Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:33 pm BST

PDB ID	:	1H3I
Title	:	Crystal structure of the Histone Methyltransferase SET7/9
Authors	:	Wilson, J.R.; Jing, C.; Walker, P.A.; Martin, S.R.; Howell, S.A.; Blackburn, G.M.; Gamblin, S.J.; Xiao, B.
Deposited on	:	2002-09-04
Resolution	:	2.10 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

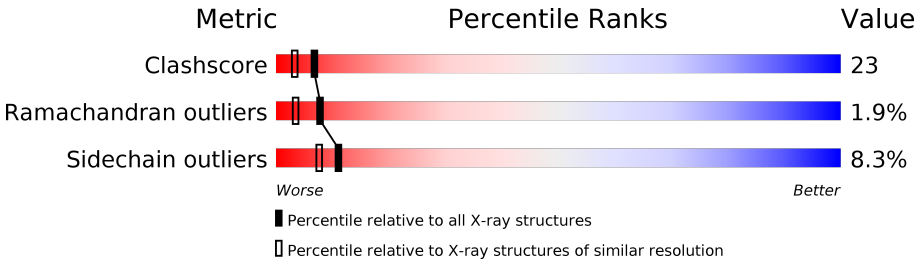
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	293	67% 28%
1	B	293	65% 27% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4935 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 H3 LYSINE 4 SPECIFIC METHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2294	1449	372	462	11			
1	B	293	Total	C	N	O	S	0	0	0
			2294	1449	372	462	11			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	173	Total	O	0	0
			173	173		
3	B	171	Total	O	0	0
			171	171		

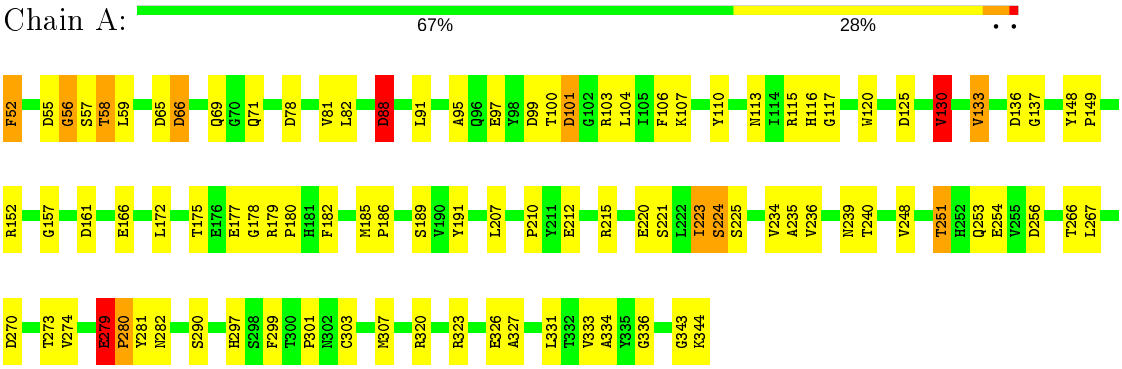
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

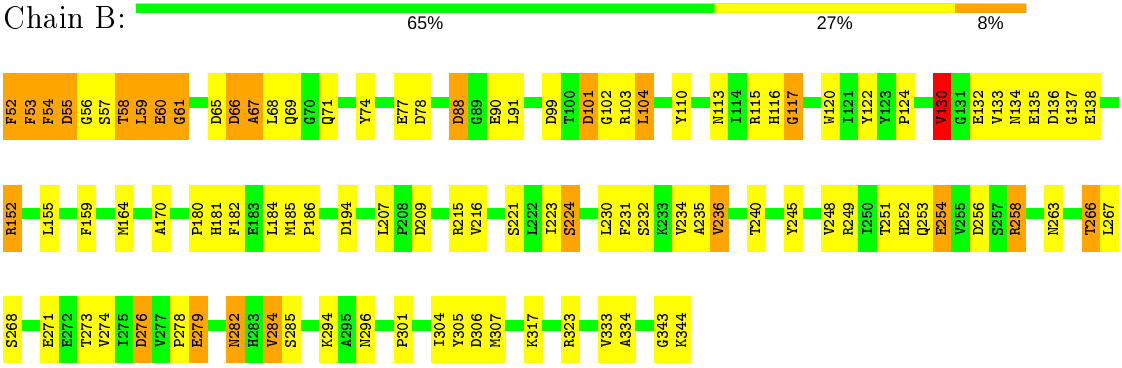
- Molecule 1: HISTONE H3 LYSINE 4 SPECIFIC METHYLTRANSFERASE

