Full wwPDB X-ray Structure Validation Report (i)

Sep 21, 2016 – 05:49 PM EDT

PDB ID	:	5DNK
Title	:	The structure of PKMT1 from Rickettsia prowazekii in complex with AdoHcy
Authors	:	Noinaj, N.; Abeykoon, A.; He, Y.; Yang, D.C.; Buchanan, S.K.
Deposited on	:	2015-09-10
Resolution	:	1.90 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:

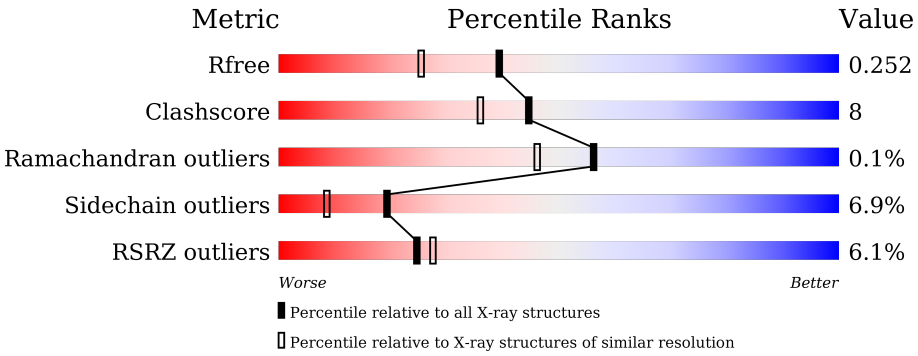
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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. 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	554	3% 76% 15% • 8%
1	B	554	8% 70% 18% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9030 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.

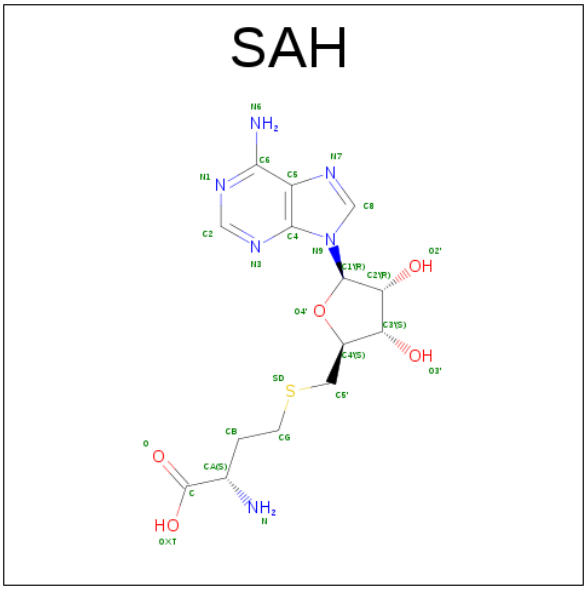
- Molecule 1 is a protein called protein lysine methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	1	0
			4065	2589	697	759	20			
1	B	502	Total	C	N	O	S	0	0	0
			3985	2538	684	743	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP O05979
B	0	GLY	-	expression tag	UNP O05979

- 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		

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

- Molecule 3 is water.

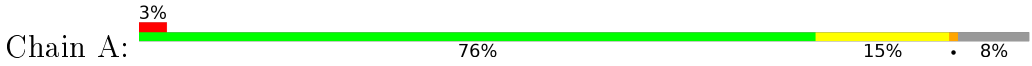
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	556	Total	O	0	0
			556	556		
3	B	372	Total	O	0	0
			372	372		

