Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 11:31 AM JST

PDB ID	:	7CHD
Title	:	AtaT complexed with acetyl-methionyl-tRNAfMet
Authors	:	Yashiro, Y.; Tomita, K.
Deposited on	:	2020-07-05
Resolution	:	3.80 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

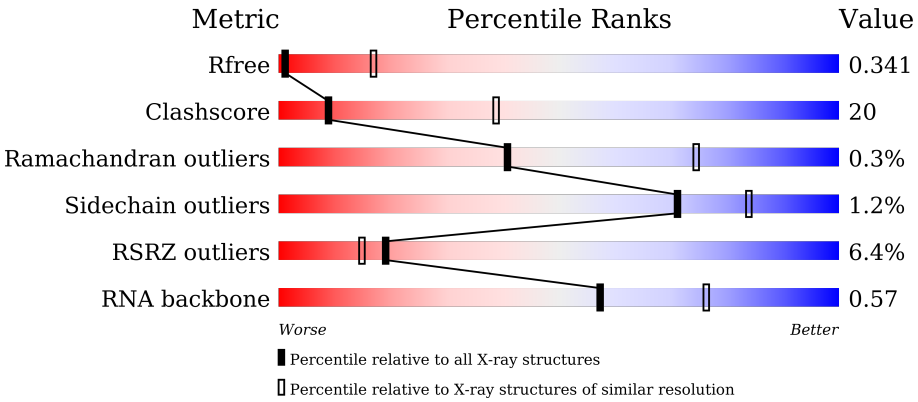
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.80 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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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 of 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% 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	183	3% 68% 25% 7%
1	B	183	4% 63% 34% •
1	C	183	5% 64% 33% •
1	D	183	3% 66% 27% • 7%

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Mol	Chain	Length	Quality of chain
1	E	183	8% 65% 27% 7%
1	F	183	7% 58% 35% 6%
1	G	183	14% 63% 28% 8%
1	H	183	9% 61% 30% 8%
2	I	77	36% 43% 17%
2	J	77	3% 35% 43% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14174 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 N-acetyltransferase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	0	0
			1351	868	232	246	5			
1	B	180	Total	C	N	O	S	0	0	0
			1441	921	253	262	5			
1	C	179	Total	C	N	O	S	0	0	0
			1429	913	248	263	5			
1	D	170	Total	C	N	O	S	0	1	0
			1352	869	232	246	5			
1	E	171	Total	C	N	O	S	0	0	0
			1358	870	234	249	5			
1	F	172	Total	C	N	O	S	0	0	0
			1366	876	235	250	5			
1	G	168	Total	C	N	O	S	0	0	0
			1335	858	230	242	5			
1	H	168	Total	C	N	O	S	0	1	0
			1336	858	230	242	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	ASP	GLY	engineered mutation	UNP Q8XED1
A	176	LEU	-	expression tag	UNP Q8XED1
A	177	GLU	-	expression tag	UNP Q8XED1
A	178	HIS	-	expression tag	UNP Q8XED1
A	179	HIS	-	expression tag	UNP Q8XED1
A	180	HIS	-	expression tag	UNP Q8XED1
A	181	HIS	-	expression tag	UNP Q8XED1
A	182	HIS	-	expression tag	UNP Q8XED1
A	183	HIS	-	expression tag	UNP Q8XED1
B	108	ASP	GLY	engineered mutation	UNP Q8XED1
B	176	LEU	-	expression tag	UNP Q8XED1
B	177	GLU	-	expression tag	UNP Q8XED1
B	178	HIS	-	expression tag	UNP Q8XED1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	179	HIS	-	expression tag	UNP Q8XED1
B	180	HIS	-	expression tag	UNP Q8XED1
B	181	HIS	-	expression tag	UNP Q8XED1
B	182	HIS	-	expression tag	UNP Q8XED1
B	183	HIS	-	expression tag	UNP Q8XED1
C	108	ASP	GLY	engineered mutation	UNP Q8XED1
C	176	LEU	-	expression tag	UNP Q8XED1
C	177	GLU	-	expression tag	UNP Q8XED1
C	178	HIS	-	expression tag	UNP Q8XED1
C	179	HIS	-	expression tag	UNP Q8XED1
C	180	HIS	-	expression tag	UNP Q8XED1
C	181	HIS	-	expression tag	UNP Q8XED1
C	182	HIS	-	expression tag	UNP Q8XED1
C	183	HIS	-	expression tag	UNP Q8XED1
D	108	ASP	GLY	engineered mutation	UNP Q8XED1
D	176	LEU	-	expression tag	UNP Q8XED1
D	177	GLU	-	expression tag	UNP Q8XED1
D	178	HIS	-	expression tag	UNP Q8XED1
D	179	HIS	-	expression tag	UNP Q8XED1
D	180	HIS	-	expression tag	UNP Q8XED1
D	181	HIS	-	expression tag	UNP Q8XED1
D	182	HIS	-	expression tag	UNP Q8XED1
D	183	HIS	-	expression tag	UNP Q8XED1
E	108	ASP	GLY	engineered mutation	UNP Q8XED1
E	176	LEU	-	expression tag	UNP Q8XED1
E	177	GLU	-	expression tag	UNP Q8XED1
E	178	HIS	-	expression tag	UNP Q8XED1
E	179	HIS	-	expression tag	UNP Q8XED1
E	180	HIS	-	expression tag	UNP Q8XED1
E	181	HIS	-	expression tag	UNP Q8XED1
E	182	HIS	-	expression tag	UNP Q8XED1
E	183	HIS	-	expression tag	UNP Q8XED1
F	108	ASP	GLY	engineered mutation	UNP Q8XED1
F	176	LEU	-	expression tag	UNP Q8XED1
F	177	GLU	-	expression tag	UNP Q8XED1
F	178	HIS	-	expression tag	UNP Q8XED1
F	179	HIS	-	expression tag	UNP Q8XED1
F	180	HIS	-	expression tag	UNP Q8XED1
F	181	HIS	-	expression tag	UNP Q8XED1
F	182	HIS	-	expression tag	UNP Q8XED1
F	183	HIS	-	expression tag	UNP Q8XED1
G	108	ASP	GLY	engineered mutation	UNP Q8XED1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	176	LEU	-	expression tag	UNP Q8XED1
G	177	GLU	-	expression tag	UNP Q8XED1
G	178	HIS	-	expression tag	UNP Q8XED1
G	179	HIS	-	expression tag	UNP Q8XED1
G	180	HIS	-	expression tag	UNP Q8XED1
G	181	HIS	-	expression tag	UNP Q8XED1
G	182	HIS	-	expression tag	UNP Q8XED1
G	183	HIS	-	expression tag	UNP Q8XED1
H	108	ASP	GLY	engineered mutation	UNP Q8XED1
H	176	LEU	-	expression tag	UNP Q8XED1
H	177	GLU	-	expression tag	UNP Q8XED1
H	178	HIS	-	expression tag	UNP Q8XED1
H	179	HIS	-	expression tag	UNP Q8XED1
H	180	HIS	-	expression tag	UNP Q8XED1
H	181	HIS	-	expression tag	UNP Q8XED1
H	182	HIS	-	expression tag	UNP Q8XED1
H	183	HIS	-	expression tag	UNP Q8XED1

- Molecule 2 is a RNA chain called RNA (77-MER).

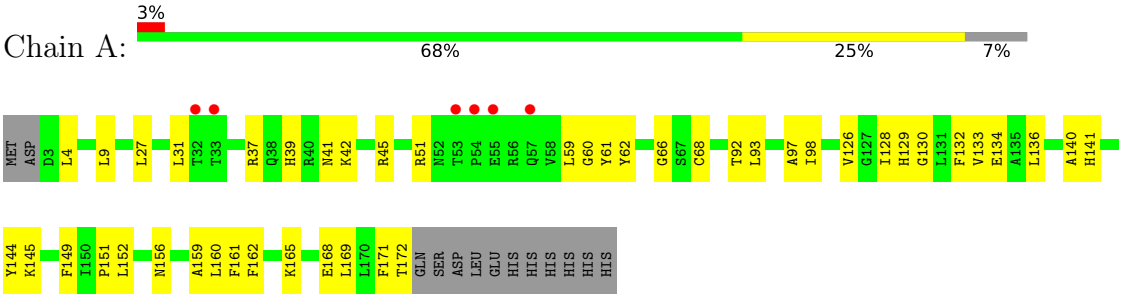
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	I	75	Total	C	N	O	P	S	0	0	0
			1603	715	289	523	75	1			
2	J	75	Total	C	N	O	P	S	0	0	0
			1603	715	289	523	75	1			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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.

