Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:15 AM GMT

PDB ID	:	3OFK
Title	:	Crystal structure of N-methyltransferase NodS from Bradyrhizobium japonicum WM9 in complex with S-adenosyl-l-homocysteine (SAH)
Authors	:	Cakici, O.; Sikorski, M.; Stepkowski, T.; Bujacz, G.; Jaskolski, M.
Deposited on	:	2010-08-15
Resolution	:	1.85 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 ⓘ symbol.

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

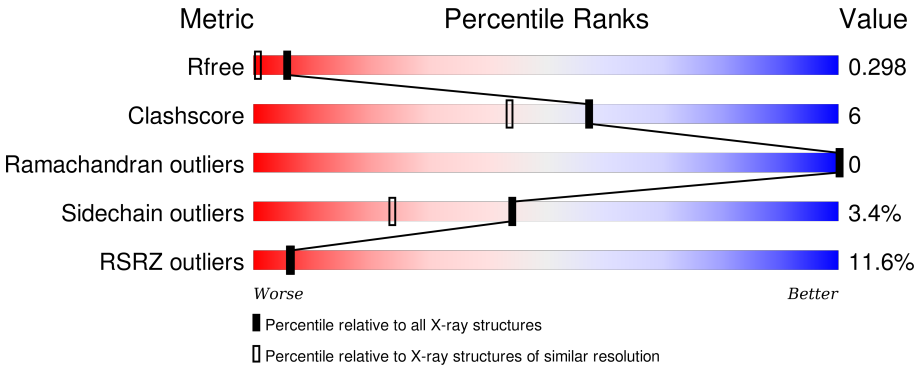
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.85 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	216	13% 85% 8% • 6%
1	B	216	10% 78% 11% • 9%
1	C	216	8% 81% 11% • 6%
1	D	216	11% 75% 9% 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7102 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 Nodulation protein S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	0	0
			1600	996	287	305	12			
1	B	196	Total	C	N	O	S	0	0	0
			1539	956	279	293	11			
1	C	202	Total	C	N	O	S	0	0	0
			1588	985	291	301	11			
1	D	181	Total	C	N	O	S	0	0	0
			1406	874	257	264	11			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP Q9AQ22
A	-5	ILE	-	EXPRESSION TAG	UNP Q9AQ22
A	-4	ASP	-	EXPRESSION TAG	UNP Q9AQ22
A	-3	PRO	-	EXPRESSION TAG	UNP Q9AQ22
A	-2	PHE	-	EXPRESSION TAG	UNP Q9AQ22
A	-1	THR	-	EXPRESSION TAG	UNP Q9AQ22
A	0	MET	-	EXPRESSION TAG	UNP Q9AQ22
A	1	VAL	-	SEE REMARK 999	UNP Q9AQ22
B	-6	GLY	-	EXPRESSION TAG	UNP Q9AQ22
B	-5	ILE	-	EXPRESSION TAG	UNP Q9AQ22
B	-4	ASP	-	EXPRESSION TAG	UNP Q9AQ22
B	-3	PRO	-	EXPRESSION TAG	UNP Q9AQ22
B	-2	PHE	-	EXPRESSION TAG	UNP Q9AQ22
B	-1	THR	-	EXPRESSION TAG	UNP Q9AQ22
B	0	MET	-	EXPRESSION TAG	UNP Q9AQ22
B	1	VAL	-	SEE REMARK 999	UNP Q9AQ22
C	-6	GLY	-	EXPRESSION TAG	UNP Q9AQ22
C	-5	ILE	-	EXPRESSION TAG	UNP Q9AQ22
C	-4	ASP	-	EXPRESSION TAG	UNP Q9AQ22
C	-3	PRO	-	EXPRESSION TAG	UNP Q9AQ22
C	-2	PHE	-	EXPRESSION TAG	UNP Q9AQ22