Chain A:



- Molecule 1: HISTONE H3 LYSINE 4 SPECIFIC METHYLTRANSFERASE

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.09Å 82.83Å 116.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	95.9 (20.00-2.10)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.210 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4935	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.45	0/2354	0.86	12/3197 (0.4%)
1	B	0.46	0/2354	0.84	13/3197 (0.4%)
All	All	0.45	0/4708	0.85	25/6394 (0.4%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	279	GLU	N-CA-C	7.25	130.58	111.00
1	B	306	ASP	CB-CG-OD2	6.90	124.51	118.30
1	B	130	VAL	CB-CA-C	-6.47	99.11	111.40
1	A	55	ASP	CB-CG-OD2	6.32	123.98	118.30
1	A	136	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	130	VAL	CB-CA-C	-5.79	100.39	111.40
1	B	88	ASP	CB-CG-OD2	5.75	123.48	118.30
1	B	276	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	256	ASP	CB-CG-OD2	5.53	123.27	118.30
1	B	209	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	279	GLU	N-CA-C	5.50	125.84	111.00
1	A	125	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	88	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	136	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	78	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	161	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	66	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	66	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	270	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	55	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	194	ASP	CB-CG-OD2	5.15	122.93	118.30
1	B	78	ASP	CB-CG-OD2	5.13	122.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	256	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	67	ALA	N-CA-C	-5.07	97.32	111.00
1	A	55	ASP	CB-CA-C	-5.03	100.34	110.40

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	2294	0	2138	88	0
1	B	2294	0	2138	128	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	173	0	0	16	0
3	B	171	0	0	14	0
All	All	4935	0	4276	207	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 23.