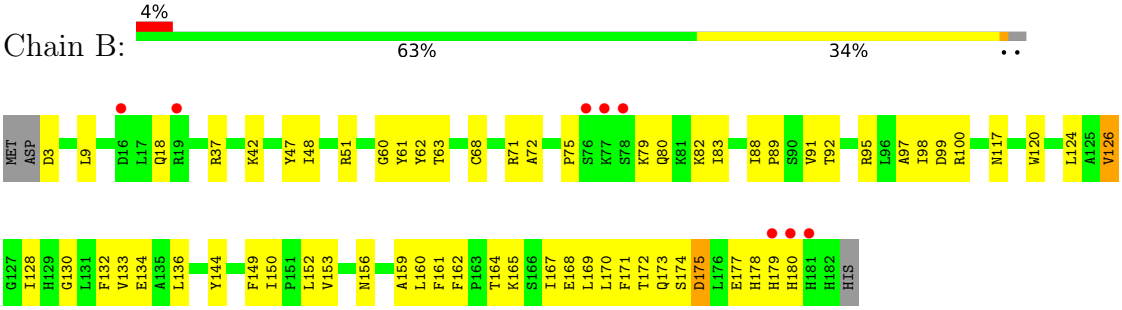
• Molecule 1: N-acetyltransferase domain-containing protein

Chain A:



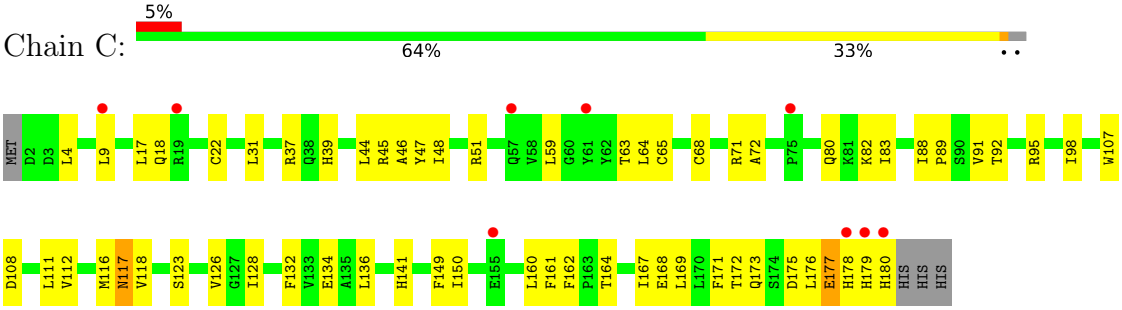
• Molecule 1: N-acetyltransferase domain-containing protein

Chain B:



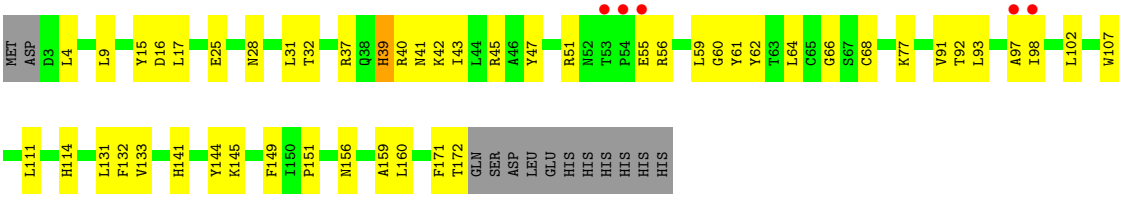
• Molecule 1: N-acetyltransferase domain-containing protein

Chain C:



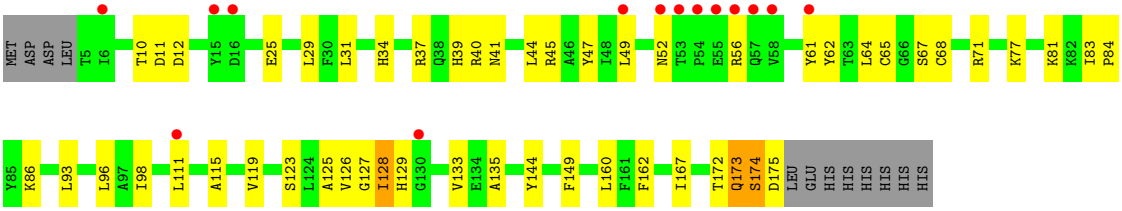
• Molecule 1: N-acetyltransferase domain-containing protein

Chain D:



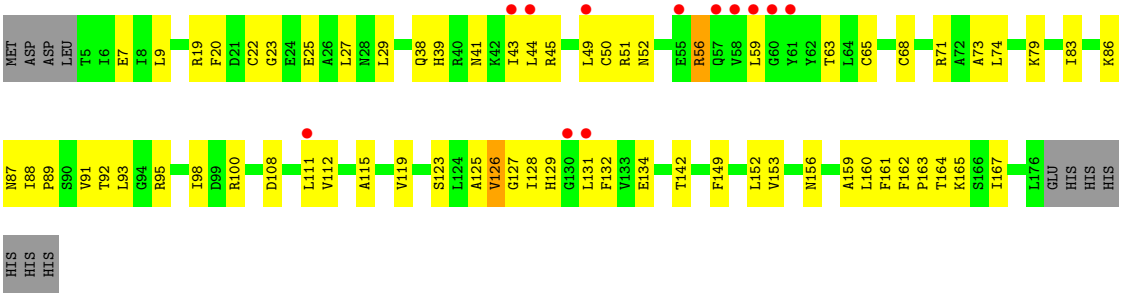
• Molecule 1: N-acetyltransferase domain-containing protein

Chain E:



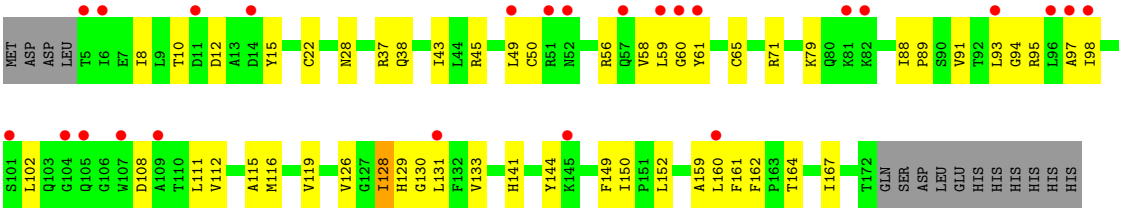
• Molecule 1: N-acetyltransferase domain-containing protein

Chain F:



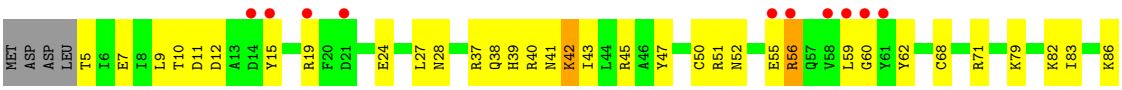
• Molecule 1: N-acetyltransferase domain-containing protein

Chain G:

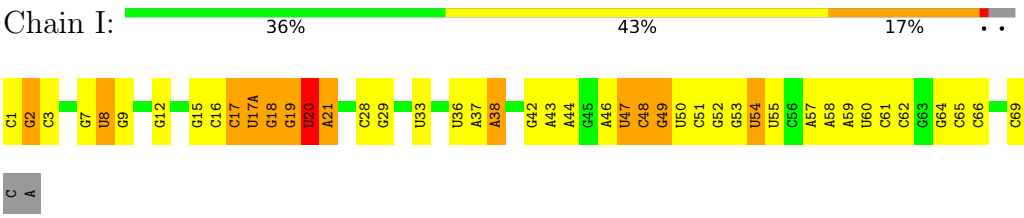


• Molecule 1: N-acetyltransferase domain-containing protein

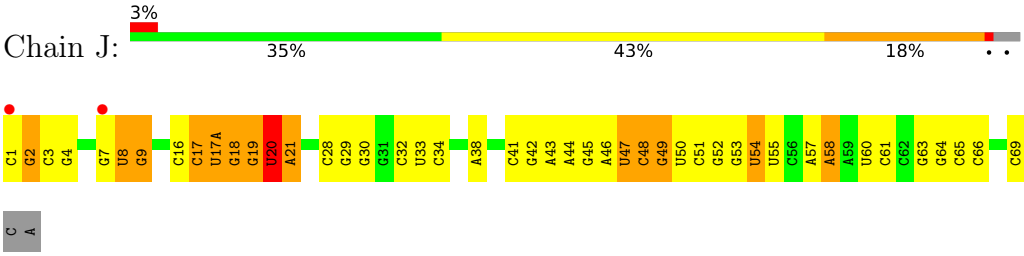
Chain H:



• Molecule 2: RNA (77-MER)



• Molecule 2: RNA (77-MER)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	269.83Å 68.28Å 136.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.21 – 3.80 48.21 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.21-3.80) 99.9 (48.21-3.80)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.286 , 0.341 0.286 , 0.341	Depositor DCC
R_{free} test set	1277 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	128.7	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 78.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	14174	wwPDB-VP
Average B, all atoms (Å^2)	139.0	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 38.51 % 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 3.6459e-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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, PSU, 5MU, H2U, OMC

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	0.27	0/1380	0.50	0/1871
1	B	0.29	0/1475	0.56	0/2000
1	C	0.29	0/1461	0.56	0/1981
1	D	0.29	0/1386	0.53	0/1879
1	E	0.27	0/1387	0.53	0/1880
1	F	0.26	0/1395	0.52	0/1891
1	G	0.26	0/1364	0.51	0/1849
1	H	0.27	0/1370	0.51	0/1857
2	I	0.32	0/1678	0.94	0/2614
2	J	0.35	0/1678	0.97	0/2614
All	All	0.29	0/14574	0.66	0/20436

There are no bond length outliers.

There are no bond angle outliers.

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	1351	0	1359	51	0
1	B	1441	0	1428	60	0
1	C	1429	0	1418	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1352	0	1358	62	0
1	E	1358	0	1361	87	0
1	F	1366	0	1372	67	0
1	G	1335	0	1344	44	0
1	H	1336	0	1345	51	0
2	I	1603	0	820	57	0
2	J	1603	0	820	58	0
All	All	14174	0	12625	545	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 20.

