



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2014 – 06:44 AM EDT

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 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/ValidationPDFNotes.html>

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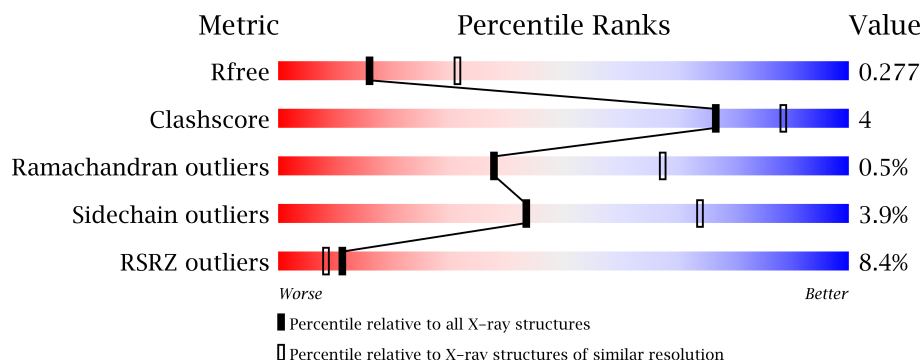
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23489  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	396	
1	B	396	
1	C	396	
1	D	396	
2	E	327	
2	F	327	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	EDO	A	401	-	X
3	EDO	A	402	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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	D	401	-	X
3	EDO	D	403	-	X
3	EDO	D	405	-	X
3	EDO	D	406	-	X
3	EDO	D	407	-	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 hydrogen and 0 are deuterium.

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:

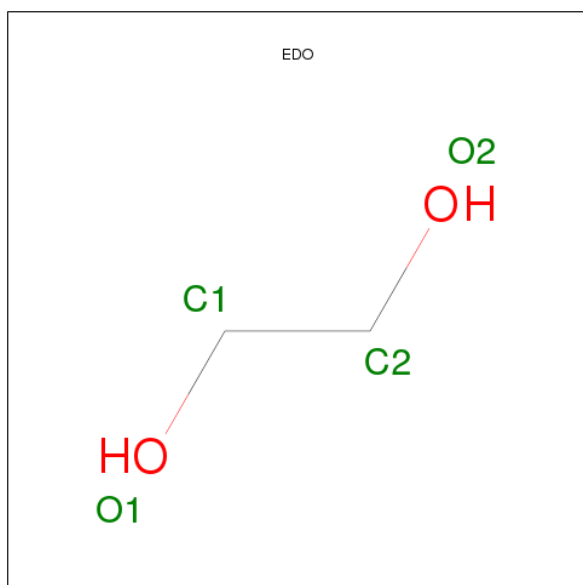
Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	EXPRESSION TAG	UNP Q9NZL9
E	-2	SER	-	EXPRESSION TAG	UNP Q9NZL9
E	-1	HIS	-	EXPRESSION TAG	UNP Q9NZL9
E	0	MET	-	EXPRESSION TAG	UNP Q9NZL9

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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:  $C_2H_6O_2$ ).



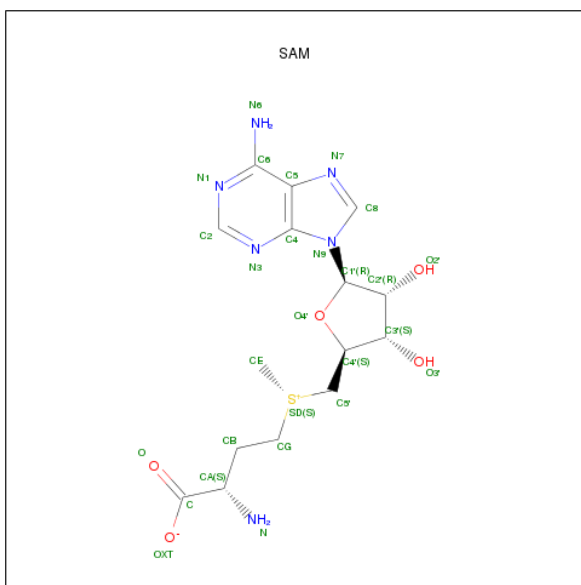
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