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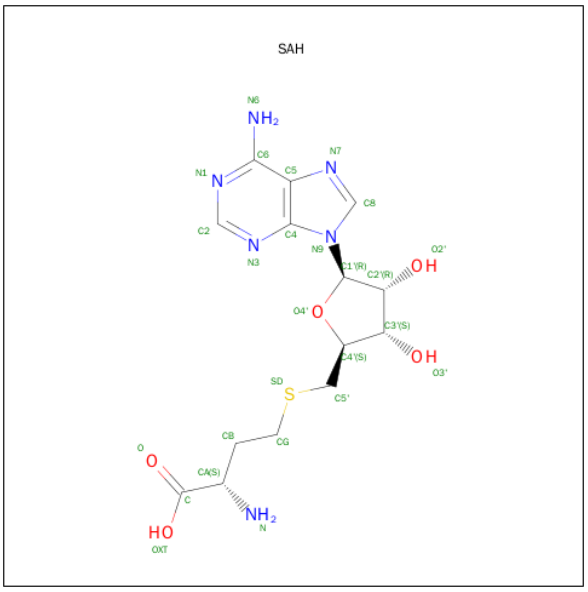
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	THR	-	EXPRESSION TAG	UNP Q9AQ22
C	0	MET	-	EXPRESSION TAG	UNP Q9AQ22
C	1	VAL	-	SEE REMARK 999	UNP Q9AQ22
D	-6	GLY	-	EXPRESSION TAG	UNP Q9AQ22
D	-5	ILE	-	EXPRESSION TAG	UNP Q9AQ22
D	-4	ASP	-	EXPRESSION TAG	UNP Q9AQ22
D	-3	PRO	-	EXPRESSION TAG	UNP Q9AQ22
D	-2	PHE	-	EXPRESSION TAG	UNP Q9AQ22
D	-1	THR	-	EXPRESSION TAG	UNP Q9AQ22
D	0	MET	-	EXPRESSION TAG	UNP Q9AQ22
D	1	VAL	-	SEE REMARK 999	UNP Q9AQ22

- 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		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is water.

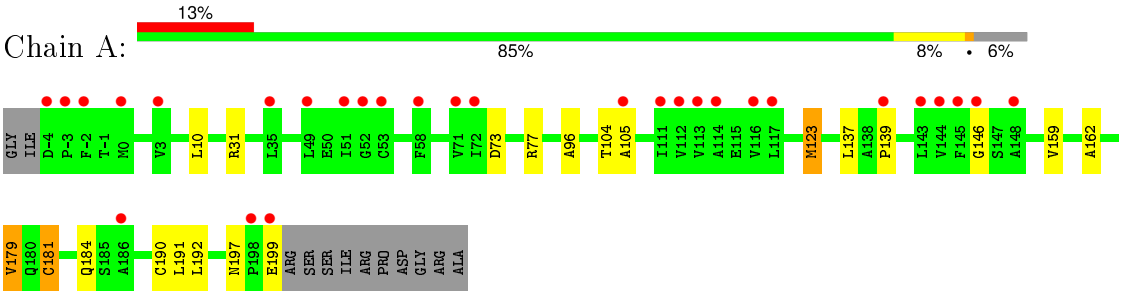
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	170	Total O 174 174	0	4
3	B	238	Total O 244 244	0	6
3	C	259	Total O 262 262	0	3
3	D	179	Total O 185 185	0	6

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.

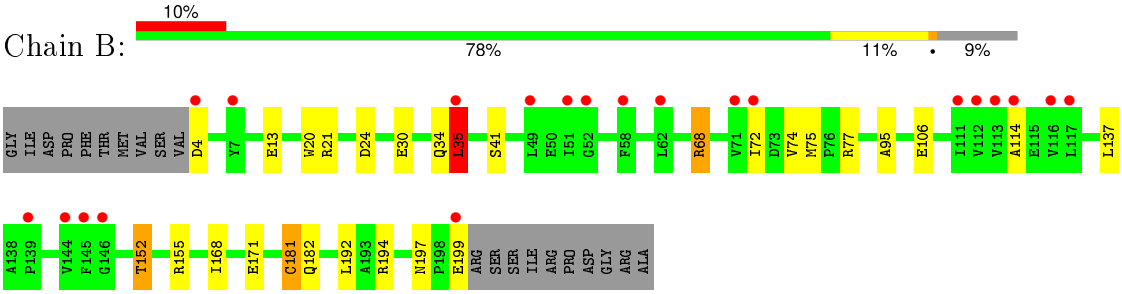
- Molecule 1: Nodulation protein S

Chain A:



