Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:16 PM GMT

PDB ID	:	1WY7
Title	:	crystal structure of a putative RNA methyltransferase PH1948 from Pyrococcus horikoshii
Authors	:	Gao, Y.G.; Yao, M.; Tanaka, I.
Deposited on	:	2005-02-08
Resolution	:	2.20 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:

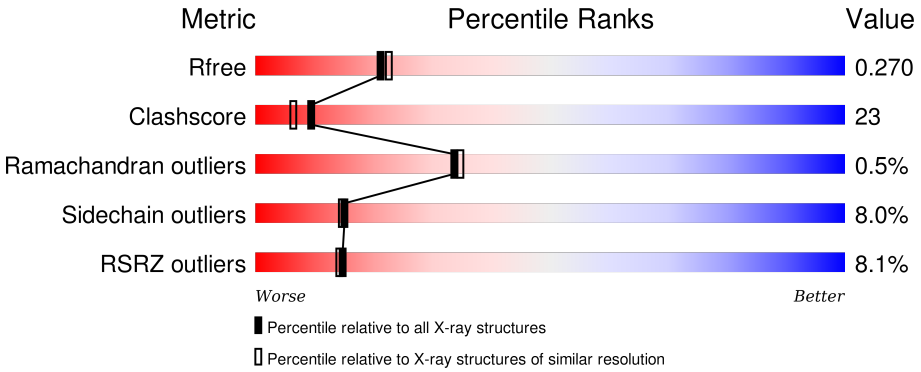
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	207	5%, 65%, 26%, 5%
1	B	207	6%, 65%, 26%
1	C	207	8%, 64%, 29%
1	D	207	12%, 60%, 33%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6823 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.

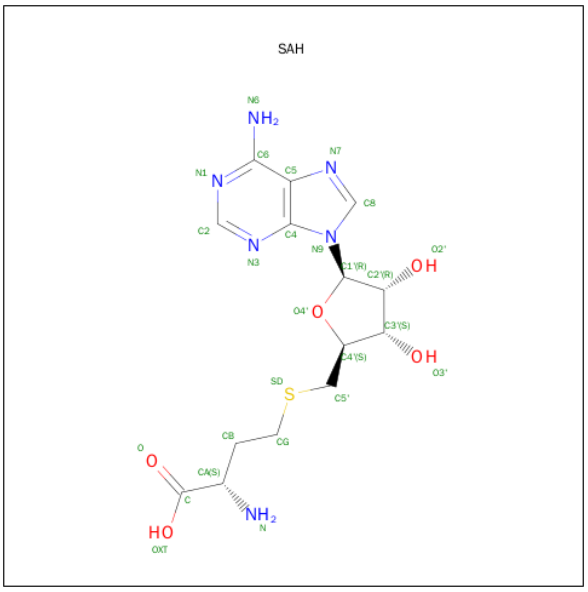
- Molecule 1 is a protein called hypothetical protein PH1948.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	Se	0	0	0
			1571	1025	269	275	1	1			
1	B	198	Total	C	N	O	S	Se	0	0	0
			1582	1033	267	279	1	2			
1	C	201	Total	C	N	O	S	Se	0	0	0
			1610	1046	276	284	1	3			
1	D	204	Total	C	N	O	S	Se	0	0	0
			1644	1077	278	285	1	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP O59611
A	2	MSE	MET	MODIFIED RESIDUE	UNP O59611
A	118	MSE	MET	MODIFIED RESIDUE	UNP O59611
B	1	MSE	MET	MODIFIED RESIDUE	UNP O59611
B	2	MSE	MET	MODIFIED RESIDUE	UNP O59611
B	118	MSE	MET	MODIFIED RESIDUE	UNP O59611
C	1	MSE	MET	MODIFIED RESIDUE	UNP O59611
C	2	MSE	MET	MODIFIED RESIDUE	UNP O59611
C	118	MSE	MET	MODIFIED RESIDUE	UNP O59611
D	1	MSE	MET	MODIFIED RESIDUE	UNP O59611
D	2	MSE	MET	MODIFIED RESIDUE	UNP O59611
D	118	MSE	MET	MODIFIED RESIDUE	UNP O59611

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

- Molecule 3 is water.

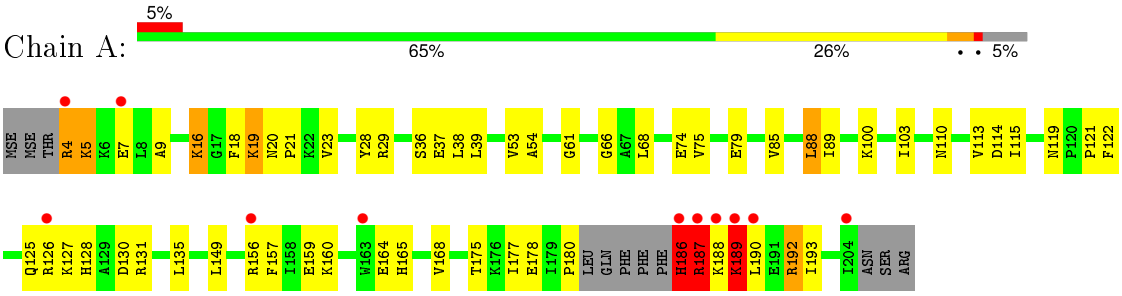
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	100	Total O 100 100	0	0
3	B	85	Total O 85 85	0	0
3	C	64	Total O 64 64	0	0
3	D	63	Total O 63 63	0	0

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.