All (545) 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:G:89:PRO:HB2	1:G:128:ILE:CG2	1.51	1.39
1:D:141:HIS:CE1	1:D:145:LYS:HE3	1.58	1.35
1:A:141:HIS:NE2	1:A:145:LYS:HE3	1.46	1.29
1:E:162:PHE:HE2	1:E:167:ILE:CG1	1.47	1.26
1:E:77:LYS:HE2	1:E:81:LYS:NZ	1.50	1.25
1:E:123:SER:CA	1:E:128:ILE:HD11	1.67	1.23
1:D:141:HIS:CE1	1:D:145:LYS:CE	2.22	1.22
1:G:89:PRO:CB	1:G:128:ILE:HG22	1.67	1.22
1:C:178:HIS:O	1:C:179:HIS:CD2	1.96	1.18
1:D:141:HIS:HE1	1:D:145:LYS:CE	1.57	1.18
1:E:123:SER:CB	1:E:128:ILE:CD1	2.22	1.17
1:E:162:PHE:CE2	1:E:167:ILE:CG1	2.28	1.16
1:E:123:SER:HA	1:E:128:ILE:CG1	1.75	1.15
1:E:123:SER:HB3	1:E:128:ILE:CD1	1.77	1.15
1:E:126:VAL:HA	1:F:45:ARG:HG3	1.27	1.13
1:E:123:SER:CA	1:E:128:ILE:CD1	2.27	1.13
1:E:123:SER:HA	1:E:128:ILE:CD1	1.78	1.12
1:E:123:SER:HB3	1:E:128:ILE:HD13	1.17	1.12
1:D:141:HIS:HE1	1:D:145:LYS:NZ	1.46	1.12
1:E:77:LYS:HE2	1:E:81:LYS:CE	1.79	1.12
1:E:123:SER:OG	1:E:128:ILE:HG12	1.51	1.11
1:H:42:LYS:HE2	1:H:45:ARG:NH2	1.65	1.10
1:G:91:VAL:HG23	1:G:128:ILE:CD1	1.81	1.09
1:E:125:ALA:O	1:E:126:VAL:HG22	1.51	1.09
1:D:145:LYS:HE2	1:D:151:PRO:HG3	1.11	1.09
1:E:162:PHE:HE2	1:E:167:ILE:HG12	1.14	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:LEU:HB3	1:F:65:CYS:SG	1.96	1.06
1:H:37:ARG:HG2	1:H:41:ASN:OD1	1.54	1.04
1:E:125:ALA:O	1:E:126:VAL:CG2	2.05	1.04
1:E:123:SER:HA	1:E:128:ILE:HD11	1.31	1.04
1:E:162:PHE:CD2	1:E:167:ILE:HD11	1.95	1.01
1:G:91:VAL:HG23	1:G:128:ILE:HD13	1.40	1.00
1:A:141:HIS:NE2	1:A:145:LYS:CE	2.24	1.00
1:E:162:PHE:CE2	1:E:167:ILE:HD11	1.95	1.00
1:E:162:PHE:CE2	1:E:167:ILE:HG12	1.95	1.00
1:B:169:LEU:O	1:B:172:THR:HG22	1.60	0.99
1:A:145:LYS:HE2	1:A:151:PRO:HG3	1.43	0.98
1:E:77:LYS:CE	1:E:81:LYS:NZ	2.27	0.97
1:C:117:ASN:HB2	1:C:171:PHE:CZ	2.01	0.96
1:D:145:LYS:HE2	1:D:151:PRO:CG	1.92	0.96
1:D:141:HIS:CE1	1:D:145:LYS:NZ	2.34	0.96
1:E:123:SER:CA	1:E:128:ILE:CG1	2.43	0.95
1:E:162:PHE:HE2	1:E:167:ILE:CD1	1.79	0.94
1:E:162:PHE:CE2	1:E:167:ILE:CD1	2.49	0.94
1:A:145:LYS:HE2	1:A:151:PRO:CG	1.96	0.94
1:E:123:SER:CB	1:E:128:ILE:HG12	1.97	0.94
1:E:77:LYS:HE2	1:E:81:LYS:HZ1	1.22	0.94
1:E:128:ILE:HD12	1:E:128:ILE:H	1.31	0.93
1:B:169:LEU:HA	1:B:172:THR:CG2	2.00	0.91
1:E:123:SER:CB	1:E:128:ILE:HD13	1.92	0.91
1:B:169:LEU:HA	1:B:172:THR:HG22	1.53	0.90
1:D:145:LYS:CE	1:D:151:PRO:HG3	2.00	0.90
1:E:123:SER:CB	1:E:128:ILE:CG1	2.49	0.90
1:A:128:ILE:HD12	1:A:128:ILE:H	1.37	0.88
1:E:123:SER:CA	1:E:128:ILE:HG12	2.01	0.88
1:E:77:LYS:CE	1:E:81:LYS:HZ1	1.84	0.87
1:A:126:VAL:HG23	1:A:128:ILE:HD11	1.56	0.86
1:C:178:HIS:O	1:C:179:HIS:HD2	1.54	0.84
1:E:123:SER:OG	1:E:128:ILE:CG1	2.24	0.84
1:H:37:ARG:CG	1:H:41:ASN:OD1	2.26	0.84
1:F:125:ALA:O	1:F:126:VAL:CG1	2.26	0.83
1:D:39:HIS:HD2	1:D:45:ARG:NH2	1.75	0.83
1:H:42:LYS:HE2	1:H:45:ARG:HH22	1.44	0.83
1:E:126:VAL:HA	1:F:45:ARG:CG	2.09	0.83
1:B:169:LEU:CA	1:B:172:THR:HG22	2.09	0.82
1:B:169:LEU:C	1:B:172:THR:HG22	1.99	0.82
1:C:168:GLU:O	1:C:172:THR:HG23	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:SER:C	1:E:128:ILE:HD11	1.99	0.82
1:H:51:ARG:HE	1:H:59:LEU:HD11	1.45	0.81
1:H:79:LYS:NZ	1:H:150:ILE:HD13	1.95	0.81
1:E:162:PHE:CE2	1:E:167:ILE:HG13	2.16	0.81
2:I:18:G:C4	2:I:58:A:C2	2.69	0.80
1:A:51:ARG:HE	1:A:59:LEU:HD11	1.43	0.80
1:C:117:ASN:HB2	1:C:171:PHE:CE2	2.18	0.79
1:H:83:ILE:HG21	1:H:88:ILE:HG12	1.65	0.79
1:A:92:THR:HG1	1:A:132:PHE:HD2	1.32	0.78
1:E:77:LYS:HE2	1:E:81:LYS:HE2	1.64	0.78
1:F:51:ARG:HE	1:F:59:LEU:HD11	1.48	0.77
1:G:91:VAL:CG2	1:G:128:ILE:CD1	2.61	0.77
2:J:1:C:H4'	2:J:2:G:OP2	1.82	0.77
1:D:39:HIS:CD2	1:D:45:ARG:CZ	2.68	0.77
1:B:117:ASN:HA	1:B:171:PHE:HE2	1.51	0.75
1:A:37:ARG:HG2	1:A:41:ASN:OD1	1.87	0.75
1:D:141:HIS:HE1	1:D:145:LYS:HZ2	1.33	0.75
1:F:125:ALA:O	1:F:126:VAL:HG12	1.85	0.74
1:D:39:HIS:CD2	1:D:45:ARG:NH2	2.56	0.74
1:E:11:ASP:HB3	1:E:40:ARG:HH21	1.53	0.74
1:A:39:HIS:O	1:A:45:ARG:NH2	2.21	0.74
1:A:128:ILE:HD12	1:A:128:ILE:N	2.02	0.73
1:E:123:SER:O	1:E:128:ILE:HD11	1.87	0.73
2:J:19:G:H5'	2:J:20:H2U:H62	1.70	0.73
1:A:126:VAL:HG23	1:A:128:ILE:CD1	2.18	0.73
1:E:128:ILE:HD12	1:E:128:ILE:N	2.04	0.73
1:H:149:PHE:HB3	1:H:160:LEU:HB3	1.69	0.73
2:J:57:A:H2'	2:J:58:A:H5'	1.70	0.73
1:C:51:ARG:HE	1:C:59:LEU:HD11	1.54	0.73
1:A:66:GLY:HA3	1:B:89:PRO:HB3	1.71	0.72
1:G:91:VAL:CG2	1:G:128:ILE:HD11	2.18	0.72
2:I:57:A:H2'	2:I:58:A:H5'	1.70	0.72
2:I:57:A:C2'	2:I:58:A:H5'	2.20	0.71
2:I:71:C:H2'	2:I:72:A:H8	1.54	0.71
1:H:19:ARG:NH1	1:H:55:GLU:OE1	2.24	0.71
2:J:21:A:O2'	2:J:46:A:N6	2.23	0.71
1:E:39:HIS:O	1:E:45:ARG:NH2	2.23	0.71
1:H:11:ASP:O	1:H:40:ARG:NH2	2.24	0.70
2:J:28:C:H2'	2:J:29:G:H8	1.55	0.70
1:C:44:LEU:HB3	1:C:65:CYS:SG	2.31	0.70
1:G:89:PRO:HB2	1:G:128:ILE:HG22	0.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:VAL:CG2	1:A:128:ILE:HD11	2.22	0.70
1:E:71:ARG:N	1:E:86:LYS:O	2.21	0.70
2:J:71:C:H2'	2:J:72:A:H8	1.56	0.69
2:I:1:C:H4'	2:I:2:G:OP2	1.91	0.69
1:E:125:ALA:C	1:E:126:VAL:CG2	2.59	0.69
1:F:149:PHE:HB3	1:F:160:LEU:HB3	1.73	0.69
1:C:123:SER:OG	1:C:128:ILE:HB	1.92	0.68
1:B:51:ARG:NH1	2:J:19:G:N7	2.41	0.68
1:E:149:PHE:HB3	1:E:160:LEU:HB3	1.75	0.68
2:I:18:G:C2	2:I:58:A:C4	2.82	0.68
2:J:57:A:C2'	2:J:58:A:H5'	2.24	0.68
1:A:141:HIS:CD2	1:A:145:LYS:HE3	2.29	0.67
1:G:91:VAL:HG23	1:G:128:ILE:HD11	1.71	0.67
2:I:19:G:H5'	2:I:20:H2U:H62	1.75	0.67
1:F:44:LEU:CB	1:F:65:CYS:SG	2.78	0.67
1:B:169:LEU:HA	1:B:172:THR:HG21	1.76	0.67
1:H:37:ARG:HD2	2:J:2:G:OP2	1.95	0.67
2:I:71:C:H2'	2:I:72:A:C8	2.30	0.67
1:E:125:ALA:C	1:E:126:VAL:HG23	2.14	0.67
1:H:79:LYS:HZ3	1:H:150:ILE:HD13	1.58	0.67
1:A:37:ARG:CG	1:A:41:ASN:OD1	2.42	0.67
1:F:125:ALA:C	1:F:126:VAL:HG13	2.15	0.66
1:H:93:LEU:HB2	1:H:131:LEU:HD11	1.77	0.66
1:A:128:ILE:H	1:A:128:ILE:CD1	2.08	0.66
1:E:162:PHE:HD2	1:E:167:ILE:HD11	1.56	0.66
2:I:69:C:H2'	2:I:70:G:H8	1.60	0.66
1:F:86:LYS:NZ	2:J:34:C:OP1	2.29	0.66
1:F:7:GLU:OE1	1:F:56:ARG:NH1	2.29	0.66
1:D:4:LEU:HD13	1:D:107:TRP:HH2	1.62	0.65
1:F:125:ALA:O	1:F:126:VAL:HG13	1.97	0.64
1:G:89:PRO:CB	1:G:128:ILE:CG2	2.46	0.64
1:C:117:ASN:OD1	1:C:171:PHE:CE2	2.50	0.64
1:F:71:ARG:N	1:F:86:LYS:O	2.30	0.64
2:I:28:C:H2'	2:I:29:G:H8	1.62	0.64
1:C:51:ARG:NH1	2:I:19:G:N7	2.46	0.64
1:G:130:GLY:HA3	1:G:162:PHE:O	1.97	0.64
1:B:136:LEU:HB3	1:F:142:THR:HG21	1.78	0.64
1:B:170:LEU:O	1:B:180:HIS:NE2	2.31	0.63
1:E:123:SER:HA	1:E:128:ILE:HG13	1.77	0.63
1:G:93:LEU:HB2	1:G:131:LEU:HD11	1.79	0.63
1:B:169:LEU:O	1:B:172:THR:CG2	2.41	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:149:PHE:HB3	1:G:160:LEU:HB3	1.79	0.63
1:F:92:THR:HA	1:F:132:PHE:O	1.99	0.63
1:B:177:GLU:O	1:B:178:HIS:HB2	1.98	0.63
1:A:68:CYS:SG	1:B:68:CYS:HB2	2.39	0.62
1:D:39:HIS:O	1:D:42:LYS:N	2.22	0.62
1:A:9:LEU:HD23	1:A:39:HIS:CG	2.34	0.62
1:A:37:ARG:HG2	1:A:37:ARG:O	2.00	0.62
2:I:17:C:OP2	2:I:17(A):U:O2'	2.11	0.62
1:H:5:THR:N	1:H:50:CYS:O	2.33	0.62
1:A:156:ASN:OD1	1:A:159:ALA:N	2.33	0.62
1:B:173:GLN:HB2	1:B:180:HIS:CE1	2.35	0.61
2:J:71:C:H2'	2:J:72:A:C8	2.35	0.61
1:D:62:TYR:OH	1:D:114:HIS:ND1	2.27	0.61
1:H:126:VAL:HG12	1:H:127:GLY:N	2.14	0.61
1:A:145:LYS:HE2	1:A:151:PRO:HG2	1.83	0.61
1:G:59:LEU:HD13	1:G:102:LEU:HD11	1.81	0.61
1:G:126:VAL:HG12	1:G:126:VAL:O	2.00	0.61
1:F:126:VAL:HG23	1:F:126:VAL:O	2.00	0.61
1:H:7:GLU:OE1	1:H:56:ARG:NH1	2.33	0.61
1:C:173:GLN:O	1:C:179:HIS:HB2	2.01	0.61
1:F:39:HIS:O	1:F:45:ARG:NH2	2.34	0.61
1:H:37:ARG:CD	2:J:2:G:OP2	2.49	0.61
1:H:129:HIS:O	1:H:164:THR:N	2.34	0.61
1:E:67:SER:HA	1:F:68:CYS:SG	2.40	0.61
1:D:156:ASN:OD1	1:D:159:ALA:N	2.33	0.60
1:H:39:HIS:O	1:H:45:ARG:NH2	2.34	0.60
1:D:39:HIS:NE2	1:D:45:ARG:NH1	2.50	0.60
1:E:125:ALA:O	1:E:126:VAL:HG23	1.95	0.60
2:I:57:A:O2'	2:I:58:A:H5'	2.02	0.60
1:D:4:LEU:HD13	1:D:107:TRP:CH2	2.37	0.60
1:G:61:TYR:CE1	1:G:97:ALA:HB3	2.36	0.60
1:A:141:HIS:NE2	1:A:145:LYS:NZ	2.49	0.60
1:C:150:ILE:N	1:C:161:PHE:O	2.35	0.59
1:G:144:TYR:HB2	1:G:160:LEU:HD22	1.83	0.59
