



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 05:27 AM GMT

PDB ID : 2OB2
Title : ppm1 in the absence of 1,8-ANS (cf 1JD)
Authors : Groves, M.R.; Mueller, I.B.; Kreplin, X.; Mueller-Dieckmann, J.
Deposited on : 2006-12-18
Resolution : 1.92 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

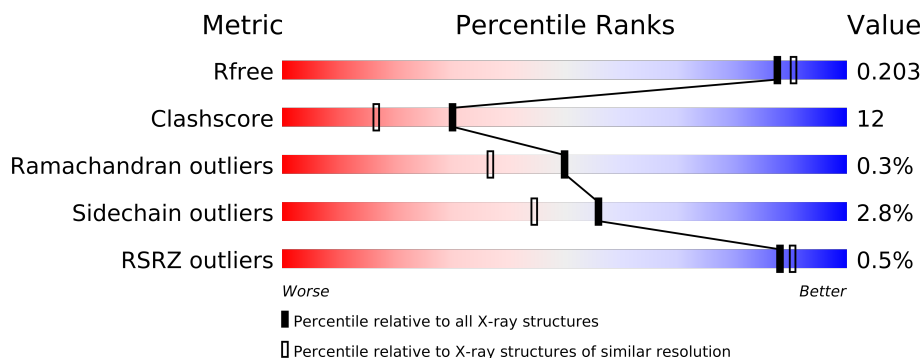
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
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) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.92 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	4387 (1.94-1.90)
Clashscore	79885	5258 (1.94-1.90)
Ramachandran outliers	78287	5193 (1.94-1.90)
Sidechain outliers	78261	5194 (1.94-1.90)
RSRZ outliers	66119	4389 (1.94-1.90)

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 ≥ 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	327	
1	B	327	
1	C	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
2	PO4	A	1001	-	X
4	GOL	A	2003	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8641 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.

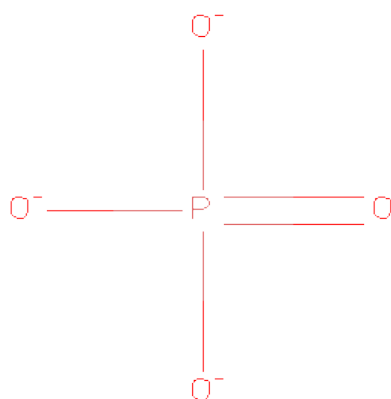
- Molecule 1 is a protein called Leucine carboxyl methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2636	1676	448	494	18			
1	B	327	Total	C	N	O	S	0	2	0
			2650	1684	451	497	18			
1	C	327	Total	C	N	O	S	0	0	0
			2636	1676	448	494	18			

There are 3 discrepancies between the modelled and reference sequences:

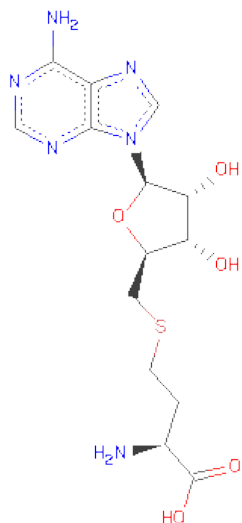
Chain	Residue	Modelled	Actual	Comment	Reference
A	202	SMC	CYS	MODIFIED RESIDUE	UNP Q04081
B	202	SMC	CYS	MODIFIED RESIDUE	UNP Q04081
C	202	SMC	CYS	MODIFIED RESIDUE	UNP Q04081

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

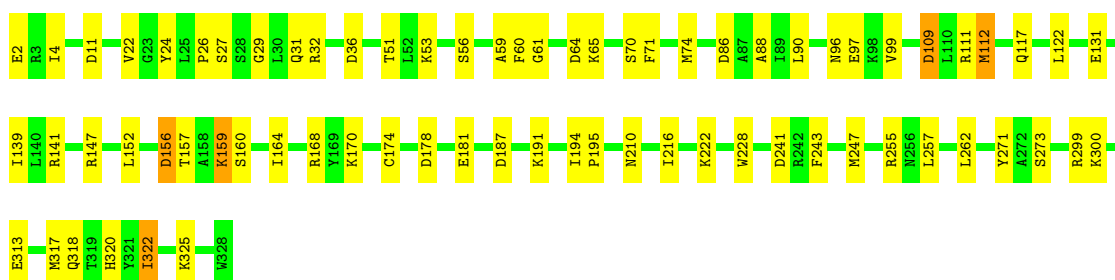
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	246	Total	O	0	0
			246	246		
5	B	232	Total	O	0	0
			232	232		
5	C	146	Total	O	0	0
			146	146		

3 Residue-property plots

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.

