



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:00 PM GMT

PDB ID : 4NDN  
Title : Structural insights of MAT enzymes: MATa2b complexed with SAM and PPNP  
Authors : Murray, B.; Antonyuk, S.V.; Marina, A.; Lu, S.C.; Mato, J.M.; Hasnain, S.S.; Rojas, A.L.  
Deposited on : 2013-10-27  
Resolution : 2.34 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

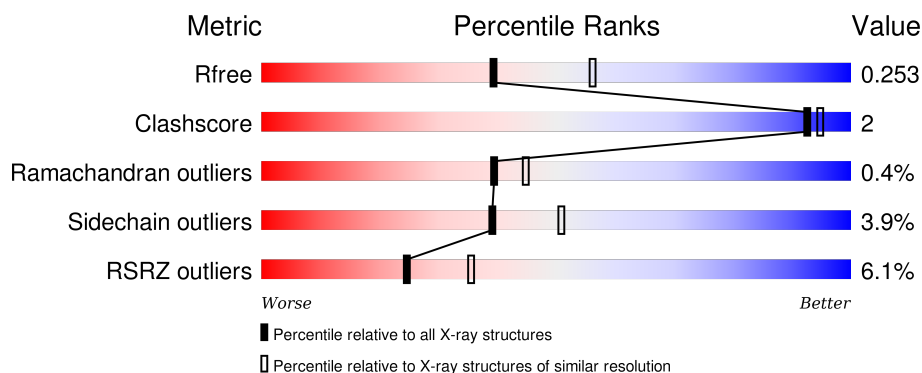
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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))
$R_{free}$	91344	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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	395	<div> <div>3%</div> <div>87% 5% 8%</div> </div>
1	B	395	<div> <div>4%</div> <div>88% 8% ..</div> </div>
1	C	395	<div> <div>9%</div> <div>83% 8% 9%</div> </div>
1	D	395	<div> <div>4%</div> <div>88% 7% ..</div> </div>
2	E	323	<div> <div>2%</div> <div>92% ...</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	323	

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
4	EDO	A	403	-	-	-	X
4	EDO	A	404	-	-	-	X
4	EDO	B	401	-	-	-	X
4	EDO	B	403	-	-	-	X
4	EDO	B	404	-	-	-	X
4	EDO	C	402	-	-	-	X
4	EDO	D	402	-	-	-	X
4	EDO	D	404	-	-	-	X
4	EDO	D	405	-	-	-	X
4	EDO	D	406	-	-	-	X
4	EDO	D	407	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17113 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	362	Total	C	N	O	S	0	0	0
			2822	1790	492	529	11			
1	B	383	Total	C	N	O	S	0	0	0
			2980	1883	520	566	11			
1	C	360	Total	C	N	O	S	0	0	0
			2809	1782	490	526	11			
1	D	382	Total	C	N	O	S	0	1	0
			2980	1882	522	565	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	309	Total	C	N	O	S	0	1	0
			2456	1551	449	446	10			
2	F	304	Total	C	N	O	S	0	1	0
			2416	1527	442	437	10			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



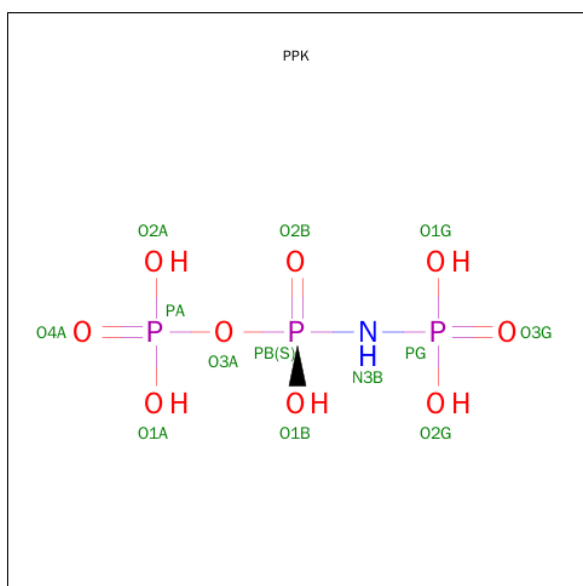
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total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

