



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:26 am GMT

PDB ID : 4KTT  
Title : Structural insights of MAT enzymes: MATa2b complexed with SAM  
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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](mailto: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.

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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

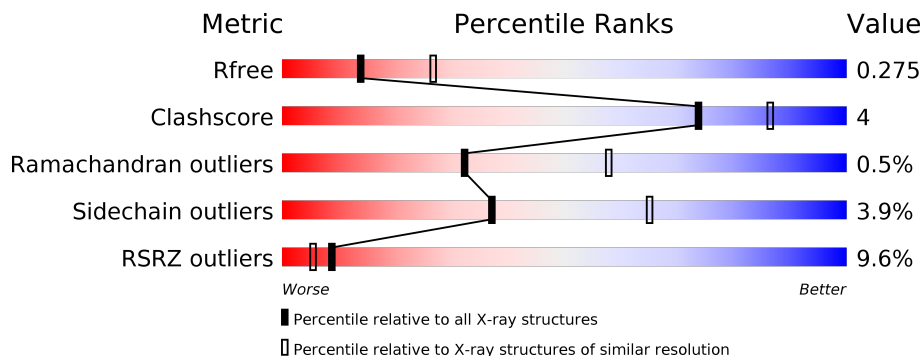
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	396	<div> <div>4%</div> <div>83% 7% 9%</div> </div>
1	B	396	<div> <div>9%</div> <div>84% 12% . .</div> </div>
1	C	396	<div> <div>11%</div> <div>77% 13% . 9%</div> </div>
1	D	396	<div> <div>6%</div> <div>85% 11% . .</div> </div>
2	E	327	<div> <div>3%</div> <div>80% 13% . 6%</div> </div>
2	F	327	<div> <div>22%</div> <div>73% 11% . 14%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	401	-	-	-	X
3	EDO	A	403	-	-	-	X
3	EDO	B	401	-	-	-	X
3	EDO	B	404	-	-	-	X
3	EDO	B	406	-	-	-	X
3	EDO	B	407	-	-	-	X
3	EDO	B	408	-	-	-	X
3	EDO	B	409	-	-	-	X
3	EDO	C	401	-	-	-	X
3	EDO	C	403	-	-	-	X
3	EDO	D	405	-	-	-	X
3	EDO	D	406	-	-	-	X
3	EDO	D	407	-	-	-	X
3	EDO	E	401	-	-	-	X
3	EDO	E	403	-	-	-	X
3	EDO	E	404	-	-	-	X
5	PO4	A	406	-	-	-	X

## 2 Entry composition

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
1	A	360	Total	C	N	O	S	0	0	0
			2811	1783	490	527	11			
1	B	382	Total	C	N	O	S	0	0	0
			2972	1877	519	565	11			
1	C	360	Total	C	N	O	S	0	0	0
			2813	1784	490	528	11			
1	D	380	Total	C	N	O	S	0	0	0
			2954	1867	517	559	11			

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
2	E	306	Total	C	N	O	S	0	0	0
			2429	1533	443	443	10			
2	F	280	Total	C	N	O	S	0	0	0
			2237	1418	406	403	10			

There are 8 discrepancies between the modelled and reference sequences:

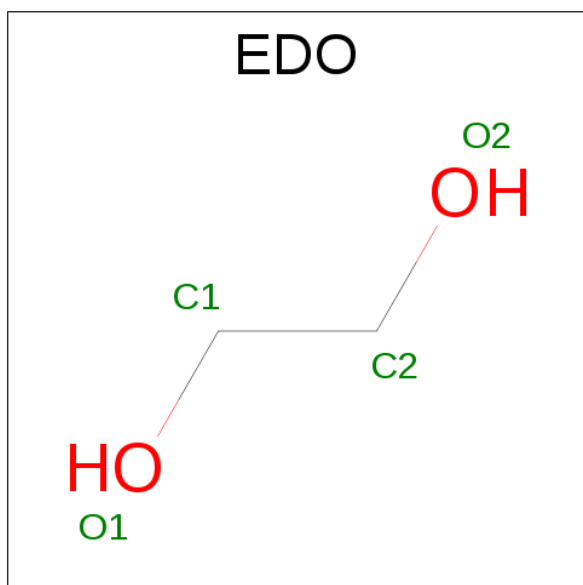
Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	EXPRESSION TAG	UNP Q9NZL9
E	-2	SER	-	EXPRESSION TAG	UNP Q9NZL9
E	-1	HIS	-	EXPRESSION TAG	UNP Q9NZL9
E	0	MET	-	EXPRESSION TAG	UNP Q9NZL9

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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:  $C_2H_6O_2$ ).