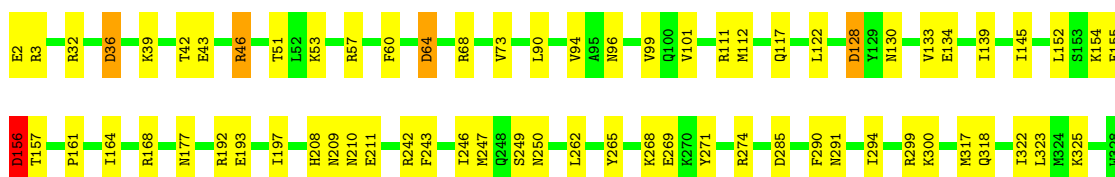
- Molecule 1: Leucine carboxyl methyltransferase 1

Chain A:



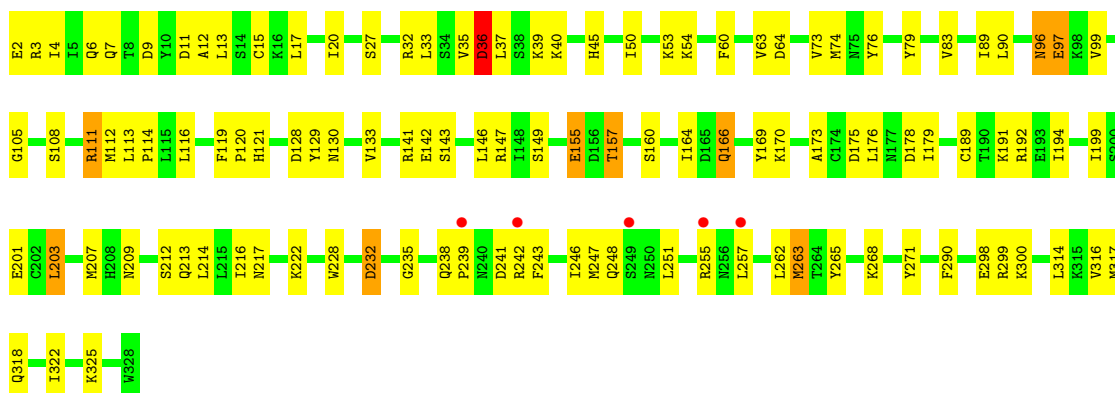
- Molecule 1: Leucine carboxyl methyltransferase 1

Chain B:



- Molecule 1: Leucine carboxyl methyltransferase 1

Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	110.62Å 110.62Å 161.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.06 – 1.92 33.05 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.06-1.92) 99.8 (33.05-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.206 , 0.268 0.178 , 0.203	Depositor DCC
R_{free} test set	4276 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 30.7	EDS
Estimated twinning fraction	0.336 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 85540 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8641	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: GOL, PO4, SAH, SMC

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	0.95	0/2677	1.01	6/3613 (0.2%)
1	B	0.93	0/2697	1.01	6/3639 (0.2%)
1	C	0.87	0/2677	0.96	8/3613 (0.2%)
All	All	0.92	0/8051	0.99	20/10865 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	ASP	CB-CG-OD2	6.78	124.41	118.30
1	C	232	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	112	MET	CG-SD-CE	6.63	110.81	100.20
1	B	111	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	64	ASP	CB-CG-OD2	6.11	123.80	118.30
1	C	11	ASP	CB-CG-OD2	5.94	123.65	118.30
1	C	36	ASP	CB-CG-OD2	5.86	123.58	118.30
1	B	285	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	36	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	178	ASP	CB-CG-OD2	5.73	123.45	118.30
1	C	128	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	128	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C	9	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	274	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	A	109	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	64	ASP	CB-CG-OD2	5.31	123.08	118.30
1	C	175	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	64	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	147	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	C	178	ASP	CB-CG-OD2	5.04	122.84	118.30

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	2636	0	2666	60	0
1	B	2650	0	2682	59	0
1	C	2636	0	2666	79	0
2	A	5	0	0	1	0
3	A	26	0	19	0	0
3	B	26	0	19	0	0
3	C	26	0	19	0	0
4	A	12	0	16	1	0
5	A	246	0	0	10	0
5	B	232	0	0	16	0
5	C	146	0	0	10	0
All	All	8641	0	8087	194	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 12.