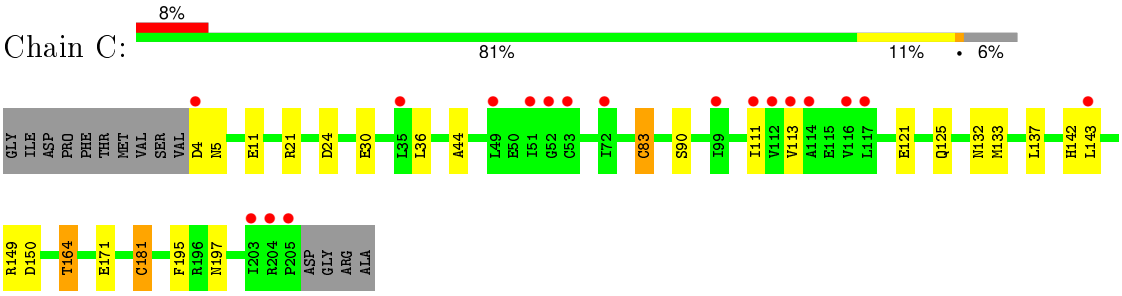
- Molecule 1: Nodulation protein S

Chain B:



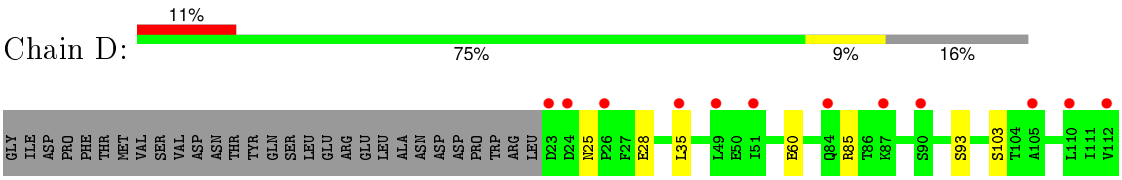
- Molecule 1: Nodulation protein S

Chain C:



- Molecule 1: Nodulation protein S

Chain D:




V113
A114
E115
V116
M123
M126
N132
L137
H142
L143
V144
F145
G146
A151
V159
T164
Q180
Q184
S185
A186
L192
N197
I203
ARG
PRO
ASP
GLY
ARG
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	81.01Å 143.30Å 75.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.70 – 1.85 29.70 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.70-1.85) 94.4 (29.70-1.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.190 , 0.238 0.250 , 0.298	Depositor DCC
R_{free} test set	1165 reflections (1.65%)	DCC
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 30.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 71694 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7102	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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: 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	0.67	1/1629 (0.1%)	0.75	1/2210 (0.0%)
1	B	1.01	2/1566 (0.1%)	0.94	3/2123 (0.1%)
1	C	0.97	2/1616 (0.1%)	0.91	0/2190
1	D	0.72	0/1429	0.78	0/1934
All	All	0.86	5/6240 (0.1%)	0.85	4/8457 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	83	CYS	CB-SG	-5.89	1.72	1.81
1	C	181	CYS	CB-SG	-5.59	1.72	1.81
1	B	181	CYS	C-N	-5.55	1.21	1.34
1	B	199	GLU	CD-OE2	5.51	1.31	1.25
1	A	181	CYS	CB-SG	-5.41	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	68	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	B	194	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	B	35	LEU	CA-CB-CG	5.12	127.07	115.30
1	A	31	ARG	NE-CZ-NH1	5.11	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1600	0	1573	17	0
1	B	1539	0	1510	14	0
1	C	1588	0	1565	29	0
1	D	1406	0	1399	14	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	C	26	0	19	0	0
2	D	26	0	19	0	0
3	A	174	0	0	1	0
3	B	244	0	0	4	0
3	C	262	0	0	11	0
3	D	185	0	0	5	0
All	All	7102	0	6123	74	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 6.