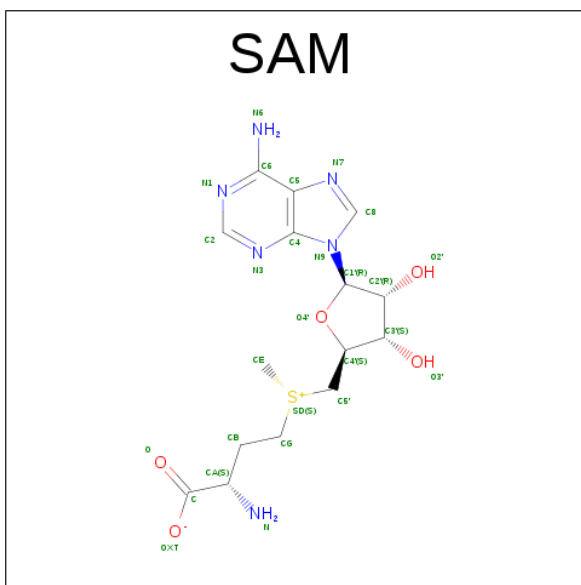
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

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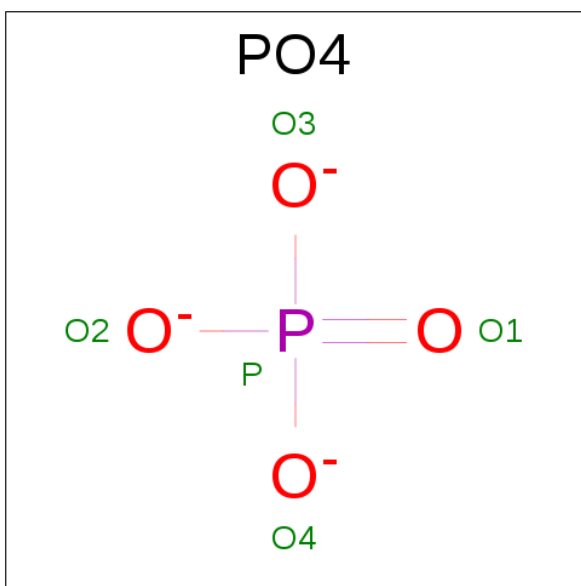
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total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

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C<sub>15</sub>H<sub>22</sub>N<sub>6</sub>O<sub>5</sub>S).



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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $\text{O}_4\text{P}$ ).



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

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

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

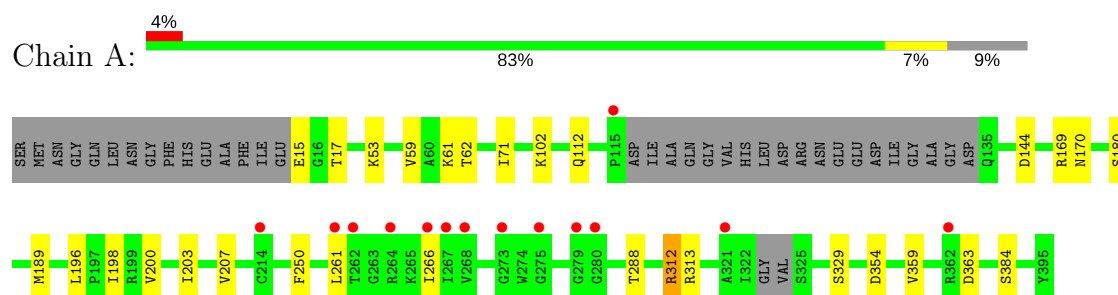
- Molecule 7 is water.

