO4	A	406	-	4,4,4	0.85	0	6,6,6	0.34	0
3	EDO	B	401	-	3,3,3	0.55	0	2,2,2	0.12	0
3	EDO	D	405	-	3,3,3	0.43	0	2,2,2	0.34	0
3	EDO	D	403	-	3,3,3	0.49	0	2,2,2	0.27	0
3	EDO	D	406	-	3,3,3	0.64	0	2,2,2	0.13	0
3	EDO	E	401	-	3,3,3	0.54	0	2,2,2	0.08	0
3	EDO	E	402	-	3,3,3	0.48	0	2,2,2	0.27	0
3	EDO	D	404	-	3,3,3	0.55	0	2,2,2	0.22	0
3	EDO	B	406	-	3,3,3	0.50	0	2,2,2	0.18	0
3	EDO	A	401	-	3,3,3	0.47	0	2,2,2	0.41	0
3	EDO	A	404	-	3,3,3	0.53	0	2,2,2	0.10	0
3	EDO	B	409	-	3,3,3	0.46	0	2,2,2	0.23	0
3	EDO	B	407	-	3,3,3	0.49	0	2,2,2	0.27	0
3	EDO	A	403	-	3,3,3	0.41	0	2,2,2	0.46	0
3	EDO	D	402	-	3,3,3	0.47	0	2,2,2	0.28	0
3	EDO	B	403	-	3,3,3	0.45	0	2,2,2	0.17	0
3	EDO	A	402	-	3,3,3	0.52	0	2,2,2	0.11	0
3	EDO	B	404	-	3,3,3	0.54	0	2,2,2	0.15	0
3	EDO	C	401	-	3,3,3	0.49	0	2,2,2	0.25	0
3	EDO	B	405	-	3,3,3	0.56	0	2,2,2	0.17	0
4	SAM	A	405	-	24,29,29	1.03	1 (4%)	23,42,42	1.50	6 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	E	404	-	-	1/1/1/1	-
3	EDO	B	402	-	-	1/1/1/1	-
4	SAM	C	404	-	-	8/12/33/33	0/3/3/3
3	EDO	C	403	-	-	1/1/1/1	-
3	EDO	D	401	-	-	0/1/1/1	-
3	EDO	E	403	-	-	1/1/1/1	-
3	EDO	D	407	-	-	1/1/1/1	-
3	EDO	F	401	-	-	1/1/1/1	-
3	EDO	C	402	-	-	1/1/1/1	-
3	EDO	B	408	-	-	0/1/1/1	-
3	EDO	B	401	-	-	1/1/1/1	-
3	EDO	D	405	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	403	-	-	1/1/1/1	-
3	EDO	D	406	-	-	1/1/1/1	-
3	EDO	E	401	-	-	1/1/1/1	-
3	EDO	E	402	-	-	1/1/1/1	-
3	EDO	D	404	-	-	1/1/1/1	-
3	EDO	B	406	-	-	1/1/1/1	-
3	EDO	A	401	-	-	0/1/1/1	-
3	EDO	A	404	-	-	0/1/1/1	-
3	EDO	B	409	-	-	1/1/1/1	-
3	EDO	B	407	-	-	1/1/1/1	-
3	EDO	A	403	-	-	1/1/1/1	-
3	EDO	D	402	-	-	0/1/1/1	-
3	EDO	B	403	-	-	1/1/1/1	-
3	EDO	A	402	-	-	1/1/1/1	-
3	EDO	B	404	-	-	0/1/1/1	-
3	EDO	C	401	-	-	1/1/1/1	-
3	EDO	B	405	-	-	1/1/1/1	-
4	SAM	A	405	-	-	5/12/33/33	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	SAM	C5-C4	2.40	1.47	1.40
