Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:21 PM GMT

PDB ID	:	3X0D
Title	:	Crystal structure of C.elegans PRMT7 in complex with SAH (P43212)
Authors	:	Hasegawa, M.; Toma-Fukai, S.; Shimizu, T.
Deposited on	:	2014-10-10
Resolution	:	2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

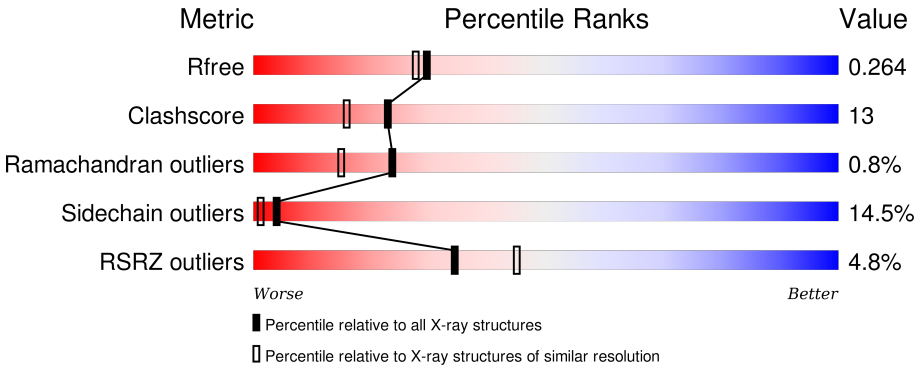
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	655	5% 68% 21% 5% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5082 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.

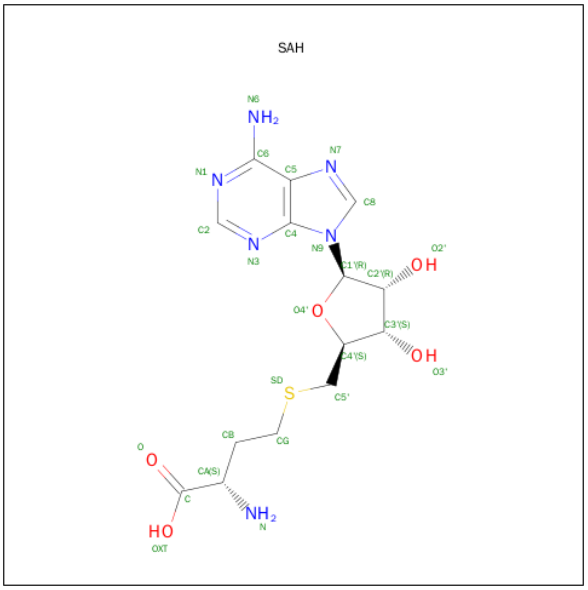
- Molecule 1 is a protein called Protein arginine N-methyltransferase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	S	0	0	0
			4964	3156	834	945	29			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP Q9XW42
A	-6	PRO	-	EXPRESSION TAG	UNP Q9XW42
A	-5	LEU	-	EXPRESSION TAG	UNP Q9XW42
A	-4	GLY	-	EXPRESSION TAG	UNP Q9XW42
A	-3	SER	-	EXPRESSION TAG	UNP Q9XW42
A	-2	GLY	-	EXPRESSION TAG	UNP Q9XW42
A	-1	ILE	-	EXPRESSION TAG	UNP Q9XW42
A	0	PRO	-	EXPRESSION TAG	UNP Q9XW42