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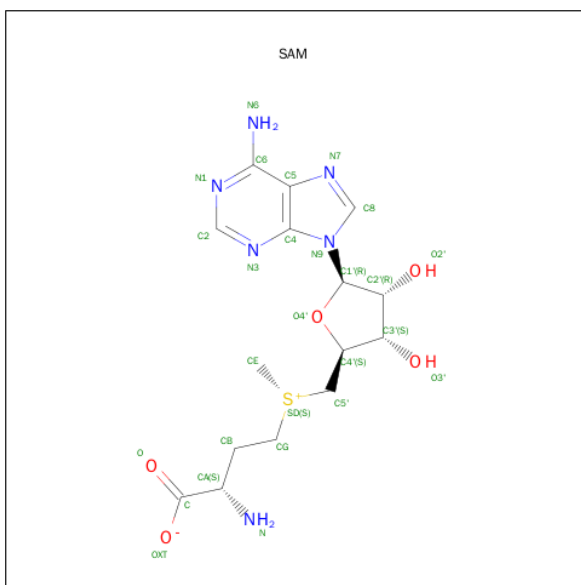
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is (DIPHOSPHONO)AMINOPHOSPHONIC ACID (three-letter code: PPK) (formula:  $\text{H}_6\text{NO}_9\text{P}_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	N	O	P	0	0
			13	1	9	3		
5	C	1	Total	N	O	P	0	0
			13	1	9	3		

- Molecule 6 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula:  $\text{C}_{15}\text{H}_{22}\text{N}_6\text{O}_5\text{S}$ ).



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

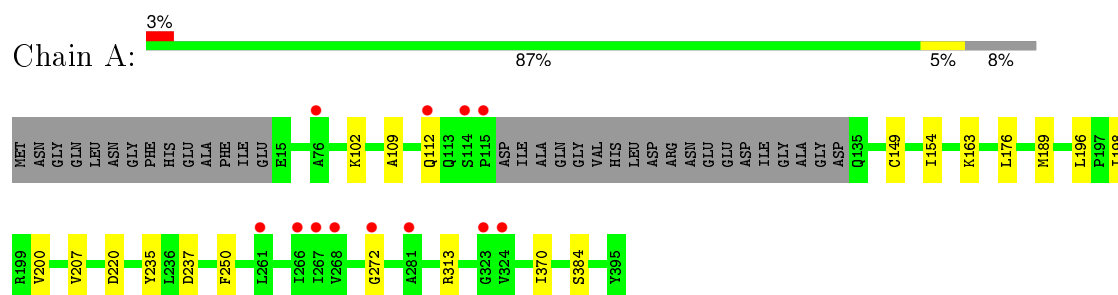
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	109	Total O 109 109	0	0
7	B	97	Total O 97 97	0	0
7	C	91	Total O 91 91	0	0
7	D	116	Total O 116 116	0	0
7	E	67	Total O 67 67	0	0
7	F	18	Total O 18 18	0	0

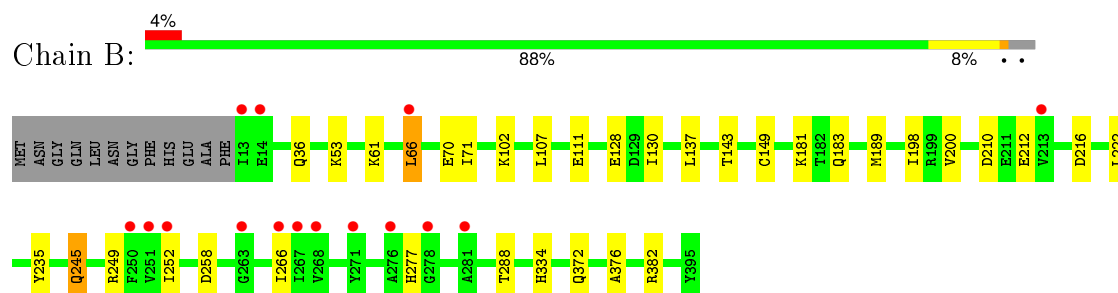
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

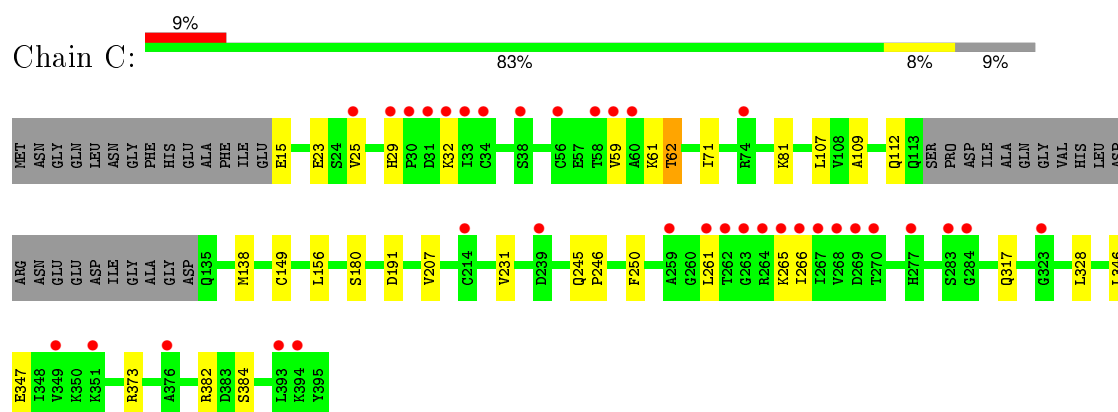
- Molecule 1: S-adenosylmethionine synthase isoform type-2



