Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:48 AM GMT

PDB ID	:	2O8J
Title	:	Human euchromatic histone methyltransferase 2
Authors	:	Min, J.; Wu, H.; Antoshenko, T.; Loppnau, P.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Plotnikov, A.N.; Structural Genomics Consortium (SGC)
Deposited on	:	2006-12-12
Resolution	:	1.80 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:

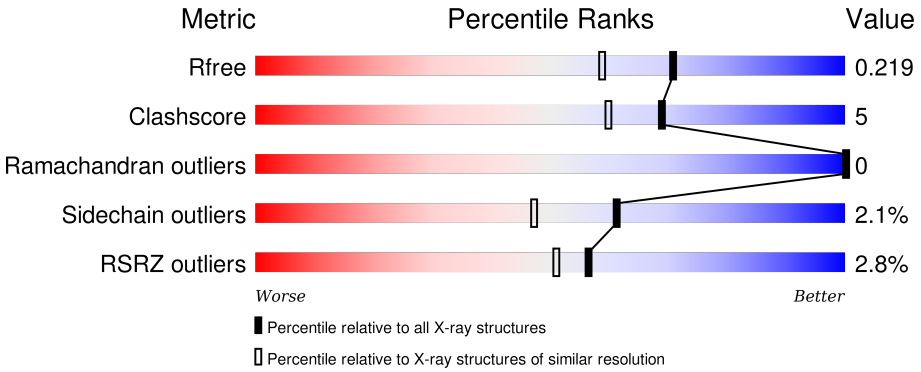
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	281	83% 7% • 10%
1	B	281	5% 86% 9% • •
1	C	281	2% 84% 8% • 7%
1	D	281	2% 81% 7% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	A	1502	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9510 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.

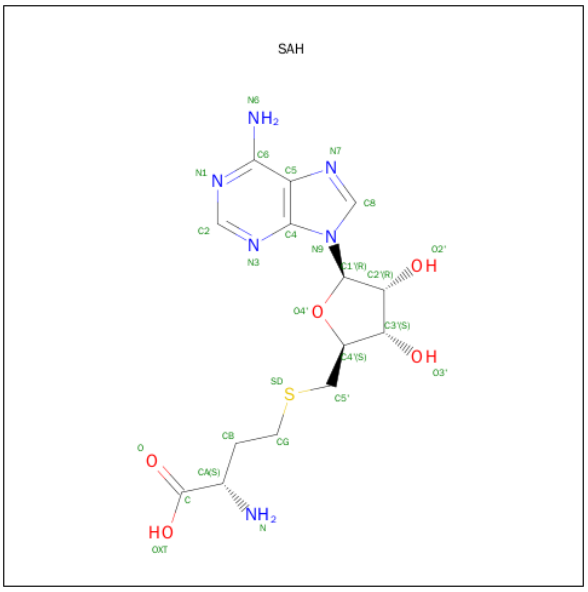
- Molecule 1 is a protein called Histone-lysine N-methyltransferase, H3 lysine-9 specific 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			2050	1281	357	389	23			
1	B	271	Total	C	N	O	S	0	0	0
			2173	1355	383	412	23			
1	C	262	Total	C	N	O	S	0	1	0
			2119	1323	371	402	23			
1	D	248	Total	C	N	O	S	0	0	0
			1985	1239	349	374	23			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

- Molecule 4 is water.