All (74) 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:159:VAL:HG22	3:D:231:HOH:O	1.50	1.08
1:C:133:MET:CE	1:C:143:LEU:HD11	1.89	1.02
1:C:133:MET:HE2	1:C:143:LEU:HD11	1.48	0.95
1:C:113:VAL:HG21	1:C:133:MET:CE	1.96	0.94
1:C:113:VAL:HG21	1:C:133:MET:HE1	1.50	0.93
1:A:123:MET:CE	1:A:159:VAL:HG12	2.01	0.90
1:D:123:MET:HE1	1:D:164:THR:HG21	1.55	0.89
1:A:123:MET:CE	1:A:159:VAL:CG1	2.54	0.86
1:D:123:MET:CE	1:D:164:THR:HG21	2.05	0.85
1:A:123:MET:HE3	1:A:159:VAL:HG12	1.60	0.82
1:C:133:MET:HE1	1:C:143:LEU:HD11	1.66	0.77
1:C:133:MET:HE2	1:C:143:LEU:CD1	2.17	0.75
1:C:149:ARG:CD	3:C:744:HOH:O	2.36	0.74
1:A:123:MET:HE3	1:A:159:VAL:CG1	2.18	0.71
1:C:11:GLU:HG2	3:C:825:HOH:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:GLU:HB2	3:C:838:HOH:O	1.92	0.68
1:D:142:HIS:HE1	3:D:236:HOH:O	1.77	0.68
1:D:132:ASN:HB3	3:D:638:HOH:O	2.00	0.62
1:B:4:ASP:N	3:B:535:HOH:O	2.33	0.61
1:C:133:MET:CE	1:C:143:LEU:CD1	2.72	0.60
1:C:113:VAL:CG2	1:C:133:MET:CE	2.76	0.60
1:C:24:ASP:HB2	3:C:766:HOH:O	2.02	0.59
1:A:105:ALA:HB3	3:A:745:HOH:O	2.03	0.57
1:A:190:CYS:SG	1:A:192:LEU:HD21	2.43	0.57
1:C:121:GLU:HB3	1:C:125:GLN:NE2	2.20	0.57
1:B:24:ASP:HB2	3:B:306[A]:HOH:O	2.04	0.57
1:B:4:ASP:N	3:B:763:HOH:O	2.38	0.57
1:A:123:MET:CE	1:A:159:VAL:HG11	2.35	0.56
1:C:21:ARG:HG2	3:C:268:HOH:O	2.05	0.56
1:D:123:MET:HE3	1:D:164:THR:HG21	1.86	0.55
1:D:123:MET:HE3	1:D:164:THR:CG2	2.37	0.55
1:D:142:HIS:CE1	3:D:236:HOH:O	2.58	0.54
1:D:123:MET:CE	1:D:164:THR:CG2	2.85	0.53
1:C:132:ASN:HB3	3:C:833:HOH:O	2.09	0.53
1:A:162:ALA:HB1	1:A:191:LEU:HB3	1.91	0.52
1:D:137:LEU:HD13	1:D:197:ASN:HB2	1.91	0.52
1:C:113:VAL:CG2	1:C:133:MET:HE3	2.39	0.51
1:A:146:GLY:HA3	1:A:192:LEU:HD22	1.93	0.50
1:C:150:ASP:OD1	1:C:164:THR:HG23	2.10	0.50
1:D:35:LEU:HD23	1:D:192:LEU:HD23	1.94	0.50
1:A:123:MET:HE1	1:A:159:VAL:HG12	1.90	0.50
1:A:179:VAL:HG23	1:A:192:LEU:HB2	1.93	0.49
1:C:111:ILE:HG21	1:C:133:MET:HE3	1.94	0.49
1:C:90:SER:C	3:C:235:HOH:O	2.51	0.48
1:C:149:ARG:HD3	3:C:744:HOH:O	2.05	0.48
1:C:21:ARG:HD2	3:C:822:HOH:O	2.15	0.47
1:C:30:GLU:HG2	1:C:181:CYS:SG	2.55	0.47
1:C:142:HIS:HA	1:C:195:PHE:O	2.14	0.46
1:C:44:ALA:HB1	3:C:273:HOH:O	2.15	0.46
1:A:190:CYS:SG	1:A:192:LEU:CD2	3.03	0.46
1:B:168:ILE:O	1:B:171:GLU:HB2	2.16	0.46
1:A:137:LEU:HD13	1:A:197:ASN:HB2	1.97	0.46
1:B:21:ARG:NH2	3:B:772:HOH:O	2.50	0.45
1:A:123:MET:HE2	1:A:159:VAL:CG1	2.45	0.45
1:B:34:GLN:HG3	1:B:181:CYS:SG	2.57	0.44
1:C:111:ILE:CG2	1:C:133:MET:HE3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:VAL:HG13	1:B:75:MET:HG2	2.00	0.44
1:B:35:LEU:HD11	1:B:114:ALA:CB	2.48	0.43
1:B:137:LEU:HD23	1:B:197:ASN:HB2	1.99	0.43
1:B:152:THR:HB	1:B:155:ARG:NH2	2.33	0.43
1:C:133:MET:HB3	1:C:133:MET:HE2	1.75	0.43
1:C:90:SER:HA	3:C:235:HOH:O	2.17	0.43
1:B:72:ILE:HG22	1:B:95:ALA:HB3	2.00	0.43
1:A:123:MET:HE2	1:A:159:VAL:HG11	2.01	0.43
1:A:73:ASP:O	1:A:96:ALA:HA	2.19	0.43
1:B:13:GLU:HG2	1:B:20:TRP:CE2	2.53	0.43
1:B:68:ARG:NH1	1:B:106:GLU:OE2	2.52	0.43
1:A:139:PRO:O	1:A:199:GLU:C	2.57	0.42
1:C:137:LEU:HD23	1:C:197:ASN:HB2	2.02	0.42
1:D:25:ASN:HB3	1:D:28:GLU:HB2	2.01	0.41
1:C:36:LEU:HD12	1:C:36:LEU:HA	1.86	0.41
1:B:35:LEU:HD23	1:B:192:LEU:HD23	2.03	0.41
1:D:60:GLU:HG3	1:D:85:ARG:HG2	2.02	0.41
1:D:151:ALA:HB3	3:D:747:HOH:O	2.21	0.41