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

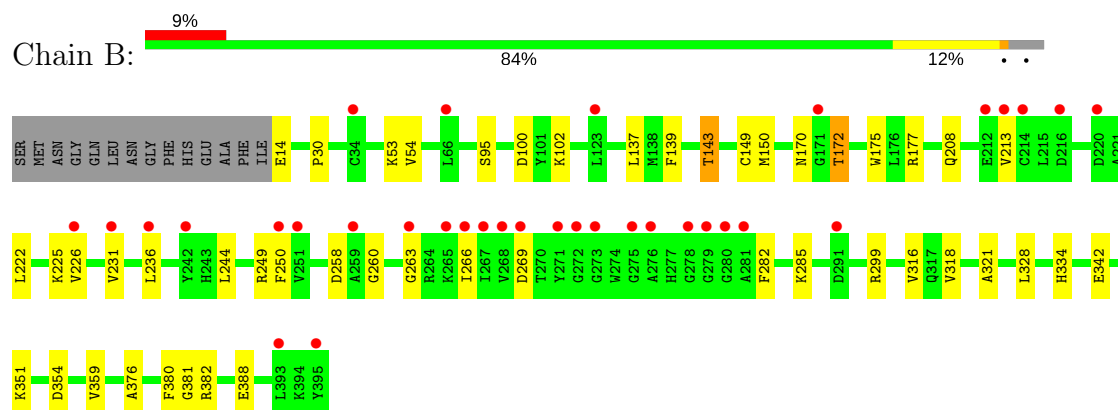
### 3 Residue-property plots [i](#)

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

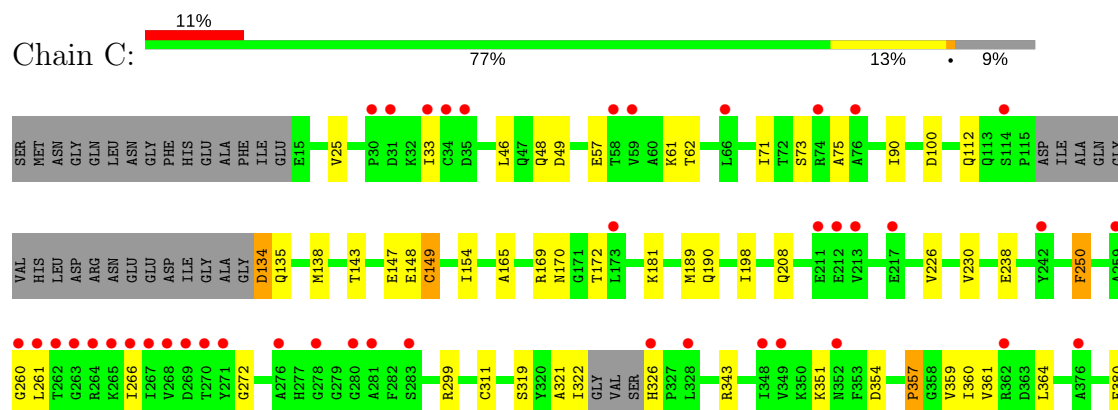
#### • Molecule 1: S-adenosylmethionine synthase isoform type-2

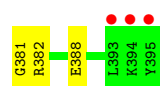


#### • Molecule 1: S-adenosylmethionine synthase isoform type-2

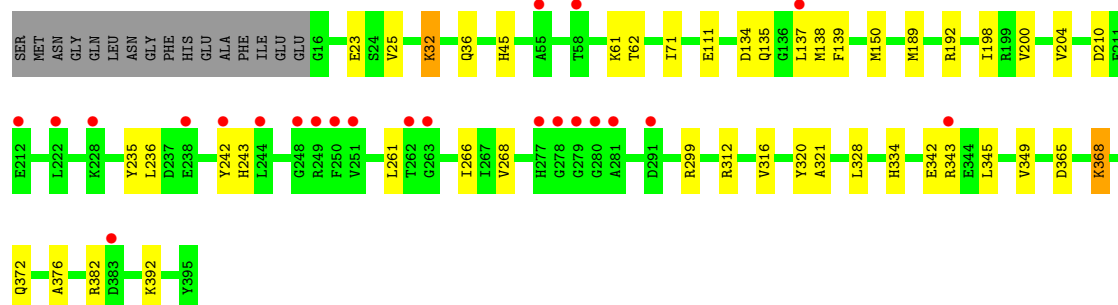
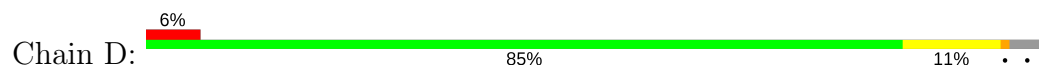


