Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 03:04 PM EDT

PDB ID	:	2NQB
Title	:	Drosophila Nucleosome Structure
Authors	:	Luger, K.; Chakravarthy, S.
Deposited on	:	2006-10-30
Resolution	:	2.30 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 (1)) were used in the production of this report:

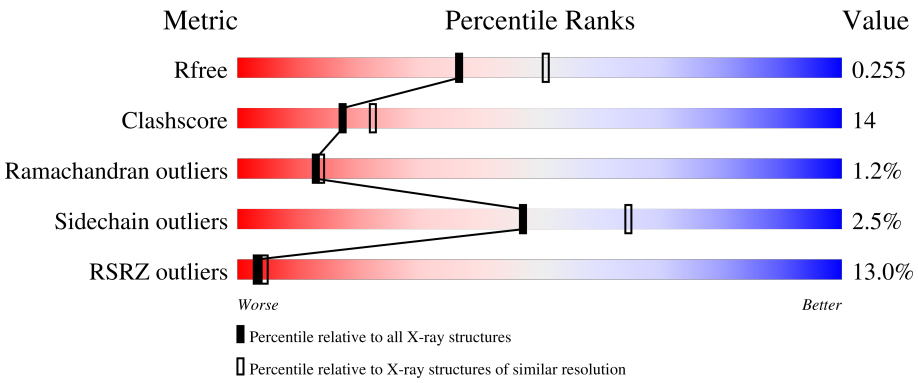
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	I	146	27% 49% 50% •
1	J	146	26% 55% 45%
2	A	135	2% 56% 14% • 27%
2	E	135	4% 61% 10% • 27%
3	B	103	6% 65% 13% • 21%

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Mol	Chain	Length	Quality of chain
3	F	103	15% 58% 21% 17%
4	C	123	4% 63% 20% 14%
4	G	123	5% 63% 21% 15%
5	D	123	8% 63% 13% 23%
5	H	123	8% 63% 11% 24%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12294 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 DNA chain called alpha-satellite DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	I	146	2990	1430	541	874	145	0	0	0
1	J	146	2990	1430	541	874	145	0	0	0

- Molecule 2 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	98	807	508	156	140	3	0	0	0
2	E	98	807	508	156	140	3	0	0	0

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	81	646	407	126	112	1	0	0	0
3	F	86	694	436	140	117	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ILE	-	expression tag	UNP P84040
F	200	ILE	-	expression tag	UNP P84040

- Molecule 4 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	106	812	512	158	141	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	G	105	803	506	156	140	1	0	0	0

- Molecule 5 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	95	751	472	136	141	2	0	0	0
			Total	C	N	O	S			
5	H	93	730	460	130	138	2	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1200	ILE	-	expression tag	UNP P02283
D	1240	THR	LYS	engineered mutation	UNP P02283
H	1400	ILE	-	expression tag	UNP P02283
H	1440	THR	LYS	engineered mutation	UNP P02283

- Molecule 6 is water.

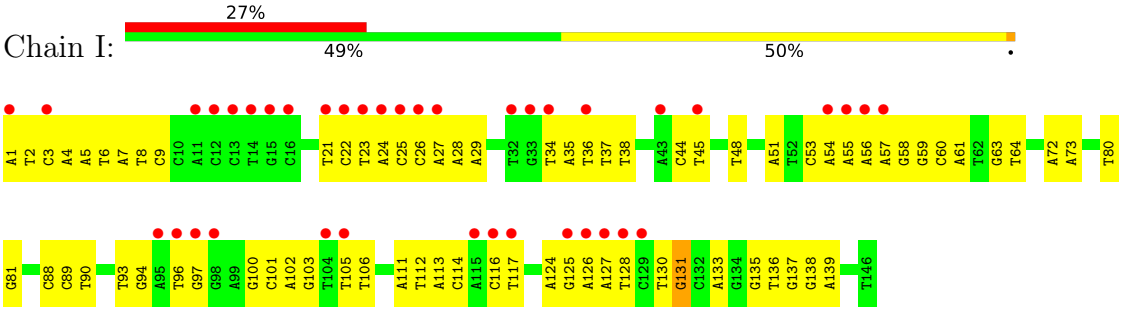
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	I	32	32	32	0	0
			Total	O		
6	J	32	32	32	0	0
			Total	O		
6	A	23	23	23	0	0
			Total	O		
6	B	16	16	16	0	0
			Total	O		
6	C	29	29	29	0	0
			Total	O		
6	D	28	28	28	0	0
			Total	O		
6	E	41	41	41	0	0
			Total	O		
6	F	26	26	26	0	0
			Total	O		
6	G	26	26	26	0	0
			Total	O		
6	H	11	11	11	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.