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	202/216 (94%)	193 (96%)	9 (4%)	0	100	100
1	B	194/216 (90%)	188 (97%)	6 (3%)	0	100	100
1	C	200/216 (93%)	192 (96%)	8 (4%)	0	100	100
1	D	179/216 (83%)	173 (97%)	6 (3%)	0	100	100
All	All	775/864 (90%)	746 (96%)	29 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	172/181 (95%)	165 (96%)	7 (4%)	37	17
1	B	164/181 (91%)	158 (96%)	6 (4%)	41	20
1	C	170/181 (94%)	166 (98%)	4 (2%)	57	39
1	D	150/181 (83%)	145 (97%)	5 (3%)	45	25
All	All	656/724 (91%)	634 (97%)	22 (3%)	44	24

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	77	ARG
1	A	104	THR
1	A	123	MET
1	A	179	VAL
1	A	181	CYS
1	A	184	GLN
1	B	30	GLU
1	B	35	LEU
1	B	41	SER
1	B	77	ARG
1	B	152	THR
1	B	182	GLN
1	C	4	ASP
1	C	5	ASN
1	C	83	CYS
1	C	164	THR
1	D	93	SER
1	D	103	SER
1	D	126	MET
1	D	180	GLN
1	D	184	GLN

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	184	GLN
1	B	184	GLN
1	C	5	ASN
1	D	142	HIS

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

4 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	217	-	20,28,28	1.26	2 (10%)	19,40,40	2.65	3 (15%)
2	SAH	B	217	-	20,28,28	1.07	2 (10%)	19,40,40	3.93	4 (21%)
2	SAH	C	217	-	20,28,28	1.30	2 (10%)	19,40,40	3.19	2 (10%)
2	SAH	D	217	-	20,28,28	1.23	2 (10%)	19,40,40	2.72	4 (21%)