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

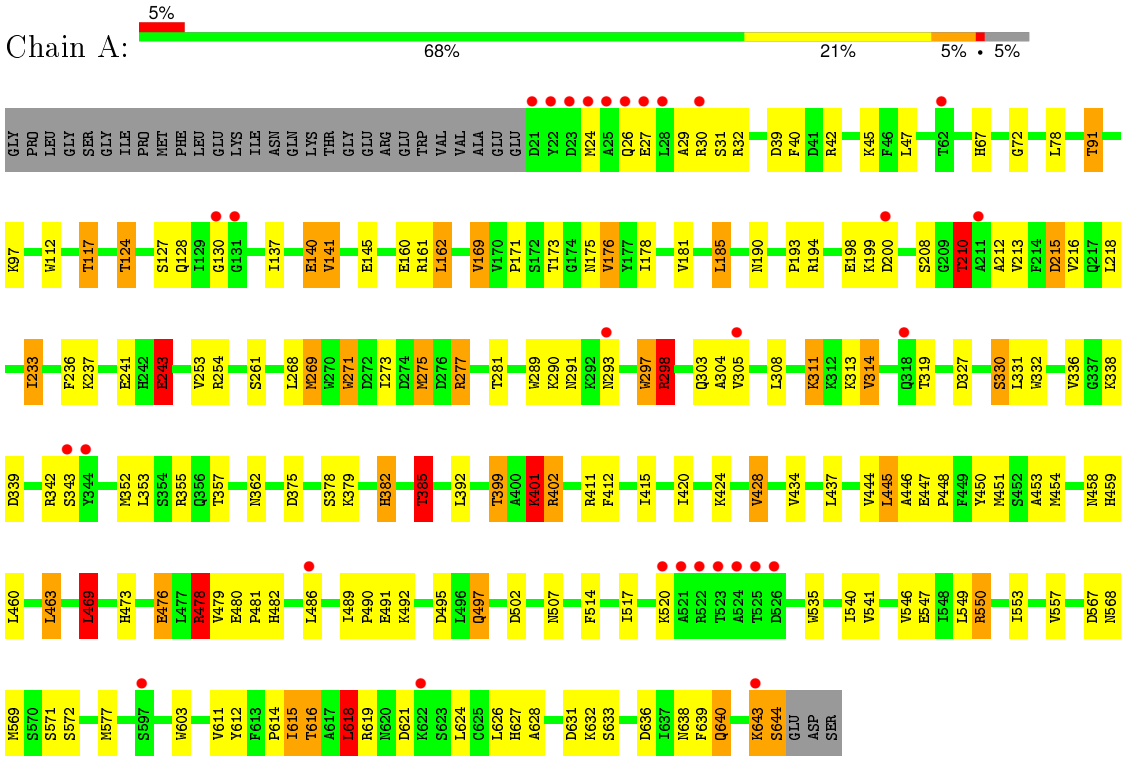
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		

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: Protein arginine N-methyltransferase 7

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	114.18Å 114.18Å 184.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.12 – 2.15 31.12 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.3 (31.12-2.15) 99.3 (31.12-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.220 , 0.266 0.218 , 0.264	Depositor DCC
R_{free} test set	3355 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	55.1	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 35.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	1 of 66186 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5082	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SAH

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	1.02	9/5074 (0.2%)	1.11	17/6855 (0.2%)

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
1	A	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	535	TRP	CD2-CE2	6.30	1.49	1.41
1	A	297	TRP	CD2-CE2	5.85	1.48	1.41
1	A	289	TRP	CD2-CE2	5.78	1.48	1.41
1	A	332	TRP	CD2-CE2	5.62	1.48	1.41
1	A	112	TRP	CD2-CE2	5.58	1.48	1.41
1	A	271	TRP	CD2-CE2	5.48	1.48	1.41
1	A	382	HIS	CG-CD2	5.37	1.44	1.35
1	A	385	THR	CB-CG2	-5.35	1.34	1.52
1	A	603	TRP	CD2-CE2	5.15	1.47	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	298	ARG	NE-CZ-NH1	13.12	126.86	120.30
1	A	298	ARG	NE-CZ-NH2	-13.02	113.79	120.30
1	A	277	ARG	NE-CZ-NH2	-10.47	115.07	120.30
1	A	277	ARG	NE-CZ-NH1	8.89	124.75	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	401	LYS	CD-CE-NZ	-6.46	96.85	111.70
1	A	473	HIS	C-N-CA	-6.00	109.69	122.30
1	A	141	VAL	CG1-CB-CG2	5.46	119.63	110.90
1	A	478	ARG	NE-CZ-NH2	5.43	123.01	120.30
1	A	215	ASP	CB-CG-OD2	5.36	123.13	118.30
1	A	298	ARG	CD-NE-CZ	5.36	131.10	123.60
1	A	469	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	402	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	185	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	298	ARG	CB-CG-CD	-5.21	98.06	111.60
1	A	473	HIS	N-CA-C	-5.14	97.12	111.00
1	A	618	LEU	CA-CB-CG	5.12	127.08	115.30
1	A	402	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	GLU	Peptide
1	A	210	THR	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	4964	0	4853	133	0
2	A	26	0	19	2	0
3	A	1	0	0	0	0
4	A	91	0	0	8	0
All	All	5082	0	4872	133	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 13.