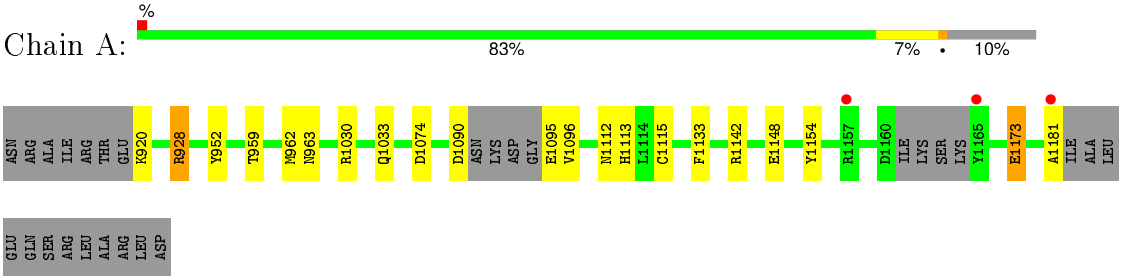
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	318	Total	O	0	0
			318	318		
4	B	210	Total	O	0	0
			210	210		
4	C	272	Total	O	0	0
			272	272		
4	D	263	Total	O	0	0
			263	263		

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.

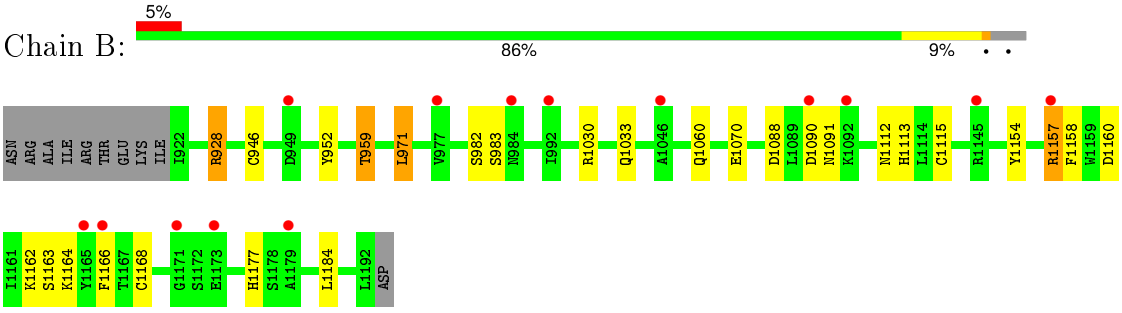
- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-9 specific 3

Chain A:



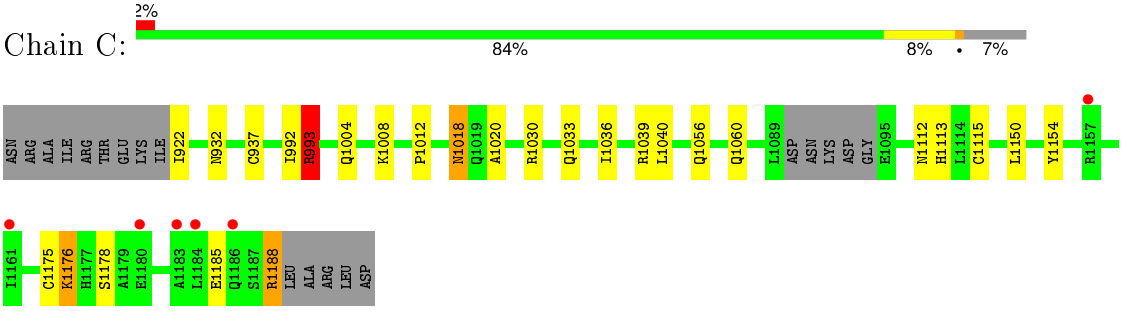
- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-9 specific 3

Chain B:



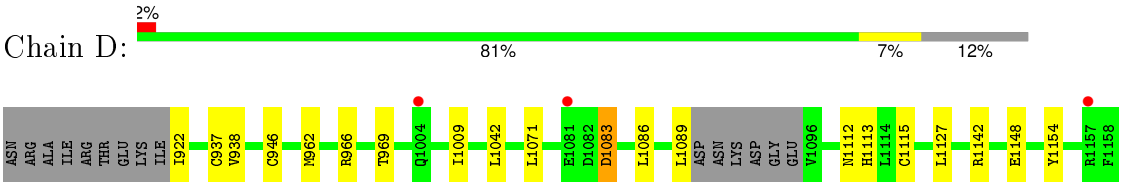
- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-9 specific 3