1:D:133:VAL:HG21	1:D:144:TYR:CE2	2.38	0.59
1:D:39:HIS:CD2	1:D:45:ARG:NH1	2.70	0.59
2:J:7:G:H4'	2:J:8:4SU:OP2	2.03	0.59
1:E:98:ILE:HD11	1:E:111:LEU:HD22	1.85	0.59
2:I:47:U:H4'	2:I:48:C:O5'	2.00	0.59
1:E:172:THR:C	1:E:174:SER:N	2.52	0.59
2:J:43:A:H2'	2:J:44:A:C8	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:HIS:HD2	1:D:45:ARG:HH22	1.48	0.59
1:H:62:TYR:HB2	1:H:93:LEU:HD11	1.84	0.59
2:I:58:A:O2'	2:I:60:U:OP2	2.21	0.59
1:B:130:GLY:HA3	1:B:162:PHE:O	2.03	0.59
1:C:149:PHE:HB3	1:C:160:LEU:HB3	1.84	0.58
1:C:176:LEU:O	1:C:178:HIS:N	2.36	0.58
2:I:7:G:H4'	2:I:8:4SU:OP2	2.02	0.58
1:B:173:GLN:HB2	1:B:180:HIS:NE2	2.18	0.58
1:F:125:ALA:C	1:F:126:VAL:CG1	2.70	0.58
2:J:28:C:H2'	2:J:29:G:C8	2.38	0.58
2:I:18:G:N3	2:I:58:A:C2	2.72	0.58
1:C:68:CYS:HB2	1:D:68:CYS:HB2	1.86	0.58
1:D:39:HIS:HE2	1:D:45:ARG:NH1	2.01	0.57
1:B:92:THR:HG1	1:B:132:PHE:HD2	1.52	0.57
1:C:17:LEU:HD23	1:C:31:LEU:HD11	1.86	0.57
1:C:134:GLU:OE2	1:C:136:LEU:HD21	2.03	0.57
1:F:123:SER:OG	1:F:128:ILE:HB	2.03	0.57
1:C:37:ARG:NH1	2:J:17(A):U:C6	2.72	0.57
1:G:129:HIS:O	1:G:164:THR:N	2.37	0.57
1:H:10:THR:OG1	1:H:12:ASP:O	2.22	0.57
1:H:50:CYS:SG	1:H:56:ARG:NH2	2.78	0.57
1:H:82:LYS:HE3	1:H:165:LYS:NZ	2.20	0.57
1:E:47:TYR:HB2	1:E:62:TYR:CZ	2.40	0.57
1:E:71:ARG:NH1	1:E:83:ILE:O	2.32	0.57
1:H:141:HIS:CD2	1:H:160:LEU:HD11	2.40	0.57
1:F:68:CYS:HB3	1:F:87:ASN:HB3	1.87	0.57
1:D:77:LYS:HZ1	2:J:4:G:P	2.28	0.56
2:I:69:C:H2'	2:I:70:G:C8	2.40	0.56
1:D:62:TYR:HB2	1:D:93:LEU:HD11	1.88	0.56
1:F:50:CYS:SG	1:F:56:ARG:NH2	2.79	0.56
1:E:10:THR:OG1	1:E:12:ASP:O	2.23	0.56
1:E:126:VAL:HG13	1:F:45:ARG:HB2	1.87	0.56
2:J:47:U:H4'	2:J:48:C:O5'	2.04	0.56
1:D:37:ARG:O	1:D:41:ASN:OD1	2.23	0.56
2:I:48:C:OP2	2:I:48:C:H6	1.88	0.56
1:C:82:LYS:HE3	1:D:43:ILE:HD11	1.86	0.56
1:C:164:THR:HA	1:C:167:ILE:HD12	1.88	0.56
1:C:89:PRO:HB3	1:D:66:GLY:HA3	1.88	0.55
1:H:79:LYS:HZ1	1:H:150:ILE:HD13	1.69	0.55
2:I:43:A:H2'	2:I:44:A:C8	2.41	0.55
1:C:117:ASN:O	1:C:117:ASN:ND2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:LEU:O	1:C:173:GLN:OE1	2.24	0.55
2:I:18:G:C4	2:I:58:A:N1	2.74	0.55
1:B:91:VAL:HG23	1:B:128:ILE:HG21	1.88	0.55
1:D:4:LEU:HA	1:D:51:ARG:HA	1.87	0.55
1:B:150:ILE:O	1:B:161:PHE:N	2.33	0.55
1:C:178:HIS:C	1:C:179:HIS:CD2	2.78	0.55
1:G:10:THR:OG1	1:G:12:ASP:O	2.25	0.55
1:G:15:TYR:OH	1:G:56:ARG:NH1	2.39	0.55
1:C:169:LEU:HB3	1:C:173:GLN:OE1	2.06	0.54
1:B:174:SER:O	1:B:175:ASP:O	2.26	0.54
1:B:89:PRO:HB2	1:B:128:ILE:HG12	1.88	0.54
1:B:117:ASN:CA	1:B:171:PHE:HE2	2.20	0.54
1:E:49:LEU:HB2	1:E:111:LEU:HD11	1.89	0.54
2:J:18:G:C4	2:J:58:A:C2	2.96	0.54
2:I:18:G:C2	2:I:58:A:C5	2.96	0.54
1:G:38:GLN:HA	1:G:43:ILE:HD12	1.88	0.54
1:B:133:VAL:HG21	1:B:144:TYR:CZ	2.43	0.54
1:F:19:ARG:NH2	2:I:12:G:O3'	2.41	0.54
1:F:164:THR:HA	1:F:167:ILE:HD12	1.90	0.54
1:G:22:CYS:H	1:G:28:ASN:HD21	1.55	0.54
2:I:16:C:O2'	2:I:17:C:O4'	2.26	0.54
2:J:58:A:O2'	2:J:60:U:OP2	2.24	0.54
1:B:126:VAL:HG23	1:B:126:VAL:O	2.07	0.54
1:G:93:LEU:HD22	1:G:131:LEU:HD21	1.89	0.53
1:F:152:LEU:HD11	1:F:161:PHE:HB2	1.90	0.53
1:H:37:ARG:HG3	2:J:1:C:H5'	1.89	0.53
1:F:93:LEU:HB2	1:F:131:LEU:HD11	1.90	0.53
1:C:51:ARG:NH1	2:I:19:G:C5	2.76	0.53
1:C:126:VAL:HG23	1:C:126:VAL:O	2.09	0.53
1:E:52:ASN:OD1	1:E:56:ARG:NH2	2.42	0.53
1:E:123:SER:CB	1:E:128:ILE:HD11	2.12	0.53
1:H:27:LEU:HD13	1:H:97:ALA:HB2	1.91	0.53
1:E:40:ARG:O	1:F:165:LYS:NZ	2.42	0.52
1:F:91:VAL:HG23	1:F:128:ILE:HG12	1.91	0.52
1:H:60:GLY:HA3	1:H:98:ILE:HD13	1.91	0.52
2:J:16:C:O2'	2:J:17:C:O4'	2.27	0.52
2:J:48:C:H6	2:J:48:C:OP2	1.91	0.52
1:H:156:ASN:OD1	1:H:159:ALA:N	2.35	0.52
1:D:17:LEU:HD22	1:D:32:THR:HA	1.90	0.52
1:E:68:CYS:HB2	1:F:68:CYS:HB2	1.92	0.52
1:F:83:ILE:HG21	1:F:88:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PHE:O	1:A:172:THR:OG1	2.27	0.52
1:F:38:GLN:HG2	1:F:43:ILE:HD12	1.92	0.52
1:H:126:VAL:CG1	1:H:127:GLY:N	2.73	0.52
1:A:141:HIS:CE1	1:A:145:LYS:HE3	2.35	0.51
1:A:60:GLY:HA3	1:A:98:ILE:HD13	1.92	0.51
1:C:39:HIS:O	1:C:45:ARG:NH2	2.43	0.51
1:E:126:VAL:CA	1:F:45:ARG:HG3	2.19	0.51
1:H:152:LEU:HD11	1:H:161:PHE:HB2	1.92	0.51
2:J:16:C:O2'	2:J:17:C:O5'	2.28	0.51
1:A:92:THR:OG1	1:A:132:PHE:CD2	2.59	0.51
1:B:150:ILE:N	1:B:161:PHE:O	2.43	0.51
1:F:52:ASN:HA	1:F:56:ARG:NH2	2.25	0.51
1:B:75:PRO:HA	1:B:153:VAL:HB	1.93	0.51
2:J:53:G:C5	2:J:54:5MU:H72	2.45	0.51
1:C:92:THR:HG1	1:C:132:PHE:HD2	1.59	0.51
1:A:42:LYS:HG3	1:B:165:LYS:NZ	2.26	0.51
1:E:25:GLU:O	1:E:29:LEU:HG	2.11	0.51
2:J:50:U:H2'	2:J:51:C:C6	2.46	0.51
1:C:63:THR:OG1	1:C:95:ARG:N	2.42	0.51
1:D:25:GLU:HA	1:D:28:ASN:HD22	1.76	0.51
2:I:50:U:H3	2:I:64:G:H1	1.59	0.51
2:J:42:G:H2'	2:J:43:A:H8	1.75	0.51
1:G:89:PRO:HB2	1:G:128:ILE:HG21	1.74	0.50
1:A:128:ILE:HG22	1:A:130:GLY:H	1.76	0.50
1:C:117:ASN:OD1	1:C:171:PHE:CD2	2.64	0.50
1:E:77:LYS:CE	1:E:81:LYS:HZ3	2.18	0.50
2:I:48:C:OP2	2:I:48:C:C6	2.65	0.50
1:E:62:TYR:HB2	1:E:93:LEU:HD11	1.92	0.50
1:A:133:VAL:HG21	1:A:144:TYR:CE2	2.47	0.50
1:E:172:THR:O	1:E:173:GLN:C	2.49	0.50
1:D:141:HIS:NE2	1:D:145:LYS:HE3	2.16	0.50
1:D:39:HIS:O	1:D:41:ASN:N	2.45	0.49
1:D:60:GLY:HA3	1:D:98:ILE:HD13	1.94	0.49
1:B:63:THR:OG1	1:B:95:ARG:N	2.45	0.49
2:J:50:U:H3	2:J:64:G:H1	1.60	0.49
1:G:8:ILE:HD11	1:G:45:ARG:NH1	2.27	0.49
2:J:44:A:H2'	2:J:45:G:C8	2.47	0.49
1:C:176:LEU:O	1:C:177:GLU:HB2	2.11	0.49
1:B:18:GLN:HG3	1:C:18:GLN:CD	2.33	0.49
1:A:27:LEU:HD13	1:A:97:ALA:HB2	1.94	0.49
1:B:156:ASN:OD1	1:B:159:ALA:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:8:ILE:HD11	1:G:45:ARG:HD3	1.95	0.49
1:E:129:HIS:NE2	1:F:41:ASN:O	2.46	0.49
1:C:47:TYR:OH	1:C:118:VAL:HG11	2.13	0.49
1:C:71:ARG:NH1	1:C:83:ILE:O	2.46	0.48
1:A:168:GLU:OE2	1:B:42:LYS:NZ	2.43	0.48
1:B:9:LEU:HB2	1:B:48:ILE:HD13	1.94	0.48
1:B:149:PHE:HB3	1:B:160:LEU:HB3	1.95	0.48
1:C:178:HIS:CG	1:C:179:HIS:N	2.82	0.48
2:J:17(A):U:H4'	2:J:18:G:OP1	2.13	0.48
1:F:86:LYS:NZ	2:J:34:C:P	2.87	0.48
1:D:145:LYS:HG3	1:D:160:LEU:HD21	1.96	0.48
2:I:17:C:OP1	2:I:61:C:H5'	2.13	0.48
2:I:53:G:C5	2:I:54:5MU:H72	2.49	0.48
1:C:150:ILE:O	1:C:161:PHE:N	2.35	0.48
1:H:71:ARG:N	1:H:86:LYS:O	2.46	0.48
1:G:164:THR:HA	1:G:167:ILE:HD12	1.95	0.48
1:G:112:VAL:HG12	1:G:116:MET:HE3	1.96	0.48
1:A:140:ALA:O	1:A:144:TYR:HD1	1.96	0.48
1:B:117:ASN:HA	1:B:171:PHE:CE2	2.41	0.48
1:B:164:THR:HA	1:B:167:ILE:HD12	1.97	0.47
1:B:178:HIS:C	1:B:179:HIS:CG	2.87	0.47
1:F:91:VAL:O	1:F:131:LEU:HD12	2.15	0.47
1:H:9:LEU:HD23	1:H:39:HIS:CG	2.50	0.47
1:A:134:GLU:OE2	1:A:136:LEU:HD21	2.14	0.47
1:D:16:ASP:HB3	1:D:55:GLU:O	2.14	0.47
1:E:31:LEU:HB2	1:E:61:TYR:CZ	2.49	0.47
1:E:62:TYR:HB3	1:E:96:LEU:HD13	1.96	0.47
1:F:134:GLU:HA	1:F:159:ALA:HA	1.95	0.47
1:G:79:LYS:NZ	1:G:150:ILE:HD13	2.29	0.47
1:B:18:GLN:HG3	1:C:18:GLN:HG3	1.97	0.47
1:D:98:ILE:HD11	1:D:111:LEU:HD22	1.97	0.47
1:E:49:LEU:HD22	1:E:111:LEU:HD11	1.96	0.47
2:I:28:C:H2'	2:I:29:G:C8	2.46	0.47
1:A:141:HIS:ND1	1:A:160:LEU:HD11	2.29	0.47
1:B:51:ARG:NH1	2:J:19:G:C5	2.83	0.47
1:D:141:HIS:CD2	1:D:160:LEU:HD11	2.50	0.47
1:D:171:PHE:O	1:D:172:THR:OG1	2.33	0.47
1:G:37:ARG:HH12	2:I:2:G:H8	1.62	0.47
1:H:165:LYS:O	1:H:169:LEU:HG	2.15	0.47
2:I:18:G:C6	2:I:58:A:C6	3.03	0.47
1:C:9:LEU:HB2	1:C:48:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:MET:HB3	1:C:167:ILE:HG23	1.96	0.47
2:I:2:G:H2'	2:I:3:C:C6	2.50	0.47
1:D:77:LYS:NZ	2:J:4:G:OP1	2.47	0.46
1:D:92:THR:HG1	1:D:132:PHE:HD2	1.59	0.46
1:E:127:GLY:H	1:F:45:ARG:HG2	1.80	0.46
1:F:74:LEU:HD13	1:F:79:LYS:HB3	1.96	0.46
2:I:49:G:C2	2:I:66:C:C2	3.04	0.46
1:F:131:LEU:HD23	1:F:149:PHE:HZ	1.80	0.46
1:C:149:PHE:CD2	1:C:162:PHE:HB2	2.51	0.46
1:D:9:LEU:HD23	1:D:39:HIS:ND1	2.31	0.46
1:F:162:PHE:HE2	1:F:167:ILE:HG12	1.80	0.46
1:D:59:LEU:HD13	1:D:102:LEU:HD11	1.98	0.46
1:E:41:ASN:O	1:F:129:HIS:NE2	2.48	0.46
1:F:162:PHE:HE2	1:F:167:ILE:CG1	2.28	0.46
1:G:37:ARG:NH1	2:I:2:G:H8	2.14	0.46
1:A:128:ILE:HG22	1:A:129:HIS:N	2.31	0.46