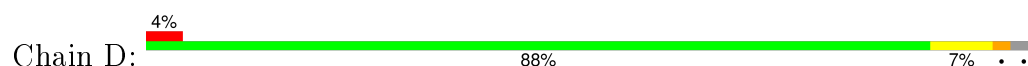
- Molecule 1: S-adenosylmethionine synthase isoform type-2



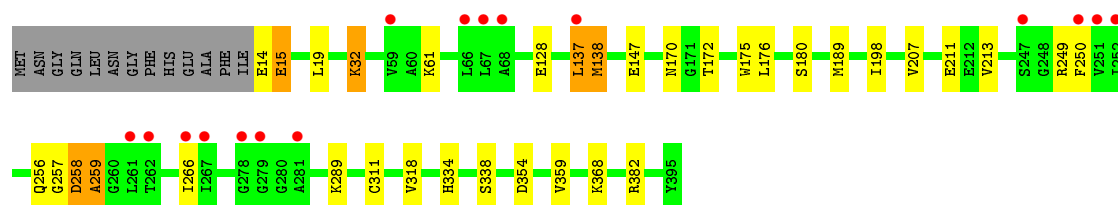
- Molecule 1: S-adenosylmethionine synthase isoform type-2



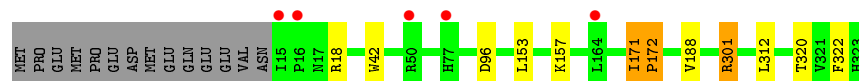
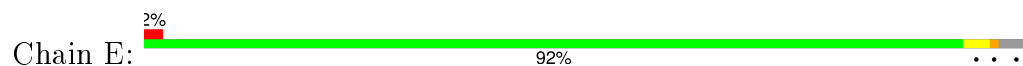
- Molecule 1: S-adenosylmethionine synthase isoform type-2



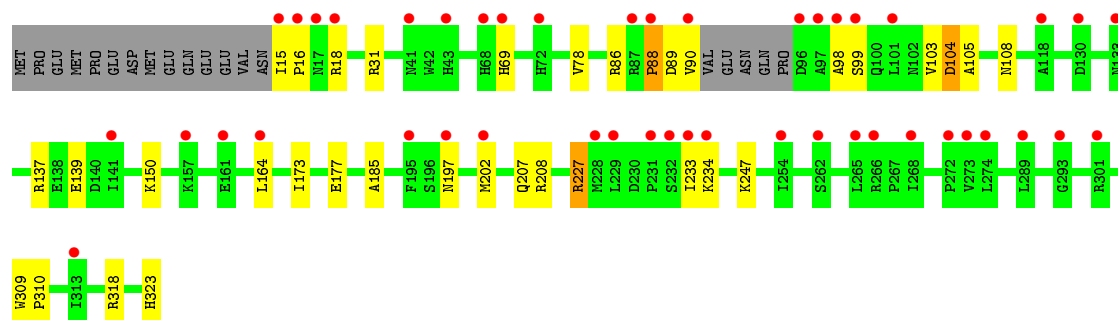
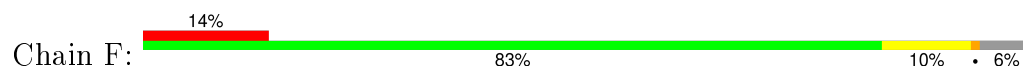




• Molecule 2: Methionine adenosyltransferase 2 subunit beta



• 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, $\alpha$ , $\beta$ , $\gamma$	72.14Å 122.18Å 298.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.78 – 2.34 47.74 – 2.34	Depositor EDS
% Data completeness (in resolution range)	96.9 (47.78-2.34) 96.9 (47.74-2.34)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.211 , 0.251 0.212 , 0.253	Depositor DCC
$R_{free}$ test set	5409 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.5	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 32.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 108283 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17113	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PPK, MG, EDO, 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	0.32	0/2879	0.54	0/3893
1	B	0.31	0/3039	0.53	0/4111
1	C	0.29	0/2865	0.53	0/3873
1	D	0.32	0/3042	0.54	0/4114
2	E	0.30	0/2518	0.50	0/3415
2	F	0.30	0/2476	0.50	0/3355
All	All	0.31	0/16819	0.52	0/22761