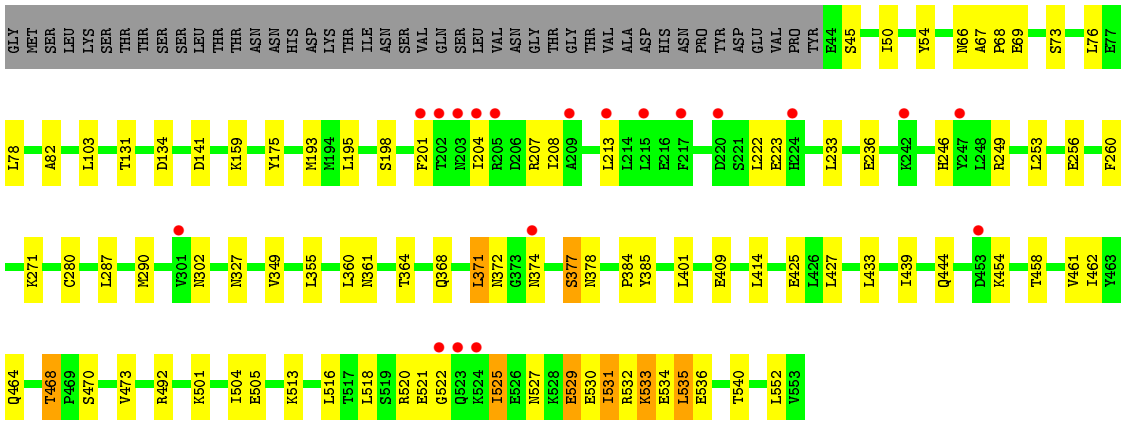
3 Residue-property plots (i)

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 lysine methyltransferase 1

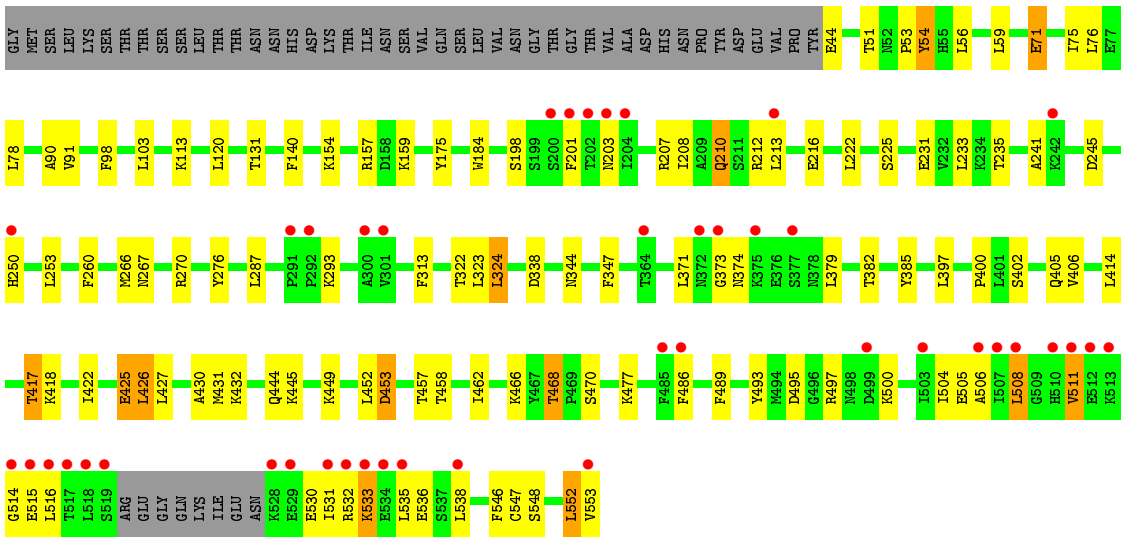
Chain A:





- Molecule 1: protein lysine methyltransferase 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.02Å 62.13Å 107.39Å 90.00° 100.88° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 48.13 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-1.90) 96.3 (48.13-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.10_2142: ???)	Depositor
R, R_{free}	0.202 , 0.249 0.205 , 0.252	Depositor DCC
R_{free} test set	1952 reflections (2.02%)	DCC
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9030	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.86% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.40	0/4149	0.63	0/5625
1	B	0.35	0/4068	0.56	0/5517
All	All	0.38	0/8217	0.60	0/11142

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	4
1	B	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	SER	Peptide
1	A	201	PHE	Peptide
1	A	260	PHE	Peptide
1	A	372	ASN	Peptide
1	B	260	PHE	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	4065	0	3994	51	0
1	B	3985	0	3905	74	0
2	A	26	0	19	1	0
2	B	26	0	19	1	0
3	A	556	0	0	10	2
3	B	372	0	0	19	1
All	All	9030	0	7937	126	2

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 8.