1:F:156:ASN:OD1	1:F:159:ALA:HB3	2.16	0.46
1:E:172:THR:C	1:E:174:SER:H	2.19	0.46
1:G:50:CYS:SG	1:G:56:ARG:NH2	2.89	0.46
1:E:47:TYR:HB2	1:E:62:TYR:CE1	2.50	0.46
2:I:50:U:H2'	2:I:51:C:C6	2.52	0.45
2:I:71:C:C2	2:I:72:A:N7	2.83	0.45
2:J:42:G:H2'	2:J:43:A:C8	2.51	0.45
1:B:178:HIS:O	1:B:179:HIS:CG	2.69	0.45
1:D:61:TYR:CE1	1:D:97:ALA:HB3	2.51	0.45
2:I:17:C:H3'	2:I:17(A):U:H6	1.80	0.45
1:B:61:TYR:CE1	1:B:97:ALA:HB3	2.51	0.45
1:E:44:LEU:HA	1:F:127:GLY:HA3	1.98	0.45
2:J:2:G:H2'	2:J:3:C:H6	1.81	0.45
1:A:9:LEU:HD23	1:A:39:HIS:CD2	2.52	0.45
1:F:129:HIS:O	1:F:164:THR:N	2.42	0.45
1:D:145:LYS:HE2	1:D:151:PRO:CB	2.45	0.45
2:J:17:C:H5"	2:J:17(A):U:P	2.57	0.45
2:J:18:G:O4'	2:J:18:G:OP2	2.34	0.45
1:B:170:LEU:HA	1:B:180:HIS:CE1	2.51	0.45
1:E:77:LYS:HG2	1:E:81:LYS:HE2	1.98	0.45
1:H:164:THR:HA	1:H:167:ILE:HD12	1.98	0.45
1:E:77:LYS:CE	1:E:81:LYS:HE2	2.40	0.45
1:D:47:TYR:HB2	1:D:62:TYR:CE1	2.52	0.45
1:G:60:GLY:HA3	1:G:98:ILE:HD13	1.99	0.45
1:H:38:GLN:HG2	1:H:43:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:VAL:HG23	1:C:128:ILE:HG21	1.97	0.45
1:D:141:HIS:CE1	1:D:145:LYS:HZ2	2.19	0.45
1:F:20:PHE:CZ	1:F:22:CYS:HB3	2.52	0.45
1:A:152:LEU:HD11	1:A:161:PHE:HB2	1.99	0.45
1:D:92:THR:OG1	1:D:132:PHE:CD2	2.68	0.45
1:H:130:GLY:HA3	1:H:162:PHE:O	2.15	0.45
2:J:64:G:H2'	2:J:65:C:O4'	2.17	0.45
1:C:4:LEU:HD11	1:C:107:TRP:CH2	2.52	0.44
1:H:7:GLU:OE2	1:H:15:TYR:HE1	1.99	0.44
1:A:37:ARG:CG	1:A:37:ARG:O	2.64	0.44
1:E:93:LEU:HB3	1:E:133:VAL:HB	1.99	0.44
2:J:17:C:OP1	2:J:61:C:H5'	2.17	0.44
1:A:4:LEU:HB3	1:A:51:ARG:HA	1.99	0.44
1:E:34:HIS:O	1:E:37:ARG:HG2	2.18	0.44
1:H:91:VAL:O	1:H:131:LEU:HD12	2.16	0.44
2:I:7:G:O2'	2:I:49:G:O5'	2.36	0.44
2:J:50:U:H2'	2:J:51:C:H6	1.81	0.44
1:B:71:ARG:HG3	1:B:88:ILE:HD11	2.00	0.44
1:D:37:ARG:HG3	1:D:41:ASN:OD1	2.17	0.44
1:E:45:ARG:HG2	1:F:127:GLY:H	1.81	0.44
1:G:37:ARG:HH11	2:I:2:G:P	2.41	0.44
1:C:176:LEU:O	1:C:177:GLU:CB	2.64	0.44
1:E:62:TYR:CZ	1:E:115:ALA:HB2	2.53	0.44
1:H:24:GLU:O	1:H:28:ASN:ND2	2.50	0.44
1:A:66:GLY:CA	1:B:89:PRO:HB3	2.45	0.44
1:D:149:PHE:HB3	1:D:160:LEU:HB3	1.99	0.44
1:F:115:ALA:O	1:F:119:VAL:HG23	2.18	0.44
2:I:18:G:OP2	2:I:18:G:O4'	2.36	0.44
1:C:39:HIS:HD2	1:C:46:ALA:H	1.65	0.44
2:I:36:U:C4	2:I:38:A:C5	3.05	0.44
2:I:64:G:H2'	2:I:65:C:O4'	2.18	0.44
1:C:178:HIS:NE2	1:C:180:HIS:CE1	2.86	0.43
2:J:63:G:H2'	2:J:64:G:H8	1.83	0.43
1:C:117:ASN:CB	1:C:171:PHE:CE2	2.96	0.43
2:J:2:G:H2'	2:J:3:C:C6	2.53	0.43
1:C:72:ALA:HA	1:C:80:GLN:NE2	2.34	0.43
1:C:123:SER:HG	1:C:128:ILE:HB	1.83	0.43
2:I:16:C:O2'	2:I:17:C:O5'	2.35	0.43
1:A:92:THR:OG1	1:A:132:PHE:HD2	1.96	0.43
1:B:120:TRP:CH2	1:B:124:LEU:HD21	2.52	0.43
1:F:98:ILE:HG13	1:F:108:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:20:H2U:H61	2:J:20:H2U:H2'	1.81	0.43
1:B:79:LYS:HB3	1:B:83:ILE:HD12	1.99	0.43
1:B:134:GLU:OE2	1:B:136:LEU:HD21	2.18	0.43
1:D:42:LYS:HD3	1:D:45:ARG:NH2	2.33	0.43
2:I:18:G:N3	2:I:58:A:N3	2.67	0.43
2:J:30:G:C2	2:J:41:C:C2	3.06	0.43
1:B:152:LEU:HD12	1:B:159:ALA:HB1	2.01	0.43
1:G:133:VAL:O	1:G:159:ALA:HA	2.19	0.43
1:H:41:ASN:HD21	2:J:1:C:P	2.42	0.43
1:F:44:LEU:HD22	1:F:63:THR:HB	2.01	0.43
2:I:17(A):U:H4'	2:I:18:G:OP1	2.17	0.43
2:I:42:G:H2'	2:I:43:A:H8	1.83	0.43
2:I:53:G:N7	2:I:54:5MU:H72	2.33	0.43
2:J:7:G:O2'	2:J:49:G:OP2	2.37	0.43
1:B:60:GLY:HA3	1:B:98:ILE:HD13	2.00	0.43
1:C:71:ARG:HA	1:C:88:ILE:HD11	2.00	0.43
1:D:91:VAL:O	1:D:131:LEU:HD12	2.18	0.43
1:E:172:THR:O	1:E:174:SER:N	2.52	0.43
1:F:89:PRO:HB2	1:F:127:GLY:O	2.19	0.43
2:I:18:G:C5	2:I:58:A:N1	2.87	0.43
1:C:68:CYS:HB2	1:D:68:CYS:SG	2.58	0.43
1:A:37:ARG:O	1:A:41:ASN:OD1	2.37	0.43
1:F:25:GLU:O	1:F:29:LEU:HG	2.19	0.43
1:H:42:LYS:HD2	1:H:42:LYS:N	2.34	0.43
1:H:51:ARG:NE	1:H:59:LEU:HD11	2.24	0.42
1:F:27:LEU:CD2	1:F:95:ARG:HH11	2.32	0.42
1:G:108:ASP:O	1:G:112:VAL:HG23	2.20	0.42
1:H:47:TYR:HB2	1:H:62:TYR:CE1	2.55	0.42
1:D:64:LEU:HD23	1:D:93:LEU:HA	2.00	0.42
1:G:94:GLY:O	1:G:95:ARG:HG3	2.19	0.42
1:H:37:ARG:O	1:H:41:ASN:N	2.37	0.42
2:J:49:G:C2	2:J:66:C:C2	3.07	0.42
1:B:18:GLN:CG	1:C:18:GLN:HG3	2.50	0.42
1:B:47:TYR:HB2	1:B:62:TYR:CE1	2.55	0.42
1:B:133:VAL:HG13	1:B:160:LEU:HB2	2.01	0.42
1:C:141:HIS:CD2	1:C:160:LEU:HD11	2.54	0.42
1:F:73:ALA:O	1:F:153:VAL:N	2.53	0.42
1:H:37:ARG:CG	2:J:1:C:H5'	2.49	0.42
1:B:175:ASP:HB2	1:B:179:HIS:CD2	2.55	0.42
1:D:77:LYS:NZ	2:J:4:G:P	2.92	0.42
1:G:141:HIS:ND1	1:G:160:LEU:HD11	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LYS:O	1:A:169:LEU:HG	2.20	0.42
1:C:37:ARG:NH1	2:J:17(A):U:N1	2.67	0.42
1:G:152:LEU:HD11	1:G:161:PHE:HB2	2.01	0.42
1:H:82:LYS:HE3	1:H:165:LYS:HZ1	1.84	0.42
1:A:149:PHE:CD2	1:A:162:PHE:HB2	2.55	0.42
1:D:15:TYR:HD1	1:D:56:ARG:HB3	1.85	0.42
1:H:52:ASN:HA	1:H:56:ARG:HH21	1.84	0.42
2:I:70:G:H2'	2:I:71:C:H6	1.84	0.42
1:A:62:TYR:HB2	1:A:93:LEU:HD11	2.01	0.41
2:J:9:G:C5	2:J:45:G:C6	3.08	0.41
2:J:18:G:C2	2:J:58:A:C4	3.08	0.41
1:B:37:ARG:NH1	2:I:17(A):U:C6	2.88	0.41
1:F:23:GLY:N	1:F:100:ARG:HD2	2.34	0.41
1:F:73:ALA:HB1	1:F:152:LEU:HB3	2.02	0.41
1:F:83:ILE:HD13	1:F:88:ILE:HG12	2.02	0.41
1:G:49:LEU:HD22	1:G:111:LEU:HD11	2.02	0.41
1:C:175:ASP:O	1:C:176:LEU:HB3	2.20	0.41
1:E:77:LYS:HE3	1:E:81:LYS:NZ	2.27	0.41
1:G:61:TYR:HE1	1:G:97:ALA:HB3	1.82	0.41
1:B:128:ILE:HG22	1:B:130:GLY:H	1.85	0.41
1:C:47:TYR:HE2	1:C:64:LEU:HD12	1.85	0.41
1:E:135:ALA:HB2	1:E:144:TYR:HE2	1.86	0.41
1:F:108:ASP:O	1:F:112:VAL:HG23	2.20	0.41
1:G:71:ARG:HG3	1:G:88:ILE:HD11	2.02	0.41
1:G:115:ALA:O	1:G:119:VAL:HG23	2.20	0.41
1:H:37:ARG:HD2	2:J:1:C:OP2	2.20	0.41
1:H:68:CYS:HA	1:H:88:ILE:O	2.21	0.41
1:D:39:HIS:O	1:D:40:ARG:C	2.58	0.41
1:E:45:ARG:HG3	1:F:125:ALA:C	2.41	0.41
1:F:63:THR:O	1:F:93:LEU:HD12	2.21	0.41
2:I:61:C:H2'	2:I:62:C:H6	1.86	0.41
2:J:48:C:OP2	2:J:48:C:C6	2.71	0.41
2:J:69:C:H2'	2:J:70:G:C8	2.55	0.41
1:A:37:ARG:HG3	1:A:41:ASN:OD1	2.19	0.41
1:A:145:LYS:CE	1:A:151:PRO:HG3	2.30	0.41
1:B:99:ASP:OD1	1:B:100:ARG:N	2.54	0.41
1:B:177:GLU:O	1:B:178:HIS:CB	2.64	0.41
2:I:50:U:H2'	2:I:51:C:H6	1.86	0.41
2:J:32:OMC:HM23	2:J:32:OMC:O2	2.21	0.41
1:A:42:LYS:NZ	1:B:168:GLU:OE2	2.53	0.41
1:D:9:LEU:HB3	1:D:39:HIS:ND1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:ILE:HA	1:E:84:PRO:HD3	1.95	0.41
1:F:49:LEU:HB2	1:F:111:LEU:HD11	2.03	0.41
1:G:150:ILE:N	1:G:161:PHE:O	2.48	0.41
2:J:65:C:O2'	2:J:66:C:H5'	2.21	0.41
1:B:79:LYS:HA	1:B:82:LYS:HB3	2.03	0.41
1:D:25:GLU:HA	1:D:28:ASN:ND2	2.36	0.41
1:C:98:ILE:HD11	1:C:111:LEU:HD22	2.02	0.40
1:E:115:ALA:O	1:E:119:VAL:HG23	2.21	0.40
1:F:9:LEU:HD23	1:F:39:HIS:CG	2.56	0.40
1:F:162:PHE:HA	1:F:163:PRO:HD3	1.94	0.40
2:I:15:G:N2	2:I:59:A:C5	2.89	0.40
2:J:53:G:N7	2:J:54:5MU:H72	2.36	0.40
1:C:108:ASP:O	1:C:112:VAL:HG23	2.21	0.40
1:E:64:LEU:HD23	1:E:93:LEU:HA	2.03	0.40
2:I:42:G:H2'	2:I:43:A:C8	2.56	0.40
1:D:17:LEU:HD23	1:D:31:LEU:HG	2.02	0.40
1:H:52:ASN:HA	1:H:56:ARG:NH2	2.36	0.40
1:A:31:LEU:HB2	1:A:61:TYR:CZ	2.56	0.40
1:A:141:HIS:CD2	1:A:145:LYS:CE	2.99	0.40
1:B:72:ALA:HA	1:B:80:GLN:OE1	2.21	0.40
1:C:89:PRO:HB3	1:D:66:GLY:CA	2.50	0.40
1:D:145:LYS:HG3	1:D:160:LEU:CD2	2.51	0.40
1:E:45:ARG:HG3	1:F:126:VAL:HA	2.04	0.40
1:F:131:LEU:HD23	1:F:149:PHE:CZ	2.57	0.40
1:G:58:VAL:O	1:G:59:LEU:HD23	2.21	0.40
2:I:20:H2U:H2'	2:I:20:H2U:H61	1.90	0.40
2:I:21:A:O2'	2:I:46:A:N6	2.54	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	168/183 (92%)	165 (98%)	3 (2%)	0	100	100
1	B	178/183 (97%)	167 (94%)	10 (6%)	1 (1%)	25	62
1	C	177/183 (97%)	172 (97%)	5 (3%)	0	100	100
1	D	169/183 (92%)	162 (96%)	6 (4%)	1 (1%)	25	62
1	E	169/183 (92%)	163 (96%)	5 (3%)	1 (1%)	25	62
1	F	170/183 (93%)	163 (96%)	6 (4%)	1 (1%)	25	62
1	G	166/183 (91%)	163 (98%)	3 (2%)	0	100	100
1	H	167/183 (91%)	163 (98%)	4 (2%)	0	100	100
All	All	1364/1464 (93%)	1318 (97%)	42 (3%)	4 (0%)	41	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	175	ASP
1	E	173	GLN
1	D	39	HIS
1	F	126	VAL

