Full wwPDB X-ray Structure Validation Report (i)

Oct 1, 2024 – 07:36 PM JST

PDB ID	:	6JR1
Title	:	Crystal structure of the human nucleosome phased with 16 selenium atoms
Authors	:	Saotome, M.; Horikoshi, N.; Urano, K.; Kujirai, T.; Yuzurihara, H.; Kurumizaka, H.; Kagawa, W.
Deposited on	:	2019-04-02
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

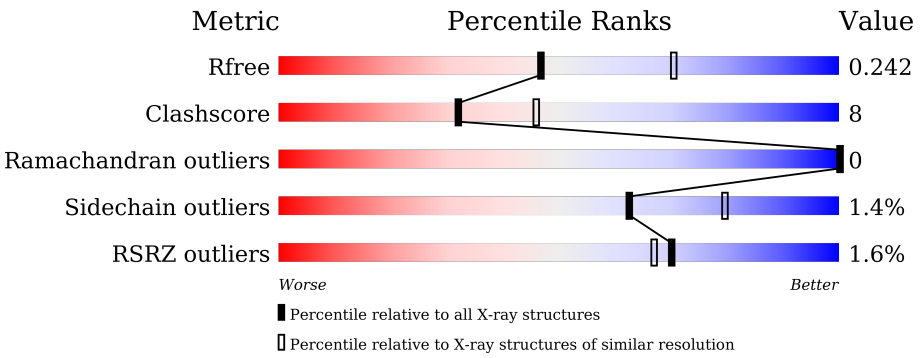
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	139	.% 60% 8% • 31%
1	E	139	.% 60% 8% • 29%
2	B	106	.% 68% 6% 26%
2	F	106	2% 73% 8% 20%
3	C	133	.% 74% 6% • 19%
3	G	133	2% 66% 13% 21%

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Mol	Chain	Length	Quality of chain
4	D	129	2% 65% 7% 28%
4	H	129	% 60% 11% 29%
5	I	146	2% 61% 39%
5	J	146	62% 36%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12557 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 H3.1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	96	790	499	151	136	2	2	0	0	0
1	E	98	810	511	157	138	2	2	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P68431
A	-2	SER	-	expression tag	UNP P68431
A	-1	HIS	-	expression tag	UNP P68431
E	-3	GLY	-	expression tag	UNP P68431
E	-2	SER	-	expression tag	UNP P68431
E	-1	HIS	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	78	622	393	120	108	1	0	0	0
2	F	85	689	434	139	115	1	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P62805
B	-2	SER	-	expression tag	UNP P62805
B	-1	HIS	-	expression tag	UNP P62805
F	-3	GLY	-	expression tag	UNP P62805
F	-2	SER	-	expression tag	UNP P62805
F	-1	HIS	-	expression tag	UNP P62805

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
3	C	108	835	524	165	144	2	0	0	0
3	G	105	810	509	158	141	2	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P04908
C	-2	SER	-	expression tag	UNP P04908
C	-1	HIS	-	expression tag	UNP P04908
C	65	MSE	LEU	engineered mutation	UNP P04908
C	85	MSE	LEU	engineered mutation	UNP P04908
G	-3	GLY	-	expression tag	UNP P04908
G	-2	SER	-	expression tag	UNP P04908
G	-1	HIS	-	expression tag	UNP P04908
G	65	MSE	LEU	engineered mutation	UNP P04908
G	85	MSE	LEU	engineered mutation	UNP P04908

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
4	D	93	725	454	130	137	4	0	0	0
4	H	92	719	451	129	135	4	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP P06899
D	-2	SER	-	expression tag	UNP P06899
D	-1	HIS	-	expression tag	UNP P06899
D	101	MSE	LEU	engineered mutation	UNP P06899
D	106	MSE	LEU	engineered mutation	UNP P06899
H	-3	GLY	-	expression tag	UNP P06899
H	-2	SER	-	expression tag	UNP P06899
H	-1	HIS	-	expression tag	UNP P06899
H	101	MSE	LEU	engineered mutation	UNP P06899
H	106	MSE	LEU	engineered mutation	UNP P06899