All (126) 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:527:ASN:ND2	1:A:529:GLU:O	2.10	0.83
1:A:208:ILE:HD11	1:A:249:ARG:HA	1.64	0.80
1:A:385:TYR:HB2	1:A:425:GLU:HG3	1.67	0.77
1:B:414:LEU:HD12	1:B:422:ILE:HD11	1.68	0.76
1:B:504:ILE:HG23	1:B:535:LEU:HD23	1.68	0.75
1:B:210:GLN:HA	1:B:213:LEU:HG	1.68	0.74
1:B:462:ILE:HG22	1:B:466:LYS:HE2	1.70	0.73
1:A:374:ASN:OD1	1:A:377:SER:N	2.20	0.72
1:B:432:LYS:NZ	3:B:712:HOH:O	2.23	0.71
1:A:527:ASN:O	1:A:531:ILE:HG23	1.91	0.70
1:B:547:CYS:SG	3:B:967:HOH:O	2.48	0.70
1:B:426:LEU:HD22	1:B:430:ALA:HB2	1.76	0.66
1:A:504:ILE:HD13	1:A:536:GLU:HG2	1.77	0.66
1:B:533:LYS:O	3:B:703:HOH:O	2.13	0.66
1:A:409:GLU:OE2	3:A:702:HOH:O	2.14	0.65
1:A:468:THR:HG23	1:A:470:SER:H	1.59	0.65
1:B:225:SER:OG	3:B:702:HOH:O	2.13	0.65
1:A:530:GLU:HA	1:A:533:LYS:HB3	1.79	0.65
1:B:505:GLU:OE2	3:B:704:HOH:O	2.14	0.65
1:A:69:GLU:O	1:A:73[A]:SER:OG	2.12	0.65
1:A:492:ARG:NH1	3:A:706:HOH:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:ARG:NH1	3:B:719:HOH:O	2.29	0.64
1:A:505:GLU:OE2	1:A:532:ARG:NH1	2.31	0.64
1:B:198:SER:HA	1:B:210:GLN:HE22	1.63	0.63
1:A:327:ASN:ND2	3:A:711:HOH:O	2.32	0.62
1:B:216:GLU:OE2	3:B:705:HOH:O	2.16	0.62
1:B:44:GLU:OE2	1:B:470:SER:OG	2.13	0.61
1:A:67:ALA:O	3:A:703:HOH:O	2.16	0.61
1:B:453:ASP:O	3:B:706:HOH:O	2.17	0.60
1:A:368:GLN:OE1	1:A:378:ASN:ND2	2.36	0.59
1:B:486:PHE:HA	1:B:516:LEU:HD11	1.85	0.58
1:B:267:ASN:ND2	3:B:725:HOH:O	2.36	0.58
1:A:525:ILE:HD11	1:A:530:GLU:C	2.23	0.57
1:B:458:THR:O	1:B:462:ILE:HG13	2.03	0.57
1:B:344:ASN:HB3	1:B:400:PRO:HB2	1.86	0.57
1:B:444:GLN:NE2	3:B:713:HOH:O	2.23	0.57
1:A:530:GLU:HA	1:A:533:LYS:HD3	1.87	0.56
2:A:601:SAH:HB1	2:A:601:SAH:H4'	1.87	0.56
1:B:453:ASP:N	1:B:453:ASP:OD1	2.36	0.56
1:A:458:THR:OG1	1:A:461:VAL:HG13	2.06	0.56
1:B:231:GLU:O	1:B:235:THR:HG23	2.05	0.56
1:A:461:VAL:HB	1:A:473:VAL:HB	1.88	0.55
1:B:131:THR:HA	1:B:159:LYS:HG2	1.88	0.54
1:B:207:ARG:HB3	1:B:250:HIS:NE2	2.24	0.53
1:A:66:ASN:OD1	3:A:703:HOH:O	2.19	0.53
1:B:198:SER:HB2	1:B:207:ARG:HE	1.74	0.53
1:B:514:GLY:HA2	1:B:515:GLU:HB2	1.89	0.53
1:B:546:PHE:HB3	1:B:552:LEU:HD13	1.90	0.52
1:A:433:LEU:HB2	1:A:439:ILE:HD12	1.92	0.52
1:B:449:LYS:NZ	3:B:735:HOH:O	2.42	0.52
1:A:531:ILE:HD12	1:A:535:LEU:HD22	1.92	0.52
1:A:533:LYS:HG2	1:A:534:GLU:N	2.24	0.51
1:B:495:ASP:OD1	3:B:707:HOH:O	2.17	0.51
1:B:468:THR:HG23	1:B:470:SER:H	1.76	0.51
1:A:50:ILE:HG12	1:A:280:CYS:HB3	1.93	0.51
1:B:374:ASN:ND2	3:B:737:HOH:O	2.44	0.51
1:A:193:MET:HG3	1:B:313:PHE:CD2	2.46	0.51
1:B:344:ASN:HD21	1:B:445:LYS:HD3	1.76	0.50
1:B:198:SER:HA	1:B:210:GLN:NE2	2.27	0.50
1:B:417:THR:HG22	1:B:418:LYS:HD3	1.93	0.50
1:B:397:LEU:HD12	1:B:548:SER:HB2	1.93	0.49
1:A:222:LEU:HD11	1:A:233:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:TYR:O	3:B:707:HOH:O	2.19	0.49
1:B:373:GLY:HA3	1:B:374:ASN:CB	2.42	0.49