All (194) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:317:MET:HE3	1:A:318:GLN:NE2	1.66	1.10
1:B:46[A]:ARG:HH21	1:B:46[A]:ARG:HB3	1.06	1.10
1:A:317:MET:HE3	1:A:318:GLN:HE21	0.98	1.09
1:C:317:MET:HE3	1:C:318:GLN:NE2	1.82	0.94
1:A:317:MET:CE	1:A:318:GLN:HE21	1.79	0.94
1:A:27:SER:H	1:A:31:GLN:HE21	1.14	0.94
1:C:317:MET:CE	1:C:318:GLN:HE21	1.82	0.93
1:C:155:GLU:HG3	1:C:157:THR:HG23	1.58	0.86
1:A:70:SER:HB3	1:A:74:MET:CE	2.07	0.85
1:B:46[A]:ARG:HH21	1:B:46[A]:ARG:CB	1.88	0.85
1:B:46[A]:ARG:HB3	1:B:46[A]:ARG:NH2	1.92	0.81
1:B:161:PRO:O	5:B:2019:HOH:O	1.98	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:242:ARG:HB2	1:B:242:ARG:NH1	1.97	0.80
1:C:2:GLU:N	5:C:1932:HOH:O	2.15	0.80
1:A:27:SER:H	1:A:31:GLN:NE2	1.80	0.79
1:B:193[B]:GLU:HG2	5:B:1988:HOH:O	1.82	0.79
1:C:12:ALA:HB2	5:C:1943:HOH:O	1.83	0.79
1:B:247:MET:HE3	1:B:262:LEU:HD21	1.63	0.78
1:A:70:SER:HB3	1:A:74:MET:HE1	1.66	0.78
1:B:247:MET:HE3	1:B:262:LEU:CD2	2.14	0.78
1:B:242:ARG:CZ	1:B:242:ARG:HB2	2.15	0.76
1:A:271:TYR:CD2	1:A:322:ILE:HD11	2.21	0.75
1:C:170:LYS:HD2	5:C:1848:HOH:O	1.86	0.75
1:B:64:ASP:O	1:B:68:ARG:HG3	1.87	0.75
1:C:317:MET:HE3	1:C:318:GLN:HE21	1.44	0.73
1:C:322:ILE:O	1:C:322:ILE:HD12	1.89	0.73
1:A:36:ASP:H	1:B:117:GLN:HE22	1.38	0.71
1:C:317:MET:CE	1:C:318:GLN:NE2	2.47	0.71
1:B:42:THR:O	1:B:46[A]:ARG:HG3	1.91	0.70
1:A:247:MET:HE3	1:A:262:LEU:HD21	1.74	0.70
1:C:263:MET:HA	1:C:263:MET:HE3	1.74	0.69
1:A:70:SER:CB	1:A:74:MET:HE2	2.23	0.68
1:C:238:GLN:O	1:C:241:ASP:HB2	1.94	0.68
1:C:242:ARG:HE	1:C:246:ILE:HD11	1.59	0.67
1:A:2:GLU:N	5:A:2213:HOH:O	2.28	0.67
1:B:156:ASP:HB3	5:B:2029:HOH:O	1.94	0.66
1:B:46[A]:ARG:HD3	5:B:1979:HOH:O	1.94	0.66
1:A:70:SER:CB	1:A:74:MET:CE	2.74	0.66
1:C:201:GLU:OE2	5:C:1884:HOH:O	2.13	0.66
1:C:3:ARG:O	1:C:7:GLN:HG3	1.96	0.65
1:B:291:ASN:HA	1:B:299:ARG:HH22	1.64	0.63
1:A:117:GLN:HE22	1:B:36:ASP:H	1.46	0.63
1:A:70:SER:HB2	1:A:74:MET:HE2	1.80	0.62
1:A:325:LYS:HE2	5:A:2046:HOH:O	1.99	0.61
1:B:247:MET:CE	1:B:262:LEU:HD21	2.29	0.61
1:A:26:PRO:HA	1:A:31:GLN:HE22	1.67	0.60
1:A:32:ARG:O	4:A:2003:GOL:H32	2.01	0.60
1:B:51:THR:HB	1:B:139:ILE:HG23	1.85	0.59
1:C:143:SER:HB3	1:C:146:LEU:HD12	1.83	0.59
1:B:192:ARG:HD3	5:B:1928:HOH:O	2.04	0.58
1:C:13:LEU:O	1:C:17:LEU:HG	2.04	0.57
1:C:105:GLY:HA3	1:C:203:LEU:HD13	1.87	0.57
1:C:166:GLN:O	5:C:1857:HOH:O	2.17	0.57
1:A:27:SER:N	1:A:31:GLN:HE21	1.96	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:232:ASP:OD2	1:C:271:TYR:OH	2.21	0.56
1:B:145:ILE:HG13	5:B:1905:HOH:O	2.06	0.56
1:B:208:HIS:HB3	5:B:1819:HOH:O	2.06	0.56
1:B:46[B]:ARG:NH2	5:B:1979:HOH:O	2.38	0.55
1:A:97:GLU:OE2	5:A:2222:HOH:O	2.18	0.55
1:C:13:LEU:HD13	1:C:108:SER:HB3	1.89	0.55
1:A:99:VAL:HG22	1:A:195:PRO:HB2	1.89	0.55
1:B:32:ARG:HG3	1:B:90:LEU:HD13	1.89	0.54
1:B:271:TYR:CZ	1:B:322:ILE:HD11	2.43	0.54
1:C:111:ARG:O	1:C:114:PRO:HD2	2.07	0.54
1:B:53:LYS:HB2	1:B:60:PHE:CD1	2.43	0.54
1:A:255:ARG:HG3	1:A:255:ARG:HH11	1.73	0.54