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	146/159 (92%)	146 (100%)	0	100	100
1	B	156/159 (98%)	154 (99%)	2 (1%)	69	82
1	C	155/159 (98%)	152 (98%)	3 (2%)	57	76
1	D	147/159 (92%)	147 (100%)	0	100	100
1	E	147/159 (92%)	143 (97%)	4 (3%)	44	69
1	F	148/159 (93%)	147 (99%)	1 (1%)	84	91
1	G	144/159 (91%)	142 (99%)	2 (1%)	67	81
1	H	145/159 (91%)	143 (99%)	2 (1%)	67	81
All	All	1188/1272 (93%)	1174 (99%)	14 (1%)	71	84

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	ASP
1	B	126	VAL
1	C	22	CYS
1	C	117	ASN
1	C	177	GLU
1	E	65	CYS
1	E	128	ILE
1	E	174	SER
1	E	175	ASP
1	F	56	ARG
1	G	65	CYS
1	G	128	ILE
1	H	42	LYS
1	H	56	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	179	HIS
1	D	141	HIS
1	E	39	HIS
1	G	28	ASN
1	H	39	HIS
1	H	80	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	I	74/77 (96%)	16 (21%)	3 (4%)
2	J	74/77 (96%)	16 (21%)	3 (4%)
All	All	148/154 (96%)	32 (21%)	6 (4%)