1:B:536:GLU:HB2	3:B:722:HOH:O	2.13	0.49
1:A:68:PRO:HG2	1:A:141:ASP:HB3	1.95	0.49
1:A:505:GLU:CD	1:A:532:ARG:HH12	2.16	0.48
1:B:208:ILE:HD12	1:B:245:ASP:HB3	1.96	0.48
1:A:349:VAL:HG12	1:A:371:LEU:HD22	1.95	0.48
1:A:520:ARG:N	1:A:521:GLU:HA	2.28	0.48
1:A:525:ILE:HG13	1:A:531:ILE:HG22	1.95	0.47
1:B:203:ASN:O	1:B:207:ARG:HB2	2.15	0.47
1:A:204:ILE:O	1:A:208:ILE:HD13	2.15	0.47
1:B:56:LEU:HD22	1:B:323:LEU:HD21	1.96	0.46
1:B:493:TYR:CZ	1:B:506:ALA:HB1	2.51	0.46
1:B:113:LYS:HE2	3:B:1010:HOH:O	2.16	0.46
1:A:525:ILE:HG13	1:A:525:ILE:O	2.14	0.46
1:B:385:TYR:HB2	1:B:425:GLU:HG3	1.98	0.45
1:A:195:LEU:HD21	1:A:253:LEU:HB2	1.97	0.45
1:A:360:LEU:O	1:A:384:PRO:HB3	2.16	0.45
1:B:508:LEU:HA	1:B:511:VAL:CG2	2.46	0.45
1:A:521:GLU:CB	1:A:522:GLY:HA2	2.46	0.45
1:B:212:ARG:NH1	1:B:245:ASP:OD1	2.45	0.45
1:B:322:THR:HG22	1:B:324:LEU:HD13	1.99	0.45
1:B:207:ARG:HB3	1:B:250:HIS:CD2	2.52	0.45
1:B:466:LYS:NZ	3:B:727:HOH:O	2.38	0.45
1:B:500:LYS:NZ	1:B:536:GLU:OE1	2.47	0.44
1:A:364:THR:N	3:A:701:HOH:O	2.51	0.44
1:B:53:PRO:HG2	1:B:75:ILE:HD13	2.00	0.44
1:B:91:VAL:HG22	1:B:120:LEU:HD21	2.00	0.44
1:A:131:THR:HA	1:A:159:LYS:HG2	2.00	0.44
1:A:271:LYS:NZ	3:A:748:HOH:O	2.50	0.44
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.86	0.43
1:A:464:GLN:O	1:A:468:THR:HG22	2.18	0.43
1:B:402:SER:OG	1:B:405:GLN:HG3	2.18	0.43
2:B:601:SAH:HB1	2:B:601:SAH:H4'	2.00	0.43
1:B:222:LEU:HD11	1:B:233:LEU:HD23	1.99	0.43
1:A:531:ILE:HG13	1:A:532:ARG:N	2.33	0.43
1:A:518:LEU:HD11	1:A:535:LEU:HD13	2.01	0.43
1:B:75:ILE:HD12	1:B:98:PHE:CE2	2.53	0.43
1:B:266:MET:O	1:B:270:ARG:HG3	2.19	0.42
1:A:134:ASP:HB2	3:A:823:HOH:O	2.19	0.42
1:B:477:LYS:NZ	3:B:747:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:SER:HB2	1:A:82:ALA:HB3	2.01	0.42
1:B:250:HIS:HA	1:B:253:LEU:HB2	2.01	0.42
1:B:449:LYS:HD3	1:B:449:LYS:HA	1.85	0.42
1:B:90:ALA:HA	1:B:98:PHE:CE1	2.55	0.42
1:A:513:LYS:HG3	3:A:857:HOH:O	2.19	0.42
1:A:361:ASN:OD1	1:A:414:LEU:HD22	2.20	0.42
1:A:525:ILE:HD11	1:A:531:ILE:N	2.35	0.42
1:B:51:THR:HG22	1:B:175:TYR:CZ	2.55	0.42
1:B:54:TYR:OH	1:B:71:GLU:OE2	2.20	0.42
1:B:71:GLU:H	1:B:71:GLU:HG2	1.40	0.42
1:B:495:ASP:OD1	1:B:497:ARG:HB2	2.20	0.41
1:B:154:LYS:HG2	1:B:157:ARG:NH1	2.35	0.41
1:B:489:PHE:CD2	1:B:516:LEU:HD12	2.56	0.41
1:B:458:THR:HG22	1:B:553:VAL:HG23	2.02	0.41
1:A:454:LYS:NZ	3:A:726:HOH:O	2.39	0.41
1:B:241:ALA:O	3:B:709:HOH:O	2.21	0.41
1:B:508:LEU:HD12	1:B:508:LEU:HA	1.77	0.41
1:A:50:ILE:CG1	1:A:280:CYS:HB3	2.51	0.40
1:B:276:TYR:CE1	1:B:322:THR:HG23	2.56	0.40
1:B:402:SER:O	1:B:406:VAL:HG23	2.22	0.40
1:B:457:THR:HG23	1:B:462:ILE:HG12	2.03	0.40
1:A:529:GLU:CD	1:A:529:GLU:H	2.24	0.40
1:B:76:LEU:HB2	1:B:140:PHE:CD2	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1029:HOH:O	3:B:719:HOH:O[1_556]	2.10	0.10
3:A:1234:HOH:O	3:A:1247:HOH:O[2_646]	2.18	0.02