#### • Molecule 1: S-adenosylmethionine synthase isoform type-2

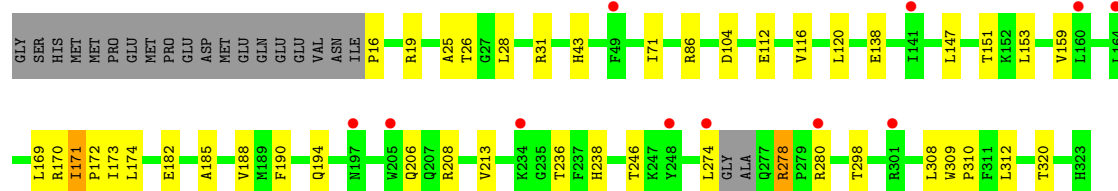
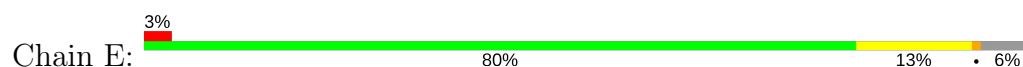




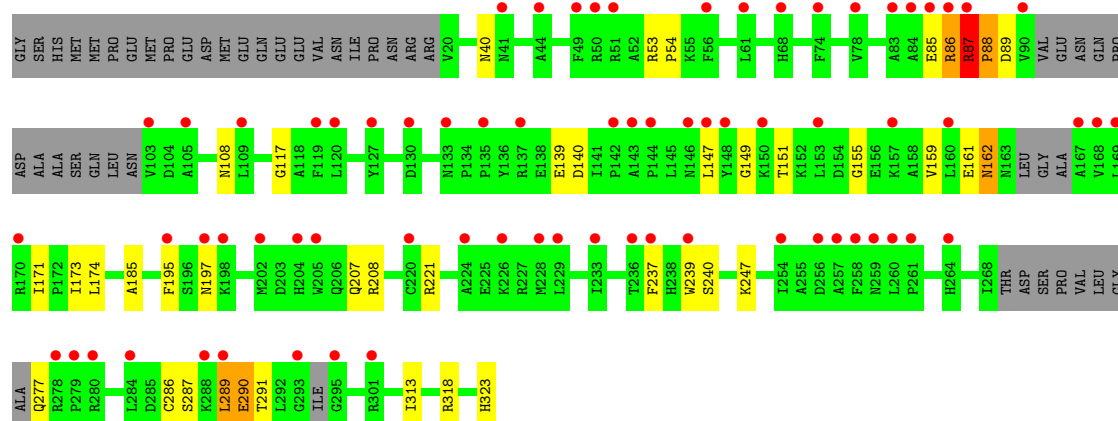
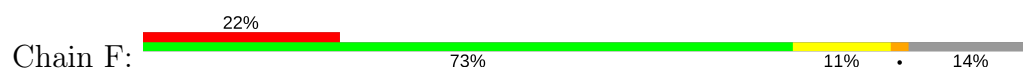
- Molecule 1: S-adenosylmethionine synthase isoform type-2



- Molecule 2: Methionine adenosyltransferase 2 subunit beta



- Molecule 2: Methionine adenosyltransferase 2 subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.10 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.218 , 0.279 0.217 , 0.275	Depositor DCC
$R_{free}$ test set	3847 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.9	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PO4, MG, SAM, EDO

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(°)	Ideal(°)
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

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:O	2:E:116:VAL:HG12	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
2:E:138:GLU:OE2	2:E:238:HIS:N	2.49	0.43
1:A:313:ARG:NH2	2:F:323:HIS:O	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
2:F:87:ARG:O	2:F:89:ASP:HB2	2.21	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
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:269:ASP:OD2	3:B:404:EDO:H11	2.22	0.40
1:B:95:SER:OG	1:C:100:ASP:OD2	2.26	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%)	44	70
1	C	354/396 (89%)	335 (95%)	18 (5%)	1 (0%)	44	70
1	D	378/396 (96%)	362 (96%)	15 (4%)	1 (0%)	44	70
2	E	302/327 (92%)	287 (95%)	14 (5%)	1 (0%)	44	70
2	F	270/327 (83%)	237 (88%)	27 (10%)	6 (2%)	8	14
All	All	2038/2238 (91%)	1920 (94%)	108 (5%)	10 (0%)	32	58