4	C	404	SAM	C5-C4	2.36	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	405	SAM	N3-C2-N1	-3.66	122.96	128.68
4	C	404	SAM	N3-C2-N1	-3.64	122.99	128.68
4	A	405	SAM	CG-SD-C5'	2.71	110.31	103.40
4	C	404	SAM	C3'-C2'-C1'	2.55	104.82	100.98
4	A	405	SAM	C3'-C2'-C1'	2.23	104.34	100.98
4	A	405	SAM	C2-N1-C6	2.23	122.57	118.75
4	C	404	SAM	C2-N1-C6	2.14	122.42	118.75
4	C	404	SAM	C4-C5-N7	-2.12	107.19	109.40
4	A	405	SAM	C4-C5-N7	-2.11	107.20	109.40
4	C	404	SAM	CG-SD-C5'	2.09	108.75	103.40
4	A	405	SAM	N6-C6-N1	2.00	122.73	118.57

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	405	SAM	C-CA-CB-CG
4	A	405	SAM	CA-CB-CG-SD
4	C	404	SAM	O-C-CA-N
4	C	404	SAM	CA-CB-CG-SD
4	C	404	SAM	CB-CG-SD-CE
4	C	404	SAM	CB-CG-SD-C5'
4	C	404	SAM	OXT-C-CA-N
3	D	405	EDO	O1-C1-C2-O2
4	C	404	SAM	OXT-C-CA-CB
4	C	404	SAM	O-C-CA-CB
3	B	405	EDO	O1-C1-C2-O2
3	D	404	EDO	O1-C1-C2-O2
3	E	402	EDO	O1-C1-C2-O2
3	A	403	EDO	O1-C1-C2-O2
3	D	406	EDO	O1-C1-C2-O2
3	B	401	EDO	O1-C1-C2-O2
3	D	403	EDO	O1-C1-C2-O2
4	A	405	SAM	O4'-C4'-C5'-SD
4	A	405	SAM	OXT-C-CA-CB
3	A	402	EDO	O1-C1-C2-O2
3	B	403	EDO	O1-C1-C2-O2
3	B	406	EDO	O1-C1-C2-O2
3	B	409	EDO	O1-C1-C2-O2
3	C	403	EDO	O1-C1-C2-O2
4	A	405	SAM	O-C-CA-CB
3	E	404	EDO	O1-C1-C2-O2
3	F	401	EDO	O1-C1-C2-O2
3	B	402	EDO	O1-C1-C2-O2
3	B	407	EDO	O1-C1-C2-O2
3	C	401	EDO	O1-C1-C2-O2
3	E	401	EDO	O1-C1-C2-O2
3	E	403	EDO	O1-C1-C2-O2
3	C	402	EDO	O1-C1-C2-O2
3	D	407	EDO	O1-C1-C2-O2
4	C	404	SAM	O4'-C4'-C5'-SD

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	405	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	EDO	1	0
3	B	404	EDO	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SAM C 404

Ligand SAM A 405

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	360/396 (90%)	0.39	15 (4%)	36	29	45, 63, 91, 112	0
1	B	382/396 (96%)	0.51	34 (8%)	9	6	47, 65, 95, 126	0
1	C	360/396 (90%)	0.79	45 (12%)	3	2	50, 72, 104, 147	0