All (133) 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:A:275:MET:HE2	1:A:275:MET:HA	1.17	1.15
1:A:199:LYS:HG2	1:A:200:ASP:HA	1.13	1.08
1:A:269:MET:HE2	1:A:304:ALA:HB3	1.31	1.08
1:A:502:ASP:OD2	1:A:616:THR:HG21	1.58	1.04
1:A:67:HIS:HE1	1:A:91:THR:CG2	1.73	1.01
1:A:379:LYS:HA	1:A:399:THR:HG23	1.43	0.99
1:A:269:MET:CE	1:A:304:ALA:HB3	1.92	0.98
1:A:489:ILE:HD13	1:A:541:VAL:HG21	1.42	0.96
1:A:450:TYR:H	1:A:459:HIS:HD2	1.12	0.95
1:A:171:PRO:HB3	1:A:275:MET:HE1	1.50	0.93
1:A:171:PRO:HB3	1:A:275:MET:CE	1.98	0.92
1:A:497:GLN:HE21	1:A:497:GLN:H	1.14	0.91
1:A:275:MET:CA	1:A:275:MET:HE2	2.00	0.91
1:A:275:MET:CE	1:A:275:MET:HA	2.02	0.89
1:A:489:ILE:CD1	1:A:541:VAL:HG21	2.04	0.88
1:A:210:THR:HB	1:A:212:ALA:H	1.38	0.87
1:A:569:MET:HA	1:A:569:MET:HE2	1.57	0.87
1:A:199:LYS:CG	1:A:200:ASP:HA	2.01	0.87
1:A:190:ASN:HD22	1:A:355:ARG:HH12	1.22	0.87
1:A:67:HIS:HE1	1:A:91:THR:HG22	1.42	0.84
1:A:450:TYR:H	1:A:459:HIS:CD2	1.95	0.84
1:A:378:SER:HB2	1:A:399:THR:HG22	1.61	0.81
1:A:67:HIS:CE1	1:A:91:THR:CG2	2.61	0.81
1:A:478:ARG:HG2	1:A:478:ARG:HH21	1.45	0.80
1:A:643:LYS:O	1:A:644:SER:HB2	1.84	0.78
1:A:480:GLU:OE2	1:A:482:HIS:HD2	1.67	0.76
1:A:489:ILE:HD13	1:A:541:VAL:CG2	2.16	0.75
1:A:569:MET:HE2	1:A:572:SER:HB2	1.67	0.75
1:A:490:PRO:HB3	1:A:569:MET:HE3	1.67	0.73
1:A:497:GLN:H	1:A:497:GLN:NE2	1.85	0.72
1:A:275:MET:CE	1:A:275:MET:CA	2.66	0.72
1:A:392:LEU:O	1:A:392:LEU:HD23	1.89	0.72
1:A:273:ILE:HD12	1:A:275:MET:HE1	1.73	0.70
1:A:117:THR:CG2	4:A:813:HOH:O	2.39	0.70
1:A:117:THR:HG22	4:A:813:HOH:O	1.93	0.69
1:A:39:ASP:OD2	1:A:298:ARG:HD3	1.94	0.68
1:A:627:HIS:HB2	1:A:640:GLN:HG2	1.74	0.68
1:A:67:HIS:HE1	1:A:91:THR:HG23	1.58	0.67
1:A:171:PRO:HB3	1:A:275:MET:HE2	1.75	0.67
1:A:497:GLN:N	1:A:497:GLN:HE21	1.90	0.66
1:A:569:MET:CE	1:A:569:MET:HA	2.24	0.66
1:A:547:GLU:OE2	1:A:550:ARG:NH1	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:MET:CE	1:A:304:ALA:CB	2.73	0.65
1:A:454:MET:H	1:A:458:ASN:HD22	1.46	0.63
1:A:569:MET:CE	1:A:572:SER:HB2	2.27	0.63
1:A:210:THR:HB	1:A:212:ALA:N	2.12	0.63
1:A:490:PRO:HB3	1:A:569:MET:CE	2.29	0.62
1:A:445:LEU:HD12	1:A:480:GLU:HB2	1.81	0.62
1:A:67:HIS:CE1	1:A:91:THR:HG22	2.29	0.62
1:A:379:LYS:CA	1:A:399:THR:HG23	2.25	0.62
1:A:489:ILE:CD1	1:A:541:VAL:CG2	2.77	0.61
1:A:169:VAL:HG13	1:A:241:GLU:HG2	1.82	0.61
1:A:269:MET:HE2	1:A:304:ALA:CB	2.18	0.61
1:A:434:VAL:CG1	1:A:469:LEU:HD13	2.32	0.60
1:A:569:MET:HE2	1:A:572:SER:CB	2.31	0.60
1:A:32:ARG:HB3	1:A:514:PHE:HZ	1.68	0.58
1:A:353:LEU:HD22	1:A:357:THR:HG21	1.84	0.58
1:A:478:ARG:CG	1:A:478:ARG:HH21	2.15	0.58
1:A:631:ASP:OD1	1:A:633:SER:HB3	2.05	0.57
1:A:434:VAL:HG13	1:A:469:LEU:HD13	1.85	0.57
1:A:615:ILE:HG22	1:A:618:LEU:HD22	1.87	0.57
1:A:375:ASP:O	1:A:399:THR:HG21	2.05	0.56
1:A:218:LEU:H	1:A:303:GLN:HE21	1.54	0.55
1:A:269:MET:C	1:A:269:MET:HE3	2.27	0.55
1:A:268:LEU:HD23	1:A:268:LEU:N	2.22	0.55
1:A:478:ARG:NH2	1:A:478:ARG:HG2	2.20	0.55
1:A:577:MET:HE1	1:A:639:PHE:CE1	2.42	0.54
1:A:399:THR:HB	4:A:814:HOH:O	2.08	0.54
1:A:411:ARG:O	1:A:415:ILE:HD12	2.07	0.54