- Molecule 5 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	I	146	2990	1431	540	874	145	0	0	0
5	J	146	2990	1431	540	874	145	0	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
6	A	1	1	1	0	0
6	C	1	1	1	0	0
6	E	1	1	1	0	0
6	G	1	1	1	0	0

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
7	E	1	1	1	0	0
7	I	3	3	3	0	0
7	J	4	4	4	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	25	25	25	0	0
8	B	29	29	29	0	0
8	C	54	54	54	0	0
8	D	45	45	45	0	0
8	E	56	56	56	0	0
8	F	52	52	52	0	0

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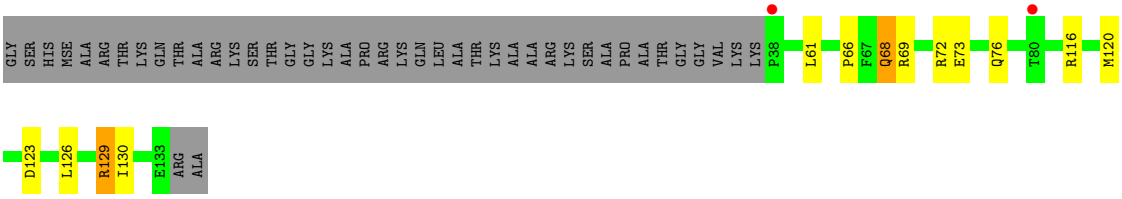
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	G	44	44	44	0	0
			Total	O		
8	H	20	20	20	0	0
			Total	O		
8	I	118	118	118	0	0
			Total	O		
8	J	122	122	122	0	0

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.

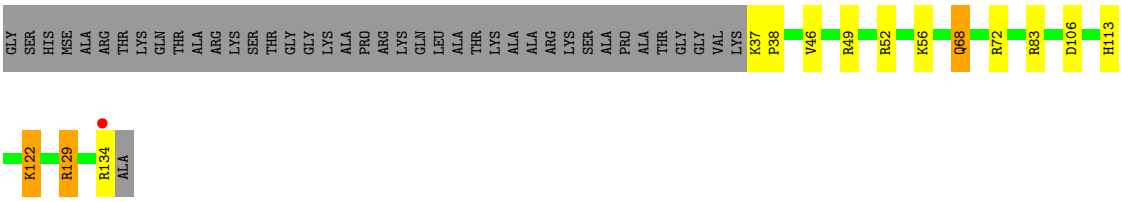
• Molecule 1: Histone H3.1

Chain A:



• Molecule 1: Histone H3.1

Chain E:

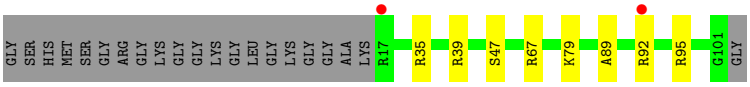


• Molecule 2: Histone H4

Chain B:

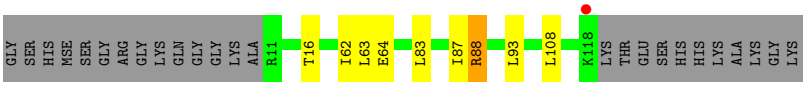
• Molecule 2: Histone H4

Chain F:



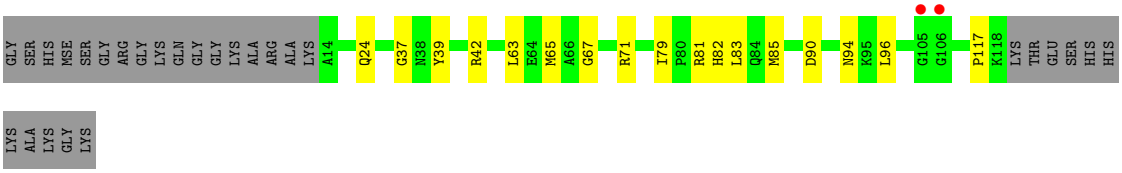
• Molecule 3: Histone H2A type 1-B/E

Chain C:



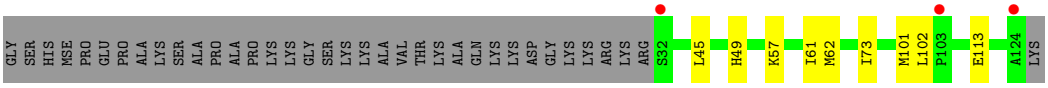
• Molecule 3: Histone H2A type 1-B/E

Chain G:



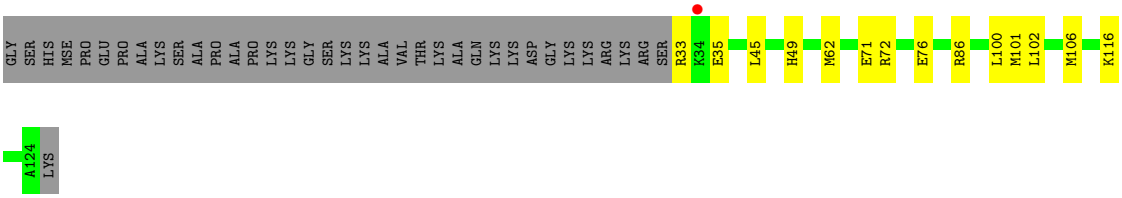
• Molecule 4: Histone H2B type 1-J

Chain D:



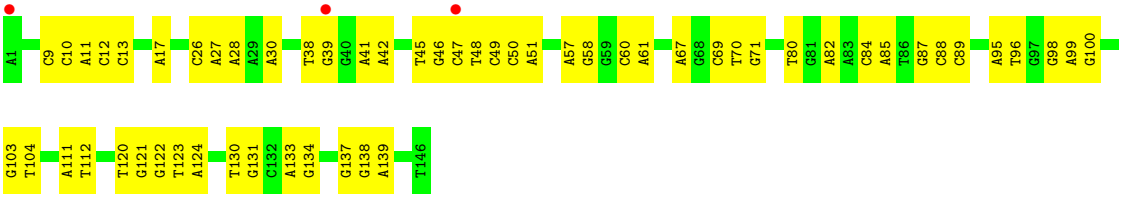
• Molecule 4: Histone H2B type 1-J

Chain H:



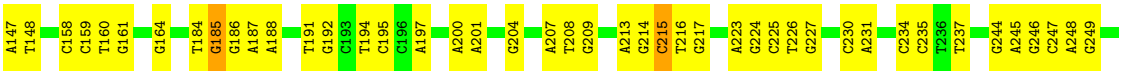
• Molecule 5: DNA (146-MER)

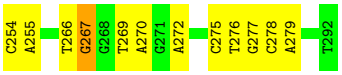
Chain I:



• Molecule 5: DNA (146-MER)

Chain J:




C254
A255
T266
G267
G268
T269
A270
G271
A272
C275
T276
G277
C278
A279
T292

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.46Å 108.54Å 170.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.74 – 2.40 47.74 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.74-2.40) 100.0 (47.74-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.209 , 0.243 0.209 , 0.242	Depositor DCC
R_{free} test set	3599 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	38.4	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12557	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 2.61% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.28	0/800	0.43	0/1070
1	E	0.28	0/820	0.46	0/1096
2	B	0.27	0/629	0.46	0/843
2	F	0.33	0/697	0.51	0/932
3	C	0.27	0/843	0.44	0/1131
3	G	0.26	0/818	0.46	0/1099
4	D	0.28	0/732	0.44	0/976
4	H	0.27	0/726	0.45	0/968
5	I	0.69	0/3354	1.00	1/5175 (0.0%)
5	J	0.71	1/3354 (0.0%)	1.02	2/5175 (0.0%)
All	All	0.54	1/12773 (0.0%)	0.82	3/18465 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	215	DC	C3'-O3'	-5.48	1.36	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	185	DG	O4'-C1'-N9	-5.84	103.91	108.00
5	I	98	DG	O4'-C1'-N9	5.53	111.87	108.00
5	J	267	DG	O4'-C1'-N9	-5.27	104.31	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	790	0	826	15	1
1	E	810	0	851	17	0
2	B	622	0	660	6	0
2	F	689	0	739	12	0
3	C	835	0	893	8	0
3	G	810	0	862	13	0
4	D	725	0	741	9	0
4	H	719	0	736	19	0
5	I	2990	0	1652	54	1
5	J	2990	0	1652	51	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
7	E	1	0	0	0	0
7	I	3	0	0	0	0
7	J	4	0	0	0	0
8	A	25	0	0	0	0
8	B	29	0	0	1	0
8	C	54	0	0	0	0
8	D	45	0	0	1	0
8	E	56	0	0	6	0
8	F	52	0	0	3	0
8	G	44	0	0	5	0
8	H	20	0	0	1	0
8	I	118	0	0	17	1
8	J	122	0	0	9	1
All	All	12557	0	9612	171	2

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 8.