All (207) 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:B:307:MET:CE	1:B:317:LYS:HE2	1.74	1.17
1:A:236:VAL:HG21	1:A:240:THR:HG21	1.32	1.11
1:B:307:MET:HE1	1:B:317:LYS:HE2	1.31	1.07
1:B:67:ALA:HB1	1:B:88:ASP:HA	1.34	1.06
1:A:69:GLN:HE22	1:A:88:ASP:HA	1.28	0.98
1:B:52:PHE:HA	1:B:55:ASP:HB2	1.45	0.97
1:B:69:GLN:HE22	1:B:88:ASP:H	1.12	0.96
1:A:266:THR:HG23	1:A:274:VAL:HG11	1.45	0.95
1:A:266:THR:HG23	1:A:274:VAL:CG1	1.97	0.95
1:B:58:THR:CG2	1:B:59:LEU:N	2.30	0.94
1:A:59:LEU:CD1	1:A:71:GLN:HG3	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLY:N	3:A:2055:HOH:O	2.03	0.92
1:B:58:THR:HG22	1:B:59:LEU:N	1.85	0.91
1:B:279:GLU:O	1:B:282:ASN:ND2	2.05	0.89
1:B:251:THR:HG22	1:B:253:GLN:H	1.37	0.89
1:B:307:MET:HE2	1:B:317:LYS:HE2	1.55	0.87
1:B:52:PHE:HA	1:B:55:ASP:CB	2.03	0.87
1:B:58:THR:CG2	1:B:59:LEU:H	1.87	0.86
1:B:343:GLY:O	1:B:344:LYS:HB2	1.75	0.85
1:A:279:GLU:HA	1:A:282:ASN:OD1	1.75	0.85
1:B:251:THR:HB	1:B:254:GLU:OE2	1.75	0.85
1:B:279:GLU:OE2	1:B:279:GLU:O	1.95	0.84
1:A:253:GLN:HG2	3:A:2123:HOH:O	1.78	0.83
1:B:58:THR:HG23	1:B:59:LEU:H	1.44	0.82
1:B:251:THR:HG23	3:B:2129:HOH:O	1.81	0.81
1:B:69:GLN:NE2	1:B:88:ASP:H	1.77	0.81
1:B:282:ASN:HD22	1:B:282:ASN:H	1.26	0.81
1:A:251:THR:HG22	1:A:254:GLU:H	1.47	0.80
1:B:103:ARG:NH1	1:B:124:PRO:HB3	1.98	0.79
1:B:307:MET:HE1	1:B:317:LYS:CE	2.12	0.79
1:A:58:THR:HB	1:B:323:ARG:CZ	2.12	0.78
1:B:133:VAL:HG11	1:B:137:GLY:HA2	1.64	0.77
1:B:60:GLU:O	1:B:61:GLY:O	2.04	0.76
1:B:103:ARG:HH11	1:B:124:PRO:HB3	1.51	0.76
1:A:266:THR:CG2	1:A:274:VAL:HG11	2.16	0.76
1:A:59:LEU:CB	1:A:71:GLN:HG3	2.16	0.75
1:B:59:LEU:HD13	1:B:71:GLN:HG2	1.69	0.74
1:A:223:ILE:HG22	1:A:223:ILE:O	1.87	0.73
1:B:59:LEU:HB3	1:B:71:GLN:HB2	1.72	0.72
1:B:236:VAL:HG21	1:B:240:THR:HG21	1.71	0.72
1:B:135:GLU:HG2	3:B:2044:HOH:O	1.89	0.71
1:B:266:THR:HG23	1:B:274:VAL:HG11	1.72	0.71
1:A:236:VAL:CG2	1:A:240:THR:HG21	2.16	0.71
1:B:344:LYS:HD3	3:B:2171:HOH:O	1.91	0.70
1:A:99:ASP:HB3	3:A:2038:HOH:O	1.92	0.70
1:A:58:THR:HB	1:B:323:ARG:NE	2.06	0.69
1:A:103:ARG:HG2	3:A:2038:HOH:O	1.92	0.69
1:B:52:PHE:HE2	3:B:2024:HOH:O	1.75	0.69
1:A:59:LEU:HD12	1:A:71:GLN:HG3	1.73	0.69
1:B:104:LEU:HD22	1:B:122:TYR:CD1	2.29	0.68
1:B:59:LEU:HD13	1:B:71:GLN:CG	2.23	0.68
1:A:58:THR:CB	1:B:323:ARG:HD3	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ARG:HD2	1:B:263:ASN:OD1	1.93	0.67
1:A:59:LEU:HD13	1:A:71:GLN:HG3	1.75	0.66
1:B:170:ALA:HB2	1:B:184:LEU:HD23	1.76	0.66
1:A:343:GLY:O	1:A:344:LYS:HB2	1.97	0.65
1:A:97:GLU:HB2	1:A:106:PHE:HB3	1.77	0.65
1:B:279:GLU:O	1:B:279:GLU:CD	2.34	0.65
1:A:58:THR:HB	1:B:323:ARG:HD3	1.79	0.65
1:A:58:THR:HB	1:B:323:ARG:CD	2.27	0.65
1:B:323:ARG:HH11	1:B:323:ARG:HG2	1.62	0.65
1:B:266:THR:HG23	1:B:274:VAL:CG1	2.28	0.64
1:B:133:VAL:CG1	1:B:137:GLY:HA2	2.27	0.64
1:A:69:GLN:NE2	1:A:88:ASP:HA	2.07	0.64
1:B:67:ALA:CB	1:B:88:ASP:HA	2.22	0.64
1:B:90:GLU:HG2	1:B:113:ASN:HD21	1.61	0.63
1:B:282:ASN:N	1:B:282:ASN:HD22	1.96	0.63
1:B:215:ARG:HG3	1:B:215:ARG:HH11	1.63	0.63
1:B:305:TYR:CE1	1:B:333:VAL:HG11	2.33	0.63