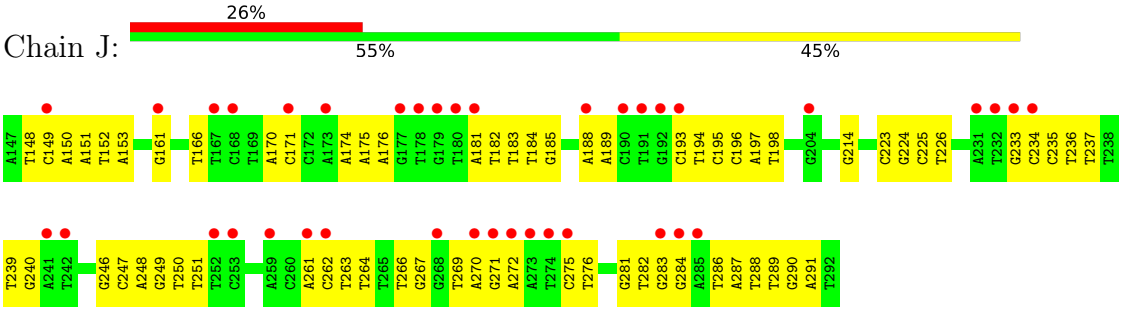
- Molecule 1: alpha-satellite DNA

Chain I:



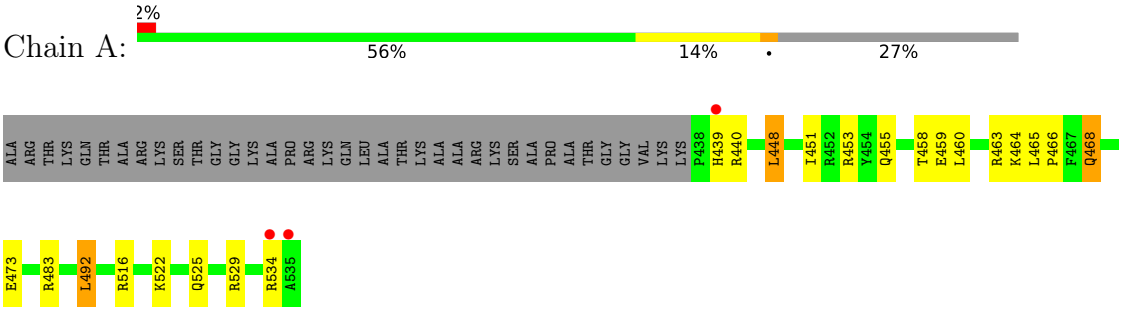
- Molecule 1: alpha-satellite DNA

Chain J:



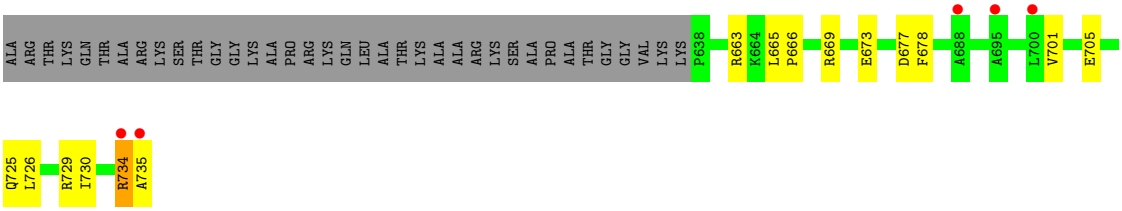
- Molecule 2: Histone H3

Chain A:



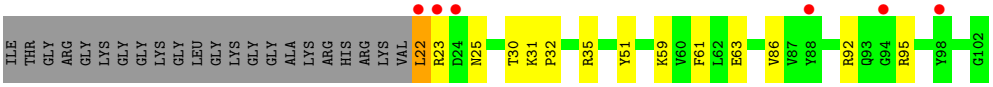
- Molecule 2: Histone H3

Chain E:



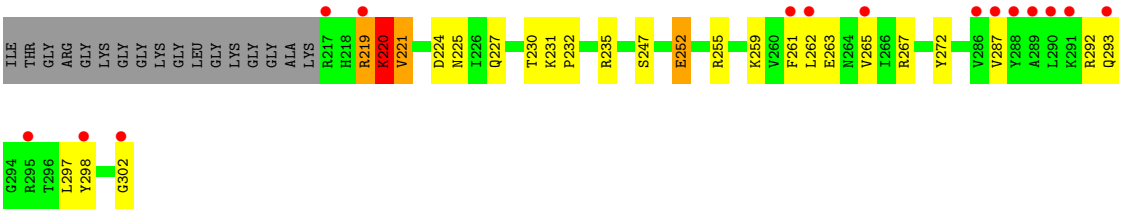
- Molecule 3: Histone H4

Chain B:



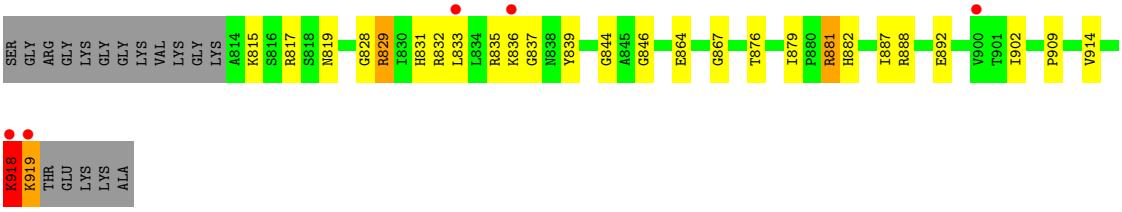
- Molecule 3: Histone H4

Chain F:



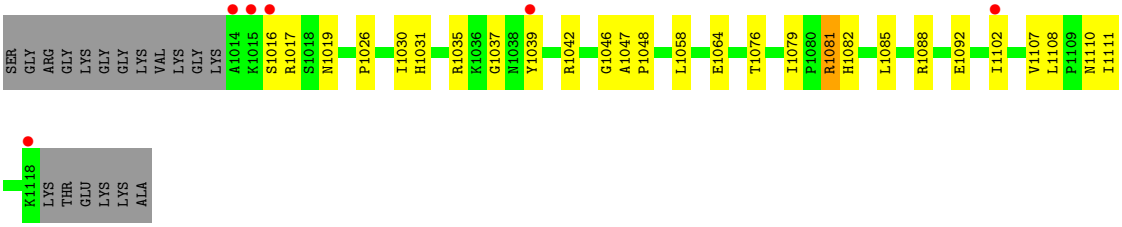
- Molecule 4: Histone H2A

Chain C:



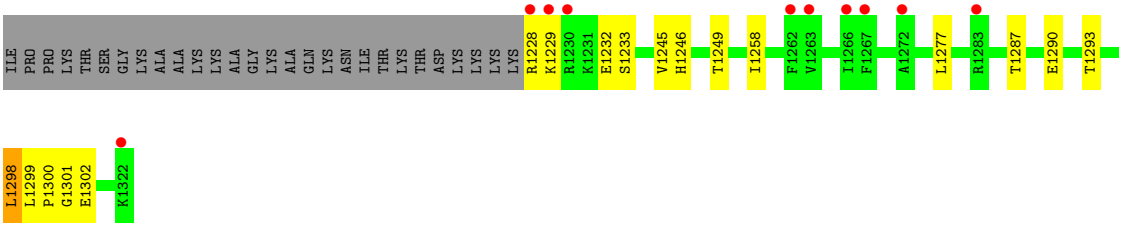
- Molecule 4: Histone H2A

Chain G:



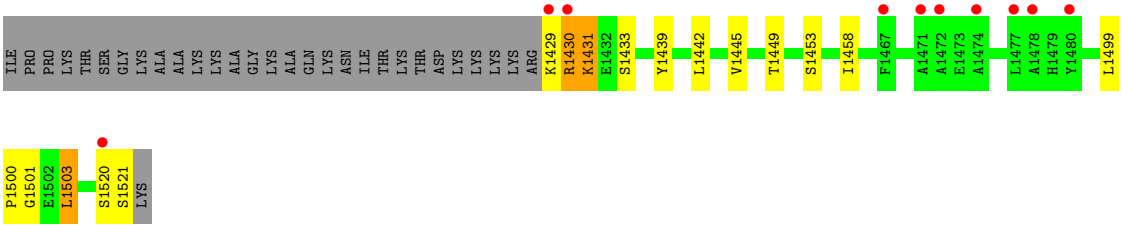
- Molecule 5: Histone H2B

Chain D:



- Molecule 5: Histone H2B

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.14Å 109.58Å 182.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 2.30 48.69 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.1 (99.00-2.30) 95.7 (48.69-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.254 0.224 , 0.255	Depositor DCC
R_{free} test set	2344 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å^2)	47.3	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 65.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12294	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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)

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	I	0.28	0/3354	0.68	0/5175
1	J	0.28	0/3354	0.67	0/5175
2	A	0.35	0/819	0.57	0/1097
2	E	0.44	0/819	0.59	0/1097
3	B	0.39	0/653	0.62	0/873
3	F	0.43	0/702	0.72	1/937 (0.1%)
4	C	0.38	0/822	0.56	0/1108
4	G	0.33	0/813	0.56	0/1097
5	D	0.41	0/762	0.57	0/1023
5	H	0.37	0/741	0.59	0/998
All	All	0.33	0/12839	0.64	1/18580 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1
1	J	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	220	LYS	N-CA-C	-5.07	97.31	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	131	DG	Sidechain
1	J	214	DG	Sidechain

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	I	2990	0	1651	87	0
1	J	2990	0	1651	82	0
2	A	807	0	844	25	0
2	E	807	0	844	13	0
3	B	646	0	687	17	0
3	F	694	0	742	33	0
4	C	812	0	866	32	0
4	G	803	0	853	27	0
5	D	751	0	779	16	0
5	H	730	0	753	12	0
6	A	23	0	0	2	0
6	B	16	0	0	4	0
6	C	29	0	0	8	0
6	D	28	0	0	1	0
6	E	41	0	0	2	0
6	F	26	0	0	12	0
6	G	26	0	0	1	0
6	H	11	0	0	0	0
6	I	32	0	0	16	0
6	J	32	0	0	11	0
All	All	12294	0	9670	299	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 14.