All (171) 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)
5:I:137:DG:N7	8:I:301:HOH:O	1.96	0.98
5:J:192:DG:N7	8:J:402:HOH:O	1.98	0.95
5:I:47:DC:H2"	5:I:48:DT:H5"	1.56	0.88
5:J:207:DA:OP2	8:J:401:HOH:O	1.91	0.88
2:F:92:ARG:HH22	4:H:101:MSE:SE	2.06	0.87
5:I:111:DA:OP2	8:I:303:HOH:O	1.98	0.82
5:I:26:DC:O2	8:I:302:HOH:O	1.98	0.79
5:J:204:DG:N3	8:J:404:HOH:O	2.16	0.79
5:I:80:DT:OP2	8:I:305:HOH:O	2.01	0.78
5:I:87:DG:OP2	8:I:304:HOH:O	2.01	0.77
5:J:164:DG:N3	8:J:405:HOH:O	2.18	0.76
5:J:213:DA:OP2	8:J:403:HOH:O	2.05	0.75
1:E:37:LYS:N	8:E:302:HOH:O	2.20	0.74
2:F:92:ARG:NH2	4:H:101:MSE:SE	2.70	0.74
1:E:72:ARG:NH2	5:J:197:DA:OP1	2.22	0.73
5:I:17:DA:N3	8:I:313:HOH:O	2.21	0.72
3:G:65:MSE:HE1	3:G:90:ASP:HB2	1.71	0.72
4:H:72:ARG:HB3	4:H:101:MSE:HE2	1.73	0.71
5:J:248:DA:H2"	5:J:249:DG:H5"	1.73	0.70
3:G:24:GLN:O	8:G:301:HOH:O	2.10	0.70
5:J:269:DT:H2"	5:J:270:DA:C8	2.27	0.69
5:I:27:DA:OP2	8:I:306:HOH:O	2.10	0.69
5:I:28:DA:OP2	8:I:307:HOH:O	2.11	0.68
5:J:226:DT:H2"	5:J:227:DG:C8	2.29	0.68
2:F:89:ALA:O	2:F:92:ARG:HB3	1.94	0.68
5:J:161:DG:N7	8:J:410:HOH:O	2.26	0.67
1:A:72:ARG:NH2	5:I:50:DC:OP1	2.27	0.67
2:F:95:ARG:NH1	8:F:202:HOH:O	2.28	0.66
2:B:27:GLN:O	8:B:201:HOH:O	2.13	0.66
5:J:186:DG:N7	8:J:413:HOH:O	2.30	0.65
3:G:71:ARG:NH2	8:G:305:HOH:O	2.31	0.64
5:J:244:DG:H2"	5:J:245:DA:N7	2.13	0.64
5:I:61:DA:OP2	8:I:308:HOH:O	2.15	0.64
5:I:57:DA:H4'	5:I:58:DG:OP1	1.97	0.64
5:J:216:DT:H2"	5:J:217:DG:C8	2.33	0.64
1:E:52:ARG:NH2	8:E:305:HOH:O	2.30	0.64
4:H:33:ARG:HG2	5:I:122:DG:H4'	1.81	0.62
5:J:244:DG:H2"	5:J:245:DA:C8	2.35	0.62
5:I:120:DT:H2"	5:I:121:DG:C8	2.36	0.61
5:I:133:DA:H2'	5:I:134:DG:C8	2.36	0.61
3:G:42:ARG:HD3	8:G:302:HOH:O	2.00	0.61
3:G:83:LEU:HD13	4:H:62:MSE:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:51:DA:OP2	8:I:309:HOH:O	2.16	0.60
1:A:116:ARG:NH2	1:A:123:ASP:OD2	2.33	0.60
3:C:83:LEU:HD13	4:D:62:MSE:HE3	1.83	0.59
4:H:33:ARG:NH1	8:H:201:HOH:O	2.29	0.59
5:I:130:DT:H2"	5:I:131:DG:C8	2.39	0.58
5:J:278:DC:H2"	5:J:279:DA:N7	2.19	0.58
5:J:275:DC:H1'	5:J:276:DT:H5'	1.84	0.58
5:J:191:DT:H2'	5:J:192:DG:C8	2.40	0.57
1:E:72:ARG:HH22	5:J:197:DA:P	2.27	0.57
5:J:147:DA:H2'	5:J:148:DT:C6	2.40	0.57
5:I:9:DC:H2"	5:I:10:DC:H5"	1.87	0.57
5:I:67:DA:OP2	8:I:310:HOH:O	2.18	0.56
5:I:88:DC:H2"	5:I:89:DC:C5	2.40	0.56
2:F:92:ARG:HH21	4:H:100:LEU:C	2.08	0.55
1:A:66:PRO:HG3	5:J:237:DT:OP1	2.06	0.55
3:G:96:LEU:HD22	4:H:106:MSE:HE1	1.87	0.55
1:E:134:ARG:HH12	3:G:94:ASN:HD21	1.53	0.55
1:A:129:ARG:NH1	1:E:106:ASP:OD1	2.41	0.54
1:E:68:GLN:NE2	8:E:306:HOH:O	2.40	0.54
1:A:73:GLU:OE1	2:B:25:ASN:ND2	2.25	0.54
5:I:30:DA:N7	8:I:318:HOH:O	2.33	0.54
5:I:123:DT:H2"	5:I:124:DA:C8	2.43	0.54
5:I:12:DC:H2'	5:I:13:DC:C6	2.42	0.53
5:J:223:DA:H2"	5:J:224:DG:C8	2.43	0.53
5:I:138:DG:N7	8:I:317:HOH:O	2.33	0.53
5:I:134:DG:OP2	8:I:311:HOH:O	2.19	0.53
3:G:117:PRO:O	8:G:304:HOH:O	2.18	0.53
5:J:158:DC:H2'	5:J:159:DC:C6	2.44	0.52
1:E:83:ARG:HG2	5:J:197:DA:H5"	1.92	0.52
5:I:99:DA:H2"	5:I:100:DG:O5'	2.09	0.52
2:F:92:ARG:HH22	4:H:101:MSE:CG	2.22	0.52
5:J:247:DC:H2"	5:J:248:DA:C8	2.45	0.51
3:C:62:ILE:HD11	3:C:87:ILE:HD11	1.92	0.51
5:I:49:DC:H6	5:I:49:DC:H5'	1.75	0.51
1:A:129:ARG:HD3	1:A:129:ARG:C	2.31	0.51
5:I:60:DC:H2"	5:I:61:DA:C8	2.46	0.51
4:D:73:ILE:HD11	4:D:101:MSE:HE1	1.92	0.51
5:J:200:DA:H2"	5:J:201:DA:C8	2.45	0.51
5:I:9:DC:H2"	5:I:10:DC:C5'	2.41	0.51
3:C:88:ARG:HB3	3:C:108:LEU:HD11	1.92	0.51
5:I:57:DA:H2"	5:I:58:DG:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:214:DG:H2"	5:J:215:DC:C6	2.46	0.50
5:I:69:DC:OP1	8:I:312:HOH:O	2.19	0.50