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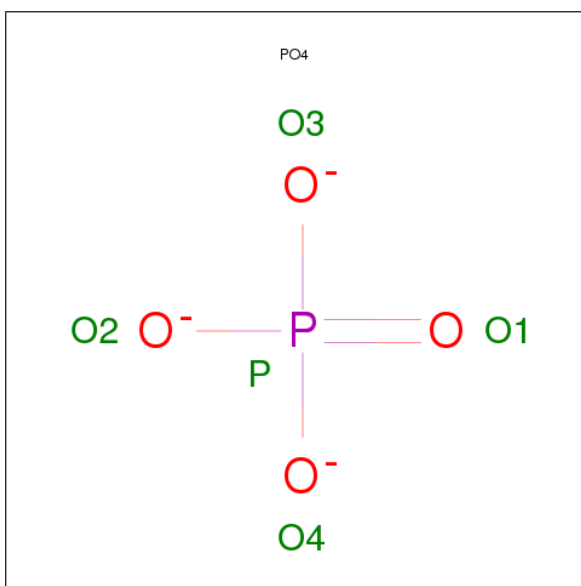
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0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

- 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	C	N	O	S	0	0
			27	15	6	5	1		
4	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

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

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

- Molecule 7 is water.

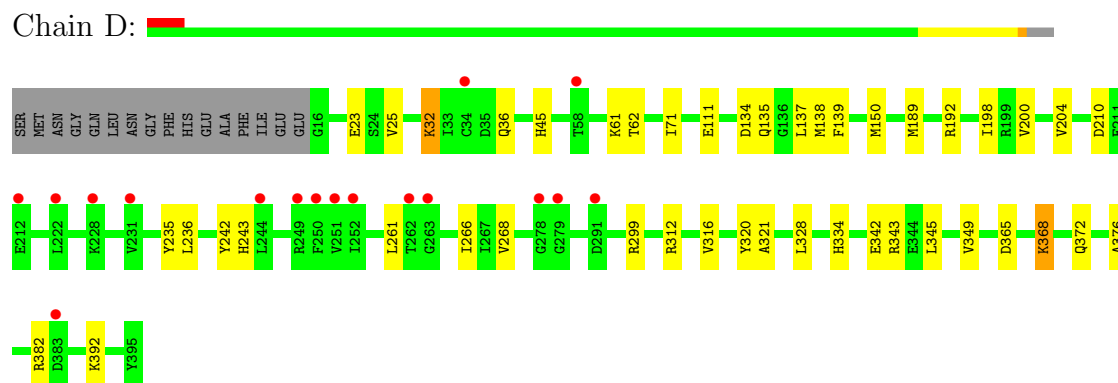
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	23	Total 23	O 23	0	0
7	B	21	Total 21	O 21	0	0
7	C	15	Total 15	O 15	0	0
7	D	35	Total 35	O 35	0	0
7	E	11	Total 11	O 11	0	0
7	F	3	Total 3	O 3	0	0





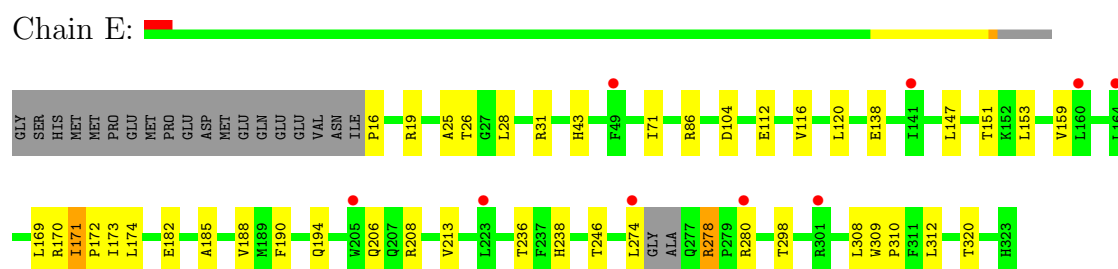
- Molecule 1: S-adenosylmethionine synthase isoform type-2

Chain D:



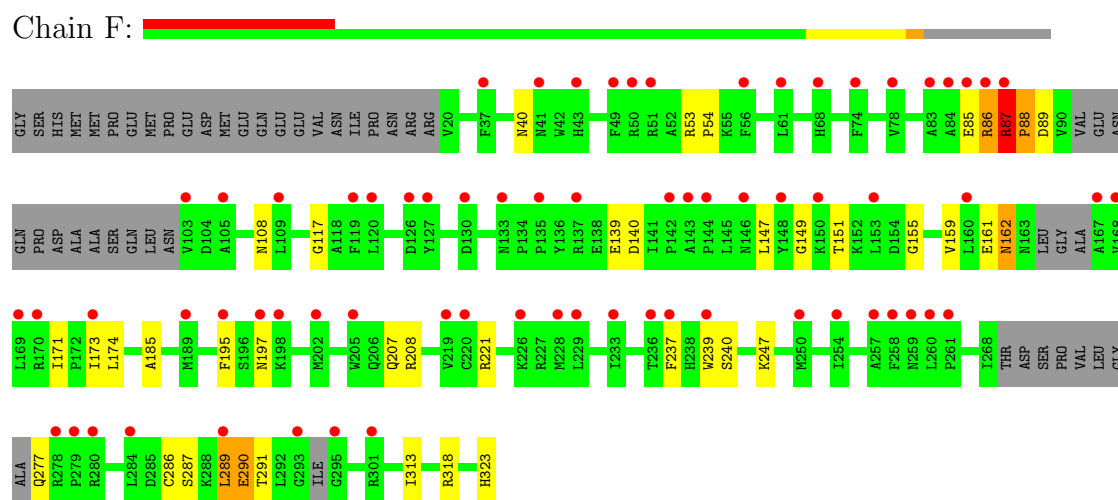
- Molecule 2: Methionine adenosyltransferase 2 subunit beta

Chain E:



- Molecule 2: Methionine adenosyltransferase 2 subunit beta

Chain F:



## 4 Data and refinement statistics

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 0.218 , 0.277	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 , 43.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 76590 reflections	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.

## 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2813	0	2818	28	0
1	D	2954	0	2950	24	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (124) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:A:59:VAL:HG22	1:A:261:LEU:CD2	2.44	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

### 5.3.1 Protein backbone ⓘ

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	380/396 (96%)	363 (96%)	16 (4%)	1 (0%)	50 77
1	C	354/396 (89%)	335 (95%)	18 (5%)	1 (0%)	50 77
1	D	378/396 (96%)	362 (96%)	15 (4%)	1 (0%)	50 77
2	E	302/327 (92%)	287 (95%)	14 (5%)	1 (0%)	50 77
2	F	270/327 (83%)	237 (88%)	27 (10%)	6 (2%)	10 18
All	All	2038/2238 (91%)	1920 (94%)	108 (5%)	10 (0%)	38 67

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%)	57 85
1	B	317/328 (97%)	306 (96%)	11 (4%)	48 77
1	C	301/328 (92%)	285 (95%)	16 (5%)	32 58
1	D	315/328 (96%)	309 (98%)	6 (2%)	69 91
2	E	260/279 (93%)	248 (95%)	12 (5%)	37 66
2	F	239/279 (86%)	225 (94%)	14 (6%)	28 52
All	All	1733/1870 (93%)	1666 (96%)	67 (4%)	43 74

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
1	D	192	ARG
1	D	343	ARG
1	D	368	LYS
1	D	392	LYS
2	E	26	THR