All (299) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:292:ARG:CB	6:F:517:HOH:O	1.65	1.32
1:J:166:DT:C5'	6:J:529:HOH:O	1.65	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:28:DA:O3'	6:I:522:HOH:O	1.63	1.12
3:F:292:ARG:HB2	6:F:517:HOH:O	1.23	1.12
3:B:35:ARG:HB2	6:B:487:HOH:O	1.55	1.03
1:J:237:DT:H4'	2:A:463:ARG:HE	1.23	1.01
4:C:914:VAL:HG13	6:C:513:HOH:O	1.61	0.99
3:F:265:VAL:N	6:F:531:HOH:O	1.78	0.97
1:J:166:DT:O4'	6:J:529:HOH:O	1.81	0.95
1:J:174:DA:H2"	1:J:175:DA:H5"	1.46	0.95
1:I:55:DA:C4	6:I:565:HOH:O	2.18	0.94
1:J:166:DT:H5'	6:J:529:HOH:O	1.40	0.94
4:C:817:ARG:HH12	4:C:831:HIS:HD2	1.13	0.91
1:I:3:DC:H5	1:J:290:DG:H1	1.16	0.91
1:I:59:DG:C6	6:I:525:HOH:O	2.22	0.91
1:I:100:DG:N7	6:I:516:HOH:O	2.02	0.90
1:I:25:DC:H2"	1:I:26:DC:H5'	1.54	0.87
1:I:55:DA:N3	6:I:565:HOH:O	2.06	0.87
3:F:292:ARG:HD3	6:F:517:HOH:O	1.77	0.85
3:B:95:ARG:HD3	6:B:486:HOH:O	1.77	0.85
1:J:261:DA:H2"	1:J:262:DC:H5"	1.59	0.84
3:F:262:LEU:O	6:F:531:HOH:O	1.94	0.84
4:G:1017:ARG:HH12	4:G:1031:HIS:CD2	1.97	0.83
4:G:1017:ARG:HH12	4:G:1031:HIS:HD2	1.23	0.83
1:I:29:DA:P	6:I:522:HOH:O	2.31	0.82
2:E:725:GLN:HG2	2:E:734:ARG:HH12	1.44	0.82
3:F:292:ARG:CD	6:F:517:HOH:O	2.20	0.82
1:I:28:DA:C3'	6:I:522:HOH:O	2.22	0.82
1:J:237:DT:H4'	2:A:463:ARG:NE	1.94	0.80
1:J:149:DC:N4	6:J:587:HOH:O	1.97	0.79
4:C:881:ARG:NH1	6:C:478:HOH:O	2.14	0.79
2:A:460:LEU:HD12	2:A:464:LYS:HE2	1.67	0.76
1:I:58:DG:N3	6:I:525:HOH:O	2.18	0.75
3:F:259:LYS:O	3:F:263:GLU:HG3	1.87	0.75
1:J:261:DA:C2'	1:J:262:DC:H5"	2.17	0.75
1:I:124:DA:H5"	5:H:1429:LYS:NZ	2.02	0.73
3:B:22:LEU:HD23	3:B:22:LEU:N	2.03	0.73
1:I:22:DC:H42	1:J:271:DG:H1	1.36	0.73
1:I:127:DA:H1'	1:I:128:DT:H5'	1.71	0.73
1:J:269:DT:H5"	5:D:1229:LYS:O	1.89	0.73
4:C:909:PRO:HD3	6:C:478:HOH:O	1.89	0.72
1:I:1:DA:H2"	1:I:2:DT:H72	1.72	0.72
1:J:149:DC:C5	6:J:587:HOH:O	2.43	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:55:DA:C1'	6:I:565:HOH:O	2.37	0.72
3:F:292:ARG:CG	6:F:517:HOH:O	2.05	0.72
1:I:3:DC:H2'	1:I:3:DC:O2	1.90	0.71
1:J:166:DT:O5'	6:J:529:HOH:O	1.86	0.71
1:I:93:DT:H2"	1:I:94:DG:H5'	1.72	0.70
1:J:174:DA:C2'	1:J:175:DA:H5"	2.20	0.70
1:J:193:DC:H2"	1:J:194:DT:H72	1.74	0.70
5:D:1287:THR:H	5:D:1290:GLU:HG2	1.57	0.70
3:F:261:PHE:O	6:F:531:HOH:O	2.10	0.69
4:C:817:ARG:HH12	4:C:831:HIS:CD2	2.02	0.69
1:J:261:DA:H2"	1:J:262:DC:C5'	2.22	0.69