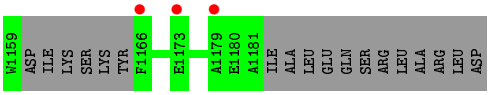
Chain C:



- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-9 specific 3

Chain D:




W1159
ASP
ILE
LYS
SER
LYS
TYR
F1166
E1173
A1179
E1180
A1181
ILE
ALA
LEU
GLU
GLN
SER
ARG
LEU
ALA
ARG
LEU
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	56.59Å 70.97Å 83.05Å 81.11° 75.13° 88.39°	Depositor
Resolution (Å)	79.31 – 1.80 48.96 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.2 (79.31-1.80) 88.5 (48.96-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.221 0.179 , 0.219	Depositor DCC
R_{free} test set	5287 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	22.1	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.7	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 105610 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9510	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.28 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.7748e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.68	0/2094	0.72	2/2830 (0.1%)
1	B	0.58	0/2219	0.64	2/3000 (0.1%)
1	C	0.68	0/2164	0.71	1/2924 (0.0%)
1	D	0.65	0/2028	0.66	0/2742
All	All	0.65	0/8505	0.68	5/11496 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	928	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	A	928	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	B	971	LEU	CA-CB-CG	5.43	127.78	115.30
1	B	928	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	C	993	ARG	NE-CZ-NH1	5.19	122.89	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2050	0	1935	17	0
1	B	2173	0	2064	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2119	0	2013	24	0
1	D	1985	0	1865	16	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	26	0	19	2	0
3	B	26	0	19	1	0
3	C	26	0	19	1	0
3	D	26	0	19	2	0
4	A	318	0	0	2	0
4	B	210	0	0	4	0
4	C	272	0	0	6	0
4	D	263	0	0	4	0
All	All	9510	0	7953	75	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 5.