5:I:84:DC:H2"	5:I:85:DA:C8	2.47	0.50
5:J:234:DC:H2"	5:J:235:DC:C5	2.46	0.50
5:J:254:DC:H2"	5:J:255:DA:C8	2.46	0.50
4:D:101:MSE:HE3	4:D:102:LEU:HD21	1.93	0.50
5:I:111:DA:H5'	8:I:316:HOH:O	2.12	0.50
5:J:159:DC:H2'	5:J:160:DT:C6	2.46	0.50
1:E:49:ARG:NH2	8:E:304:HOH:O	2.28	0.49
4:H:33:ARG:NH2	4:H:35:GLU:OE2	2.45	0.49
5:J:187:DA:H2"	5:J:188:DA:C8	2.47	0.49
5:J:266:DT:H2"	5:J:267:DG:N7	2.28	0.49
1:A:68:GLN:O	1:A:72:ARG:HG3	2.13	0.49
2:F:67:ARG:NH2	8:F:207:HOH:O	2.44	0.49
1:E:68:GLN:O	1:E:72:ARG:HG3	2.14	0.48
5:J:277:DG:H2"	5:J:278:DC:C6	2.48	0.48
5:J:187:DA:H2"	5:J:188:DA:H8	1.78	0.48
1:E:122:LYS:NZ	8:E:301:HOH:O	2.16	0.48
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.49	0.47
5:I:70:DT:H2"	5:I:71:DG:C8	2.49	0.47
5:I:88:DC:H2"	5:I:89:DC:C6	2.50	0.47
5:J:147:DA:H2"	5:J:148:DT:H5'	1.96	0.47
5:I:133:DA:H2"	5:I:134:DG:O4'	2.14	0.47
4:D:62:MSE:HA	4:D:62:MSE:HE2	1.95	0.47
5:J:277:DG:H4'	5:J:278:DC:OP1	2.14	0.47
3:G:37:GLY:HA3	3:G:39:TYR:CE2	2.51	0.46
5:J:230:DC:H2"	5:J:231:DA:C8	2.50	0.46
1:A:68:GLN:HE21	1:A:72:ARG:NH1	2.13	0.46
1:E:49:ARG:HD3	8:E:314:HOH:O	2.15	0.46
5:J:245:DA:H4'	5:J:246:DG:OP1	2.16	0.46
3:C:64:GLU:O	4:D:49:HIS:HE1	1.98	0.46
5:J:224:DG:H2"	5:J:225:DC:C6	2.51	0.46
4:H:116:LYS:HB2	4:H:116:LYS:HE3	1.74	0.45
5:I:45:DT:H2'	5:I:46:DG:C8	2.52	0.45
5:I:38:DT:H2"	5:I:39:DG:C8	2.51	0.45
5:I:41:DA:H2"	5:I:42:DA:H8	1.81	0.45
5:I:103:DG:H1'	5:I:104:DT:H5'	1.97	0.45
3:G:81:ARG:HE	3:G:85:MSE:HE3	1.81	0.45
8:G:307:HOH:O	4:H:71:GLU:HG2	2.15	0.45
5:J:225:DC:H2"	5:J:226:DT:H72	1.98	0.45
2:F:92:ARG:NH1	4:H:76:GLU:OE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:208:DT:H2"	5:J:209:DG:C8	2.52	0.45
1:A:130:ILE:HD12	1:E:106:ASP:HB3	1.98	0.45
3:C:16:THR:HA	5:I:30:DA:H5"	1.99	0.45
5:I:41:DA:H2"	5:I:42:DA:C8	2.52	0.45
5:I:111:DA:H2'	5:I:112:DT:H72	1.99	0.45
1:E:46:VAL:HG21	5:I:82:DA:H3'	1.98	0.45
4:D:57:LYS:O	4:D:61:ILE:HD12	2.18	0.44
3:G:67:GLY:HA3	4:H:49:HIS:CD2	2.53	0.44
2:F:79:LYS:HD3	5:I:100:DG:OP1	2.18	0.44
4:H:62:MSE:HA	4:H:62:MSE:HE2	1.98	0.44
5:I:133:DA:H3'	8:I:311:HOH:O	2.17	0.44
5:J:248:DA:C2'	5:J:249:DG:H5"	2.45	0.44
2:F:95:ARG:HD3	8:F:202:HOH:O	2.17	0.44
5:J:224:DG:H2"	5:J:225:DC:C5	2.53	0.44
3:C:93:LEU:HD23	3:C:93:LEU:HA	1.89	0.44
2:B:31:LYS:HG3	2:B:51:TYR:CE1	2.53	0.43
5:I:111:DA:H2'	5:I:112:DT:C7	2.48	0.43
1:A:69:ARG:HD2	2:B:25:ASN:OD1	2.19	0.43
3:C:62:ILE:HD13	4:D:62:MSE:HE1	2.01	0.43
3:G:63:LEU:HD13	4:H:45:LEU:HB2	2.01	0.43
2:B:31:LYS:HG3	2:B:51:TYR:CZ	2.53	0.43
5:I:10:DC:H2"	5:I:11:DA:H8	1.84	0.43
5:I:49:DC:H5'	5:I:49:DC:C6	2.54	0.43
5:J:159:DC:H2'	5:J:160:DT:C5	2.53	0.43
1:A:126:LEU:HD22	1:E:113:HIS:CG	2.53	0.43
1:E:129:ARG:HD3	1:E:129:ARG:C	2.39	0.42
1:A:116:ARG:CZ	1:A:120:MSE:HE2	2.48	0.42
1:A:72:ARG:HH22	5:I:50:DC:P	2.42	0.42
3:C:63:LEU:HD13	4:D:45:LEU:HB2	2.01	0.42
2:F:92:ARG:CZ	4:H:100:LEU:HB3	2.50	0.42
4:H:102:LEU:HD22	4:H:106:MSE:HE3	2.01	0.42
5:J:247:DC:H2"	5:J:248:DA:H8	1.84	0.42
2:F:35:ARG:O	2:F:39:ARG:HG2	2.20	0.41
5:I:49:DC:H1'	5:I:50:DC:H5'	2.02	0.41
5:J:215:DC:H2"	5:J:216:DT:H72	2.02	0.41
5:I:95:DA:H2"	5:I:96:DT:H5'	2.02	0.41
4:D:113:GLU:OE2	8:D:202:HOH:O	2.21	0.41
1:E:37:LYS:HA	1:E:38:PRO:HD2	1.95	0.41
4:H:86:ARG:NH2	5:J:187:DA:OP2	2.54	0.41
1:A:61:LEU:HD23	2:B:37:LEU:HD23	2.03	0.41
5:J:184:DT:H2"	5:J:185:DG:N7	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:194:DT:H1'	5:J:195:DC:H5"	2.02	0.41
1:A:69:ARG:NH2	5:J:237:DT:OP2	2.54	0.41
5:J:204:DG:H1'	8:J:404:HOH:O	2.21	0.41
5:I:133:DA:H8	5:I:133:DA:H5"	1.86	0.40
5:J:272:DA:H5"	8:J:416:HOH:O	2.21	0.40
5:I:49:DC:H2"	5:I:50:DC:C6	2.57	0.40