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 ⓘ

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%)	50	77
1	B	317/328 (97%)	306 (96%)	11 (4%)	41	68
1	C	301/328 (92%)	285 (95%)	16 (5%)	26	50
1	D	315/328 (96%)	309 (98%)	6 (2%)	62	84
2	E	260/279 (93%)	248 (95%)	12 (5%)	31	58
2	F	239/279 (86%)	225 (94%)	14 (6%)	23	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1733/1870 (93%)	1666 (96%)	67 (4%)	37 65

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

Some 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 carbohydrates 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	A	401	-	3,3,3	0.47	0	2,2,2	0.43	0
3	EDO	A	402	-	3,3,3	0.52	0	2,2,2	0.13	0
3	EDO	A	403	-	3,3,3	0.40	0	2,2,2	0.49	0
3	EDO	A	404	-	3,3,3	0.52	0	2,2,2	0.12	0
4	SAM	A	405	-	21,29,29	1.79	2 (9%)	17,42,42	2.00	3 (17%)
5	PO4	A	406	-	4,4,4	0.77	0	6,6,6	0.31	0
3	EDO	B	401	-	3,3,3	0.54	0	2,2,2	0.10	0
3	EDO	B	402	-	3,3,3	0.42	0	2,2,2	0.41	0
3	EDO	B	403	-	3,3,3	0.44	0	2,2,2	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	B	404	-	3,3,3	0.53	0	2,2,2	0.14	0
3	EDO	B	405	-	3,3,3	0.55	0	2,2,2	0.19	0
3	EDO	B	406	-	3,3,3	0.49	0	2,2,2	0.21	0
3	EDO	B	407	-	3,3,3	0.48	0	2,2,2	0.29	0
3	EDO	B	408	-	3,3,3	0.52	0	2,2,2	0.11	0
3	EDO	B	409	-	3,3,3	0.46	0	2,2,2	0.26	0
3	EDO	C	401	-	3,3,3	0.49	0	2,2,2	0.27	0
3	EDO	C	402	-	3,3,3	0.47	0	2,2,2	0.32	0
3	EDO	C	403	-	3,3,3	0.49	0	2,2,2	0.08	0
4	SAM	C	404	-	21,29,29	1.61	2 (9%)	17,42,42	2.01	3 (17%)
5	PO4	C	405	-	4,4,4	0.67	0	6,6,6	0.61	0
3	EDO	D	401	-	3,3,3	0.49	0	2,2,2	0.26	0
3	EDO	D	402	-	3,3,3	0.46	0	2,2,2	0.30	0
3	EDO	D	403	-	3,3,3	0.49	0	2,2,2	0.29	0
3	EDO	D	404	-	3,3,3	0.54	0	2,2,2	0.22	0
3	EDO	D	405	-	3,3,3	0.42	0	2,2,2	0.36	0
3	EDO	D	406	-	3,3,3	0.63	0	2,2,2	0.12	0
3	EDO	D	407	-	3,3,3	0.43	0	2,2,2	0.31	0
3	EDO	E	401	-	3,3,3	0.53	0	2,2,2	0.06	0
3	EDO	E	402	-	3,3,3	0.47	0	2,2,2	0.30	0
3	EDO	E	403	-	3,3,3	0.40	0	2,2,2	0.37	0
3	EDO	E	404	-	3,3,3	0.48	0	2,2,2	0.14	0
3	EDO	F	401	-	3,3,3	0.52	0	2,2,2	0.25	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
3	EDO	A	401	-	-	0/1/1/1	0/0/0/0
3	EDO	A	402	-	-	0/1/1/1	0/0/0/0
3	EDO	A	403	-	-	0/1/1/1	0/0/0/0
3	EDO	A	404	-	-	0/1/1/1	0/0/0/0
4	SAM	A	405	-	-	0/8/33/33	0/3/3/3
5	PO4	A	406	-	-	0/0/0/0	0/0/0/0
3	EDO	B	401	-	-	0/1/1/1	0/0/0/0
3	EDO	B	402	-	-	0/1/1/1	0/0/0/0
3	EDO	B	403	-	-	0/1/1/1	0/0/0/0