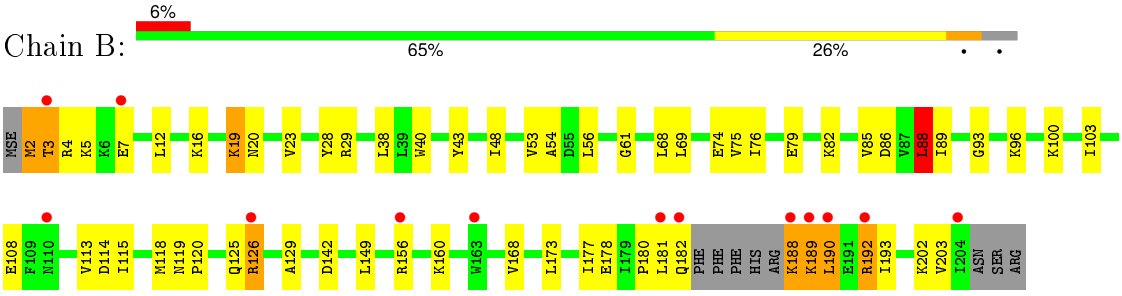
- Molecule 1: hypothetical protein PH1948

Chain A:



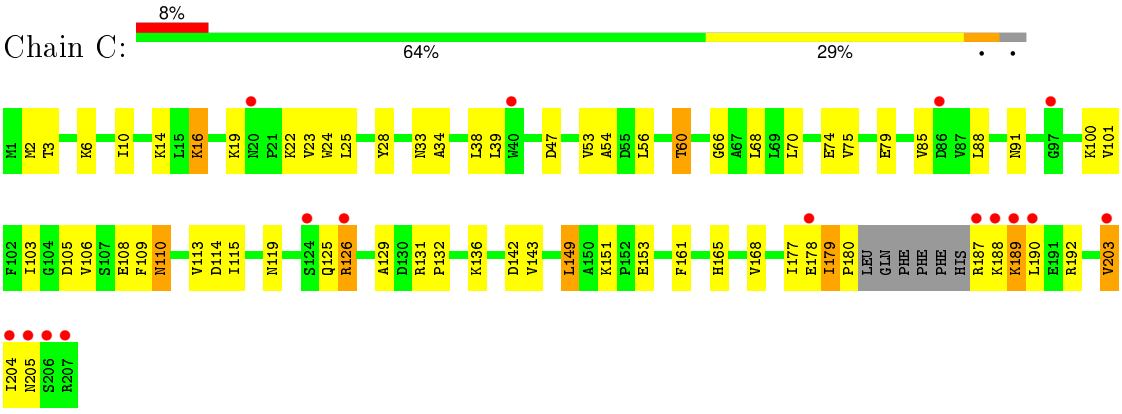
- Molecule 1: hypothetical protein PH1948

Chain B:



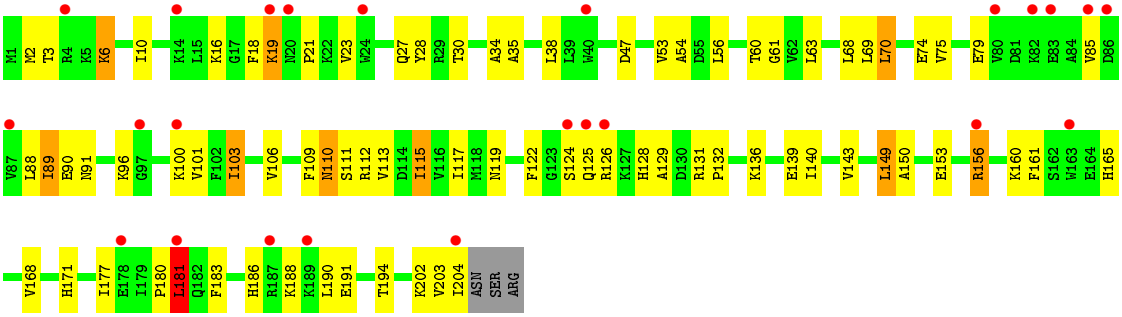
- Molecule 1: hypothetical protein PH1948

Chain C:



- Molecule 1: hypothetical protein PH1948

Chain D:


M1 M2 T3 R4 K5 K6 I10 K14 L15 K16 G17 F18 K19 N20 P21 K22 V23 W24 Q27 Y28 R29 T30 A34 A35 L38 L39 W40 D47 V53 A54 D55 L56 T60 G61 V62 L63 L68 L69 L70 E74 V75 E79 V80 D81 K82 E83 A84 V85 D86
V87 L88 I89 E90 N91 K96 G97 K100 V101 F102 I103 V106 F109 M110 S111 R112 V113 D114 I115 V116 I117 M118 N119 F122 G123 S124 Q125 R126 K127 H128 A129 D130 R131 P132 K136 E139 I140 V143 L149 A150 E153 R156 K160 F161 S162 W163 E164 H165
V168 H171 I177 E178 I179 P180 L181 Q182 F183 H186 R187 K188 K189 L190 E191 T194 K202 V203 I204 ASN SER ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	206.97Å 43.14Å 118.24Å 90.00° 92.08° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 9.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (10.00-2.20) 99.4 (9.99-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	4.59 (at 2.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.242 , 0.268 0.244 , 0.270	Depositor DCC
R_{free} test set	5285 reflections (9.99%)	DCC
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.46 , 75.3	EDS
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 52894 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6823	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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	0.47	1/1603 (0.1%)	0.70	3/2157 (0.1%)
1	B	0.44	0/1613	0.64	1/2171 (0.0%)
1	C	0.42	0/1640	0.64	0/2202
1	D	0.43	0/1679	0.66	1/2258 (0.0%)
All	All	0.44	1/6535 (0.0%)	0.66	5/8788 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	HIS	CB-CG	6.98	1.62	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	181	LEU	CA-CB-CG	6.09	129.30	115.30
1	A	186	HIS	CA-CB-CG	6.07	123.91	113.60
1	A	187	ARG	C-N-CA	-5.46	108.04	121.70
1	A	88	LEU	CA-CB-CG	5.05	126.91	115.30
1	B	88	LEU	CA-CB-CG	5.03	126.86	115.30

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	1571	0	1629	94	4
1	B	1582	0	1644	65	1
1	C	1610	0	1674	71	0
1	D	1644	0	1704	71	0
2	A	26	0	19	3	0
2	B	26	0	19	1	0
2	C	26	0	19	0	0
2	D	26	0	19	2	0
3	A	100	0	0	1	0
3	B	85	0	0	7	3
3	C	64	0	0	3	0
3	D	63	0	0	4	0
All	All	6823	0	6727	299	4

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 23.