1:C:97:GLU:OE2	1:C:121:HIS:CD2	2.62	0.53
1:B:130:ASN:O	1:B:134:GLU:HG2	2.09	0.53
1:C:53:LYS:HB2	1:C:60:PHE:CD1	2.43	0.53
1:A:255:ARG:HG3	1:A:255:ARG:NH1	2.24	0.53
1:A:53:LYS:HA	1:A:60:PHE:HB2	1.89	0.53
1:C:50:ILE:O	1:C:53:LYS:HB3	2.08	0.52
1:C:209:ASN:ND2	1:C:265:TYR:OH	2.38	0.52
1:B:243:PHE:HE2	1:B:247:MET:HE1	1.74	0.52
1:C:79:TYR:O	1:C:83:VAL:HG13	2.09	0.52
1:C:155:GLU:CG	1:C:157:THR:HG23	2.34	0.52
1:A:11:ASP:OD2	1:A:255:ARG:NH2	2.40	0.52
1:A:61:GLY:O	1:A:65:LYS:HG3	2.10	0.52
1:C:130:ASN:HA	1:C:133:VAL:HG22	1.92	0.52
1:C:238:GLN:NE2	5:C:1920:HOH:O	2.36	0.51
1:C:141:ARG:O	1:C:147:ARG:HD3	2.10	0.51
1:B:145:ILE:HG12	5:B:1830:HOH:O	2.09	0.51
1:A:131:GLU:CD	1:A:131:GLU:H	2.14	0.51
1:C:32:ARG:HG3	1:C:90:LEU:HD13	1.91	0.51
1:B:323:LEU:HD23	5:B:1999:HOH:O	2.10	0.51
1:B:246:ILE:O	1:B:250:ASN:HB2	2.11	0.51
1:A:86:ASP:O	1:A:90:LEU:HG	2.11	0.50
1:C:247:MET:CE	1:C:262:LEU:HD21	2.41	0.50
1:A:51:THR:HB	1:A:139:ILE:HG23	1.93	0.50
1:B:317:MET:CE	1:B:318:GLN:HE21	2.24	0.50
1:A:29:GLY:HA3	5:A:2233:HOH:O	2.12	0.50
1:A:271:TYR:CE2	1:A:322:ILE:HD11	2.46	0.50
1:C:27:SER:OG	1:C:298:GLU:OE2	2.30	0.49
1:C:116:LEU:HD11	1:C:169:TYR:HB2	1.94	0.49
1:C:248:GLN:HG2	5:C:1851:HOH:O	2.12	0.49
1:C:317:MET:HE2	1:C:318:GLN:HE21	1.71	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:243:PHE:HE2	1:A:247:MET:HE1	1.78	0.48
1:B:128:ASP:HB3	1:B:133:VAL:HG13	1.95	0.48
1:A:36:ASP:H	1:B:117:GLN:NE2	2.10	0.48
1:A:299:ARG:NH2	5:A:2190:HOH:O	2.43	0.48
1:A:4:ILE:HG22	1:A:257:LEU:HD13	1.96	0.48
1:C:76:TYR:HB3	1:C:314:LEU:HD11	1.95	0.48
1:C:247:MET:HE2	1:C:262:LEU:HD21	1.94	0.48
1:A:29:GLY:CA	5:A:2233:HOH:O	2.62	0.48
1:A:191:LYS:HB2	1:A:194:ILE:HG13	1.96	0.48
1:B:39:LYS:HE3	1:B:43:GLU:OE2	2.14	0.47
1:B:155:GLU:O	1:B:157:THR:HG23	2.14	0.47
1:C:251:LEU:HD13	1:C:257:LEU:HD23	1.96	0.47
1:A:170:LYS:NZ	5:A:2063:HOH:O	2.44	0.47
1:B:154:LYS:NZ	5:B:1983:HOH:O	2.18	0.47
1:A:247:MET:HE3	1:A:262:LEU:CD2	2.43	0.47
1:A:174:CYS:HA	1:A:181:GLU:OE2	2.15	0.47
1:B:247:MET:HE3	1:B:262:LEU:HD22	1.96	0.47
1:C:36:ASP:O	1:C:40:LYS:HG3	2.15	0.47
1:B:122:LEU:O	1:B:168:ARG:HD2	2.15	0.47
1:C:73:VAL:HG12	1:C:317:MET:CE	2.45	0.47
1:C:192:ARG:NH2	1:C:222:LYS:HA	2.30	0.47
1:C:113:LEU:HD22	1:C:149:SER:OG	2.14	0.47
1:C:216:ILE:HA	1:C:228:TRP:CH2	2.50	0.47
1:C:316:VAL:HG21	5:C:1881:HOH:O	2.15	0.46
1:B:243:PHE:CE2	1:B:247:MET:HE1	2.50	0.46
1:A:141:ARG:CZ	1:A:156:ASP:HA	2.45	0.46
1:C:213:GLN:HE21	1:C:217:ASN:ND2	2.14	0.46
1:C:170:LYS:HD3	1:C:189:CYS:HB2	1.97	0.46
1:C:243:PHE:HE2	1:C:247:MET:HE1	1.80	0.46
1:C:322:ILE:C	1:C:322:ILE:HD12	2.36	0.46
1:C:143:SER:CB	1:C:146:LEU:HD12	2.45	0.46
1:A:313:GLU:OE1	5:A:2219:HOH:O	2.20	0.46
1:C:15:CYS:SG	1:C:74:MET:CE	3.04	0.46
1:B:290:PHE:HA	1:B:294:ILE:HG12	1.99	0.45
1:C:263:MET:HA	1:C:263:MET:CE	2.43	0.45
1:A:247:MET:CE	1:A:262:LEU:HD21	2.44	0.45
1:A:241:ASP:OD2	1:A:320:HIS:NE2	2.30	0.45
1:C:13:LEU:HD23	1:C:63:VAL:HG21	1.99	0.44