1:A:476:GLU:H	1:A:476:GLU:CD	2.11	0.53
1:A:460:LEU:HD22	1:A:463:LEU:HD22	1.89	0.53
1:A:261:SER:HA	1:A:314:VAL:O	2.08	0.53
1:A:385:THR:HG21	4:A:809:HOH:O	2.09	0.53
1:A:497:GLN:N	1:A:497:GLN:NE2	2.54	0.52
1:A:233:ILE:CD1	1:A:254:ARG:HB3	2.40	0.52
1:A:269:MET:O	1:A:269:MET:HE3	2.10	0.52
1:A:32:ARG:HB3	1:A:514:PHE:CZ	2.44	0.52
1:A:26:GLN:O	1:A:29:ALA:HB3	2.10	0.52
1:A:626:LEU:HD23	1:A:626:LEU:C	2.29	0.52
1:A:479:VAL:HG22	1:A:553:ILE:HG21	1.92	0.51
1:A:67:HIS:CE1	1:A:91:THR:HG23	2.37	0.51
1:A:117:THR:HG23	4:A:813:HOH:O	2.08	0.51
1:A:632:LYS:O	1:A:632:LYS:HG2	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:LYS:CB	1:A:401:LYS:HZ3	2.23	0.51
1:A:353:LEU:HD22	1:A:357:THR:CG2	2.41	0.50
1:A:297:TRP:CE3	1:A:495:ASP:HB3	2.47	0.50
1:A:420:ILE:HG21	1:A:428:VAL:HG22	1.94	0.50
1:A:490:PRO:CB	1:A:569:MET:CE	2.90	0.49
1:A:479:VAL:CG2	1:A:553:ILE:HG21	2.43	0.49
1:A:193:PRO:HA	1:A:362:ASN:ND2	2.27	0.49
1:A:193:PRO:HA	1:A:362:ASN:HD21	1.77	0.48
1:A:275:MET:CE	1:A:275:MET:N	2.77	0.48
1:A:612:TYR:CE2	1:A:614:PRO:HA	2.49	0.48
1:A:160:GLU:HG3	1:A:243:GLU:HG2	1.95	0.48
1:A:453:ALA:HB1	1:A:458:ASN:HB2	1.95	0.47
1:A:492:LYS:HE3	1:A:571:SER:O	2.14	0.47
1:A:42:ARG:HH11	1:A:140:GLU:HG3	1.78	0.47
1:A:643:LYS:O	1:A:644:SER:CB	2.59	0.47
1:A:124:THR:O	1:A:161:ARG:NH2	2.48	0.47
1:A:178:ILE:HA	1:A:268:LEU:O	2.15	0.47
1:A:311:LYS:NZ	1:A:311:LYS:HB3	2.30	0.47
1:A:171:PRO:CB	1:A:275:MET:CE	2.83	0.47
1:A:577:MET:CE	1:A:639:PHE:CE1	2.97	0.47
1:A:627:HIS:O	1:A:639:PHE:HA	2.16	0.45
1:A:446:ALA:O	1:A:481:PRO:HD3	2.16	0.45
1:A:171:PRO:CB	1:A:275:MET:HE2	2.43	0.45
1:A:297:TRP:CD2	1:A:495:ASP:HB3	2.52	0.45
1:A:78:LEU:HD22	2:A:701:SAH:HN2	1.82	0.45
1:A:176:VAL:HG13	1:A:236:PHE:HB2	1.99	0.44
1:A:399:THR:HG23	1:A:399:THR:O	2.17	0.44
1:A:628:ALA:HA	1:A:638:ASN:O	2.17	0.44
1:A:327:ASP:OD1	1:A:330:SER:HB2	2.18	0.44
1:A:378:SER:HB2	1:A:399:THR:CG2	2.40	0.44
1:A:569:MET:CE	1:A:572:SER:CB	2.92	0.44
1:A:491:GLU:O	1:A:572:SER:HB3	2.18	0.43
1:A:385:THR:CG2	4:A:801:HOH:O	2.66	0.43
1:A:161:ARG:HB3	1:A:162:LEU:HD13	2.00	0.43
1:A:175:ASN:ND2	1:A:237:LYS:HG2	2.33	0.43
1:A:385:THR:HG23	4:A:801:HOH:O	2.18	0.43
1:A:311:LYS:HZ3	1:A:311:LYS:HB3	1.84	0.43
1:A:72:GLY:O	2:A:701:SAH:HB1	2.19	0.43
1:A:507:ASN:ND2	4:A:848:HOH:O	2.51	0.43
1:A:567:ASP:O	1:A:568:ASN:HB2	2.19	0.43
1:A:271:TRP:CZ3	1:A:273:ILE:HG12	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:MET:HE3	1:A:275:MET:N	2.34	0.42
1:A:401:LYS:HG3	1:A:401:LYS:HZ2	1.62	0.42
1:A:194:ARG:CG	1:A:194:ARG:HH11	2.33	0.42
1:A:145:GLU:OE1	1:A:215:ASP:OD1	2.38	0.42
1:A:447:GLU:N	1:A:448:PRO:HA	2.35	0.41
1:A:352:MET:HG2	1:A:412:PHE:CZ	2.56	0.41
1:A:382:HIS:CG	1:A:402:ARG:HD3	2.56	0.40
1:A:137:ILE:HB	1:A:169:VAL:HB	2.02	0.40
1:A:169:VAL:HG22	1:A:171:PRO:O	2.22	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	622/655 (95%)	588 (94%)	29 (5%)	5 (1%)	24 15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	643	LYS
1	A	243	GLU
1	A	619	ARG
1	A	130	GLY
1	A	291	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	543/569 (95%)	464 (86%)	79 (14%)	4 1