All (75) 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:1113:HIS:HD2	1:A:1154:TYR:H	1.08	0.93
1:C:1113:HIS:HD2	1:C:1154:TYR:H	1.16	0.91
1:D:1112:ASN:HD21	3:D:1517:SAH:HN1	1.22	0.86
1:B:946:CYS:HB2	4:B:1695:HOH:O	1.75	0.86
1:B:1112:ASN:HD21	3:B:1509:SAH:HN1	1.24	0.84
1:A:1112:ASN:HD21	3:A:1505:SAH:HN1	1.26	0.83
1:D:1113:HIS:HD2	1:D:1154:TYR:H	1.24	0.82
1:A:1142:ARG:NH2	1:A:1148:GLU:OE2	2.14	0.81
1:C:1039:ARG:H	1:C:1056:GLN:HE21	1.25	0.80
1:B:1113:HIS:HD2	1:B:1154:TYR:H	1.29	0.80
1:C:1112:ASN:HD21	3:C:1513:SAH:HN1	1.28	0.78
1:A:1113:HIS:CD2	1:A:1154:TYR:H	1.99	0.77
1:D:1083:ASP:HB2	1:D:1086:LEU:HD12	1.65	0.75
1:C:1113:HIS:CD2	1:C:1154:TYR:H	2.06	0.70
1:C:1018:ASN:HD22	1:C:1020:ALA:H	1.41	0.68
1:C:1008:LYS:HE2	4:C:1629:HOH:O	1.96	0.66
1:C:1004:GLN:HG3	4:C:1744:HOH:O	1.96	0.65
1:D:1113:HIS:CD2	1:D:1154:TYR:H	2.15	0.58
1:A:963:ASN:HB2	4:C:1585:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1173:GLU:CD	1:A:1173:GLU:H	2.09	0.56
1:A:920:LYS:N	4:A:1805:HOH:O	2.39	0.56
1:B:1030:ARG:HH11	1:B:1033:GLN:HE22	1.54	0.55
1:B:928:ARG:NH2	1:B:952:TYR:O	2.39	0.55
1:D:922:ILE:N	4:D:1737:HOH:O	2.38	0.55
1:A:1112:ASN:HD22	3:A:1505:SAH:C8	2.20	0.55
1:C:922:ILE:HG23	1:C:937:CYS:O	2.06	0.54
1:A:928:ARG:NH2	1:A:952:TYR:O	2.37	0.54
1:C:1030:ARG:HH11	1:C:1033:GLN:HE22	1.55	0.54
1:C:1039:ARG:H	1:C:1056:GLN:NE2	2.03	0.53
1:D:937:CYS:HG	1:D:946:CYS:HG	1.54	0.53
1:B:959:THR:CG2	1:B:1070:GLU:OE2	2.57	0.52
1:B:928:ARG:HH21	1:B:952:TYR:HB3	1.75	0.51
1:B:1157:ARG:HH11	1:B:1157:ARG:CG	2.24	0.51
1:B:1157:ARG:HD2	4:B:1613:HOH:O	2.10	0.51
1:B:959:THR:HG21	1:B:1070:GLU:OE2	2.11	0.50
1:A:1113:HIS:HD2	1:A:1154:TYR:N	1.92	0.50
1:A:1030:ARG:HH11	1:A:1033:GLN:HE22	1.59	0.50
1:B:1113:HIS:HE1	1:B:1115:CYS:SG	2.36	0.49
1:B:959:THR:HG22	4:B:1694:HOH:O	2.11	0.48
1:C:1185:GLU:OE1	1:C:1188:ARG:HD3	2.13	0.48
1:B:1160:ASP:O	1:B:1164:LYS:HE2	2.13	0.48
1:A:959:THR:HG22	1:D:969:THR:HG23	1.95	0.48
1:C:993:ARG:HH11	1:C:993:ARG:CG	2.27	0.48
1:B:1157:ARG:NH1	1:B:1157:ARG:HG3	2.29	0.48
1:B:1157:ARG:HH11	1:B:1157:ARG:HG3	1.78	0.47
1:C:993:ARG:HH11	1:C:993:ARG:HB2	1.79	0.47
1:C:1030:ARG:HH11	1:C:1033:GLN:NE2	2.13	0.47
1:A:962:MET:HB3	1:A:1133:PHE:CZ	2.50	0.47
1:D:1113:HIS:HE1	1:D:1115:CYS:SG	2.37	0.46
1:D:922:ILE:HG12	4:D:1737:HOH:O	2.15	0.46
1:D:1112:ASN:HD22	3:D:1517:SAH:C8	2.29	0.46
1:A:1074:ASP:HB2	1:A:1096:VAL:O	2.15	0.46
1:D:922:ILE:HD13	1:D:938:VAL:HG12	1.98	0.46
1:C:1040:LEU:HD22	1:C:1150:LEU:HD11	1.98	0.46
1:D:1142:ARG:NH1	1:D:1148:GLU:OE2	2.46	0.45
1:C:1176:LYS:HB3	1:C:1176:LYS:HE3	1.70	0.45
1:C:1008:LYS:HG3	4:C:1706:HOH:O	2.14	0.45
1:A:1113:HIS:HE1	1:A:1115:CYS:SG	2.40	0.45
1:A:1030:ARG:HH11	1:A:1033:GLN:NE2	2.15	0.44
1:C:932:ASN:HB2	1:C:1036:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:962:MET:HG3	1:D:1071:LEU:HB3	1.99	0.44
1:C:1113:HIS:HE1	1:C:1115:CYS:SG	2.41	0.43
1:B:1168:CYS:HB2	1:B:1177:HIS:HB2	2.00	0.43
1:D:1009:ILE:CA	4:D:1739:HOH:O	2.66	0.43
1:D:966:ARG:NH1	4:D:1561:HOH:O	2.44	0.43
1:C:993:ARG:HH11	1:C:993:ARG:HG3	1.84	0.42
1:C:1060:GLN:HG2	4:C:1577:HOH:O	2.19	0.42
1:B:1060:GLN:HG2	4:B:1621:HOH:O	2.18	0.42
1:C:992:ILE:HD12	1:C:1012:PRO:HB3	2.02	0.42
1:A:1181:ALA:HB1	4:A:1752:HOH:O	2.18	0.42
1:D:937:CYS:HA	1:D:1042:LEU:O	2.20	0.41
1:C:1008:LYS:CE	4:C:1629:HOH:O	2.62	0.41
1:C:1175:CYS:SG	1:C:1178:SER:HB3	2.60	0.41
1:B:1158:PHE:CZ	1:B:1162:LYS:HG3	2.55	0.41
1:B:1163:SER:HA	1:B:1166:PHE:O	2.21	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	248/281 (88%)	233 (94%)	15 (6%)	0	100	100
1	B	269/281 (96%)	256 (95%)	13 (5%)	0	100	100
1	C	259/281 (92%)	250 (96%)	9 (4%)	0	100	100
1	D	242/281 (86%)	230 (95%)	12 (5%)	0	100	100
All	All	1018/1124 (91%)	969 (95%)	49 (5%)	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	229/252 (91%)	226 (99%)	3 (1%)	76	68
1	B	241/252 (96%)	232 (96%)	9 (4%)	41	23
1	C	237/252 (94%)	233 (98%)	4 (2%)	68	57
1	D	220/252 (87%)	217 (99%)	3 (1%)	74	65
All	All	927/1008 (92%)	908 (98%)	19 (2%)	61	49