1:A:58:THR:HG21	3:A:2004:HOH:O	1.98	0.63
1:B:53:PHE:H	1:B:53:PHE:HD1	1.49	0.61
1:B:152:ARG:NH2	3:B:2053:HOH:O	2.33	0.61
1:B:254:GLU:O	1:B:258:ARG:HG2	2.02	0.60
1:A:69:GLN:HE22	1:A:88:ASP:CA	2.07	0.60
1:B:59:LEU:HD23	1:B:60:GLU:H	1.67	0.60
1:A:59:LEU:CD1	1:A:71:GLN:CG	2.79	0.60
1:B:155:LEU:HD13	1:B:164:MET:HE1	1.83	0.60
1:A:103:ARG:NH1	3:A:2041:HOH:O	2.34	0.59
1:B:216:VAL:CG2	1:B:230:LEU:HG	2.33	0.58
1:B:53:PHE:HE1	1:B:102:GLY:HA3	1.68	0.58
1:A:59:LEU:HD13	1:A:71:GLN:CG	2.33	0.58
1:A:266:THR:CG2	1:A:274:VAL:CG1	2.77	0.58
1:B:216:VAL:HG21	1:B:230:LEU:HG	1.84	0.58
1:B:223:ILE:O	1:B:224:SER:HB3	2.04	0.58
1:B:69:GLN:HE22	1:B:88:ASP:N	1.93	0.58
1:B:267:LEU:HD23	1:B:268:SER:N	2.18	0.58
1:B:130:VAL:HG11	1:B:180:PRO:HG3	1.86	0.57
1:A:185:MET:HG3	1:A:186:PRO:HD2	1.86	0.56
1:A:326:GLU:HG2	1:A:327:ALA:N	2.20	0.56
1:A:253:GLN:CG	3:A:2123:HOH:O	2.44	0.56
1:B:251:THR:HB	1:B:254:GLU:CD	2.26	0.56
1:B:284:VAL:HG13	1:B:294:LYS:HE3	1.87	0.56
1:B:304:ILE:HG13	3:B:2146:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:HD23	1:B:60:GLU:N	2.21	0.56
1:B:271:GLU:HG3	3:B:2128:HOH:O	2.05	0.56
1:A:59:LEU:HB3	1:A:71:GLN:HG3	1.86	0.56
1:B:116:HIS:O	1:B:117:GLY:O	2.24	0.56
1:B:52:PHE:HA	1:B:55:ASP:HB3	1.86	0.55
1:B:285:SER:HA	3:B:2137:HOH:O	2.05	0.55
1:A:301:PRO:HG3	1:A:334:ALA:HB2	1.89	0.54
1:B:104:LEU:HD22	1:B:122:TYR:CE1	2.42	0.54
1:B:110:TYR:CE2	1:B:115:ARG:HG2	2.42	0.54
1:A:110:TYR:CE2	1:A:115:ARG:HG2	2.43	0.53
1:A:191:TYR:CZ	1:A:210:PRO:HG3	2.44	0.53
1:B:53:PHE:N	1:B:53:PHE:CD1	2.76	0.53
1:B:67:ALA:HB1	1:B:88:ASP:CA	2.23	0.53
1:A:299:PHE:CG	1:B:68:LEU:HD22	2.44	0.53
1:B:185:MET:HG3	1:B:186:PRO:HD2	1.91	0.53
1:B:77:GLU:HG3	3:B:2006:HOH:O	2.08	0.53
1:B:90:GLU:OE1	1:B:113:ASN:ND2	2.42	0.53
1:B:267:LEU:HD23	1:B:267:LEU:C	2.29	0.52
1:B:301:PRO:HG3	1:B:334:ALA:HB2	1.91	0.52
1:B:323:ARG:HH11	1:B:323:ARG:CG	2.21	0.52
1:A:236:VAL:HG21	1:A:240:THR:CG2	2.23	0.52
1:A:65:ASP:O	1:A:66:ASP:HB2	2.09	0.52
1:A:130:VAL:HG11	1:A:180:PRO:HG3	1.91	0.52
1:A:101:ASP:OD2	1:A:101:ASP:N	2.43	0.51
1:A:115:ARG:HG3	3:A:2054:HOH:O	2.09	0.51
1:A:175:THR:C	1:A:177:GLU:H	2.14	0.51
1:A:234:VAL:HG12	1:A:235:ALA:N	2.26	0.51
1:A:251:THR:HG23	3:A:2124:HOH:O	2.09	0.51
1:B:134:ASN:ND2	3:B:2044:HOH:O	2.43	0.51
1:A:91:LEU:HB2	1:A:113:ASN:HA	1.93	0.51
1:B:116:HIS:CG	1:B:117:GLY:H	2.27	0.51
1:B:251:THR:HG22	1:B:252:HIS:N	2.26	0.51
1:A:185:MET:CG	1:A:186:PRO:HD2	2.41	0.50
1:A:212:GLU:OE1	1:A:290:SER:HA	2.11	0.50
1:B:159:PHE:CZ	1:B:164:MET:HG3	2.46	0.50
1:A:133:VAL:CG1	1:A:137:GLY:HA2	2.41	0.50
1:B:110:TYR:OH	1:B:115:ARG:HD3	2.11	0.50
1:A:172:LEU:HD13	1:A:182:PHE:CE2	2.47	0.50
1:B:251:THR:HG22	1:B:253:GLN:N	2.17	0.50
1:A:191:TYR:OH	1:A:210:PRO:HG3	2.12	0.50
1:B:234:VAL:CG1	1:B:235:ALA:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:TRP:CD2	1:B:130:VAL:HG13	2.47	0.49
1:B:52:PHE:CD2	1:B:52:PHE:N	2.80	0.49
1:A:107:LYS:NZ	3:A:2044:HOH:O	2.45	0.49
1:A:175:THR:C	1:A:177:GLU:N	2.66	0.49
1:B:91:LEU:HB2	1:B:113:ASN:HA	1.95	0.49
1:B:133:VAL:CG1	1:B:134:ASN:N	2.76	0.49