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	MET
1	A	27	GLU
1	A	30	ARG
1	A	31	SER
1	A	40	PHE
1	A	45	LYS
1	A	47	LEU
1	A	91	THR
1	A	97	LYS
1	A	117	THR
1	A	124	THR
1	A	127	SER
1	A	128	GLN
1	A	140	GLU
1	A	141	VAL
1	A	162	LEU
1	A	169	VAL
1	A	173	THR
1	A	176	VAL
1	A	181	VAL
1	A	185	LEU
1	A	208	SER
1	A	210	THR
1	A	213	VAL
1	A	216	VAL
1	A	233	ILE
1	A	243	GLU
1	A	253	VAL
1	A	269	MET
1	A	275	MET
1	A	277	ARG
1	A	281	THR
1	A	290	LYS
1	A	293	ASN
1	A	298	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	305	VAL
1	A	308	LEU
1	A	311	LYS
1	A	313	LYS
1	A	314	VAL
1	A	319	THR
1	A	330	SER
1	A	331	LEU
1	A	336	VAL
1	A	338	LYS
1	A	339	ASP
1	A	342	ARG
1	A	343	SER
1	A	385	THR
1	A	399	THR
1	A	401	LYS
1	A	424	LYS
1	A	428	VAL
1	A	437	LEU
1	A	444	VAL
1	A	445	LEU
1	A	451	MET
1	A	463	LEU
1	A	469	LEU
1	A	476	GLU
1	A	478	ARG
1	A	486	LEU
1	A	497	GLN
1	A	517	ILE
1	A	520	LYS
1	A	540	ILE
1	A	546	VAL
1	A	549	LEU
1	A	550	ARG
1	A	557	VAL
1	A	611	VAL
1	A	615	ILE
1	A	616	THR
1	A	618	LEU
1	A	621	ASP
1	A	624	LEU
1	A	636	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	640	GLN
1	A	644	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	67	HIS
1	A	175	ASN
1	A	190	ASN
1	A	293	ASN
1	A	303	GLN
1	A	317	ASN
1	A	335	ASN
1	A	362	ASN
1	A	421	HIS
1	A	455	ASN
1	A	458	ASN
1	A	459	HIS
1	A	482	HIS
1	A	497	GLN
1	A	507	ASN