4:C:902:ILE:HG23	5:D:1258:ILE:HD13	1.75	0.69
1:I:3:DC:H5	1:J:290:DG:N1	1.90	0.68
3:B:59:LYS:O	3:B:63:GLU:HG3	1.94	0.67
3:F:262:LEU:C	6:F:531:HOH:O	2.29	0.67
2:A:463:ARG:HG2	2:A:463:ARG:HH11	1.59	0.67
5:D:1277:LEU:HD21	5:D:1293:THR:HB	1.75	0.67
4:C:919:LYS:HD3	4:C:919:LYS:N	2.10	0.67
2:E:725:GLN:HG2	2:E:734:ARG:NH1	2.09	0.67
1:I:48:DT:H6	1:I:48:DT:H5'	1.60	0.66
1:J:151:DA:H1'	1:J:152:DT:H5"	1.78	0.66
1:J:246:DG:N7	6:J:304:HOH:O	2.29	0.65
1:I:58:DG:C2	6:I:525:HOH:O	2.49	0.65
5:H:1430:ARG:O	5:H:1431:LYS:HG3	1.97	0.64
1:J:151:DA:H2"	1:J:152:DT:H5'	1.79	0.64
1:I:21:DT:H2"	1:I:22:DC:O5'	1.97	0.63
3:B:22:LEU:O	3:B:23:ARG:HG3	1.99	0.63
1:I:59:DG:N1	6:I:525:HOH:O	2.30	0.63
1:J:275:DC:H2'	1:J:276:DT:H71	1.81	0.62
1:I:28:DA:H1'	1:I:29:DA:H5"	1.82	0.62
4:C:833:LEU:HD23	4:C:836:LYS:HD3	1.81	0.62
2:A:525:GLN:HG2	2:A:534:ARG:CZ	2.29	0.62
1:J:239:DT:H2"	1:J:240:DG:C8	2.34	0.62
1:J:248:DA:H2"	1:J:249:DG:C8	2.34	0.62
3:B:31:LYS:HB3	3:B:32:PRO:HD3	1.81	0.61
4:G:1017:ARG:NH1	4:G:1031:HIS:HD2	1.97	0.61
3:F:298:TYR:HA	3:F:302:GLY:O	2.00	0.61
4:C:844:GLY:C	6:C:499:HOH:O	2.38	0.61
4:C:817:ARG:NH1	4:C:831:HIS:HD2	1.92	0.61
4:G:1035:ARG:HH11	4:G:1035:ARG:HG2	1.65	0.61
1:I:2:DT:H2"	1:I:3:DC:H5'	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:124:DA:H5"	5:H:1429:LYS:HZ3	1.66	0.60
4:C:828:GLY:N	6:C:576:HOH:O	2.35	0.60
1:I:89:DC:H2"	1:I:90:DT:H71	1.83	0.60
4:C:835:ARG:HG2	4:C:835:ARG:HH11	1.66	0.59
4:G:1111:ILE:HD12	4:G:1111:ILE:N	2.17	0.59
1:I:51:DA:H5'	2:A:483:ARG:NH1	2.17	0.59
1:I:124:DA:H2"	1:I:125:DG:C8	2.38	0.59
3:F:224:ASP:OD1	3:F:227:GLN:HG2	2.03	0.59
1:J:239:DT:H2"	1:J:240:DG:H8	1.68	0.59
4:G:1081:ARG:NH2	4:G:1107:VAL:O	2.35	0.59
1:I:5:DA:H2"	1:I:6:DT:C5'	2.34	0.58
3:F:231:LYS:HB3	3:F:232:PRO:HD3	1.84	0.58
4:C:918:LYS:HB2	4:C:918:LYS:NZ	2.18	0.58
2:A:451:ILE:O	2:A:455:GLN:HG3	2.03	0.58
1:I:5:DA:H2"	1:I:6:DT:H5'	1.86	0.58
1:I:28:DA:C2'	1:I:29:DA:H5"	2.33	0.58
3:F:293:GLN:HG3	6:F:480:HOH:O	2.03	0.58
1:I:1:DA:H2"	1:I:2:DT:C7	2.35	0.57
2:E:673:GLU:OE1	3:F:225:ASN:ND2	2.35	0.57
1:J:151:DA:H2"	1:J:152:DT:C5'	2.34	0.57
1:I:28:DA:H2"	1:I:29:DA:H5"	1.86	0.57
2:A:460:LEU:CD1	2:A:464:LYS:HE2	2.35	0.56
1:I:135:DG:H2"	1:I:136:DT:OP2	2.06	0.56
4:C:846:GLY:N	6:C:499:HOH:O	2.35	0.56
1:J:225:DC:H2"	1:J:226:DT:H71	1.88	0.56
4:C:815:LYS:HD3	4:C:819:ASN:HD22	1.70	0.56
2:E:726:LEU:O	2:E:730:ILE:HG12	2.06	0.56