1:C:239:PRO:HA	5:C:1919:HOH:O	2.17	0.44
1:A:117:GLN:NE2	1:B:36:ASP:H	2.12	0.44
1:B:2:GLU:HG3	5:B:2002:HOH:O	2.18	0.44
1:B:325:LYS:HE3	1:B:325:LYS:HB2	1.81	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:20:ILE:CD1	1:C:45:HIS:CG	3.00	0.44
1:B:96:ASN:O	1:B:99:VAL:HG23	2.17	0.44
1:B:193[B]:GLU:CG	5:B:1988:HOH:O	2.50	0.44
1:B:3:ARG:HG3	5:B:1984:HOH:O	2.17	0.44
1:B:268:LYS:NZ	5:B:1962:HOH:O	2.43	0.44
1:B:243:PHE:CE2	1:B:247:MET:CE	3.00	0.44
1:C:96:ASN:N	1:C:96:ASN:HD22	2.16	0.44
1:A:88:ALA:HB2	1:A:325:LYS:HD3	2.00	0.43
1:B:317:MET:HE3	1:B:318:GLN:NE2	2.33	0.43
1:C:35:VAL:HG12	1:C:39:LYS:HE2	1.99	0.43
1:A:159:LYS:O	1:A:160:SER:C	2.56	0.43
1:A:222:LYS:HE3	5:A:2170:HOH:O	2.18	0.43
1:A:96:ASN:HB2	1:A:99:VAL:HG21	1.99	0.43
1:C:133:VAL:HG21	1:C:173:ALA:HB2	2.00	0.43
1:C:4:ILE:HG23	1:C:255:ARG:HG2	2.01	0.43
1:C:176:LEU:HD23	1:C:176:LEU:HA	1.81	0.43
1:B:209:ASN:ND2	1:B:265:TYR:OH	2.52	0.43
1:B:101:VAL:HG22	1:B:197:ILE:HB	2.00	0.43
1:A:29:GLY:N	5:A:2233:HOH:O	2.50	0.43
1:A:71:PHE:N	1:A:71:PHE:CD2	2.87	0.42
1:C:119:PHE:HA	1:C:120:PRO:HD3	1.82	0.42
1:C:290:PHE:O	1:C:299:ARG:NH1	2.53	0.42
1:C:199:ILE:HD13	1:C:199:ILE:HG21	1.84	0.42
1:B:269:GLU:O	5:B:1859:HOH:O	2.22	0.42
1:B:177:ASN:HD22	1:B:211:GLU:HB3	1.85	0.42
1:A:109:ASP:OD2	1:A:111:ARG:NH1	2.53	0.42
1:A:216:ILE:HA	1:A:228:TRP:CH2	2.54	0.42
1:C:89:ILE:HD11	1:C:199:ILE:HD11	2.01	0.42
1:C:325:LYS:HE3	1:C:325:LYS:HB2	1.91	0.42
1:B:73:VAL:O	1:B:317:MET:HE1	2.19	0.41
1:C:36:ASP:OD2	1:C:40:LYS:HE3	2.20	0.41
1:C:54:LYS:HE3	1:C:142:GLU:CD	2.40	0.41
1:C:243:PHE:CE2	1:C:247:MET:CE	3.03	0.41
1:B:90:LEU:O	1:B:94:VAL:HG23	2.21	0.41
1:A:56:SER:HB3	1:A:59:ALA:HB3	2.02	0.41
1:A:122:LEU:O	1:A:168:ARG:HD2	2.20	0.41
1:C:222:LYS:HB3	1:C:222:LYS:HE3	1.86	0.41
1:C:6:GLN:HE21	1:C:129:TYR:HB3	1.85	0.41
1:C:207:MET:HE2	1:C:212:SER:CA	2.50	0.41
1:A:71:PHE:CZ	1:A:74:MET:HB2	2.56	0.41
1:B:242:ARG:NH1	1:B:242:ARG:CB	2.77	0.41
1:C:235:GLY:HA3	1:C:263:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:290:PHE:O	1:B:299:ARG:NH2	2.54	0.41
1:C:97:GLU:OE2	1:C:121:HIS:CG	2.74	0.41
1:A:164:ILE:O	1:A:170:LYS:HA	2.21	0.41
1:A:300:LYS:HG3	2:A:1001:PO4:O4	2.20	0.41
1:C:300:LYS:HD2	5:C:1820:HOH:O	2.20	0.41
1:C:191:LYS:HB2	1:C:194:ILE:HD12	2.03	0.40
1:C:164:ILE:CG2	1:C:166:GLN:HB2	2.51	0.40
1:C:243:PHE:HE2	1:C:247:MET:CE	2.33	0.40
1:B:291:ASN:HA	1:B:299:ARG:NH2	2.34	0.40
1:A:152:LEU:HD21	1:A:164:ILE:HG23	2.02	0.40
1:C:179:ILE:HG21	1:C:214:LEU:HD21	2.03	0.40
1:C:33:LEU:HD22	1:C:37:LEU:HG	2.04	0.40
1:A:22:VAL:HG11	1:A:24:TYR:HE1	1.86	0.40
1:B:152:LEU:HD21	1:B:164:ILE:HG23	2.04	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	324/327 (99%)	310 (96%)	13 (4%)	1 (0%)	50	37
1	B	326/327 (100%)	318 (98%)	7 (2%)	1 (0%)	50	37
1	C	324/327 (99%)	312 (96%)	11 (3%)	1 (0%)	50	37
All	All	974/981 (99%)	940 (96%)	31 (3%)	3 (0%)	50	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	ASP
1	C	97	GLU
1	A	273	SER