All (2) 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)
8:I:317:HOH:O	8:J:515:HOH:O[1_655]	2.01	0.19
1:A:76:GLN:NE2	5:I:139:DA:OP1[3_746]	2.19	0.01

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	94/139 (68%)	94 (100%)	0	0	100	100
1	E	96/139 (69%)	96 (100%)	0	0	100	100
2	B	76/106 (72%)	74 (97%)	2 (3%)	0	100	100
2	F	83/106 (78%)	81 (98%)	2 (2%)	0	100	100
3	C	106/133 (80%)	104 (98%)	2 (2%)	0	100	100
3	G	103/133 (77%)	101 (98%)	2 (2%)	0	100	100
4	D	91/129 (70%)	90 (99%)	1 (1%)	0	100	100
4	H	90/129 (70%)	89 (99%)	1 (1%)	0	100	100
All	All	739/1014 (73%)	729 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/110 (76%)	82 (98%)	2 (2%)	44	64
1	E	86/110 (78%)	82 (95%)	4 (5%)	22	38
2	B	64/81 (79%)	63 (98%)	1 (2%)	58	76
2	F	71/81 (88%)	70 (99%)	1 (1%)	62	79
3	C	85/99 (86%)	84 (99%)	1 (1%)	67	82
3	G	83/99 (84%)	83 (100%)	0	100	100
4	D	79/102 (78%)	79 (100%)	0	100	100
4	H	78/102 (76%)	78 (100%)	0	100	100
All	All	630/784 (80%)	621 (99%)	9 (1%)	62	79