All (299) 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:187:ARG:N	1:A:187:ARG:CD	1.70	1.46
1:A:186:HIS:CB	1:A:187:ARG:HD2	1.52	1.39
1:A:187:ARG:H	1:A:187:ARG:CD	1.32	1.29
1:A:186:HIS:HB3	1:A:187:ARG:CD	1.65	1.24
1:A:187:ARG:CZ	1:A:188:LYS:HD2	1.72	1.19
1:A:187:ARG:N	1:A:187:ARG:HD3	0.88	1.03
1:A:187:ARG:NH2	1:A:188:LYS:HD2	1.75	1.00
1:A:186:HIS:C	1:A:187:ARG:HD3	1.88	0.94
1:C:47:ASP:O	1:C:115:ILE:HD13	1.68	0.93
1:A:186:HIS:C	1:A:187:ARG:CD	2.42	0.88
1:C:178:GLU:HG2	1:C:192:ARG:HG2	1.54	0.88
1:A:180:PRO:HA	1:A:190:LEU:HD23	1.56	0.88
1:D:28:TYR:HB3	1:D:181:LEU:HD11	1.57	0.87
1:A:187:ARG:NH1	1:A:188:LYS:HD2	1.89	0.86
1:A:128:HIS:HB3	1:A:131:ARG:HD3	1.56	0.86
1:C:126:ARG:HG3	1:C:129:ALA:HB2	1.56	0.85
1:C:125:GLN:HE21	1:C:125:GLN:HA	1.41	0.85
1:A:187:ARG:CZ	1:A:188:LYS:CD	2.52	0.84
1:A:178:GLU:HB3	1:A:190:LEU:HD13	1.59	0.84
1:B:19:LYS:HD3	1:B:20:ASN:N	1.93	0.84
1:A:189:LYS:NZ	1:A:189:LYS:HB2	1.92	0.84
1:A:186:HIS:CA	1:A:187:ARG:HD2	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:VAL:HG12	1:D:204:ILE:HG13	1.58	0.83
1:A:178:GLU:HG2	1:A:192:ARG:HG3	1.60	0.83
1:C:74:GLU:OE1	1:C:100:LYS:HE3	1.79	0.82
1:B:180:PRO:HB3	1:B:188:LYS:NZ	1.94	0.81
1:D:85:VAL:O	1:D:89:ILE:HG13	1.81	0.80
1:C:187:ARG:HG3	1:C:188:LYS:H	1.47	0.79
1:A:189:LYS:HZ3	1:A:189:LYS:HB2	1.45	0.79
1:A:180:PRO:HG3	1:A:190:LEU:CD2	2.12	0.79
1:C:125:GLN:NE2	1:C:125:GLN:HA	1.97	0.79
1:B:189:LYS:HZ2	1:B:189:LYS:HA	1.47	0.78
1:D:126:ARG:HG3	1:D:129:ALA:HB2	1.66	0.78
1:C:178:GLU:HB3	1:C:190:LEU:HD21	1.65	0.78
1:C:187:ARG:HG3	1:C:188:LYS:N	1.99	0.78
1:A:187:ARG:HB3	1:B:7:GLU:OE2	1.84	0.77
1:A:16:LYS:N	1:A:16:LYS:HD2	1.99	0.77
1:B:3:THR:HG23	1:B:4:ARG:H	1.49	0.77
1:D:101:VAL:HG12	1:D:103:ILE:CD1	2.16	0.75
1:B:189:LYS:HA	1:B:189:LYS:NZ	2.00	0.75
1:D:74:GLU:OE1	1:D:100:LYS:HE3	1.88	0.74
1:A:178:GLU:CB	1:A:190:LEU:HD13	2.18	0.73
1:C:189:LYS:CD	1:C:189:LYS:H	2.02	0.72
1:C:23:VAL:HG22	3:C:1059:HOH:O	1.90	0.72
1:B:190:LEU:O	1:B:190:LEU:HD22	1.90	0.72
1:A:189:LYS:CB	1:A:189:LYS:NZ	2.50	0.72
1:C:101:VAL:HG12	1:C:103:ILE:HD11	1.70	0.71
1:C:28:TYR:CD1	1:C:179:ILE:HG21	2.25	0.70
1:C:103:ILE:HD12	1:C:103:ILE:N	2.07	0.70
1:A:19:LYS:N	1:A:19:LYS:HD3	2.06	0.69
1:B:126:ARG:HG3	1:B:129:ALA:HB2	1.73	0.69
1:A:180:PRO:HG3	1:A:190:LEU:HD21	1.74	0.69
1:A:128:HIS:HB3	1:A:131:ARG:CD	2.22	0.68
1:A:186:HIS:CA	1:A:187:ARG:CD	2.70	0.68
1:D:3:THR:HG21	3:D:1051:HOH:O	1.93	0.68
1:B:190:LEU:HD13	1:B:190:LEU:N	2.09	0.67
1:C:3:THR:HG23	1:C:6:LYS:H	1.59	0.67
1:C:14:LYS:HA	1:C:14:LYS:HZ3	1.60	0.67
1:C:203:VAL:HG12	1:C:204:ILE:HG13	1.76	0.67
1:A:186:HIS:N	1:A:187:ARG:NH1	2.43	0.67
1:B:2:MSE:HE2	1:B:5:LYS:NZ	2.10	0.67
1:C:189:LYS:H	1:C:189:LYS:CE	2.09	0.66
1:B:180:PRO:HB3	1:B:188:LYS:HZ2	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:LYS:HG3	1:D:90:GLU:OE2	1.95	0.66
1:B:74:GLU:OE1	1:B:100:LYS:HE2	1.95	0.66
1:A:187:ARG:NH2	1:A:188:LYS:CD	2.57	0.65
1:B:2:MSE:N	1:B:2:MSE:HE3	2.11	0.65
1:C:101:VAL:HG12	1:C:103:ILE:CD1	2.25	0.65
1:A:186:HIS:HB3	1:A:187:ARG:HD2	0.73	0.65
1:A:125:GLN:C	1:A:126:ARG:HD2	2.17	0.65
1:D:180:PRO:O	1:D:181:LEU:HD13	1.97	0.64
1:D:3:THR:HG23	1:D:6:LYS:H	1.62	0.64
1:A:125:GLN:O	1:A:126:ARG:HD2	1.96	0.64
1:B:2:MSE:HE2	1:B:5:LYS:HZ1	1.63	0.64
1:B:188:LYS:HD3	1:B:189:LYS:N	2.13	0.64
1:A:19:LYS:H	1:A:19:LYS:HD3	1.60	0.64
1:A:85:VAL:O	1:A:89:ILE:HG12	1.97	0.64
1:D:101:VAL:HG12	1:D:103:ILE:HD13	1.80	0.62
1:A:19:LYS:CD	1:A:20:ASN:H	2.12	0.61
1:D:16:LYS:O	1:D:60:THR:HG21	2.00	0.61
1:D:181:LEU:HD22	1:D:181:LEU:O	2.00	0.61
1:D:150:ALA:HB3	1:D:194:THR:HG22	1.81	0.61
1:D:28:TYR:HB3	1:D:181:LEU:CD1	2.29	0.61
1:A:187:ARG:C	1:A:188:LYS:CG	2.69	0.60
1:B:190:LEU:H	1:B:190:LEU:HD13	1.64	0.60
1:B:190:LEU:HD21	1:B:192:ARG:HH11	1.66	0.60
1:C:189:LYS:H	1:C:189:LYS:HE3	1.66	0.60
1:B:4:ARG:HG2	1:B:4:ARG:HH11	1.66	0.60
1:A:187:ARG:NH1	1:A:188:LYS:HG3	2.17	0.60
1:D:161:PHE:O	1:D:165:HIS:HD2	1.85	0.60
1:C:14:LYS:HA	1:C:14:LYS:NZ	2.16	0.60
1:B:190:LEU:O	1:B:192:ARG:HD2	2.02	0.59
1:A:156:ARG:HG2	1:A:160:LYS:HE2	1.85	0.59
1:C:2:MSE:SE	1:C:10:ILE:HD12	2.53	0.59
1:D:168:VAL:HG13	1:D:203:VAL:HG22	1.85	0.58
1:A:29:ARG:HA	2:A:1001:SAH:N	2.18	0.58
1:B:180:PRO:HB3	1:B:188:LYS:HZ1	1.68	0.58
1:A:189:LYS:HZ3	1:A:189:LYS:CB	2.13	0.57