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	88	PRO	Peptide

### 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	2822	0	2832	11	0
1	B	2980	0	2973	16	0
1	C	2809	0	2820	13	0
1	D	2980	0	2975	22	0
2	E	2456	0	2431	4	0
2	F	2416	0	2394	10	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	18	0	0
4	B	20	0	30	0	0
4	C	8	0	12	0	0
4	D	24	0	36	0	0
4	E	4	0	6	0	0
5	A	13	0	1	0	0
5	C	13	0	1	0	0
6	A	27	0	22	0	0
6	C	27	0	22	1	0
7	A	109	0	0	0	0
7	B	97	0	0	0	0
7	C	91	0	0	0	0
7	D	116	0	0	0	0
7	E	67	0	0	0	0
7	F	18	0	0	0	0
All	All	17113	0	16573	67	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:MET:HB2	1:D:198:ILE:HD11	1.77	0.66
1:B:36:GLN:HE21	1:B:372:GLN:HE21	1.52	0.56
1:A:313:ARG:NH2	2:F:323:HIS:O	2.35	0.56
1:C:59:VAL:HG13	1:C:261:LEU:HD23	1.88	0.55
1:A:109:ALA:HB1	1:B:61:LYS:CE	2.37	0.54
1:B:376:ALA:O	1:B:382:ARG:NH2	2.41	0.53
2:E:301[A]:ARG:HH11	2:E:301[A]:ARG:HG2	1.73	0.53
1:A:189:MET:HB2	1:A:198:ILE:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:GLN:HA	1:B:245:GLN:HE21	1.74	0.52
1:C:71:ILE:O	1:C:112:GLN:HA	2.11	0.51
2:F:31[B]:ARG:NH2	2:F:177:GLU:O	2.43	0.51
1:D:15:GLU:N	1:D:15:GLU:OE1	2.44	0.50
1:D:138:MET:CE	1:D:318:VAL:HG23	2.42	0.49
1:A:109:ALA:HB1	1:B:61:LYS:HE3	1.94	0.49
1:D:176:LEU:HD22	1:D:207:VAL:HG21	1.95	0.49
1:C:109:ALA:HB1	1:D:61:LYS:HE2	1.94	0.48
1:B:66:LEU:HD12	1:B:107:LEU:HB2	1.95	0.48
1:D:175:TRP:CG	1:D:213:VAL:HG11	2.48	0.48
1:D:138:MET:HE3	1:D:318:VAL:HG23	1.95	0.48
1:D:170:ASN:OD1	1:D:172:THR:HG23	2.13	0.48
2:F:227:ARG:HG2	2:F:233:ILE:HB	1.95	0.47
1:B:200:VAL:HG23	1:B:235:TYR:HB3	1.96	0.47
1:D:311:CYS:HB3	1:D:338:SER:HB2	1.96	0.47
1:A:176:LEU:HD22	1:A:207:VAL:HG21	1.97	0.47
1:B:143:THR:O	1:B:149:CYS:HA	2.14	0.47
1:B:266:ILE:HD12	1:B:277:HIS:CE1	2.50	0.47
1:C:29:HIS:CE1	1:C:265:LYS:HE2	2.50	0.47
1:C:61:LYS:O	1:C:62:THR:C	2.53	0.46
1:C:317:GLN:NE2	1:D:19:LEU:O	2.48	0.46
1:C:156:LEU:HD22	1:C:231:VAL:HG22	1.98	0.46
1:D:213:VAL:O	1:D:249:ARG:NH2	2.49	0.46
6:C:405:SAM:N	1:D:289:LYS:HE3	2.31	0.46
1:C:23:GLU:HG2	1:D:137:LEU:HD21	1.98	0.45
1:A:109:ALA:HB2	1:C:107:LEU:HD23	1.99	0.44
2:E:18:ARG:HB3	2:E:42:TRP:CE3	2.52	0.44
1:D:180:SER:HB3	1:D:207:VAL:HG23	1.99	0.44
1:A:109:ALA:HB1	1:B:61:LYS:HE2	1.99	0.44
1:A:154:ILE:HD12	1:A:272:GLY:HA3	2.00	0.44
2:F:103:VAL:HA	2:F:105:ALA:H	1.83	0.44
2:F:173:ILE:HD11	2:F:185:ALA:HB3	2.00	0.43
1:B:130:ILE:CD1	1:B:288:THR:HG22	2.48	0.43
1:A:154:ILE:HD12	1:A:272:GLY:CA	2.48	0.43
2:E:320:THR:HG23	2:E:322:PHE:O	2.18	0.43
1:B:70:GLU:HA	1:B:111:GLU:O	2.19	0.43
1:C:180:SER:HB3	1:C:207:VAL:HG23	1.99	0.43
2:F:90:VAL:HG13	2:F:208:ARG:NH1	2.34	0.42
1:D:258:ASP:O	1:D:259:ALA:CB	2.67	0.42
1:D:354:ASP:HB3	1:D:359:VAL:HG11	2.00	0.42
2:E:171:ILE:HA	2:E:172:PRO:HD3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:TRP:CD1	1:D:213:VAL:HG11	2.54	0.42
1:A:200:VAL:HG23	1:A:235:TYR:HB3	2.02	0.42
1:D:258:ASP:O	1:D:259:ALA:HB3	2.20	0.41
1:B:252:ILE:HG23	1:B:252:ILE:O	2.20	0.41
2:F:103:VAL:HA	2:F:104:ASP:CB	2.50	0.41
2:F:15:ILE:N	2:F:16:PRO:HD2	2.35	0.41
1:C:245:GLN:N	1:C:246:PRO:CD	2.83	0.41
1:B:181:LYS:HE3	1:B:183:GLN:HE21	1.86	0.41
1:D:32:LYS:HE2	1:D:32:LYS:HA	2.02	0.41
1:D:256:GLN:HA	1:D:257:GLY:HA2	1.81	0.41
2:F:309:TRP:CG	2:F:310:PRO:HD3	2.56	0.41
1:C:266:ILE:HD11	1:D:266:ILE:HD11	2.03	0.41
1:A:237:ASP:OD1	1:A:237:ASP:C	2.60	0.40
1:B:53:LYS:O	1:B:71:ILE:HA	2.22	0.40
1:C:25:VAL:CG2	1:C:32:LYS:HD3	2.51	0.40
2:F:90:VAL:HG13	2:F:208:ARG:HH12	1.85	0.40
1:D:14:GLU:OE2	1:D:14:GLU:N	2.55	0.40
1:B:189:MET:HB2	1:B:198:ILE:HD11	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	358/395 (91%)	345 (96%)	13 (4%)	0	100	100
1	B	381/395 (96%)	365 (96%)	16 (4%)	0	100	100
1	C	356/395 (90%)	343 (96%)	12 (3%)	1 (0%)	46	54
1	D	381/395 (96%)	370 (97%)	10 (3%)	1 (0%)	46	54
2	E	308/323 (95%)	294 (96%)	13 (4%)	1 (0%)	46	54
2	F	301/323 (93%)	284 (94%)	12 (4%)	5 (2%)	11	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2085/2226 (94%)	2001 (96%)	76 (4%)	8 (0%)	39	45