3:F:219:ARG:O	3:F:220:LYS:HB2	2.05	0.56
1:I:126:DA:H1'	1:I:127:DA:H5'	1.88	0.56
1:I:124:DA:H5"	5:H:1429:LYS:HZ2	1.70	0.55
1:J:270:DA:H2"	1:J:271:DG:O5'	2.06	0.55
2:A:463:ARG:HG2	2:A:463:ARG:NH1	2.21	0.55
2:A:465:LEU:HB3	2:A:466:PRO:HD3	1.89	0.55
1:I:1:DA:C2'	1:I:2:DT:H72	2.36	0.55
1:J:235:DC:C6	1:J:236:DT:H72	2.42	0.55
2:A:492:LEU:HD13	3:B:86:VAL:HG13	1.89	0.55
1:I:72:DA:H2"	1:I:73:DA:H5'	1.89	0.55
4:G:1092:GLU:HB3	5:H:1503:LEU:HD22	1.88	0.55
6:A:545:HOH:O	4:G:1111:ILE:HD11	2.08	0.54
3:F:265:VAL:HG23	6:F:426:HOH:O	2.07	0.54
4:C:828:GLY:CA	6:C:576:HOH:O	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:126:DA:H2"	1:I:127:DA:OP2	2.07	0.54
1:I:23:DT:H2"	1:I:24:DA:OP2	2.06	0.53
1:J:175:DA:H2"	1:J:176:DA:C8	2.43	0.53
1:J:286:DT:H2"	1:J:287:DA:O5'	2.07	0.53
4:G:1031:HIS:CD2	4:G:1048:PRO:HG3	2.43	0.53
3:B:92:ARG:NH2	5:D:1298:LEU:HD13	2.24	0.53
4:G:1035:ARG:HG2	4:G:1035:ARG:NH1	2.24	0.53
1:I:138:DG:H2"	1:I:139:DA:OP2	2.09	0.53
1:J:188:DA:H2"	1:J:189:DA:C8	2.44	0.52
1:I:8:DT:H1'	1:I:9:DC:H5'	1.91	0.52
1:I:36:DT:H2"	1:I:37:DT:OP2	2.08	0.52
2:E:665:LEU:HB3	2:E:666:PRO:HD3	1.91	0.52
1:J:225:DC:H2"	1:J:226:DT:C7	2.40	0.52
2:E:701:VAL:O	2:E:705:GLU:HG3	2.09	0.52
1:J:275:DC:C2'	1:J:276:DT:H71	2.40	0.52
2:A:453:ARG:HD2	6:A:548:HOH:O	2.09	0.52
1:I:6:DT:H2"	1:I:7:DA:C8	2.45	0.51
1:J:288:DT:H1'	1:J:289:DT:H5"	1.92	0.51
1:I:112:DT:OP2	4:G:1035:ARG:NH2	2.41	0.51
1:J:170:DA:H2"	1:J:171:DC:OP2	2.10	0.51
1:I:57:DA:H2"	1:I:58:DG:C8	2.46	0.51
1:J:283:DG:H2"	1:J:284:DG:C8	2.45	0.51
1:I:5:DA:H1'	1:I:6:DT:H5"	1.92	0.51
3:B:22:LEU:N	3:B:22:LEU:CD2	2.74	0.51
1:I:55:DA:N9	6:I:565:HOH:O	2.30	0.51
2:A:525:GLN:HG2	2:A:534:ARG:NH2	2.26	0.51
1:I:48:DT:H5'	1:I:48:DT:C6	2.44	0.50
1:J:149:DC:C2'	1:J:150:DA:C8	2.94	0.50
1:J:270:DA:N1	6:J:508:HOH:O	2.35	0.50
4:C:832:ARG:O	4:C:836:LYS:HG2	2.11	0.50
3:F:252:GLU:OE1	3:F:255:ARG:HD2	2.12	0.50
1:I:101:DC:H2"	1:I:102:DA:C8	2.46	0.50
2:A:492:LEU:HD13	3:B:86:VAL:CG1	2.41	0.50
1:I:27:DA:H1'	1:I:28:DA:H5'	1.92	0.50
2:E:677:ASP:OD1	6:E:736:HOH:O	2.18	0.50
2:A:458:THR:HG21	4:G:1081:ARG:HG2	1.93	0.50
1:I:88:DC:H2"	1:I:89:DC:C6	2.46	0.50
1:I:53:DC:N4	1:J:240:DG:H1	2.10	0.49
4:C:864:GLU:OE2	5:D:1245:VAL:HB	2.12	0.49
4:G:1110:ASN:C	4:G:1111:ILE:HD12	2.33	0.49
3:F:230:THR:HB	3:F:232:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:261:DA:H1'	1:J:262:DC:H5"	1.94	0.48