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

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 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	0.52	0	2,2,2	0.47	0
3	EDO	A	402	-	3,3,3	0.57	0	2,2,2	0.17	0
3	EDO	A	403	-	3,3,3	0.46	0	2,2,2	0.53	0
3	EDO	A	404	-	3,3,3	0.57	0	2,2,2	0.16	0
4	SAM	A	405	-	26,29,29	1.78	3 (11%)	38,42,42	2.28	8 (21%)
5	PO4	A	406	-	4,4,4	0.22	0	6,6,6	0.28	0
3	EDO	B	401	-	3,3,3	0.59	0	2,2,2	0.08	0
3	EDO	B	402	-	3,3,3	0.47	0	2,2,2	0.45	0
3	EDO	B	403	-	3,3,3	0.49	0	2,2,2	0.23	0
3	EDO	B	404	-	3,3,3	0.58	0	2,2,2	0.14	0
3	EDO	B	405	-	3,3,3	0.60	0	2,2,2	0.23	0
3	EDO	B	406	-	3,3,3	0.54	0	2,2,2	0.25	0
3	EDO	B	407	-	3,3,3	0.54	0	2,2,2	0.33	0
3	EDO	B	408	-	3,3,3	0.57	0	2,2,2	0.14	0
3	EDO	B	409	-	3,3,3	0.51	0	2,2,2	0.30	0
3	EDO	C	401	-	3,3,3	0.54	0	2,2,2	0.31	0
3	EDO	C	402	-	3,3,3	0.52	0	2,2,2	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	C	403	-	3,3,3	0.54	0	2,2,2	0.11	0
4	SAM	C	404	-	26,29,29	1.70	4 (15%)	38,42,42	2.09	8 (21%)
5	PO4	C	405	-	4,4,4	0.25	0	6,6,6	0.30	0
3	EDO	D	401	-	3,3,3	0.54	0	2,2,2	0.30	0
3	EDO	D	402	-	3,3,3	0.51	0	2,2,2	0.35	0
3	EDO	D	403	-	3,3,3	0.54	0	2,2,2	0.33	0
3	EDO	D	404	-	3,3,3	0.59	0	2,2,2	0.24	0
3	EDO	D	405	-	3,3,3	0.48	0	2,2,2	0.40	0
3	EDO	D	406	-	3,3,3	0.67	0	2,2,2	0.11	0
3	EDO	D	407	-	3,3,3	0.48	0	2,2,2	0.35	0
3	EDO	E	401	-	3,3,3	0.58	0	2,2,2	0.05	0
3	EDO	E	402	-	3,3,3	0.52	0	2,2,2	0.34	0
3	EDO	E	403	-	3,3,3	0.45	0	2,2,2	0.41	0
3	EDO	E	404	-	3,3,3	0.53	0	2,2,2	0.12	0
3	EDO	F	401	-	3,3,3	0.57	0	2,2,2	0.29	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	-	-	0/13/33/33	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
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	-	-	0/13/33/33	0/3/3/3
5	PO4	C	405	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	SAM	CG-SD	-7.29	1.66	1.80
4	C	404	SAM	CG-SD	-5.74	1.69	1.80
4	C	404	SAM	C4-N9	-3.41	1.32	1.37
4	A	405	SAM	C5-C4	3.01	1.47	1.40
4	C	404	SAM	C5-C4	2.96	1.47	1.40
4	A	405	SAM	C4-N9	-2.36	1.34	1.37
4	C	404	SAM	O4'-C1'	2.08	1.43	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	SAM	C5-C4-N3	-7.95	118.23	125.98
4	A	405	SAM	N3-C2-N1	-6.74	122.96	128.89
4	C	404	SAM	N3-C2-N1	-6.71	122.99	128.89
4	C	404	SAM	C5-C4-N3	-6.63	119.52	125.98
4	A	405	SAM	N3-C4-N9	5.95	135.60	125.39
4	C	404	SAM	N3-C4-N9	4.98	133.93	125.39
4	A	405	SAM	C2-N3-C4	2.81	121.36	113.27
4	C	404	SAM	C2-N3-C4	2.51	120.51	113.27
4	C	404	SAM	C3'-C2'-C1'	2.49	104.82	100.92
4	A	405	SAM	C5'-SD-CG	2.43	110.31	102.90
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	CG-CB-CA	2.20	115.45	112.22
4	A	405	SAM	C3'-C2'-C1'	2.18	104.34	100.92
4	A	405	SAM	C2-N1-C6	2.14	122.57	118.76