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	295/295 (100%)	289 (98%)	6 (2%)	68	60
1	B	297/295 (101%)	289 (97%)	8 (3%)	57	46
1	C	295/295 (100%)	283 (96%)	12 (4%)	41	27
All	All	887/885 (100%)	861 (97%)	26 (3%)	56	43

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	MET
1	A	156	ASP
1	A	157	THR
1	A	159	LYS
1	A	210	ASN
1	A	322	ILE
1	B	46[A]	ARG
1	B	46[B]	ARG
1	B	57	ARG
1	B	112	MET
1	B	156	ASP
1	B	210	ASN
1	B	249	SER
1	B	300	LYS
1	C	36	ASP
1	C	96	ASN
1	C	99	VAL
1	C	111	ARG
1	C	112	MET
1	C	155	GLU
1	C	157	THR
1	C	160	SER
1	C	166	GLN
1	C	203	LEU
1	C	263	MET
1	C	268	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	31	GLN
1	A	117	GLN
1	A	121	HIS
1	A	177	ASN
1	A	209	ASN
1	A	210	ASN
1	A	318	GLN
1	B	117	GLN
1	B	121	HIS
1	B	177	ASN
1	B	209	ASN
1	B	210	ASN
1	B	318	GLN
1	C	96	ASN
1	C	121	HIS
1	C	177	ASN
1	C	209	ASN
1	C	217	ASN
1	C	250	ASN
1	C	318	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	SMC	A	202	1	6,6,7	5.81	1 (16%)	4,6,8	2.78	3 (75%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SMC	B	202	1	6,6,7	6.63	1 (16%)	4,6,8	2.92	3 (75%)
1	SMC	C	202	1	6,6,7	9.24	3 (50%)	4,6,8	1.26	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
1	SMC	A	202	1	-	0/3/5/7	0/0/0/0
1	SMC	B	202	1	-	0/3/5/7	0/0/0/0
1	SMC	C	202	1	-	0/3/5/7	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	202	SMC	O-C	22.38	1.26	1.11
1	B	202	SMC	O-C	16.07	1.22	1.11
1	A	202	SMC	O-C	13.99	1.21	1.11
1	C	202	SMC	CB-SG	-2.37	1.78	1.80
1	C	202	SMC	CA-C	2.24	1.52	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	SMC	CS-SG-CB	3.76	107.48	101.14
1	A	202	SMC	CS-SG-CB	3.66	107.31	101.14
1	A	202	SMC	C-CA-N	-3.44	110.39	113.83
1	B	202	SMC	C-CA-N	-3.10	110.73	113.83
1	B	202	SMC	CA-CB-SG	-3.05	109.95	113.86
1	A	202	SMC	CA-CB-SG	-2.17	111.08	113.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	A	1001	-	4,4,4	0.33	0	6,6,6	0.30	0
3	SAH	A	1801	-	28,28,28	1.07	3 (10%)	40,40,40	2.40	12 (30%)
4	GOL	A	2002	-	5,5,5	0.55	0	5,5,5	0.58	0
4	GOL	A	2003	-	5,5,5	0.35	0	5,5,5	1.18	0
3	SAH	B	1802	-	28,28,28	1.00	3 (10%)	40,40,40	2.68	14 (35%)
3	SAH	C	1803	-	28,28,28	1.18	3 (10%)	40,40,40	2.57	11 (27%)