1:D:150:ALA:CB	1:D:194:THR:HG22	2.34	0.57
1:D:183:PHE:HB2	1:D:186:HIS:O	2.04	0.57
1:A:186:HIS:C	1:A:187:ARG:HD2	2.17	0.57
1:B:190:LEU:CD2	1:B:192:ARG:HH11	2.18	0.57
1:C:54:ALA:HB2	1:C:113:VAL:HG11	1.85	0.57
1:D:69:LEU:O	1:D:69:LEU:HD13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ALA:HB2	1:C:177:ILE:HG21	1.87	0.57
1:C:189:LYS:H	1:C:189:LYS:HD3	1.70	0.57
1:A:180:PRO:CA	1:A:190:LEU:HD23	2.33	0.56
1:A:16:LYS:HD2	1:A:16:LYS:H	1.70	0.56
1:A:5:LYS:HE2	3:A:1020:HOH:O	2.06	0.56
1:C:101:VAL:CG1	1:C:103:ILE:HD11	2.35	0.55
1:C:110:ASN:O	1:C:110:ASN:ND2	2.32	0.55
1:A:38:LEU:C	1:A:38:LEU:HD23	2.27	0.55
1:A:19:LYS:HG2	1:A:20:ASN:N	2.21	0.55
1:B:142:ASP:OD2	1:B:202:LYS:HD2	2.06	0.55
1:A:28:TYR:O	2:A:1001:SAH:HG1	2.07	0.55
1:B:85:VAL:O	1:B:89:ILE:HG12	2.07	0.55
1:A:187:ARG:NH1	1:A:188:LYS:CD	2.65	0.54
1:A:135:LEU:HD21	1:A:165:HIS:CE1	2.43	0.54
1:A:74:GLU:OE1	1:A:100:LYS:NZ	2.41	0.54
1:B:40:TRP:NE1	3:B:1037:HOH:O	2.30	0.54
1:A:19:LYS:CG	1:A:20:ASN:N	2.71	0.54
1:A:114:ASP:C	1:A:115:ILE:HD12	2.29	0.53
1:B:156:ARG:HD3	1:B:160:LYS:NZ	2.24	0.53
1:D:61:GLY:HA3	1:D:88:LEU:HD22	1.90	0.53
1:A:177:ILE:HD11	1:A:193:ILE:HD11	1.90	0.53
1:B:54:ALA:HB2	1:B:113:VAL:HG11	1.91	0.53
1:B:173:LEU:HD22	1:D:171:HIS:CD2	2.44	0.53
1:A:159:GLU:HG2	3:C:1023:HOH:O	2.09	0.53
1:A:54:ALA:HB2	1:A:113:VAL:HG11	1.90	0.53
1:B:126:ARG:CG	1:B:129:ALA:HB2	2.38	0.53
1:D:136:LYS:O	1:D:140:ILE:HG12	2.08	0.53
1:D:180:PRO:C	1:D:181:LEU:HD13	2.30	0.53
1:B:188:LYS:HD2	1:B:190:LEU:HD12	1.90	0.52
1:A:187:ARG:C	1:A:188:LYS:HG3	2.29	0.52
1:B:19:LYS:HD3	1:B:20:ASN:H	1.74	0.52
1:D:79:GLU:O	1:D:103:ILE:HA	2.09	0.52
1:B:178:GLU:HB3	1:B:190:LEU:HD23	1.91	0.52
1:C:16:LYS:HB3	1:C:16:LYS:NZ	2.24	0.52
1:A:186:HIS:N	1:A:187:ARG:HH11	2.08	0.52
1:B:188:LYS:HD3	1:B:188:LYS:C	2.30	0.52
1:D:27:GLN:HG2	2:D:1004:SAH:H3'	1.92	0.52
1:A:160:LYS:O	1:A:164:GLU:HG3	2.09	0.52
1:D:18:PHE:HB2	1:D:21:PRO:HG3	1.92	0.52
1:D:103:ILE:N	1:D:103:ILE:HD13	2.25	0.52
1:D:183:PHE:CE1	1:D:191:GLU:HB2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:PRO:HA	1:A:190:LEU:CD2	2.35	0.51
1:C:60:THR:HG23	1:C:91:ASN:ND2	2.25	0.51
1:C:125:GLN:HE21	1:C:125:GLN:CA	2.13	0.51
1:C:178:GLU:HB3	1:C:190:LEU:CD2	2.39	0.51
1:B:76:ILE:HG12	1:B:100:LYS:HE3	1.91	0.50
1:C:151:LYS:HE2	1:C:153:GLU:OE1	2.10	0.50
1:D:2:MSE:SE	1:D:10:ILE:HD12	2.61	0.50
1:B:114:ASP:C	1:B:115:ILE:HD12	2.32	0.50
1:D:18:PHE:CE2	1:D:27:GLN:HB3	2.47	0.50
1:D:30:THR:HG22	1:D:35:ALA:HB2	1.92	0.50
1:C:34:ALA:HB2	1:C:177:ILE:CG2	2.42	0.50
1:C:189:LYS:HE3	1:C:190:LEU:H	1.77	0.50
1:A:187:ARG:O	1:A:188:LYS:HG2	2.11	0.50
1:C:60:THR:HG23	1:C:91:ASN:HD22	1.75	0.50
1:A:122:PHE:CG	1:A:149:LEU:HD13	2.46	0.50
1:C:189:LYS:N	1:C:189:LYS:HD3	2.27	0.50
1:A:79:GLU:O	1:A:103:ILE:HA	2.12	0.49
1:D:181:LEU:HD12	3:D:1022:HOH:O	2.12	0.49
1:C:2:MSE:HG3	1:C:6:LYS:HZ3	1.77	0.49
1:D:131:ARG:HB2	1:D:132:PRO:HD3	1.95	0.49
1:B:190:LEU:CD1	1:B:190:LEU:N	2.74	0.49
1:A:68:LEU:HD22	1:A:75:VAL:HG21	1.95	0.49
1:C:189:LYS:CD	1:C:189:LYS:N	2.73	0.49
1:C:114:ASP:O	1:C:115:ILE:HG13	2.12	0.49
1:A:180:PRO:HG3	1:A:190:LEU:HD22	1.91	0.49
1:B:93:GLY:O	1:B:96:LYS:HD3	2.12	0.49
1:D:168:VAL:HG13	1:D:203:VAL:CG2	2.43	0.49
1:C:79:GLU:O	1:C:103:ILE:HA	2.13	0.49
1:B:43:TYR:HB2	1:B:48:ILE:HD12	1.95	0.49
1:A:178:GLU:HB3	1:A:190:LEU:HB3	1.96	0.48
1:D:16:LYS:O	1:D:60:THR:CG2	2.60	0.48
1:D:109:PHE:CZ	1:D:111:SER:HB3	2.49	0.48
1:B:38:LEU:HD23	1:B:38:LEU:C	2.33	0.48
1:B:82:LYS:HE2	1:B:86:ASP:OD1	2.13	0.48
1:B:3:THR:HG23	1:B:4:ARG:N	2.23	0.48
1:C:6:LYS:NZ	1:C:6:LYS:HB3	2.28	0.48
1:A:4:ARG:HG3	1:A:37:GLU:OE1	2.13	0.48
1:C:114:ASP:C	1:C:115:ILE:HG13	2.34	0.48
1:D:63:LEU:HB3	1:D:117:ILE:HD12	1.96	0.48
1:A:88:LEU:HD12	1:A:89:ILE:HD13	1.95	0.48
1:B:4:ARG:NH1	3:B:1016:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLY:HA3	1:B:88:LEU:HD22	1.95	0.47
1:C:24:TRP:CD1	1:C:25:LEU:HG	2.49	0.47
1:C:125:GLN:NE2	1:C:125:GLN:CA	2.69	0.47
1:D:110:ASN:N	1:D:110:ASN:HD22	2.13	0.47
1:D:181:LEU:CD2	1:D:181:LEU:O	2.62	0.47
1:C:6:LYS:HZ3	1:C:6:LYS:HB3	1.80	0.47
1:A:122:PHE:CD2	1:A:149:LEU:CD1	2.97	0.47
1:D:38:LEU:C	1:D:38:LEU:HD23	2.36	0.47
1:C:60:THR:HG23	1:C:60:THR:O	2.13	0.47
1:D:153:GLU:CD	1:D:153:GLU:H	2.17	0.47
1:B:7:GLU:HG3	3:B:1051:HOH:O	2.14	0.47
1:A:4:ARG:O	1:A:5:LYS:C	2.53	0.47