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
2	SAH	A	701	-	20,28,28	1.71	4 (20%)	19,40,40	3.56	11 (57%)

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	SAH	A	701	-	-	0/7/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	SAH	C2-N3	2.20	1.36	1.32
2	A	701	SAH	C5-C4	2.90	1.47	1.40
2	A	701	SAH	C8-N7	3.19	1.40	1.34
2	A	701	SAH	O4'-C1'	5.03	1.47	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	SAH	N3-C2-N1	-10.27	121.03	128.89
2	A	701	SAH	C1'-N9-C4	-5.27	118.99	126.94
2	A	701	SAH	O4'-C1'-N9	-4.07	99.58	108.10
2	A	701	SAH	O3'-C3'-C4'	-3.26	101.28	111.05
2	A	701	SAH	C4'-C5'-SD	-2.03	107.26	113.53
2	A	701	SAH	C2'-C3'-C4'	2.06	106.84	102.61
2	A	701	SAH	CB-CA-N	2.19	116.74	110.52
2	A	701	SAH	C2-N1-C6	3.32	124.70	118.77
2	A	701	SAH	C4'-O4'-C1'	3.39	113.44	109.72
2	A	701	SAH	C2'-C1'-N9	4.16	120.64	114.29
2	A	701	SAH	O4'-C4'-C5'	4.22	120.34	108.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	SAH	2	0

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^{th} 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	624/655 (95%)	-0.04	30 (4%) 34 45	38, 58, 100, 130	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	TYR	6.5
1	A	26	GLN	5.7
1	A	23	ASP	5.5
1	A	525	THR	5.0
1	A	526	ASP	4.3
1	A	28	LEU	4.0
1	A	24	MET	4.0
1	A	27	GLU	3.8
1	A	523	THR	3.6
1	A	21	ASP	3.5
1	A	521	ALA	3.5
1	A	344	TYR	3.4
1	A	30	ARG	3.3
1	A	211	ALA	3.1
1	A	524	ALA	3.1
1	A	131	GLY	3.1
1	A	597	SER	3.1
1	A	25	ALA	3.0
1	A	62	THR	2.8
1	A	318	GLN	2.7
1	A	486	LEU	2.5
1	A	130	GLY	2.5
1	A	622	LYS	2.4
1	A	520	LYS	2.4
1	A	522	ARG	2.2
1	A	200	ASP	2.2
1	A	343	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	305	VAL	2.1
1	A	643	LYS	2.0
1	A	293	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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^2)	Q<0.9
2	SAH	A	701	26/26	0.97	0.10	-1.33	40,50,60,65	0
3	ZN	A	702	1/1	0.99	0.02	-2.12	66,66,66,66	0

6.5 Other polymers (i)

There are no such residues in this entry.