3	EDO	B	404	-	-	0/1/1/1	0/0/0/0
3	EDO	B	405	-	-	0/1/1/1	0/0/0/0
3	EDO	B	406	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	407	-	-	0/1/1/1	0/0/0/0
3	EDO	B	408	-	-	0/1/1/1	0/0/0/0
3	EDO	B	409	-	-	0/1/1/1	0/0/0/0
3	EDO	C	401	-	-	0/1/1/1	0/0/0/0
3	EDO	C	402	-	-	0/1/1/1	0/0/0/0
3	EDO	C	403	-	-	0/1/1/1	0/0/0/0
4	SAM	C	404	-	-	0/8/33/33	0/3/3/3
5	PO4	C	405	-	-	0/0/0/0	0/0/0/0
3	EDO	D	401	-	-	0/1/1/1	0/0/0/0
3	EDO	D	402	-	-	0/1/1/1	0/0/0/0
3	EDO	D	403	-	-	0/1/1/1	0/0/0/0
3	EDO	D	404	-	-	0/1/1/1	0/0/0/0
3	EDO	D	405	-	-	0/1/1/1	0/0/0/0
3	EDO	D	406	-	-	0/1/1/1	0/0/0/0
3	EDO	D	407	-	-	0/1/1/1	0/0/0/0
3	EDO	E	401	-	-	0/1/1/1	0/0/0/0
3	EDO	E	402	-	-	0/1/1/1	0/0/0/0
3	EDO	E	403	-	-	0/1/1/1	0/0/0/0
3	EDO	E	404	-	-	0/1/1/1	0/0/0/0
3	EDO	F	401	-	-	0/1/1/1	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	SAM	CG-SD	-6.64	1.66	1.80
4	C	404	SAM	CG-SD	-5.24	1.69	1.80
4	C	404	SAM	C5-C4	2.96	1.47	1.40
4	A	405	SAM	C5-C4	3.01	1.47	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	SAM	N3-C2-N1	-6.77	122.96	128.86
4	C	404	SAM	N3-C2-N1	-6.74	122.99	128.86
4	C	404	SAM	C4-C5-N7	-2.29	107.19	109.41
4	A	405	SAM	C4-C5-N7	-2.28	107.20	109.41
4	C	404	SAM	C2-N1-C6	2.09	122.42	118.77
4	A	405	SAM	C2-N1-C6	2.17	122.57	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	EDO	1	0
3	B	404	EDO	3	0
3	D	405	EDO	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	360/396 (90%)	0.39	14 (3%)	40 32	45, 63, 91, 112	0
1	B	382/396 (96%)	0.51	34 (8%)	10 6	47, 65, 95, 126	0
1	C	360/396 (90%)	0.79	45 (12%)	4 2	50, 72, 104, 147	0
1	D	380/396 (95%)	0.41	23 (6%)	22 16	44, 60, 85, 109	0
2	E	306/327 (93%)	0.26	11 (3%)	43 35	53, 74, 99, 133	0
2	F	280/327 (85%)	1.23	72 (25%)	1 0	56, 113, 139, 154	0
All	All	2068/2238 (92%)	0.58	199 (9%)	9 5	44, 69, 120, 154	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	150	LYS	6.8
2	F	289	LEU	6.4
2	F	233	ILE	5.7
2	F	229	LEU	5.4
2	F	280	ARG	5.0
1	B	251	VAL	4.9
1	B	242	TYR	4.7
2	F	239	TRP	4.7
2	F	103	VAL	4.6
2	F	86	ARG	4.5
1	C	263	GLY	4.4
2	F	169	LEU	4.4
1	D	251	VAL	4.4
2	E	274	LEU	4.3
1	C	267	ILE	4.3
1	B	123	LEU	4.1
2	E	141	ILE	4.1
2	F	197	ASN	4.1
2	F	220	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	279	GLY	3.8
2	F	130	ASP	3.8
1	C	266	ILE	3.8
1	C	34	CYS	3.8
2	F	228	MET	3.8
1	C	393	LEU	3.7
1	B	266	ILE	3.7
2	F	68	HIS	3.7
1	C	265	LYS	3.7