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	C	404	SAM	C2-N1-C6	2.06	122.42	118.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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%)	0.33	12 (3%) 44 41	45, 63, 91, 112	0
1	B	382/396 (96%)	0.48	25 (6%) 18 15	47, 65, 95, 126	0
1	C	360/396 (90%)	0.74	41 (11%) 6 4	50, 72, 104, 147	0
1	D	380/396 (95%)	0.36	17 (4%) 32 28	44, 60, 85, 109	0
2	E	306/327 (93%)	0.24	9 (2%) 49 46	53, 74, 99, 133	0
2	F	280/327 (85%)	1.19	70 (25%) 1 1	56, 113, 139, 154	0
All	All	2068/2238 (92%)	0.54	174 (8%) 11 8	44, 69, 120, 154	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	220	CYS	6.3
2	F	150	LYS	5.9
2	F	169	LEU	5.9
2	F	289	LEU	5.6
2	F	229	LEU	5.0
2	E	141	ILE	4.8
2	F	239	TRP	4.7
2	E	274	LEU	4.6
2	F	86	ARG	4.5
2	F	233	ILE	4.4
1	C	34	CYS	4.3
1	D	251	VAL	4.3
2	F	143	ALA	4.2
1	B	242	TYR	4.2
1	C	393	LEU	4.1
1	C	267	ILE	4.0
2	F	197	ASN	4.0
2	F	127	TYR	3.9
1	C	263	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
2	F	295	GLY	3.8
1	C	395	TYR	3.8
1	B	123	LEU	3.8
2	F	103	VAL	3.8
2	F	109	LEU	3.8
1	B	266	ILE	3.7
2	F	144	PRO	3.7
2	F	78	VAL	3.7
1	C	326	HIS	3.7
2	F	280	ARG	3.6
2	F	301	ARG	3.6
1	B	251	VAL	3.6
2	F	119	PHE	3.6
1	D	262	THR	3.5
2	F	120	LEU	3.4
2	F	228	MET	3.4
1	C	265	LYS	3.4
1	C	31	ASP	3.4
2	F	195	PHE	3.4
1	D	244	LEU	3.3
2	F	279	PRO	3.3
1	A	279	GLY	3.2
1	C	266	ILE	3.2
2	F	254	ILE	3.2
2	F	170	ARG	3.2
2	F	130	ASP	3.2
2	F	153	LEU	3.2
2	F	51	ARG	3.1
2	F	226	LYS	3.1
2	F	278	ARG	3.1
1	C	114	SER	3.1
2	F	258	PHE	3.0
2	F	260	LEU	3.0
1	C	328	LEU	3.0
1	C	35	ASP	3.0
2	F	160	LEU	3.0
1	B	263	GLY	3.0
1	B	281	ALA	3.0
1	C	33	ILE	3.0
2	F	50	ARG	2.9
2	F	198	LYS	2.9
1	C	261	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	259	ALA	2.9
2	F	74	PHE	2.9
1	C	394	LYS	2.9
1	B	395	TYR	2.9
2	F	205	TRP	2.8
2	F	68	HIS	2.8
1	C	242	TYR	2.8
2	F	261	PRO	2.8
1	D	263	GLY	2.8
2	F	236	THR	2.8
1	A	34	CYS	2.8
2	F	284	LEU	2.8
1	C	30	PRO	2.8
2	E	205	TRP	2.8
1	D	279	GLY	2.8
2	F	173	ILE	2.8
1	D	58	THR	2.7
1	B	214	CYS	2.7
2	F	167	ALA	2.7
1	A	267	ILE	2.7
2	F	83	ALA	2.7
2	F	49	PHE	2.7
1	B	231	VAL	2.7
1	B	280	GLY	2.7
1	C	269	ASP	2.7
1	C	268	VAL	2.6
2	F	202	MET	2.6
1	B	34	CYS	2.5
1	D	249	ARG	2.5
2	E	280	ARG	2.5
2	F	41	ASN	2.5
2	F	146	ASN	2.5
1	B	267	ILE	2.5
1	C	283	SER	2.5
2	F	142	PRO	2.5
1	C	264	ARG	2.5
1	B	226	VAL	2.5
1	D	383	ASP	2.5
2	F	84	ALA	2.5
1	D	222	LEU	2.5
1	B	393	LEU	2.5
1	C	58	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	135	PRO	2.5
2	F	133	ASN	2.4
1	C	281	ALA	2.4
2	F	293	GLY	2.4
1	A	261	LEU	2.4
1	C	115	PRO	2.4
2	E	223	LEU	2.4