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	217	-	-	0/7/31/31	0/3/3/3
2	SAH	B	217	-	-	0/7/31/31	0/3/3/3
2	SAH	C	217	-	-	0/7/31/31	0/3/3/3
2	SAH	D	217	-	-	0/7/31/31	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	217	SAH	C2-N1	2.11	1.37	1.33
2	D	217	SAH	C2-N1	2.47	1.38	1.33
2	C	217	SAH	O4'-C1'	2.64	1.44	1.41
2	A	217	SAH	C2-N1	2.98	1.39	1.33
2	B	217	SAH	C2-N3	3.10	1.37	1.32
2	C	217	SAH	C2-N3	3.22	1.37	1.32
2	A	217	SAH	C2-N3	4.17	1.39	1.32
2	D	217	SAH	C2-N3	4.34	1.39	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	217	SAH	N3-C2-N1	-16.24	116.46	128.89
2	C	217	SAH	N3-C2-N1	-12.76	119.13	128.89
2	D	217	SAH	N3-C2-N1	-10.65	120.74	128.89
2	A	217	SAH	N3-C2-N1	-10.38	120.95	128.89
2	C	217	SAH	C4'-O4'-C1'	-2.57	106.89	109.72
2	B	217	SAH	C4'-O4'-C1'	-2.45	107.03	109.72
2	A	217	SAH	C5'-SD-CG	-2.24	95.68	102.41
2	D	217	SAH	N6-C6-N1	2.06	123.63	119.20
2	D	217	SAH	C2'-C1'-N9	2.19	117.63	114.29
2	B	217	SAH	O4'-C4'-C3'	2.32	109.83	105.15
2	D	217	SAH	C4'-O4'-C1'	2.34	112.29	109.72
2	B	217	SAH	C2-N1-C6	2.37	123.01	118.77
2	A	217	SAH	C2'-C1'-N9	2.55	118.19	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	204/216 (94%)	0.85	29 (14%) 4 3	29, 46, 70, 98	0
1	B	196/216 (90%)	0.67	21 (10%) 8 7	19, 35, 55, 67	0
1	C	202/216 (93%)	0.55	18 (8%) 12 11	19, 33, 57, 84	0
1	D	181/216 (83%)	0.73	23 (12%) 5 5	30, 42, 65, 84	0
All	All	783/864 (90%)	0.70	91 (11%) 6 6	19, 39, 64, 98	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	VAL	5.7
1	D	112	VAL	5.4
1	B	113	VAL	5.1
1	A	51	ILE	4.8
1	D	114	ALA	4.7
1	B	51	ILE	4.7
1	D	113	VAL	4.7
1	A	112	VAL	4.6
1	A	113	VAL	4.5
1	D	51	ILE	4.5
1	C	205	PRO	4.2
1	D	184	GLN	4.0
1	B	112	VAL	4.0
1	A	-2	PHE	4.0
1	A	198	PRO	3.9
1	B	114	ALA	3.9
1	A	-4	ASP	3.9
1	B	35	LEU	3.8
1	A	199	GLU	3.7
1	A	114	ALA	3.7
1	C	112	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	145	PHE	3.5
1	A	117	LEU	3.5
1	A	52	GLY	3.5
1	D	84	GLN	3.5
1	A	186	ALA	3.4
1	A	116	VAL	3.4
1	C	51	ILE	3.4
1	C	113	VAL	3.4
1	C	4	ASP	3.3
1	C	35	LEU	3.3
1	B	144	VAL	3.3
1	C	116	VAL	3.3
1	B	52	GLY	3.2
1	D	105	ALA	3.2
1	D	35	LEU	3.2
1	D	143	LEU	3.1
1	D	87	LYS	3.1
1	D	145	PHE	3.1
1	B	4	ASP	3.0
1	D	49	LEU	3.0
1	B	58	PHE	2.9
1	D	144	VAL	2.9
1	A	145	PHE	2.9
1	C	49	LEU	2.9
1	B	116	VAL	2.9
1	A	72	ILE	2.9
1	A	71	VAL	2.9
1	C	114	ALA	2.9
1	A	35	LEU	2.8
1	C	203	ILE	2.8
1	B	111	ILE	2.7
1	D	24	ASP	2.7
1	A	146	GLY	2.7
1	A	53	CYS	2.7
1	A	144	VAL	2.7
1	A	58	PHE	2.7
1	D	185	SER	2.6
1	C	204	ARG	2.6
1	A	-3	PRO	2.6
1	A	105	ALA	2.6
1	D	203	ILE	2.6
1	A	49	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	146	GLY	2.5
1	B	62	LEU	2.5
1	C	99	ILE	2.4
1	B	49	LEU	2.4
1	B	71	VAL	2.4
1	D	23	ASP	2.4
1	B	7	TYR	2.3
1	C	72	ILE	2.3
1	A	139	PRO	2.3
1	D	90	SER	2.3
1	D	116	VAL	2.3
1	B	146	GLY	2.3
1	C	53	CYS	2.3
1	C	52	GLY	2.3
1	A	143	LEU	2.2
1	D	110	LEU	2.2
1	C	143	LEU	2.2
1	B	199	GLU	2.2
1	D	186	ALA	2.2
1	C	111	ILE	2.2
1	B	139	PRO	2.2
1	A	111	ILE	2.2
1	B	117	LEU	2.2
1	A	0	MET	2.1
1	D	26	PRO	2.1
1	B	72	ILE	2.1
1	C	117	LEU	2.1
1	A	148	ALA	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	C	217	26/26	0.96	0.19	0.21	21,24,27,29	0
2	SAH	B	217	26/26	0.95	0.19	0.21	18,26,32,36	0
2	SAH	D	217	26/26	0.95	0.16	-0.02	32,38,40,42	0
2	SAH	A	217	26/26	0.95	0.17	-0.07	26,32,35,37	0

6.5 Other polymers (i)

There are no such residues in this entry.