2	F	144	PRO	3.7
2	F	295	GLY	3.7
2	F	205	TRP	3.6
1	B	214	CYS	3.6
2	F	143	ALA	3.6
1	A	267	ILE	3.5
2	F	51	ARG	3.5
1	D	262	THR	3.5
2	F	278	ARG	3.5
2	F	301	ARG	3.5
2	F	279	PRO	3.4
1	C	326	HIS	3.4
2	F	195	PHE	3.4
2	F	226	LYS	3.4
1	D	279	GLY	3.3
2	F	153	LEU	3.3
1	C	328	LEU	3.2
2	F	260	LEU	3.2
2	F	236	THR	3.2
1	C	264	ARG	3.2
1	C	31	ASP	3.2
2	F	160	LEU	3.2
1	A	214	CYS	3.2
1	D	244	LEU	3.2
1	B	281	ALA	3.2
1	C	259	ALA	3.2
1	C	242	TYR	3.1
2	F	120	LEU	3.1
1	B	263	GLY	3.1
2	F	258	PHE	3.1
2	F	78	VAL	3.1
1	B	279	GLY	3.1
2	F	167	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	119	PHE	3.0
1	C	114	SER	3.0
2	E	164	LEU	3.0
2	F	293	GLY	3.0
2	F	50	ARG	3.0
2	F	168	VAL	3.0
1	B	280	GLY	3.0
2	F	170	ARG	3.0
2	E	205	TRP	3.0
1	B	278	GLY	3.0
2	F	137	ARG	3.0
1	B	276	ALA	3.0
2	F	127	TYR	2.9
1	C	280	GLY	2.9
1	D	278	GLY	2.9
1	D	263	GLY	2.9
1	C	33	ILE	2.9
1	C	261	LEU	2.9
1	C	281	ALA	2.9
2	F	198	LYS	2.9
2	F	41	ASN	2.8
1	C	268	VAL	2.8
1	C	395	TYR	2.8
2	F	83	ALA	2.8
1	D	58	THR	2.7
1	C	269	ASP	2.7
2	F	146	ASN	2.7
1	B	273	GLY	2.7
1	C	35	ASP	2.7
1	B	213	VAL	2.7
1	C	66	LEU	2.7
1	B	267	ILE	2.7
1	C	394	LYS	2.7
2	F	44	ALA	2.6
2	F	87	ARG	2.6
2	F	109	LEU	2.6
2	F	284	LEU	2.6
1	D	383	ASP	2.6
1	D	280	GLY	2.6
2	F	49	PHE	2.6
1	A	280	GLY	2.6
1	B	236	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	283	SER	2.6
2	F	259	ASN	2.6
1	A	362	ARG	2.6
1	C	260	GLY	2.6
1	C	270	THR	2.5
2	F	257	ALA	2.5
1	C	30	PRO	2.5
1	B	393	LEU	2.5
2	F	204	HIS	2.5
2	F	133	ASN	2.5
1	A	321	ALA	2.5
2	F	74	PHE	2.5
2	F	135	PRO	2.5
2	F	142	PRO	2.5
1	A	268	VAL	2.4
1	B	259	ALA	2.4
2	F	148	TYR	2.4
2	F	254	ILE	2.4
1	C	58	THR	2.4
1	D	281	ALA	2.4
2	F	157	LYS	2.4
2	F	202	MET	2.4
1	B	272	GLY	2.4
1	A	115	PRO	2.4
1	B	395	TYR	2.4
2	F	105	ALA	2.4
1	B	226	VAL	2.4
1	C	362	ARG	2.4
1	C	376	ALA	2.4
1	D	228	LYS	2.3
1	D	249	ARG	2.3
1	D	291	ASP	2.3
1	A	264	ARG	2.3
2	F	90	VAL	2.3
2	F	84	ALA	2.3
1	D	212	GLU	2.3
2	F	224	ALA	2.3
1	C	213	VAL	2.3
1	A	266	ILE	2.3
1	C	348	ILE	2.3
2	E	248	TYR	2.3
1	C	349	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	262	THR	2.3
1	B	216	ASP	2.2
1	D	55	ALA	2.2
1	A	261	LEU	2.2
1	D	222	LEU	2.2
1	C	212	GLU	2.2
2	F	237	PHE	2.2
2	E	280	ARG	2.2
2	F	61	LEU	2.2
1	B	271	TYR	2.2
1	B	275	GLY	2.2
1	C	59	VAL	2.2
2	F	56	PHE	2.2
1	C	352	ASN	2.2
1	B	231	VAL	2.2
2	F	261	PRO	2.2
1	B	268	VAL	2.2
1	B	212	GLU	2.2
2	F	264	HIS	2.2