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	89	ASP
2	F	104	ASP
1	D	259	ALA
2	F	88	PRO
1	C	62	THR
2	F	98	ALA
2	F	86	ARG
2	E	172	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	302/327 (92%)	293 (97%)	9 (3%)	48	61
1	B	318/327 (97%)	306 (96%)	12 (4%)	40	51
1	C	300/327 (92%)	288 (96%)	12 (4%)	38	49
1	D	318/327 (97%)	306 (96%)	12 (4%)	40	51
2	E	263/276 (95%)	255 (97%)	8 (3%)	48	61
2	F	258/276 (94%)	242 (94%)	16 (6%)	23	26
All	All	1759/1860 (95%)	1690 (96%)	69 (4%)	39	51

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LYS
1	A	112	GLN
1	A	149	CYS
1	A	163	LYS

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Mol	Chain	Res	Type
1	A	196	LEU
1	A	220	ASP
1	A	250	PHE
1	A	370	ILE
1	A	384	SER
1	B	66	LEU
1	B	102	LYS
1	B	128	GLU
1	B	137	LEU
1	B	210	ASP
1	B	212	GLU
1	B	216	ASP
1	B	222	LEU
1	B	245	GLN
1	B	249	ARG
1	B	258	ASP
1	B	334	HIS
1	C	15	GLU
1	C	81	LYS
1	C	138	MET
1	C	149	CYS
1	C	191	ASP
1	C	250	PHE
1	C	328	LEU
1	C	346	LEU
1	C	347	GLU
1	C	373	ARG
1	C	382	ARG
1	C	384	SER
1	D	15	GLU
1	D	32	LYS
1	D	128	GLU
1	D	137	LEU
1	D	138	MET
1	D	147	GLU
1	D	211	GLU
1	D	250	PHE
1	D	258	ASP
1	D	334	HIS
1	D	368	LYS
1	D	382	ARG
2	E	96	ASP