1:B:23:VAL:O	1:B:125:GLN:HG3	2.14	0.47
1:B:126:ARG:CD	1:B:129:ALA:HB2	2.46	0.46
1:D:79:GLU:OE2	2:D:1004:SAH:O2'	2.30	0.46
1:A:156:ARG:CG	1:A:160:LYS:HE2	2.46	0.46
1:C:105:ASP:HB3	1:C:108:GLU:HG3	1.97	0.46
1:A:178:GLU:HB3	1:A:190:LEU:CD1	2.38	0.46
1:A:19:LYS:CG	1:A:20:ASN:H	2.27	0.46
1:A:122:PHE:CD2	1:A:149:LEU:HD13	2.50	0.46
1:C:187:ARG:CG	1:C:188:LYS:H	2.13	0.46
1:D:54:ALA:HB2	1:D:113:VAL:HG11	1.97	0.46
1:C:47:ASP:C	1:C:115:ILE:HD13	2.31	0.46
1:B:4:ARG:HD3	1:B:40:TRP:CH2	2.51	0.46
1:B:4:ARG:HG2	1:B:4:ARG:NH1	2.31	0.46
1:A:4:ARG:HB3	1:A:4:ARG:NH1	2.30	0.46
1:D:112:ARG:NH1	1:D:139:GLU:O	2.48	0.46
1:A:187:ARG:H	1:A:187:ARG:HH11	1.63	0.46
1:B:79:GLU:O	1:B:103:ILE:HA	2.15	0.46
1:B:2:MSE:HA	1:B:5:LYS:HE2	1.98	0.45
1:D:202:LYS:NZ	3:D:1023:HOH:O	2.49	0.45
1:C:2:MSE:HG3	1:C:6:LYS:NZ	2.31	0.45
1:C:131:ARG:HB2	1:C:132:PRO:HD3	1.98	0.45
1:D:203:VAL:C	1:D:204:ILE:HG13	2.35	0.45
1:D:53:VAL:HG13	1:D:115:ILE:HG22	1.99	0.45
1:A:187:ARG:O	1:A:188:LYS:CG	2.64	0.45
1:A:180:PRO:CA	1:A:190:LEU:CD2	2.93	0.45
1:C:56:LEU:HG	1:C:106:VAL:HG23	1.98	0.45
1:D:16:LYS:HE2	1:D:90:GLU:OE1	2.17	0.45
1:C:22:LYS:HD3	1:C:24:TRP:CZ2	2.52	0.45
1:A:180:PRO:CG	1:A:190:LEU:CD2	2.88	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:PHE:O	1:D:136:LYS:NZ	2.47	0.45
1:D:60:THR:CG2	1:D:91:ASN:ND2	2.80	0.45
1:C:2:MSE:CG	1:C:6:LYS:HZ3	2.29	0.45
1:D:60:THR:O	1:D:60:THR:HG22	2.17	0.45
1:D:23:VAL:O	1:D:125:GLN:HG3	2.16	0.45
1:A:187:ARG:NH1	1:A:188:LYS:CG	2.80	0.45
1:B:156:ARG:HD3	1:B:160:LYS:HZ2	1.82	0.45
1:D:34:ALA:HB2	1:D:177:ILE:CG2	2.47	0.44
1:C:38:LEU:HD23	1:C:38:LEU:C	2.38	0.44
1:D:47:ASP:OD1	1:D:143:VAL:HG11	2.18	0.44
1:D:156:ARG:HH11	1:D:160:LYS:HB2	1.82	0.44
1:A:187:ARG:CZ	1:A:188:LYS:CG	2.95	0.44
1:A:16:LYS:N	1:A:16:LYS:CD	2.78	0.44
1:D:160:LYS:HE3	1:D:160:LYS:HB2	1.78	0.44
1:A:18:PHE:HB2	1:A:21:PRO:HG3	2.00	0.44
1:B:190:LEU:HD21	1:B:192:ARG:NH1	2.32	0.44
1:D:89:ILE:H	1:D:89:ILE:HG13	1.63	0.44
1:B:189:LYS:HZ2	1:B:190:LEU:H	1.65	0.43
1:D:122:PHE:CD1	1:D:149:LEU:HD13	2.53	0.43
1:C:85:VAL:HG21	1:C:103:ILE:HG13	2.00	0.43
1:A:53:VAL:O	1:A:75:VAL:HA	2.19	0.43
1:B:177:ILE:HD11	1:B:193:ILE:HD11	2.00	0.43
1:B:4:ARG:HD3	1:B:40:TRP:HH2	1.83	0.43
1:A:4:ARG:CG	1:A:37:GLU:OE1	2.66	0.43
1:C:88:LEU:C	1:C:88:LEU:HD13	2.39	0.43
1:C:153:GLU:H	1:C:153:GLU:CD	2.22	0.43
1:D:128:HIS:HB3	1:D:131:ARG:HD2	2.00	0.43
1:C:109:PHE:O	1:C:136:LYS:HD2	2.19	0.43
1:C:39:LEU:HD13	1:C:66:GLY:HA3	2.01	0.43
1:C:2:MSE:HG3	1:C:6:LYS:HE2	2.00	0.43
1:A:131:ARG:NH1	1:A:157:PHE:CE2	2.87	0.43
1:D:69:LEU:C	1:D:69:LEU:HD13	2.39	0.43
1:D:190:LEU:HD22	1:D:190:LEU:N	2.34	0.43
1:D:19:LYS:CE	1:D:19:LYS:HA	2.49	0.43
1:D:53:VAL:O	1:D:75:VAL:HA	2.19	0.42
1:C:149:LEU:HB2	3:C:1025:HOH:O	2.19	0.42
1:C:103:ILE:N	1:C:103:ILE:CD1	2.77	0.42
1:D:115:ILE:HD11	3:D:1063:HOH:O	2.18	0.42
1:D:88:LEU:C	1:D:88:LEU:HD13	2.39	0.42
1:A:61:GLY:HA3	1:A:88:LEU:HD22	2.02	0.42
1:C:23:VAL:O	1:C:125:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:ASP:OD1	1:C:205:ASN:OD1	2.37	0.42
1:B:118:MSE:HG3	1:B:120:PRO:HD3	2.01	0.42
1:A:19:LYS:HE2	1:A:20:ASN:H	1.84	0.42
1:B:126:ARG:HB3	3:B:1063:HOH:O	2.19	0.42
1:B:168:VAL:HG13	1:B:203:VAL:HG22	2.02	0.42
1:D:19:LYS:HA	1:D:19:LYS:NZ	2.35	0.41
1:D:56:LEU:HG	1:D:106:VAL:HG23	2.02	0.41
1:A:39:LEU:HD13	1:A:66:GLY:HA3	2.02	0.41
1:C:161:PHE:O	1:C:165:HIS:HD2	2.03	0.41
1:A:178:GLU:O	1:A:180:PRO:HD3	2.20	0.41
1:B:53:VAL:O	1:B:75:VAL:HA	2.21	0.41
1:A:29:ARG:HA	2:A:1001:SAH:HN2	1.83	0.41
1:D:128:HIS:HB3	1:D:131:ARG:CD	2.51	0.41
1:B:189:LYS:HZ2	1:B:189:LYS:CA	2.26	0.41
1:A:121:PRO:O	1:A:130:ASP:HB3	2.20	0.41
1:D:203:VAL:HG12	1:D:204:ILE:CG1	2.39	0.41
1:B:88:LEU:HD13	1:B:88:LEU:C	2.41	0.41
1:D:70:LEU:HD12	1:D:70:LEU:HA	1.91	0.41
1:A:23:VAL:O	1:A:125:GLN:HG3	2.21	0.41
1:B:188:LYS:HA	3:B:1062:HOH:O	2.21	0.41
1:A:9:ALA:HB2	1:A:36:SER:OG	2.21	0.41
1:C:85:VAL:CG1	1:C:101:VAL:HG11	2.51	0.41
1:B:12:LEU:O	1:B:29:ARG:NH1	2.54	0.41
1:C:168:VAL:HG13	1:C:203:VAL:HG22	2.03	0.40
1:B:108:GLU:OE1	3:B:1060:HOH:O	2.20	0.40
1:B:28:TYR:O	2:B:1002:SAH:HG1	2.21	0.40
1:A:187:ARG:CZ	1:A:188:LYS:HG3	2.51	0.40
1:B:181:LEU:HB3	3:B:1061:HOH:O	2.20	0.40
1:C:47:ASP:OD1	1:C:143:VAL:HG11	2.21	0.40
1:C:179:ILE:HA	1:C:180:PRO:HD3	1.82	0.40
1:C:53:VAL:O	1:C:75:VAL:HA	2.20	0.40