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	129	ARG
2	B	47	SER
3	C	88	ARG
1	E	56	LYS
1	E	68	GLN
1	E	122	LYS
1	E	129	ARG
2	F	47	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	94/139 (67%)	-0.10	2 (2%)	63	60	23, 35, 58, 70	0
1	E	96/139 (69%)	-0.45	1 (1%)	79	76	18, 28, 44, 68	0
2	B	78/106 (73%)	-0.19	1 (1%)	74	71	23, 33, 46, 73	0
2	F	85/106 (80%)	-0.30	2 (2%)	59	56	19, 25, 41, 84	0
3	C	106/133 (79%)	-0.16	1 (0%)	81	78	21, 30, 54, 78	0
3	G	103/133 (77%)	-0.19	2 (1%)	66	62	22, 33, 54, 68	0
4	D	89/129 (68%)	-0.16	3 (3%)	48	45	20, 28, 51, 62	0
4	H	88/129 (68%)	-0.25	1 (1%)	77	75	21, 31, 49, 62	0
5	I	146/146 (100%)	0.14	3 (2%)	63	60	32, 54, 99, 111	0
5	J	146/146 (100%)	0.17	0	100	100	33, 54, 99, 107	0
All	All	1031/1306 (78%)	-0.12	16 (1%)	70	67	18, 35, 76, 111	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	92	ARG	4.0
1	A	38	PRO	3.6
5	I	1	DA	3.1
4	D	124	ALA	3.1
4	D	103	PRO	3.0
2	F	17	ARG	3.0
1	E	134	ARG	2.9
2	B	24	ASP	2.9
3	C	118	LYS	2.7
4	H	34	LYS	2.5
3	G	105	GLY	2.5
5	I	39	DG	2.5
4	D	32	SER	2.5

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Mol	Chain	Res	Type	RSRZ
5	I	47	DC	2.2
3	G	106	GLY	2.1
1	A	80	THR	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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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
7	MN	I	203	1/1	0.82	0.11	90,90,90,90	0
7	MN	J	303	1/1	0.94	0.06	62,62,62,62	0
7	MN	J	301	1/1	0.96	0.07	75,75,75,75	0
6	CL	A	201	1/1	0.97	0.12	49,49,49,49	0
6	CL	G	201	1/1	0.98	0.05	31,31,31,31	0
6	CL	E	202	1/1	0.98	0.04	47,47,47,47	0
7	MN	J	304	1/1	0.98	0.05	52,52,52,52	0
7	MN	E	201	1/1	0.99	0.02	26,26,26,26	0
7	MN	J	302	1/1	0.99	0.03	41,41,41,41	0
7	MN	I	201	1/1	0.99	0.06	63,63,63,63	0
6	CL	C	201	1/1	0.99	0.03	33,33,33,33	0
7	MN	I	202	1/1	1.00	0.03	44,44,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.