1:A:99:ASP:O	1:A:101:ASP:N	2.46	0.48
1:A:58:THR:HB	1:B:323:ARG:NH1	2.27	0.48
1:A:99:ASP:O	1:A:101:ASP:O	2.30	0.48
1:A:239:ASN:OD1	1:A:320:ARG:HD3	2.14	0.48
1:B:133:VAL:CG1	1:B:137:GLY:CA	2.91	0.48
1:A:179:ARG:NH1	3:A:2090:HOH:O	2.45	0.48
1:B:234:VAL:HG12	1:B:235:ALA:N	2.29	0.47
1:B:279:GLU:HA	1:B:282:ASN:ND2	2.29	0.47
1:A:116:HIS:C	3:A:2055:HOH:O	2.48	0.47
1:A:336:GLY:HA2	1:B:74:TYR:CE1	2.49	0.47
1:A:59:LEU:HB2	1:A:71:GLN:HG3	1.94	0.47
1:B:251:THR:CB	1:B:254:GLU:OE2	2.57	0.47
1:B:221:SER:OG	1:B:296:ASN:ND2	2.48	0.47
1:B:323:ARG:NH1	1:B:323:ARG:CG	2.77	0.47
1:B:52:PHE:CD1	3:B:2010:HOH:O	2.65	0.46
1:A:110:TYR:OH	1:A:115:ARG:HD3	2.16	0.46
1:B:155:LEU:HD13	1:B:164:MET:CE	2.45	0.46
1:A:59:LEU:HB3	1:A:71:GLN:CG	2.45	0.46
1:A:82:LEU:HD11	1:A:95:ALA:HB1	1.96	0.46
1:B:133:VAL:HG11	1:B:137:GLY:CA	2.40	0.46
1:B:279:GLU:C	1:B:282:ASN:ND2	2.68	0.46
1:B:279:GLU:CD	1:B:282:ASN:HD21	2.19	0.46
1:B:59:LEU:HB3	1:B:71:GLN:CB	2.43	0.46
1:A:157:GLY:HA3	1:A:166:GLU:O	2.16	0.45
1:A:333:VAL:HG12	1:A:334:ALA:N	2.29	0.45
1:B:236:VAL:CG2	1:B:240:THR:HG21	2.45	0.45
1:A:253:GLN:NE2	3:A:2125:HOH:O	2.49	0.45
1:B:138:GLU:HG2	3:B:2055:HOH:O	2.16	0.45
1:B:59:LEU:HD13	1:B:71:GLN:HG3	1.97	0.45
1:B:101:ASP:CG	1:B:103:ARG:HH21	2.20	0.45
1:B:307:MET:CE	1:B:317:LYS:CE	2.68	0.44
1:B:52:PHE:HD2	1:B:52:PHE:N	2.16	0.44
1:A:326:GLU:HG2	1:A:327:ALA:H	1.82	0.44
1:B:54:PHE:N	1:B:54:PHE:CD1	2.83	0.44
1:A:133:VAL:HG11	1:A:137:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LEU:HB3	1:B:164:MET:HE1	2.00	0.44
1:B:234:VAL:HG13	3:B:2106:HOH:O	2.18	0.43
1:B:59:LEU:HD23	1:B:61:GLY:N	2.33	0.43
1:A:52:PHE:N	1:A:52:PHE:CD2	2.87	0.43
1:B:216:VAL:HG21	1:B:230:LEU:CG	2.49	0.42
1:A:52:PHE:N	1:A:52:PHE:HD2	2.17	0.42
1:A:56:GLY:HA2	3:A:2028:HOH:O	2.19	0.42
1:A:297:HIS:HA	1:A:333:VAL:O	2.20	0.42
1:B:276:ASP:C	1:B:278:PRO:HD3	2.40	0.42
1:A:234:VAL:HG12	1:A:235:ALA:H	1.84	0.42
1:B:67:ALA:HB2	1:B:88:ASP:OD2	2.20	0.42
1:A:148:TYR:HB3	1:A:149:PRO:CD	2.50	0.42
1:A:148:TYR:HB3	1:A:149:PRO:HD2	2.02	0.42
1:B:232:SER:OG	1:B:234:VAL:O	2.37	0.41
1:A:236:VAL:HG22	1:A:240:THR:OG1	2.21	0.41
1:B:133:VAL:HG12	1:B:134:ASN:O	2.20	0.41
1:A:116:HIS:O	1:A:133:VAL:HG12	2.20	0.41
1:B:116:HIS:O	1:B:133:VAL:HB	2.20	0.41
1:B:251:THR:CG2	1:B:252:HIS:N	2.82	0.41
1:A:106:PHE:CZ	1:A:115:ARG:HD2	2.55	0.41
1:B:65:ASP:O	1:B:66:ASP:HB2	2.19	0.41
1:B:248:VAL:CG1	1:B:249:ARG:N	2.83	0.41
1:A:224:SER:OG	1:A:225:SER:N	2.52	0.41
1:A:280:PRO:CD	1:A:281:TYR:H	2.32	0.41
1:A:307:MET:HE3	3:A:2159:HOH:O	2.19	0.41
1:B:216:VAL:HG23	1:B:231:PHE:O	2.21	0.41
1:A:120:TRP:CD2	1:A:130:VAL:HG13	2.56	0.41
1:A:303:CYS:SG	1:A:331:LEU:HD22	2.60	0.41
1:A:215:ARG:NE	3:A:2111:HOH:O	2.21	0.41
1:B:181:HIS:HB3	3:B:2066:HOH:O	2.21	0.41
1:A:81:VAL:HG21	1:B:304:ILE:HD11	2.03	0.40
1:B:180:PRO:HB2	1:B:182:PHE:CE1	2.56	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	291/293 (99%)	265 (91%)	19 (6%)	7 (2%)	6 2
1	B	291/293 (99%)	273 (94%)	14 (5%)	4 (1%)	11 6
All	All	582/586 (99%)	538 (92%)	33 (6%)	11 (2%)	8 3