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Mol	Chain	Res	Type
2	E	153	LEU
2	E	157	LYS
2	E	171	ILE
2	E	188	VAL
2	E	301[A]	ARG
2	E	301[B]	ARG
2	E	312	LEU
2	F	18	ARG
2	F	69	HIS
2	F	78	VAL
2	F	99	SER
2	F	108	ASN
2	F	137	ARG
2	F	139	GLU
2	F	150	LYS
2	F	164	LEU
2	F	197	ASN
2	F	202	MET
2	F	207	GLN
2	F	227	ARG
2	F	234	LYS
2	F	247	LYS
2	F	318	ARG

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

Mol	Chain	Res	Type
1	A	190	GLN
1	B	183	GLN
1	B	245	GLN
1	B	372	GLN
1	C	48	GLN
1	C	352	ASN
2	F	197	ASN
2	F	207	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 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	$\# Z  > 2$
4	EDO	A	403	-	3,3,3	0.48	0	2,2,2	0.30	0
4	EDO	A	404	-	3,3,3	0.45	0	2,2,2	0.40	0
4	EDO	A	405	-	3,3,3	0.47	0	2,2,2	0.38	0
5	PPK	A	406	3	11,12,12	2.75	6 (54%)	14,20,20	1.09	0
6	SAM	A	407	-	21,29,29	1.59	2 (9%)	17,42,42	2.50	5 (29%)
4	EDO	B	401	-	3,3,3	0.46	0	2,2,2	0.41	0
4	EDO	B	402	-	3,3,3	0.67	0	2,2,2	0.08	0
4	EDO	B	403	-	3,3,3	0.47	0	2,2,2	0.38	0
4	EDO	B	404	-	3,3,3	0.51	0	2,2,2	0.33	0
4	EDO	B	405	-	3,3,3	0.46	0	2,2,2	0.38	0
4	EDO	C	402	-	3,3,3	0.43	0	2,2,2	0.42	0
4	EDO	C	403	-	3,3,3	0.56	0	2,2,2	0.19	0
5	PPK	C	404	3	11,12,12	2.74	5 (45%)	14,20,20	1.07	1 (7%)
6	SAM	C	405	-	21,29,29	1.78	2 (9%)	17,42,42	2.24	2 (11%)
4	EDO	D	402	-	3,3,3	0.49	0	2,2,2	0.34	0
4	EDO	D	403	-	3,3,3	0.50	0	2,2,2	0.39	0
4	EDO	D	404	-	3,3,3	0.48	0	2,2,2	0.46	0
4	EDO	D	405	-	3,3,3	0.60	0	2,2,2	0.25	0
4	EDO	D	406	-	3,3,3	0.47	0	2,2,2	0.43	0
4	EDO	D	407	-	3,3,3	0.51	0	2,2,2	0.23	0
4	EDO	E	401	-	3,3,3	0.49	0	2,2,2	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	A	404	-	-	0/1/1/1	0/0/0/0
4	EDO	A	405	-	-	0/1/1/1	0/0/0/0
5	PPK	A	406	3	-	0/6/12/12	0/0/0/0
6	SAM	A	407	-	-	0/8/33/33	0/3/3/3
4	EDO	B	401	-	-	0/1/1/1	0/0/0/0
4	EDO	B	402	-	-	0/1/1/1	0/0/0/0
4	EDO	B	403	-	-	0/1/1/1	0/0/0/0
4	EDO	B	404	-	-	0/1/1/1	0/0/0/0
4	EDO	B	405	-	-	0/1/1/1	0/0/0/0
4	EDO	C	402	-	-	0/1/1/1	0/0/0/0
4	EDO	C	403	-	-	0/1/1/1	0/0/0/0
5	PPK	C	404	3	-	1/6/12/12	0/0/0/0
6	SAM	C	405	-	-	0/8/33/33	0/3/3/3
4	EDO	D	402	-	-	0/1/1/1	0/0/0/0
4	EDO	D	403	-	-	0/1/1/1	0/0/0/0
4	EDO	D	404	-	-	0/1/1/1	0/0/0/0
4	EDO	D	405	-	-	0/1/1/1	0/0/0/0
4	EDO	D	406	-	-	0/1/1/1	0/0/0/0
4	EDO	D	407	-	-	0/1/1/1	0/0/0/0
4	EDO	E	401	-	-	0/1/1/1	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	405	SAM	CG-SD	-6.69	1.66	1.80
6	A	407	SAM	CG-SD	-5.72	1.68	1.80
5	A	406	PPK	PB-O1B	2.01	1.62	1.56
5	A	406	PPK	PG-O3G	2.41	1.48	1.46
5	C	404	PPK	PG-O3G	2.41	1.48	1.46
5	A	406	PPK	PB-O2B	2.60	1.49	1.46
6	A	407	SAM	C5-C4	2.68	1.46	1.40
6	C	405	SAM	C5-C4	2.82	1.46	1.40
5	A	406	PPK	PB-O3A	3.00	1.62	1.59
5	C	404	PPK	PB-O2B	3.07	1.49	1.46
5	C	404	PPK	PB-O3A	3.20	1.63	1.59
5	C	404	PPK	PG-N3B	4.61	1.75	1.63
5	C	404	PPK	PB-N3B	4.81	1.76	1.63
5	A	406	PPK	PG-N3B	4.88	1.76	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	406	PPK	PB-N3B	5.02	1.76	1.63