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
2	PO4	A	1001	-	-	0/0/0/0	0/0/0/0
3	SAH	A	1801	-	-	0/15/31/31	0/1/3/3
4	GOL	A	2002	-	-	0/4/4/4	0/0/0/0
4	GOL	A	2003	-	-	0/4/4/4	0/0/0/0
3	SAH	B	1802	-	-	0/15/31/31	0/1/3/3
3	SAH	C	1803	-	-	0/15/31/31	0/1/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1803	SAH	C2-N3	3.47	1.39	1.32
3	C	1803	SAH	C2-N1	2.94	1.39	1.33
3	C	1803	SAH	C4-N3	2.72	1.39	1.35
3	A	1801	SAH	C2-N3	2.58	1.37	1.32
3	B	1802	SAH	C2-N3	2.54	1.37	1.32
3	B	1802	SAH	C4-N3	2.42	1.39	1.35
3	A	1801	SAH	C2-N1	2.30	1.38	1.33
3	B	1802	SAH	C2-N1	2.05	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1801	SAH	O4'-C1'	-2.04	1.38	1.41

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1803	SAH	N3-C2-N1	-11.06	119.46	128.71
3	B	1802	SAH	N3-C2-N1	-10.48	119.95	128.71
3	A	1801	SAH	N3-C2-N1	-9.08	121.12	128.71
3	B	1802	SAH	O4'-C1'-N9	8.16	116.03	108.44
3	A	1801	SAH	O4'-C1'-C2'	-5.23	98.75	106.77
3	C	1803	SAH	C5'-SD-CG	-4.76	88.22	102.42
3	C	1803	SAH	N3-C4-N9	4.45	133.47	125.43
3	A	1801	SAH	C5'-SD-CG	-4.15	90.05	102.42
3	C	1803	SAH	O4'-C1'-C2'	-4.02	100.61	106.77
3	A	1801	SAH	C-CA-N	3.81	115.67	109.36
3	C	1803	SAH	OXT-C-O	-3.66	115.79	124.07
3	A	1801	SAH	N3-C4-N9	3.66	132.03	125.43
3	C	1803	SAH	O4'-C1'-N9	3.58	111.77	108.44
3	B	1802	SAH	C1'-N9-C4	-3.55	120.50	126.64
3	B	1802	SAH	C8-N9-C4	2.80	109.04	106.90
3	C	1803	SAH	C8-N9-C4	2.78	109.02	106.90
3	B	1802	SAH	N3-C4-N9	2.70	130.30	125.43
3	A	1801	SAH	N7-C8-N9	-2.69	106.75	114.36
3	A	1801	SAH	OXT-C-O	-2.66	118.05	124.07
3	B	1802	SAH	C2-N1-C6	2.65	123.56	118.77
3	B	1802	SAH	O4'-C4'-C3'	2.63	110.49	105.17
3	B	1802	SAH	O4'-C4'-C5'	-2.58	102.03	108.91
3	B	1802	SAH	C3'-C2'-C1'	2.57	104.93	100.91
3	C	1803	SAH	N7-C8-N9	-2.57	107.09	114.36
3	A	1801	SAH	O4'-C1'-N9	2.56	110.82	108.44
3	C	1803	SAH	C5-C4-N3	-2.52	120.22	125.70
3	A	1801	SAH	C8-N9-C4	2.49	108.80	106.90
3	B	1802	SAH	O2'-C2'-C1'	2.47	118.71	111.23
3	B	1802	SAH	C4-C5-N7	-2.37	107.50	109.52
3	B	1802	SAH	N7-C8-N9	-2.28	107.90	114.36
3	C	1803	SAH	C2-N3-C4	2.26	120.44	114.01
3	C	1803	SAH	CB-CG-SD	-2.11	109.51	113.57
3	A	1801	SAH	C3'-C2'-C1'	2.10	104.19	100.91
3	A	1801	SAH	C8-N7-C5	2.09	110.05	103.58
3	B	1802	SAH	OXT-C-O	-2.08	119.38	124.07
3	B	1802	SAH	C8-N9-C1'	2.07	130.46	126.38
3	A	1801	SAH	C6-C5-C4	2.05	121.01	117.25