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	509/554 (92%)	498 (98%)	11 (2%)	0	100	100
1	B	498/554 (90%)	484 (97%)	13 (3%)	1 (0%)	52	42
All	All	1007/1108 (91%)	982 (98%)	24 (2%)	1 (0%)	56	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	201	PHE

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	444/504 (88%)	414 (93%)	30 (7%)	20	9
1	B	435/504 (86%)	404 (93%)	31 (7%)	18	8
All	All	879/1008 (87%)	818 (93%)	61 (7%)	19	8

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	TYR
1	A	76	LEU
1	A	78	LEU
1	A	175	TYR
1	A	207	ARG
1	A	213	LEU
1	A	223	GLU
1	A	236	GLU
1	A	246	HIS
1	A	256	GLU
1	A	287	LEU
1	A	290	MET
1	A	302	ASN

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Mol	Chain	Res	Type
1	A	355	LEU
1	A	371	LEU
1	A	377	SER
1	A	401	LEU
1	A	427	LEU
1	A	444	GLN
1	A	462	ILE
1	A	468	THR
1	A	501	LYS
1	A	516	LEU
1	A	525	ILE
1	A	529	GLU
1	A	531	ILE
1	A	533	LYS
1	A	535	LEU
1	A	540	THR
1	A	552	LEU
1	B	54	TYR
1	B	59	LEU
1	B	71	GLU
1	B	78	LEU
1	B	103	LEU
1	B	184	TRP
1	B	210	GLN
1	B	287	LEU
1	B	293	LYS
1	B	324	LEU
1	B	338	ASP
1	B	347	PHE
1	B	371	LEU
1	B	379	LEU
1	B	382	THR
1	B	417	THR
1	B	425	GLU
1	B	426	LEU
1	B	427	LEU
1	B	431	MET
1	B	452	LEU
1	B	453	ASP
1	B	468	THR
1	B	508	LEU
1	B	511	VAL