2	F	137	ARG	2.4
1	C	222	LEU	2.4
1	D	252	ILE	2.4
1	D	278	GLY	2.4
2	F	87	ARG	2.3
2	F	168	VAL	2.3
1	B	176	LEU	2.3
1	C	260	GLY	2.3
2	F	43	HIS	2.3
1	C	262	THR	2.3
1	C	270	THR	2.3
2	F	189	MET	2.3
1	B	279	GLY	2.3
1	C	66	LEU	2.3
1	B	276	ALA	2.3
2	F	37	PHE	2.3
1	D	212	GLU	2.3
2	F	237	PHE	2.3
2	F	259	ASN	2.2
1	B	278	GLY	2.2
2	F	105	ALA	2.2
1	A	262	THR	2.2
1	A	362	ARG	2.2
2	F	250	MET	2.2
2	F	257	ALA	2.2
1	A	214	CYS	2.2
1	A	280	GLY	2.2
1	C	362	ARG	2.2
2	E	160	LEU	2.2
1	A	322	ILE	2.2
1	C	271	TYR	2.2
1	C	310	LEU	2.2
1	C	134	ASP	2.2
2	F	219	VAL	2.2
1	B	236	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	291	ASP	2.1
1	B	283	SER	2.1
1	B	265	LYS	2.1
1	C	376	ALA	2.1
2	F	85	GLU	2.1
1	B	262	THR	2.1
2	E	301	ARG	2.1
2	F	56	PHE	2.1
2	F	126	ASP	2.1
1	C	300	TRP	2.1
1	D	231	VAL	2.1
1	B	272	GLY	2.1
2	E	49	PHE	2.1
1	D	228	LYS	2.1
1	C	373	ARG	2.0
1	B	268	VAL	2.0
1	C	59	VAL	2.0
1	B	220	ASP	2.0
1	C	212	GLU	2.0
1	A	268	VAL	2.0
2	F	148	TYR	2.0
1	D	250	PHE	2.0
1	D	34	CYS	2.0
2	F	61	LEU	2.0
1	C	29	HIS	2.0
1	C	211	GLU	2.0
2	E	164	LEU	2.0
1	A	266	ILE	2.0
1	A	115	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	B	409	4/4	0.37	19.81	83,83,83,88	0
3	EDO	D	406	4/4	0.62	17.96	63,67,69,73	0
3	EDO	B	407	4/4	0.82	8.09	85,89,89,91	0
3	EDO	A	401	4/4	0.37	6.92	77,80,86,86	0
3	EDO	C	401	4/4	0.50	6.72	71,72,72,73	0
3	EDO	B	406	4/4	0.62	5.88	82,86,87,87	0
5	PO4	A	406	5/5	0.56	5.75	113,116,126,129	0
3	EDO	B	408	4/4	0.50	5.37	72,72,73,76	0
3	EDO	D	405	4/4	0.31	5.31	72,76,80,86	0
3	EDO	A	403	4/4	0.28	5.14	69,70,71,73	0
3	EDO	E	404	4/4	0.27	4.97	88,89,90,96	0
3	EDO	B	401	4/4	0.40	4.93	68,78,78,83	0
3	EDO	D	407	4/4	0.27	4.84	78,82,85,89	0
3	EDO	B	404	4/4	0.54	4.29	68,71,73,76	0
3	EDO	A	402	4/4	0.26	3.08	68,69,71,71	0
3	EDO	E	403	4/4	0.18	2.60	71,71,73,73	0
3	EDO	D	401	4/4	0.29	2.03	88,88,89,89	0
3	EDO	D	403	4/4	0.17	2.02	78,80,81,82	0
3	EDO	A	404	4/4	0.19	1.55	73,79,81,84	0
3	EDO	B	402	4/4	0.24	1.41	79,83,87,94	0
3	EDO	B	405	4/4	0.24	1.37	77,83,84,86	0
3	EDO	C	403	4/4	0.22	1.23	95,96,97,99	0
4	SAM	C	404	27/27	0.23	0.91	56,66,82,84	0
3	EDO	D	404	4/4	0.22	0.86	80,86,86,87	0
3	EDO	E	401	4/4	0.19	0.84	66,72,72,75	0
4	SAM	A	405	27/27	0.18	0.71	54,62,83,94	0
5	PO4	C	405	5/5	0.36	0.62	82,87,94,99	0
6	MG	B	410	1/1	0.31	0.45	60,60,60,60	0
3	EDO	B	403	4/4	0.18	0.04	64,65,65,67	0
3	EDO	D	402	4/4	0.16	-0.01	85,87,88,88	0
3	EDO	C	402	4/4	0.20	-0.47	77,82,83,88	0
3	EDO	E	402	4/4	0.18	-1.60	97,97,98,99	0
3	EDO	F	401	4/4	0.18	-2.22	91,94,95,95	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.