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1090	ASP
1	A	1095	GLU
1	A	1173	GLU
1	B	959	THR
1	B	971	LEU
1	B	982	SER
1	B	983	SER
1	B	1088	ASP
1	B	1090	ASP
1	B	1091	ASN
1	B	1157	ARG
1	B	1184	LEU
1	C	993	ARG
1	C	1018	ASN
1	C	1176	LYS
1	C	1188	ARG
1	D	1083	ASP
1	D	1089	LEU
1	D	1127	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	932	ASN
1	A	1004	GLN
1	A	1033	GLN
1	A	1112	ASN
1	A	1113	HIS
1	B	1033	GLN
1	B	1112	ASN
1	B	1113	HIS
1	C	1018	ASN
1	C	1033	GLN
1	C	1056	GLN
1	C	1112	ASN
1	C	1113	HIS
1	D	1112	ASN
1	D	1113	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

Of 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 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	$\#\|Z\|>2$
3	SAH	A	1505	-	20,28,28	1.06	1 (5%)	19,40,40	2.85	3 (15%)
3	SAH	B	1509	-	20,28,28	1.15	2 (10%)	19,40,40	3.08	3 (15%)
3	SAH	C	1513	-	20,28,28	1.16	2 (10%)	19,40,40	2.95	1 (5%)
3	SAH	D	1517	-	20,28,28	1.07	2 (10%)	19,40,40	2.60	1 (5%)