1	D	380/396 (95%)	0.41	23 (6%)	21	16	44, 60, 85, 109	0
2	E	306/327 (93%)	0.26	9 (2%)	51	45	53, 74, 99, 133	0
2	F	280/327 (85%)	1.23	72 (25%)	0	0	56, 113, 139, 154	0
All	All	2068/2238 (92%)	0.58	198 (9%)	8	5	44, 69, 120, 154	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	150	LYS	6.7
2	F	289	LEU	6.2
2	F	233	ILE	5.7
2	F	229	LEU	5.3
1	B	251	VAL	4.9
2	F	280	ARG	4.9
2	F	103	VAL	4.7
2	F	239	TRP	4.7
1	B	242	TYR	4.6
2	F	86	ARG	4.6
2	F	169	LEU	4.4
1	C	267	ILE	4.4
1	D	251	VAL	4.4
1	C	263	GLY	4.4
2	E	274	LEU	4.3
2	E	141	ILE	4.3
2	F	197	ASN	4.2
1	B	123	LEU	4.1
1	C	393	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
2	F	130	ASP	3.9
2	F	228	MET	3.9
1	C	34	CYS	3.8
2	F	205	TRP	3.8
1	C	266	ILE	3.8
1	A	279	GLY	3.8
1	C	326	HIS	3.7
1	C	265	LYS	3.7
1	B	266	ILE	3.7
2	F	220	CYS	3.7
2	F	295	GLY	3.7
2	F	144	PRO	3.7
1	B	214	CYS	3.6
2	F	68	HIS	3.6
2	F	143	ALA	3.6
2	F	278	ARG	3.5
2	F	301	ARG	3.5
2	F	51	ARG	3.5
1	D	262	THR	3.5
2	F	160	LEU	3.5
2	F	279	PRO	3.4
1	A	267	ILE	3.4
2	F	260	LEU	3.4
2	F	226	LYS	3.4
2	F	119	PHE	3.3
1	D	244	LEU	3.3
2	F	195	PHE	3.3
1	C	328	LEU	3.3
1	D	279	GLY	3.3
2	F	78	VAL	3.3
2	F	153	LEU	3.3
1	B	281	ALA	3.2
1	C	31	ASP	3.2
2	F	120	LEU	3.2
1	C	264	ARG	3.2
1	C	259	ALA	3.1
2	F	236	THR	3.1
1	B	279	GLY	3.1
1	B	263	GLY	3.1
2	F	293	GLY	3.1
2	F	167	ALA	3.1
2	F	127	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	168	VAL	3.0
1	C	242	TYR	3.0
2	E	205	TRP	3.0
1	B	280	GLY	3.0
2	F	137	ARG	3.0
1	D	263	GLY	3.0
1	B	276	ALA	3.0
1	B	278	GLY	3.0
1	A	214	CYS	3.0
2	F	258	PHE	3.0
2	F	170	ARG	3.0
1	C	33	ILE	2.9
1	C	280	GLY	2.9
1	D	278	GLY	2.9
2	F	50	ARG	2.9
1	C	114	SER	2.9
1	C	268	VAL	2.9
2	F	198	LYS	2.9
1	C	261	LEU	2.9
1	C	281	ALA	2.9
2	E	164	LEU	2.9
2	F	41	ASN	2.9
1	C	395	TYR	2.8
1	C	66	LEU	2.8
1	C	269	ASP	2.8
2	F	109	LEU	2.8
2	F	146	ASN	2.7
1	B	267	ILE	2.7
1	D	58	THR	2.7
1	C	394	LYS	2.7
1	C	35	ASP	2.7