All (4) 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)
1:A:188:LYS:NZ	3:B:1031:HOH:O[1_545]	0.54	1.66
1:A:188:LYS:CE	3:B:1031:HOH:O[1_545]	1.35	0.85
1:A:188:LYS:CD	3:B:1031:HOH:O[1_545]	2.05	0.15
1:A:186:HIS:N	1:B:125:GLN:OE1[1_545]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	192/207 (93%)	186 (97%)	4 (2%)	2 (1%)	19	16
1	B	194/207 (94%)	188 (97%)	5 (3%)	1 (0%)	34	35
1	C	197/207 (95%)	192 (98%)	4 (2%)	1 (0%)	34	35
1	D	202/207 (98%)	194 (96%)	8 (4%)	0	100	100
All	All	785/828 (95%)	760 (97%)	21 (3%)	4 (0%)	34	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	LYS
1	C	203	VAL
1	B	3	THR
1	A	5	LYS

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	169/177 (96%)	156 (92%)	13 (8%)	16	16
1	B	171/177 (97%)	156 (91%)	15 (9%)	12	12
1	C	174/177 (98%)	162 (93%)	12 (7%)	19	20
1	D	177/177 (100%)	162 (92%)	15 (8%)	13	13
All	All	691/708 (98%)	636 (92%)	55 (8%)	15	15