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
3	SAH	A	1505	-	-	0/7/31/31	0/3/3/3
3	SAH	B	1509	-	-	0/7/31/31	0/3/3/3
3	SAH	C	1513	-	-	0/7/31/31	0/3/3/3
3	SAH	D	1517	-	-	0/7/31/31	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1513	SAH	C2-N1	2.25	1.38	1.33
3	D	1517	SAH	C2-N1	2.36	1.38	1.33
3	B	1509	SAH	C2-N1	2.47	1.38	1.33
3	D	1517	SAH	C2-N3	3.28	1.38	1.32
3	A	1505	SAH	C2-N3	3.42	1.38	1.32
3	B	1509	SAH	C2-N3	3.53	1.38	1.32
3	C	1513	SAH	C2-N3	3.58	1.38	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1509	SAH	N3-C2-N1	-12.53	119.30	128.89
3	C	1513	SAH	N3-C2-N1	-12.14	119.60	128.89
3	A	1505	SAH	N3-C2-N1	-11.31	120.24	128.89
3	D	1517	SAH	N3-C2-N1	-10.55	120.81	128.89
3	A	1505	SAH	C2'-C1'-N9	-2.82	109.98	114.29
3	B	1509	SAH	C2'-C1'-N9	-2.28	110.81	114.29
3	A	1505	SAH	C1'-N9-C4	-2.01	123.90	126.94
3	B	1509	SAH	C4'-O4'-C1'	2.62	112.60	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1505	SAH	2	0
3	B	1509	SAH	1	0
3	C	1513	SAH	1	0
3	D	1517	SAH	2	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	254/281 (90%)	-0.13	3 (1%) 81 78	12, 19, 37, 44	0
1	B	271/281 (96%)	0.25	14 (5%) 31 25	17, 29, 42, 51	0
1	C	262/281 (93%)	0.01	6 (2%) 64 59	11, 20, 38, 51	0
1	D	248/281 (88%)	-0.01	6 (2%) 62 57	13, 21, 39, 48	0
All	All	1035/1124 (92%)	0.04	29 (2%) 56 51	11, 22, 39, 51	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1157	ARG	4.6
1	A	1181	ALA	4.5
1	A	1165	TYR	4.5
1	C	1184	LEU	3.7
1	B	1145	ARG	3.7
1	D	1081	GLU	3.5
1	A	1157	ARG	3.4
1	D	1173	GLU	3.1
1	D	1166	PHE	3.1
1	C	1180	GLU	3.0
1	B	1166	PHE	3.0
1	B	1165	TYR	2.9
1	B	1173	GLU	2.8
1	C	1183	ALA	2.7
1	B	984	ASN	2.6
1	C	1161	ILE	2.6
1	B	1046	ALA	2.6
1	B	977	VAL	2.5
1	D	1004	GLN	2.4
1	B	1157	ARG	2.4
1	B	1171	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1179	ALA	2.4
1	B	1092	LYS	2.3
1	B	1090	ASP	2.1
1	D	1179	ALA	2.1
1	B	992	ILE	2.1
1	C	1186	GLN	2.1
1	C	1157	ARG	2.1
1	B	949	ASP	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	ZN	A	1502	1/1	1.00	0.10	2.11	17,17,17,17	0
2	ZN	C	1510	1/1	1.00	0.11	1.84	15,15,15,15	0
2	ZN	D	1514	1/1	1.00	0.11	0.96	17,17,17,17	0
2	ZN	C	1511	1/1	1.00	0.10	0.64	16,16,16,16	0
2	ZN	C	1509	1/1	1.00	0.10	0.34	17,17,17,17	0
3	SAH	B	1509	26/26	0.91	0.14	0.21	26,27,31,34	0
2	ZN	D	1515	1/1	1.00	0.10	0.11	18,18,18,18	0
3	SAH	A	1505	26/26	0.96	0.09	0.02	18,22,25,28	0
2	ZN	A	1503	1/1	1.00	0.09	-0.14	17,17,17,17	0
3	SAH	D	1517	26/26	0.95	0.10	-0.16	23,26,29,32	0
3	SAH	C	1513	26/26	0.96	0.08	-0.55	16,19,25,31	0
2	ZN	C	1512	1/1	0.97	0.07	-0.65	26,26,26,26	0
2	ZN	D	1513	1/1	1.00	0.08	-1.33	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	B	1506	1/1	0.99	0.09	-1.39	24,24,24,24	0
2	ZN	A	1504	1/1	0.99	0.06	-1.68	27,27,27,27	0
2	ZN	D	1516	1/1	0.98	0.05	-1.88	31,31,31,31	0
2	ZN	B	1507	1/1	0.99	0.07	-1.92	27,27,27,27	0
2	ZN	B	1508	1/1	0.97	0.04	-1.94	29,29,29,29	0
2	ZN	B	1505	1/1	0.99	0.07	-2.38	26,26,26,26	0
2	ZN	A	1501	1/1	1.00	0.07	-2.98	18,18,18,18	0

6.5 Other polymers

There are no such residues in this entry.