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	407	SAM	N3-C2-N1	-8.07	122.72	128.89
6	C	405	SAM	N3-C2-N1	-7.66	123.03	128.89
6	C	405	SAM	C4-C5-N7	-3.24	106.50	109.48
6	A	407	SAM	C1'-N9-C4	-2.69	122.89	126.94
6	A	407	SAM	C2'-C1'-N9	-2.60	110.32	114.29
5	C	404	PPK	O1G-PG-O3G	-2.04	108.07	113.49
6	A	407	SAM	C4-C5-N7	-2.00	107.64	109.48
6	A	407	SAM	C2-N1-C6	2.55	123.31	118.77

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	404	PPK	O3G-PG-N3B-PB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	405	SAM	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	362/395 (91%)	0.13	12 (3%)	50	61	32, 47, 71, 109	0
1	B	383/395 (96%)	0.27	15 (3%)	43	55	34, 48, 74, 120	0
1	C	360/395 (91%)	0.50	35 (9%)	10	16	36, 56, 81, 93	0
1	D	382/395 (96%)	0.14	16 (4%)	40	52	32, 44, 69, 104	0
2	E	309/323 (95%)	0.05	5 (1%)	74	83	41, 57, 83, 106	0
2	F	304/323 (94%)	0.83	45 (14%)	3	5	46, 83, 111, 130	0
All	All	2100/2226 (94%)	0.31	128 (6%)	25	35	32, 52, 92, 130	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	15	ILE	6.3
2	E	15	ILE	6.3
2	F	99	SER	6.2
2	F	96	ASP	5.7
1	B	13	ILE	5.5
2	F	101	LEU	5.1
1	A	115	PRO	5.1
2	F	88	PRO	5.0
2	F	87	ARG	4.8
2	F	229	LEU	4.7
1	C	268	VAL	4.7
1	D	250	PHE	4.4
1	D	251	VAL	4.4
2	F	228	MET	4.3
2	F	231	PRO	4.2
2	F	273	VAL	4.2
1	B	266	ILE	4.1
2	F	301	ARG	4.1
1	A	114	SER	4.1