2	F	44	ALA	2.7
2	F	49	PHE	2.7
1	B	236	LEU	2.7
2	F	284	LEU	2.7
2	F	202	MET	2.7
2	F	259	ASN	2.6
1	B	273	GLY	2.6
1	D	383	ASP	2.6
1	A	362	ARG	2.6
2	F	87	ARG	2.6
1	C	283	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	280	GLY	2.6
1	B	213	VAL	2.6
2	F	157	LYS	2.6
1	C	260	GLY	2.6
2	F	83	ALA	2.5
1	C	270	THR	2.5
2	F	257	ALA	2.5
1	D	280	GLY	2.5
1	B	393	LEU	2.5
2	F	204	HIS	2.5
2	F	74	PHE	2.5
2	F	133	ASN	2.5
2	F	142	PRO	2.5
1	A	268	VAL	2.4
1	B	259	ALA	2.4
1	D	228	LYS	2.4
2	F	254	ILE	2.4
1	C	30	PRO	2.4
1	B	395	TYR	2.4
1	B	272	GLY	2.4
1	C	58	THR	2.4
1	C	376	ALA	2.4
1	D	281	ALA	2.4
1	D	212	GLU	2.4
1	A	321	ALA	2.4
1	D	291	ASP	2.4
2	F	105	ALA	2.4
2	E	248	TYR	2.3
2	F	148	TYR	2.3
1	B	226	VAL	2.3
1	C	213	VAL	2.3
2	F	135	PRO	2.3
1	A	115	PRO	2.3
1	A	266	ILE	2.3
1	D	249	ARG	2.3
2	F	90	VAL	2.3
2	F	224	ALA	2.3
1	A	264	ARG	2.2
1	B	275	GLY	2.2
1	C	59	VAL	2.2
1	A	262	THR	2.2
2	F	56	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	275	GLY	2.2
1	C	349	VAL	2.2
1	C	362	ARG	2.2
2	E	280	ARG	2.2
1	A	261	LEU	2.2
1	D	222	LEU	2.2
1	B	231	VAL	2.2
1	B	268	VAL	2.2
2	E	49	PHE	2.2
1	B	216	ASP	2.2
1	B	271	TYR	2.2
1	C	74	ARG	2.2
1	C	276	ALA	2.2
1	B	220	ASP	2.2
1	D	55	ALA	2.2
1	C	278	GLY	2.2
1	D	248	GLY	2.2
2	F	261	PRO	2.2
2	F	61	LEU	2.2
1	B	171	GLY	2.1
2	F	85	GLU	2.1
1	B	34	CYS	2.1
1	B	212	GLU	2.1
1	C	217	GLU	2.1
2	F	84	ALA	2.1
1	C	212	GLU	2.1
1	C	352	ASN	2.1
1	C	348	ILE	2.1
2	E	301	ARG	2.1
2	F	147	LEU	2.1
2	F	237	PHE	2.1
1	D	277	HIS	2.1
2	F	264	HIS	2.1
1	D	238	GLU	2.1
1	B	269	ASP	2.1
2	F	256	ASP	2.1
1	D	137	LEU	2.1
1	C	262	THR	2.1
1	A	34	CYS	2.1
1	D	242	TYR	2.0
1	A	273	GLY	2.0
1	D	250	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	64	MET	2.0
1	B	265	LYS	2.0
1	B	283	SER	2.0
2	F	288	LYS	2.0
1	B	250	PHE	2.0
1	B	264	ARG	2.0
1	C	271	TYR	2.0
1	D	343	ARG	2.0
2	E	160	LEU	2.0
1	C	211	GLU	2.0