1	B	220	ASP	2.2
2	F	256	ASP	2.2
2	E	301	ARG	2.2
1	C	276	ALA	2.1
1	A	275	GLY	2.1
1	C	74	ARG	2.1
1	C	278	GLY	2.1
2	F	85	GLU	2.1
1	B	34	CYS	2.1
1	D	250	PHE	2.1
2	E	49	PHE	2.1
1	D	137	LEU	2.1
2	F	147	LEU	2.1
1	D	277	HIS	2.1
1	C	262	THR	2.1
1	B	269	ASP	2.1
1	D	248	GLY	2.1
1	C	76	ALA	2.1
1	B	265	LYS	2.1
1	B	291	ASP	2.1
1	B	250	PHE	2.1
2	E	160	LEU	2.1
1	C	271	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	173	LEU	2.0
1	C	217	GLU	2.0
1	A	273	GLY	2.0
1	B	171	GLY	2.0
2	E	234	LYS	2.0
1	D	242	TYR	2.0
2	E	197	ASN	2.0
1	D	343	ARG	2.0
1	B	66	LEU	2.0
1	C	211	GLU	2.0
1	D	238	GLU	2.0
2	F	288	LYS	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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	EDO	D	406	4/4	0.81	0.65	15.52	63,67,69,73	0
3	EDO	B	409	4/4	0.87	0.36	15.21	83,83,83,88	0
3	EDO	B	407	4/4	0.86	0.89	8.70	85,89,89,91	0
3	EDO	A	401	4/4	0.78	0.41	7.37	77,80,86,86	0
3	EDO	B	406	4/4	0.86	0.72	6.80	82,86,87,87	0
3	EDO	C	401	4/4	0.95	0.55	6.65	71,72,72,73	0
3	EDO	D	407	4/4	0.93	0.33	6.12	78,82,85,89	0
3	EDO	D	405	4/4	0.87	0.36	6.01	72,76,80,86	0
5	PO4	A	406	5/5	0.70	0.56	4.95	113,116,126,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	B	401	4/4	0.86	0.38	4.66	68,78,78,83	0
3	EDO	B	408	4/4	0.88	0.51	4.31	72,72,73,76	0
3	EDO	A	403	4/4	0.75	0.28	3.98	69,70,71,73	0
3	EDO	B	404	4/4	0.87	0.48	3.31	68,71,73,76	0
3	EDO	E	403	4/4	0.91	0.22	3.23	71,71,73,73	0
3	EDO	E	404	4/4	0.75	0.25	2.56	88,89,90,96	0
3	EDO	C	403	4/4	0.84	0.26	2.34	95,96,97,99	0
3	EDO	E	401	4/4	0.93	0.23	2.06	66,72,72,75	0
3	EDO	B	405	4/4	0.90	0.28	1.98	77,83,84,86	0
3	EDO	A	402	4/4	0.94	0.22	1.87	68,69,71,71	0
3	EDO	D	404	4/4	0.76	0.27	1.78	80,86,86,87	0
3	EDO	A	404	4/4	0.91	0.22	1.44	73,79,81,84	0
3	EDO	B	402	4/4	0.88	0.24	1.22	79,83,87,94	0
4	SAM	C	404	27/27	0.91	0.25	0.99	56,66,82,84	0
3	EDO	B	403	4/4	0.95	0.20	0.94	64,65,65,67	0
3	EDO	D	401	4/4	0.88	0.21	0.82	88,88,89,89	0
5	PO4	C	405	5/5	0.88	0.39	0.78	82,87,94,99	0
4	SAM	A	405	27/27	0.94	0.19	0.77	54,62,83,94	0
3	EDO	D	402	4/4	0.85	0.19	0.32	85,87,88,88	0
3	EDO	C	402	4/4	0.92	0.21	-0.37	77,82,83,88	0
6	MG	B	410	1/1	0.93	0.22	-1.28	60,60,60,60	0
3	EDO	D	403	4/4	0.86	0.14	-	78,80,81,82	0
3	EDO	E	402	4/4	0.82	0.18	-	97,97,98,99	0
3	EDO	F	401	4/4	0.71	0.16	-	91,94,95,95	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.