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	7	GLU
1	A	16	LYS
1	A	19	LYS
1	A	110	ASN
1	A	119	ASN
1	A	127	LYS
1	A	168	VAL
1	A	175	THR
1	A	186	HIS
1	A	187	ARG
1	A	189	LYS
1	A	192	ARG
1	B	2	MSE
1	B	16	LYS
1	B	19	LYS
1	B	56	LEU
1	B	68	LEU
1	B	69	LEU
1	B	88	LEU
1	B	119	ASN
1	B	126	ARG
1	B	149	LEU
1	B	182	GLN
1	B	188	LYS
1	B	189	LYS
1	B	190	LEU
1	B	192	ARG
1	C	16	LYS
1	C	19	LYS
1	C	33	ASN
1	C	60	THR
1	C	68	LEU
1	C	70	LEU
1	C	110	ASN
1	C	119	ASN
1	C	126	ARG
1	C	149	LEU
1	C	179	ILE
1	C	189	LYS
1	D	6	LYS
1	D	19	LYS

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Mol	Chain	Res	Type
1	D	68	LEU
1	D	70	LEU
1	D	89	ILE
1	D	96	LYS
1	D	103	ILE
1	D	110	ASN
1	D	115	ILE
1	D	119	ASN
1	D	124	SER
1	D	149	LEU
1	D	156	ARG
1	D	181	LEU
1	D	188	LYS