1	C	76	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	PO4	A	406	5/5	0.69	0.56	113,116,126,129	0
3	EDO	F	401	4/4	0.71	0.17	91,94,95,95	0
3	EDO	E	404	4/4	0.75	0.25	88,89,90,96	0
3	EDO	D	404	4/4	0.76	0.28	80,86,86,87	0
3	EDO	A	403	4/4	0.76	0.28	69,70,71,73	0
3	EDO	A	401	4/4	0.79	0.41	77,80,86,86	0
3	EDO	D	406	4/4	0.81	0.64	63,67,69,73	0
3	EDO	E	402	4/4	0.83	0.18	97,97,98,99	0
3	EDO	C	403	4/4	0.85	0.26	95,96,97,99	0
3	EDO	D	402	4/4	0.85	0.19	85,87,88,88	0
3	EDO	B	406	4/4	0.85	0.72	82,86,87,87	0
3	EDO	B	407	4/4	0.85	0.89	85,89,89,91	0

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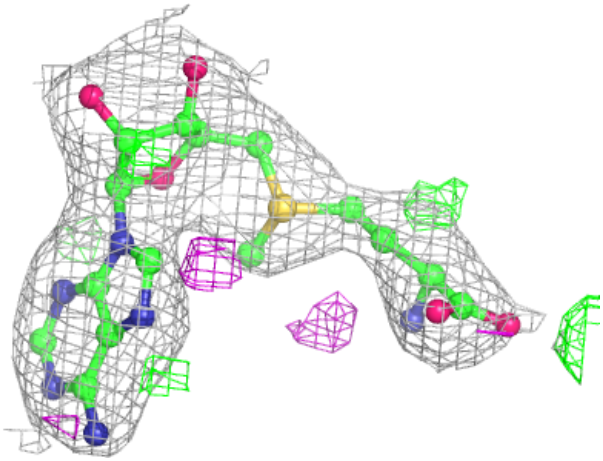
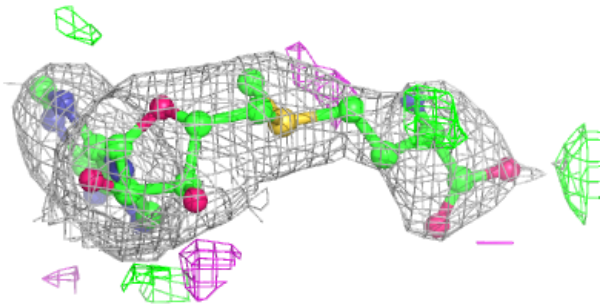
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	B	401	4/4	0.86	0.38	68,78,78,83	0
3	EDO	D	403	4/4	0.86	0.14	78,80,81,82	0
3	EDO	D	405	4/4	0.87	0.37	72,76,80,86	0
3	EDO	B	404	4/4	0.87	0.49	68,71,73,76	0
3	EDO	B	409	4/4	0.87	0.37	83,83,83,88	0
3	EDO	B	402	4/4	0.88	0.24	79,83,87,94	0
5	PO4	C	405	5/5	0.88	0.40	82,87,94,99	0
3	EDO	B	408	4/4	0.89	0.51	72,72,73,76	0
3	EDO	D	401	4/4	0.89	0.21	88,88,89,89	0
3	EDO	B	405	4/4	0.90	0.27	77,83,84,86	0
3	EDO	E	403	4/4	0.91	0.22	71,71,73,73	0
4	SAM	C	404	27/27	0.91	0.25	56,66,82,84	0
3	EDO	A	404	4/4	0.92	0.23	73,79,81,84	0
3	EDO	C	402	4/4	0.92	0.22	77,82,83,88	0
6	MG	B	410	1/1	0.92	0.22	60,60,60,60	0
3	EDO	D	407	4/4	0.93	0.34	78,82,85,89	0
3	EDO	E	401	4/4	0.93	0.22	66,72,72,75	0
3	EDO	A	402	4/4	0.94	0.22	68,69,71,71	0
4	SAM	A	405	27/27	0.94	0.19	54,62,83,94	0
3	EDO	C	401	4/4	0.95	0.55	71,72,72,73	0
3	EDO	B	403	4/4	0.95	0.20	64,65,65,67	0

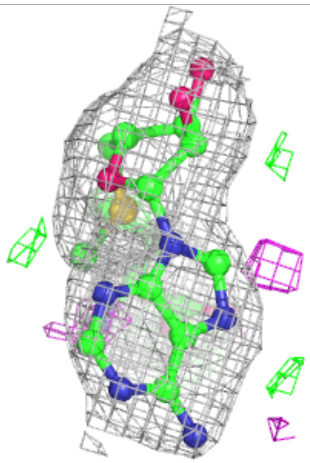
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SAM C 404:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

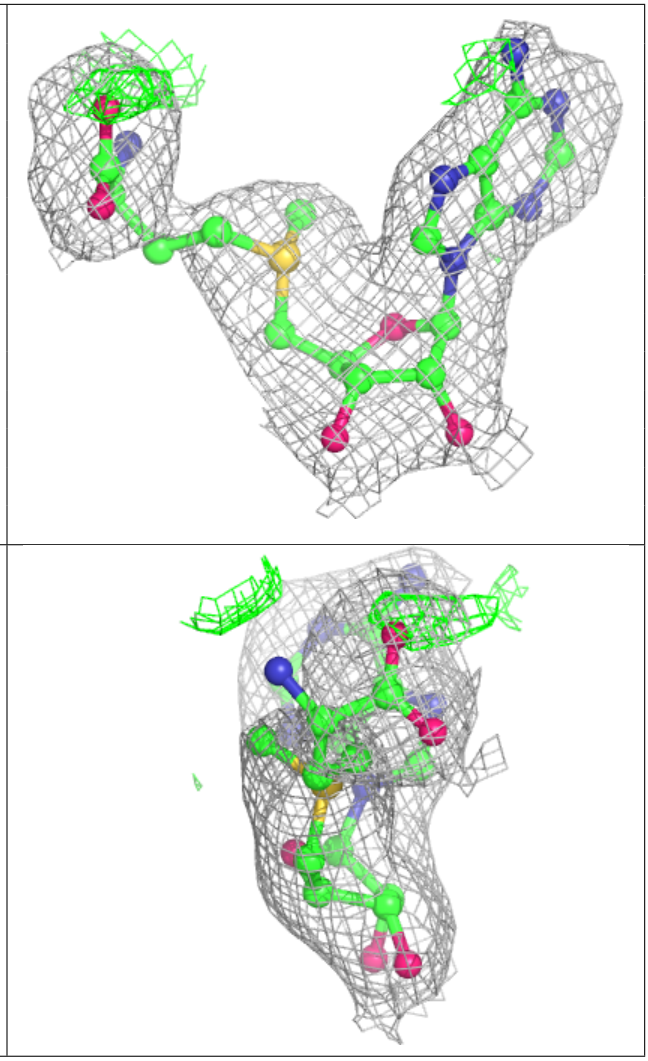






Electron density around SAM A 405:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.