All (32) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	I	2	G
2	I	8	4SU
2	I	9	G
2	I	17	C

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Mol	Chain	Res	Type
2	I	17(A)	U
2	I	18	G
2	I	19	G
2	I	20	H2U
2	I	21	A
2	I	33	U
2	I	37	A
2	I	38	A
2	I	48	C
2	I	49	G
2	I	52	G
2	I	72	A
2	J	2	G
2	J	8	4SU
2	J	9	G
2	J	17	C
2	J	17(A)	U
2	J	18	G
2	J	19	G
2	J	20	H2U
2	J	21	A
2	J	33	U
2	J	38	A
2	J	48	C
2	J	49	G
2	J	52	G
2	J	58	A
2	J	72	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	I	17	C
2	I	19	G
2	I	47	U
2	J	17	C
2	J	19	G
2	J	47	U

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

10 non-standard protein/DNA/RNA residues 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	OMC	I	32	2	19,22,23	0.32	0	26,31,34	0.58	0
2	OMC	J	32	2	19,22,23	0.35	0	26,31,34	0.64	0
2	PSU	I	55	2	18,21,22	1.06	1 (5%)	22,30,33	1.63	4 (18%)
2	H2U	I	20	2	18,21,22	1.08	3 (16%)	21,30,33	1.94	1 (4%)
2	H2U	J	20	2	18,21,22	1.06	3 (16%)	21,30,33	1.63	1 (4%)
2	4SU	J	8	2	18,21,22	0.52	0	26,30,33	0.52	0
2	PSU	J	55	2	18,21,22	1.07	1 (5%)	22,30,33	1.66	4 (18%)
2	5MU	I	54	2	19,22,23	1.42	5 (26%)	28,32,35	1.94	5 (17%)
2	5MU	J	54	2	19,22,23	1.41	6 (31%)	28,32,35	1.95	5 (17%)
2	4SU	I	8	2	18,21,22	0.53	0	26,30,33	0.52	0