4:G:1026:PRO:O	4:G:1030:ILE:HG12	2.13	0.48
1:I:26:DC:O2	5:D:1228:ARG:NH2	2.43	0.48
1:I:55:DA:H2"	1:I:56:DA:C8	2.49	0.48
1:I:90:DT:OP2	2:E:669:ARG:NH2	2.43	0.48
1:J:193:DC:H2"	1:J:194:DT:C7	2.43	0.48
1:I:53:DC:H42	1:J:240:DG:H1	1.61	0.48
1:I:116:DC:H2"	1:I:117:DT:OP2	2.13	0.48
1:J:250:DT:H2"	1:J:251:DT:H71	1.96	0.47
1:I:28:DA:C1'	1:I:29:DA:H5"	2.44	0.47
5:H:1520:SER:O	5:H:1521:SER:HB3	2.15	0.47
1:J:248:DA:H5"	6:J:348:HOH:O	2.15	0.47
5:D:1277:LEU:HD21	5:D:1293:THR:CB	2.44	0.47
1:J:250:DT:C2'	1:J:251:DT:H71	2.44	0.47
1:J:184:DT:H2"	1:J:185:DG:N7	2.29	0.47
1:I:130:DT:H2"	1:I:131:DG:N7	2.30	0.46
2:E:729:ARG:O	2:E:735:ALA:HB2	2.15	0.46
1:I:44:DC:H2"	1:I:45:DT:OP2	2.15	0.46
4:C:892:GLU:HG3	6:C:429:HOH:O	2.15	0.46
1:J:246:DG:H2"	1:J:247:DC:C5	2.50	0.46
3:B:61:PHE:HE1	6:B:486:HOH:O	1.98	0.46
3:F:287:VAL:HG11	3:F:302:GLY:HA3	1.98	0.46
1:I:80:DT:OP2	6:I:341:HOH:O	2.20	0.46
4:C:835:ARG:HG2	4:C:835:ARG:NH1	2.31	0.46
1:I:22:DC:H2'	1:I:23:DT:C5	2.51	0.46
3:F:252:GLU:OE1	3:F:252:GLU:HA	2.16	0.46
1:J:261:DA:C1'	1:J:262:DC:H5"	2.46	0.45
2:A:525:GLN:HG2	2:A:534:ARG:NH1	2.32	0.45
4:C:918:LYS:HB2	4:C:918:LYS:HZ3	1.81	0.45
3:F:220:LYS:O	3:F:221:VAL:C	2.55	0.45
4:G:1079:ILE:HG12	4:G:1082:HIS:CE1	2.51	0.45
1:J:195:DC:H1'	1:J:196:DC:C6	2.51	0.45
2:A:529:ARG:HA	2:A:534:ARG:HB3	1.97	0.45
5:H:1439:TYR:O	5:H:1442:LEU:HB3	2.16	0.45
1:J:149:DC:H2"	1:J:150:DA:C8	2.51	0.45
1:J:233:DG:H2"	1:J:234:DC:OP2	2.15	0.45
4:G:1076:THR:O	5:H:1449:THR:HG23	2.16	0.45
1:J:152:DT:H2"	1:J:153:DA:C8	2.52	0.45
1:J:235:DC:H2"	1:J:236:DT:OP2	2.17	0.45
1:J:174:DA:H4'	5:H:1430:ARG:HD2	1.99	0.44
1:J:181:DA:H2"	1:J:182:DT:OP2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:60:DC:H2"	1:I:61:DA:C8	2.52	0.44
1:J:148:DT:H2"	1:J:149:DC:O5'	2.17	0.44
1:I:81:DG:P	3:F:235:ARG:HH12	2.41	0.44
1:J:271:DG:C2	1:J:272:DA:N6	2.85	0.44
4:C:892:GLU:OE1	5:D:1302:GLU:HB3	2.17	0.44
2:A:516:ARG:NH2	2:A:522:LYS:HE3	2.32	0.44
4:C:829:ARG:NH2	5:D:1233:SER:O	2.51	0.44
3:F:292:ARG:HB3	3:F:292:ARG:CZ	2.48	0.43
4:G:1064:GLU:OE1	5:H:1445:VAL:HG13	2.18	0.43
2:E:678:PHE:CE1	3:F:267:ARG:HG3	2.53	0.43
1:J:271:DG:H1'	1:J:272:DA:N7	2.34	0.43
1:J:281:DG:H2"	1:J:282:DT:O5'	2.18	0.43
2:A:468:GLN:HE21	2:A:468:GLN:HB2	1.48	0.43
3:B:30:THR:HB	3:B:32:PRO:HD2	2.01	0.43
1:I:3:DC:H2"	1:I:4:DA:C8	2.53	0.43