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Mol	Chain	Res	Type
1	B	530	GLU
1	B	531	ILE
1	B	532	ARG
1	B	533	LYS
1	B	538	LEU
1	B	552	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	368	GLN
1	A	378	ASN
1	B	210	GLN
1	B	420	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	SAH	A	601	-	22,28,28	0.96	1 (4%)	18,40,40	2.85	3 (16%)
2	SAH	B	601	-	22,28,28	0.97	2 (9%)	18,40,40	3.03	3 (16%)

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	601	-	-	0/7/31/31	0/3/3/3
2	SAH	B	601	-	-	0/7/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	SAH	O4'-C4'	-2.00	1.40	1.45
2	B	601	SAH	C2-N3	3.07	1.37	1.32
2	A	601	SAH	C2-N3	3.20	1.37	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	SAH	N3-C2-N1	-11.90	119.52	128.87
2	A	601	SAH	N3-C2-N1	-11.41	119.91	128.87
2	B	601	SAH	C5'-SD-CG	-2.80	93.92	102.42
2	B	601	SAH	C1'-N9-C4	-2.78	123.70	126.81
2	A	601	SAH	C1'-N9-C4	-2.29	124.25	126.81
2	A	601	SAH	C5'-SD-CG	-2.10	96.03	102.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	SAH	1	0
2	B	601	SAH	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^{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	510/554 (92%)	-0.06	19 (3%)	45	49	11, 26, 69, 119	0
1	B	502/554 (90%)	0.26	43 (8%)	13	14	16, 36, 83, 132	0
All	All	1012/1108 (91%)	0.10	62 (6%)	25	27	11, 31, 77, 132	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	202	THR	13.6
1	B	300	ALA	7.6
1	A	204	ILE	4.8
1	B	529	GLU	4.8
1	B	506	ALA	4.7
1	A	523	GLN	4.3
1	B	517	THR	4.2
1	B	364	THR	4.1
1	B	204	ILE	4.1
1	A	202	THR	4.0
1	A	201	PHE	3.9
1	B	511	VAL	3.8
1	B	201	PHE	3.8
1	B	531	ILE	3.8
1	B	519	SER	3.8
1	B	516	LEU	3.7
1	B	250	HIS	3.4
1	B	301	VAL	3.3
1	B	518	LEU	3.3
1	B	503	ILE	3.3
1	A	205	ARG	3.2
1	B	538	LEU	3.2
1	B	375	LYS	3.2
1	B	532	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	533	LYS	3.1
1	B	200	SER	3.0
1	B	508	LEU	3.0
1	A	242	LYS	3.0
1	B	553	VAL	2.9
1	B	535	LEU	2.8
1	B	528	LYS	2.8
1	A	215	LEU	2.7
1	B	291	PRO	2.7
1	B	510	HIS	2.7
1	A	374	ASN	2.7
1	A	213	LEU	2.7
1	B	485	PHE	2.7
1	A	522	GLY	2.7
1	A	224	HIS	2.6
1	B	292	PRO	2.5
1	B	486	PHE	2.5
1	A	301	VAL	2.5
1	B	534	GLU	2.4
1	A	220	ASP	2.4
1	B	514	GLY	2.4
1	A	209	ALA	2.3
1	A	217	PHE	2.3
1	B	213	LEU	2.3
1	A	453	ASP	2.3
1	B	242	LYS	2.2
1	A	247	TYR	2.2
1	B	377	SER	2.2
1	B	203	ASN	2.2
1	B	499	ASP	2.1
1	B	512	GLU	2.1
1	A	203	ASN	2.1
1	B	373	GLY	2.1
1	A	524	LYS	2.1
1	B	513	LYS	2.1
1	B	515	GLU	2.1
1	B	507	ILE	2.0
1	B	372	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	B	601	26/26	0.97	0.08	-0.30	14,22,32,34	0
2	SAH	A	601	26/26	0.96	0.08	-0.66	12,17,25,29	0

6.5 Other polymers (i)

There are no such residues in this entry.