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Mol	Chain	Res	Type	RSRZ
2	F	98	ALA	4.0
1	A	323	GLY	3.9
1	B	267	ILE	3.9
1	B	250	PHE	3.9
2	F	69	HIS	3.9
2	F	16	PRO	3.8
1	C	323	GLY	3.7
2	F	97	ALA	3.7
1	D	252	ILE	3.6
2	F	141	ILE	3.5
1	C	34	CYS	3.4
1	C	267	ILE	3.4
1	B	268	VAL	3.4
1	D	261	LEU	3.3
2	F	43	HIS	3.2
1	C	59	VAL	3.2
1	D	137	LEU	3.2
1	C	283	SER	3.2
1	D	247	SER	3.2
2	F	274	LEU	3.1
2	F	118	ALA	3.0
1	A	266	ILE	3.0
1	C	266	ILE	3.0
1	C	214	CYS	2.9
2	F	195	PHE	2.9
1	D	266	ILE	2.9
1	C	33	ILE	2.9
1	D	262	THR	2.8
1	C	259	ALA	2.8
2	F	266	ARG	2.8
1	C	74	ARG	2.7
2	F	254	ILE	2.7
2	F	164	LEU	2.7
1	D	279	GLY	2.7
1	C	263	GLY	2.7
1	D	59	VAL	2.6
2	F	157	LYS	2.6
1	A	281	ALA	2.6
1	A	267	ILE	2.6
1	C	262	THR	2.6
1	D	267	ILE	2.6
2	F	233	ILE	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	393	LEU	2.6
2	F	234	LYS	2.5
1	D	281	ALA	2.5
1	C	30	PRO	2.5
1	C	264	ARG	2.5
1	C	265	LYS	2.5
1	D	278	GLY	2.5
1	C	56	CYS	2.5
2	E	16	PRO	2.5
2	E	77	HIS	2.5
1	B	281	ALA	2.5
1	B	251	VAL	2.5
2	F	17	ASN	2.4
1	C	261	LEU	2.4
2	F	130	ASP	2.4
1	B	263	GLY	2.4
1	A	324	VAL	2.4
1	B	252	ILE	2.4
1	C	29	HIS	2.4
1	A	76	ALA	2.4
2	F	18	ARG	2.4
1	C	349	VAL	2.4
1	C	376	ALA	2.4
2	F	161	GLU	2.4
2	E	164	LEU	2.4
1	C	38	SER	2.4
2	F	197	ASN	2.3
2	F	265	LEU	2.3
2	F	262	SER	2.3
2	F	268	ILE	2.3
2	F	90	VAL	2.3
1	A	268	VAL	2.3
2	F	272	PRO	2.3
1	C	32	LYS	2.3
1	C	394	LYS	2.3
1	C	25	VAL	2.3
1	B	278	GLY	2.2
1	D	67	LEU	2.2
1	C	58	THR	2.2
1	C	270	THR	2.2
1	B	276	ALA	2.2
2	F	133	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	202	MET	2.2
2	F	68	HIS	2.2
2	F	72	HIS	2.2
1	C	239	ASP	2.2
2	F	232	SER	2.2
1	B	271	TYR	2.1
2	E	50	ARG	2.1
1	B	14	GLU	2.1
2	F	289	LEU	2.1
1	C	60	ALA	2.1
2	F	41	ASN	2.1
1	B	66	LEU	2.1
1	C	269	ASP	2.1
1	C	351	LYS	2.1
2	F	313	ILE	2.1
1	A	261	LEU	2.0
1	D	66	LEU	2.0
1	A	112	GLN	2.0
1	B	213	VAL	2.0
1	C	284	GLY	2.0
2	F	293	GLY	2.0
1	C	277	HIS	2.0
1	A	272	GLY	2.0
1	C	31	ASP	2.0
1	D	68	ALA	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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	C	402	4/4	0.90	0.58	19.55	70,70,71,72	0
4	EDO	A	403	4/4	0.85	0.23	15.74	63,65,67,71	0
4	EDO	D	406	4/4	0.85	0.29	8.45	68,68,70,75	0
4	EDO	B	404	4/4	0.78	0.28	8.25	73,75,75,76	0
4	EDO	D	405	4/4	0.79	0.30	5.19	57,57,58,60	0
4	EDO	B	401	4/4	0.74	0.28	4.06	75,76,78,81	0
4	EDO	D	402	4/4	0.74	0.29	4.00	69,70,71,71	0
4	EDO	B	403	4/4	0.94	0.17	3.95	55,56,56,57	0
4	EDO	D	404	4/4	0.88	0.24	3.47	69,69,70,70	0
4	EDO	D	407	4/4	0.96	0.32	2.87	70,71,72,73	0
4	EDO	A	404	4/4	0.87	0.23	2.60	65,67,68,71	0
4	EDO	A	405	4/4	0.81	0.22	1.62	75,77,77,79	0
4	EDO	D	403	4/4	0.84	0.20	1.15	66,67,67,68	0
6	SAM	A	407	27/27	0.93	0.15	0.63	38,43,56,57	0
4	EDO	B	405	4/4	0.94	0.14	0.55	56,59,59,61	0
4	EDO	E	401	4/4	0.95	0.12	0.32	45,45,45,45	0
6	SAM	C	405	27/27	0.94	0.17	0.28	41,48,56,57	0
3	MG	D	401	1/1	0.98	0.20	-0.13	32,32,32,32	0
5	PPK	C	404	13/13	0.94	0.15	-1.22	52,61,67,73	0
5	PPK	A	406	13/13	0.94	0.14	-1.30	56,63,72,74	0
3	MG	C	401	1/1	0.98	0.15	-1.97	43,43,43,43	0
3	MG	A	401	1/1	0.94	0.04	-3.35	44,44,44,44	0
4	EDO	B	402	4/4	0.76	0.26	-	46,47,47,48	0
3	MG	A	402	1/1	0.99	0.19	-	37,37,37,37	0
4	EDO	C	403	4/4	0.72	0.25	-	65,68,68,70	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.