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	OMC	I	32	2	-	0/9/27/28	0/2/2/2
2	OMC	J	32	2	-	0/9/27/28	0/2/2/2
2	PSU	I	55	2	-	0/7/25/26	0/2/2/2
2	H2U	I	20	2	-	3/7/38/39	0/2/2/2
2	H2U	J	20	2	-	3/7/38/39	0/2/2/2
2	4SU	J	8	2	-	0/7/25/26	0/2/2/2
2	PSU	J	55	2	-	0/7/25/26	0/2/2/2
2	5MU	I	54	2	-	0/7/25/26	0/2/2/2
2	5MU	J	54	2	-	0/7/25/26	0/2/2/2
2	4SU	I	8	2	-	0/7/25/26	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	55	PSU	C6-C5	3.50	1.39	1.35
2	J	55	PSU	C6-C5	3.46	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	54	5MU	C6-C5	2.78	1.39	1.34
2	I	20	H2U	C2-N3	-2.76	1.33	1.38
2	J	54	5MU	C6-C5	2.73	1.39	1.34
2	J	20	H2U	C2-N3	-2.71	1.33	1.38
2	I	54	5MU	C4-N3	-2.59	1.34	1.38
2	J	54	5MU	C4-N3	-2.58	1.34	1.38
2	I	20	H2U	C4-N3	-2.33	1.33	1.37
2	J	20	H2U	C4-N3	-2.31	1.33	1.37
2	I	54	5MU	C4-C5	2.29	1.48	1.44
2	J	54	5MU	C4-C5	2.29	1.48	1.44
2	I	54	5MU	C2-N1	2.28	1.42	1.38
2	J	54	5MU	C2-N1	2.22	1.42	1.38
2	I	54	5MU	C6-N1	-2.22	1.34	1.38
2	J	54	5MU	C6-N1	-2.17	1.34	1.38
2	J	20	H2U	C2-N1	-2.16	1.32	1.35
2	I	20	H2U	C2-N1	-2.11	1.32	1.35
2	J	54	5MU	C2-N3	-2.02	1.34	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	20	H2U	C4-N3-C2	-8.18	119.00	125.79
2	J	20	H2U	C4-N3-C2	-6.58	120.33	125.79
2	J	54	5MU	C4-N3-C2	-4.71	121.25	127.35
2	I	54	5MU	C4-N3-C2	-4.68	121.30	127.35
2	J	54	5MU	N3-C2-N1	4.68	121.10	114.89
2	I	54	5MU	N3-C2-N1	4.66	121.08	114.89
2	J	55	PSU	C4-N3-C2	-4.42	119.98	126.34
2	I	55	PSU	C4-N3-C2	-4.34	120.08	126.34
2	J	54	5MU	C5-C4-N3	4.07	118.79	115.31
2	J	55	PSU	N1-C2-N3	4.02	119.68	115.13
2	I	54	5MU	O4-C4-C5	-4.00	120.27	124.90
2	I	54	5MU	C5-C4-N3	4.00	118.72	115.31
2	I	55	PSU	N1-C2-N3	3.94	119.60	115.13
2	J	54	5MU	O4-C4-C5	-3.86	120.42	124.90
2	J	54	5MU	C5-C6-N1	-3.30	119.94	123.34
2	I	54	5MU	C5-C6-N1	-3.29	119.95	123.34
2	J	55	PSU	O2-C2-N1	-2.44	120.10	122.79
2	I	55	PSU	O2-C2-N1	-2.35	120.20	122.79
2	J	55	PSU	C6-N1-C2	-2.10	120.53	122.68
2	I	55	PSU	C6-N1-C2	-2.09	120.55	122.68

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	20	H2U	O4'-C4'-C5'-O5'
2	I	20	H2U	C3'-C4'-C5'-O5'
2	J	20	H2U	O4'-C4'-C5'-O5'
2	J	20	H2U	C3'-C4'-C5'-O5'
2	I	20	H2U	C4'-C5'-O5'-P
2	J	20	H2U	C4'-C5'-O5'-P

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	32	OMC	1	0
2	I	20	H2U	2	0
2	J	20	H2U	2	0
2	J	8	4SU	1	0
2	I	54	5MU	2	0
2	J	54	5MU	2	0
2	I	8	4SU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	170/183 (92%)	0.11	6 (3%) 44 36	64, 127, 173, 193	0
1	B	180/183 (98%)	0.15	8 (4%) 34 29	57, 105, 165, 185	0
1	C	179/183 (97%)	0.18	9 (5%) 28 25	62, 101, 165, 198	0
1	D	170/183 (92%)	0.08	5 (2%) 51 42	71, 128, 178, 191	0
1	E	171/183 (93%)	0.42	14 (8%) 11 9	112, 165, 201, 221	0
1	F	172/183 (93%)	0.43	12 (6%) 16 12	108, 169, 211, 232	0
1	G	168/183 (91%)	0.70	25 (14%) 2 2	114, 176, 223, 248	0
1	H	168/183 (91%)	0.39	16 (9%) 8 7	101, 148, 199, 230	0
2	I	70/77 (90%)	0.34	0 100 100	103, 126, 196, 237	0
2	J	70/77 (90%)	0.43	2 (2%) 51 42	91, 125, 181, 222	0
All	All	1518/1618 (93%)	0.31	97 (6%) 19 15	57, 139, 201, 248	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	60	GLY	9.8
1	F	130	GLY	8.0
1	H	61	TYR	6.2
1	G	59	LEU	5.7
1	H	97	ALA	5.4
1	G	61	TYR	5.3
1	A	54	PRO	5.2
1	F	55	GLU	5.0
1	C	178	HIS	4.9
1	E	16	ASP	4.9
1	D	54	PRO	4.9
1	E	61	TYR	4.7
1	G	81	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	61	TYR	4.4
1	G	49	LEU	4.3
1	H	98	ILE	4.3
1	H	60	GLY	4.2
1	E	55	GLU	4.2
1	E	57	GLN	4.1
1	G	98	ILE	3.9
1	H	55	GLU	3.9
1	G	97	ALA	3.7
1	E	130	GLY	3.6
1	A	55	GLU	3.6
1	F	58	VAL	3.4
1	F	44	LEU	3.4
1	D	55	GLU	3.4
1	B	181	HIS	3.4
1	G	104	GLY	3.4
1	F	57	GLN	3.3
1	G	82	LYS	3.3
1	G	101	SER	3.3
1	G	52	ASN	3.3
1	E	52	ASN	3.2
1	G	96	LEU	3.2
1	H	134	GLU	3.1
1	C	75	PRO	3.1
2	J	7	G	3.0
1	B	19	ARG	3.0
1	H	14	ASP	3.0
1	C	180	HIS	2.9
1	H	19	ARG	2.9
1	C	57	GLN	2.8
1	C	179	HIS	2.8
1	G	160	LEU	2.7
1	G	5	THR	2.7
1	H	144	TYR	2.6
1	G	14	ASP	2.6
1	F	43	ILE	2.6
1	B	76	SER	2.6
1	E	111	LEU	2.6
1	H	15	TYR	2.6
1	D	53	THR	2.6
1	C	61	TYR	2.5
1	F	59	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	49	LEU	2.5
1	G	109	ALA	2.4
1	E	15	TYR	2.4
1	E	53	THR	2.4
1	C	9	LEU	2.4
1	G	11	ASP	2.4
1	H	102	LEU	2.4
1	B	179	HIS	2.4
1	B	16	ASP	2.4
1	A	32	THR	2.4
1	C	155	GLU	2.3
1	A	57	GLN	2.3
2	J	1	C	2.3
1	E	58	VAL	2.3
1	G	107	TRP	2.3
1	B	180	HIS	2.3
1	A	53	THR	2.3
1	G	51	ARG	2.2
1	G	6	ILE	2.2
1	G	57	GLN	2.2
1	G	131	LEU	2.2
1	F	111	LEU	2.2
1	G	145	LYS	2.2
1	E	49	LEU	2.2
1	B	78	SER	2.2
1	F	131	LEU	2.1
1	D	97	ALA	2.1
1	G	93	LEU	2.1
1	D	98	ILE	2.1
1	F	60	GLY	2.1
1	H	107	TRP	2.1
1	H	59	LEU	2.1
1	H	21	ASP	2.1
1	G	105	GLN	2.1
1	H	58	VAL	2.1
1	H	56	ARG	2.1
1	C	19	ARG	2.1
1	B	77	LYS	2.0
1	E	54	PRO	2.0
1	A	33	THR	2.0
1	E	6	ILE	2.0
1	E	56	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. 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	B-factors(Å^2)	Q<0.9
2	H2U	I	20	20/21	0.81	0.24	102,114,123,125	0
2	H2U	J	20	20/21	0.84	0.20	101,112,125,130	0
2	4SU	J	8	20/21	0.86	0.40	108,124,136,137	0
2	5MU	J	54	21/22	0.88	0.24	124,136,144,153	0
2	5MU	I	54	21/22	0.90	0.20	126,135,142,149	0
2	PSU	J	55	20/21	0.90	0.15	118,136,145,146	0
2	4SU	I	8	20/21	0.91	0.38	103,115,130,130	0
2	PSU	I	55	20/21	0.93	0.12	122,134,145,150	0
2	OMC	I	32	21/22	0.94	0.24	126,145,151,153	0
2	OMC	J	32	21/22	0.94	0.18	120,129,139,141	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.