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	327/327 (100%)	-0.49	0 100 100	7, 14, 28, 41	0
1	B	327/327 (100%)	-0.47	0 100 100	7, 14, 30, 43	0
1	C	327/327 (100%)	-0.15	5 (1%) 70 72	5, 15, 34, 41	0
All	All	981/981 (100%)	-0.37	5 (0%) 88 90	5, 14, 32, 43	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	239	PRO	2.6
1	C	255	ARG	2.5
1	C	242	ARG	2.5
1	C	249	SER	2.4
1	C	257	LEU	2.2

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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SMC	B	202	7/8	0.08	1.35	6,10,12,16	0
1	SMC	A	202	7/8	0.07	0.55	9,11,12,17	0
1	SMC	C	202	7/8	0.07	-2.26	7,9,11,15	0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PO4	A	1001	5/5	0.16	2.61	47,48,51,51	0
4	GOL	A	2003	6/6	0.09	2.07	22,27,28,30	0
4	GOL	A	2002	6/6	0.10	0.56	9,14,15,20	0
3	SAH	C	1803	26/26	0.08	-0.30	10,17,22,23	0
3	SAH	A	1801	26/26	0.07	-0.44	2,4,6,8	0
3	SAH	B	1802	26/26	0.06	-0.81	2,4,6,8	0

6.5 Other polymers ⓘ

There are no such residues in this entry.