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	GLU
1	B	56	GLY
1	B	61	GLY
1	B	117	GLY
1	A	100	THR
1	A	56	GLY
1	A	178	GLY
1	A	224	SER
1	B	224	SER
1	A	280	PRO
1	A	223	ILE

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	247/247 (100%)	228 (92%)	19 (8%)	13 9
1	B	247/247 (100%)	225 (91%)	22 (9%)	9 6
All	All	494/494 (100%)	453 (92%)	41 (8%)	11 7

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	PHE

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Mol	Chain	Res	Type
1	A	57	SER
1	A	58	THR
1	A	88	ASP
1	A	101	ASP
1	A	104	LEU
1	A	130	VAL
1	A	133	VAL
1	A	152	ARG
1	A	189	SER
1	A	207	LEU
1	A	220	GLU
1	A	221	SER
1	A	248	VAL
1	A	251	THR
1	A	267	LEU
1	A	273	THR
1	A	279	GLU
1	A	323	ARG
1	B	52	PHE
1	B	53	PHE
1	B	54	PHE
1	B	57	SER
1	B	58	THR
1	B	59	LEU
1	B	60	GLU
1	B	99	ASP
1	B	101	ASP
1	B	104	LEU
1	B	130	VAL
1	B	132	GLU
1	B	152	ARG
1	B	207	LEU
1	B	236	VAL
1	B	245	TYR
1	B	254	GLU
1	B	258	ARG
1	B	266	THR
1	B	273	THR
1	B	282	ASN
1	B	284	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	204	ASN
1	A	253	GLN
1	B	69	GLN
1	B	134	ASN
1	B	192	HIS
1	B	282	ASN
1	B	296	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.