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	110	ASN
1	A	119	ASN
1	A	125	GLN
1	A	165	HIS
1	B	119	ASN
1	B	125	GLN
1	B	165	HIS
1	C	33	ASN
1	C	119	ASN
1	C	125	GLN
1	C	165	HIS
1	D	110	ASN
1	D	119	ASN
1	D	125	GLN
1	D	165	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	1001	-	20,28,28	0.90	2 (10%)	19,40,40	1.96	5 (26%)
2	SAH	B	1002	-	20,28,28	1.02	2 (10%)	19,40,40	1.90	5 (26%)
2	SAH	C	1003	-	20,28,28	0.85	1 (5%)	19,40,40	1.40	2 (10%)
2	SAH	D	1004	-	20,28,28	1.16	2 (10%)	19,40,40	1.50	5 (26%)

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	1001	-	-	0/7/31/31	0/3/3/3
2	SAH	B	1002	-	-	0/7/31/31	0/3/3/3
2	SAH	C	1003	-	-	0/7/31/31	0/3/3/3
2	SAH	D	1004	-	-	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)
2	D	1004	SAH	C5'-SD	-3.34	1.74	1.81
2	B	1002	SAH	C5'-SD	-2.14	1.77	1.81
2	A	1001	SAH	C4-N3	2.01	1.38	1.35
2	A	1001	SAH	C2-N3	2.04	1.35	1.32
2	D	1004	SAH	C2-N3	2.12	1.35	1.32
2	C	1003	SAH	C2-N3	2.13	1.36	1.32
2	B	1002	SAH	C2-N3	2.24	1.36	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1002	SAH	C4'-O4'-C1'	-3.64	105.72	109.72
2	B	1002	SAH	O3'-C3'-C4'	-2.69	102.98	111.05
2	A	1001	SAH	C4'-O4'-C1'	-2.62	106.84	109.72
2	A	1001	SAH	O3'-C3'-C4'	-2.47	103.65	111.05
2	D	1004	SAH	C4'-O4'-C1'	-2.41	107.07	109.72
2	C	1003	SAH	C4'-O4'-C1'	-2.41	107.07	109.72
2	D	1004	SAH	O3'-C3'-C4'	-2.35	103.99	111.05
2	B	1002	SAH	C1'-N9-C4	-2.31	123.45	126.94
2	A	1001	SAH	C1'-N9-C4	-2.12	123.75	126.94
2	D	1004	SAH	C1'-N9-C4	-2.06	123.83	126.94
2	D	1004	SAH	C2'-C3'-C4'	2.00	106.73	102.61
2	C	1003	SAH	O2'-C2'-C3'	2.64	120.40	111.83
2	D	1004	SAH	O2'-C2'-C3'	2.83	121.05	111.83
2	A	1001	SAH	O2'-C2'-C3'	3.00	121.58	111.83
2	B	1002	SAH	O2'-C2'-C3'	3.13	122.00	111.83
2	B	1002	SAH	CB-CG-SD	4.17	121.61	113.57
2	A	1001	SAH	CB-CG-SD	5.34	123.88	113.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	SAH	3	0
2	B	1002	SAH	1	0
2	D	1004	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	195/207 (94%)	0.16	11 (5%) 28 27	24, 37, 63, 98	0
1	B	196/207 (94%)	0.25	13 (6%) 22 21	22, 38, 67, 88	0
1	C	198/207 (95%)	0.53	16 (8%) 15 14	29, 46, 70, 96	0
1	D	201/207 (97%)	0.56	24 (11%) 6 6	28, 47, 67, 80	0
All	All	790/828 (95%)	0.38	64 (8%) 15 14	22, 42, 68, 98	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	124	SER	11.7
1	B	181	LEU	10.3
1	C	207	ARG	7.7
1	C	205	ASN	6.8
1	B	3	THR	6.7
1	A	186	HIS	6.4
1	A	187	ARG	6.4
1	C	206	SER	6.0
1	D	126	ARG	5.7
1	A	204	ILE	5.4
1	B	204	ILE	5.3
1	D	97	GLY	5.1
1	C	188	LYS	4.8
1	B	188	LYS	4.7
1	A	4	ARG	4.7
1	C	86	ASP	4.6
1	D	204	ILE	4.6
1	B	182	GLN	4.6
1	C	190	LEU	4.5
1	A	188	LYS	4.4
1	D	156	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	24	TRP	4.2
1	B	190	LEU	3.9
1	D	125	GLN	3.8
1	C	97	GLY	3.7
1	C	187	ARG	3.7
1	D	80	VAL	3.7
1	C	204	ILE	3.6
1	A	189	LYS	3.6
1	A	126	ARG	3.3
1	A	190	LEU	3.3
1	C	126	ARG	3.3
1	D	187	ARG	3.2
1	D	86	ASP	3.0
1	C	124	SER	3.0
1	C	203	VAL	2.9
1	B	110	ASN	2.9
1	C	20	ASN	2.9
1	D	87	VAL	2.8
1	B	189	LYS	2.8
1	D	85	VAL	2.7
1	A	7	GLU	2.7
1	A	156	ARG	2.6
1	D	100	LYS	2.5
1	B	163	TRP	2.5
1	C	189	LYS	2.5
1	D	83	GLU	2.5
1	D	181	LEU	2.5
1	B	156	ARG	2.5
1	A	163	TRP	2.5
1	D	19	LYS	2.4
1	D	14	LYS	2.3
1	B	126	ARG	2.3
1	D	82	LYS	2.3
1	D	163	TRP	2.3
1	D	178	GLU	2.2
1	C	178	GLU	2.2
1	B	192	ARG	2.2
1	D	40	TRP	2.2
1	D	20	ASN	2.2
1	D	189	LYS	2.1
1	B	7	GLU	2.0
1	C	40	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	4	ARG	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	1002	26/26	0.86	0.15	1.56	32,37,54,57	0
2	SAH	A	1001	26/26	0.90	0.15	1.31	33,38,50,52	0
2	SAH	D	1004	26/26	0.83	0.19	0.75	49,62,71,72	0
2	SAH	C	1003	26/26	0.87	0.15	0.31	40,52,68,70	0

6.5 Other polymers (i)

There are no such residues in this entry.