3:F:297:LEU:O	3:F:302:GLY:O	2.36	0.43
1:I:136:DT:H1'	1:I:137:DG:H5'	2.01	0.43
4:G:1016:SER:OG	4:G:1019:ASN:ND2	2.52	0.43
4:G:1102:ILE:HG23	5:H:1458:ILE:HD13	2.00	0.43
1:J:246:DG:H5"	2:A:483:ARG:HD2	2.00	0.43
1:J:263:DT:C2'	1:J:264:DT:H71	2.48	0.43
4:G:1047:ALA:N	4:G:1048:PRO:HD2	2.34	0.43
1:J:184:DT:H4'	4:G:1042:ARG:NH2	2.34	0.43
1:I:54:DA:N3	6:I:565:HOH:O	2.50	0.43
1:I:125:DG:H2"	1:I:126:DA:OP2	2.19	0.43
1:I:133:DA:C2	1:J:161:DG:N2	2.86	0.43
1:J:193:DC:C2'	1:J:194:DT:H72	2.46	0.43
1:J:266:DT:H2"	1:J:267:DG:C8	2.54	0.43
1:J:290:DG:H2"	1:J:291:DA:OP2	2.19	0.43
4:C:887:ILE:HD12	4:C:902:ILE:HD11	2.01	0.43
4:G:1058:LEU:HD23	4:G:1058:LEU:HA	1.91	0.43
1:I:2:DT:H1'	1:I:3:DC:H5"	2.01	0.42
1:I:113:DA:H2"	1:I:114:DC:O5'	2.19	0.42
4:C:837:GLY:HA3	4:C:839:TYR:CE1	2.55	0.42
5:D:1277:LEU:HD21	5:D:1293:THR:CG2	2.48	0.42
1:I:96:DT:H2"	1:I:97:DG:C8	2.55	0.42
4:C:879:ILE:HG12	4:C:882:HIS:CE1	2.55	0.42
6:E:770:HOH:O	3:F:261:PHE:HD1	2.02	0.42
1:J:262:DC:C2'	1:J:263:DT:H71	2.50	0.42
3:F:272:TYR:OH	3:F:292:ARG:HD2	2.19	0.42
1:I:22:DC:N3	1:J:271:DG:N2	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:102:DA:H2"	1:I:103:DG:OP2	2.20	0.42
2:A:458:THR:CG2	4:G:1081:ARG:HG2	2.50	0.42
1:I:34:DT:H2"	1:I:35:DA:O5'	2.19	0.42
4:C:919:LYS:HD3	4:C:919:LYS:H	1.81	0.42
2:E:663:ARG:HA	2:E:663:ARG:NE	2.35	0.42
1:J:249:DG:H2"	1:J:250:DT:OP2	2.18	0.42
5:D:1299:LEU:HA	5:D:1300:PRO:HD3	1.76	0.42
5:D:1300:PRO:HG3	6:D:479:HOH:O	2.20	0.42
3:F:230:THR:CB	3:F:232:PRO:HD2	2.50	0.42
1:I:111:DA:H2"	1:I:112:DT:OP2	2.20	0.42
1:J:182:DT:H2"	1:J:183:DT:OP2	2.20	0.42
1:I:126:DA:H1'	1:I:127:DA:C5'	2.50	0.42
1:J:270:DA:N6	6:J:508:HOH:O	2.45	0.42
3:B:35:ARG:NE	6:B:487:HOH:O	2.48	0.42
4:G:1037:GLY:HA3	4:G:1039:TYR:CE1	2.55	0.42
1:I:25:DC:H2"	1:I:26:DC:C5'	2.39	0.41
1:I:59:DG:C5	6:I:525:HOH:O	2.66	0.41
1:J:149:DC:H2'	1:J:150:DA:C8	2.54	0.41
3:F:297:LEU:O	3:F:302:GLY:C	2.58	0.41
4:G:1111:ILE:N	4:G:1111:ILE:CD1	2.83	0.41
1:I:105:DT:H2"	1:I:106:DT:OP2	2.20	0.41
1:J:166:DT:P	6:J:529:HOH:O	2.70	0.41
1:J:197:DA:H1'	1:J:198:DT:H5'	2.02	0.41
4:G:1085:LEU:HD23	4:G:1108:LEU:HD23	2.01	0.41
1:I:136:DT:H2"	1:I:137:DG:O5'	2.20	0.41
1:J:237:DT:P	3:B:23:ARG:HH12	2.42	0.41
5:H:1499:LEU:HA	5:H:1500:PRO:HD3	1.90	0.41
2:A:448:LEU:HD12	2:A:448:LEU:HA	1.89	0.41
2:E:663:ARG:HA	2:E:663:ARG:HE	1.85	0.41
1:J:237:DT:H4'	2:A:463:ARG:CZ	2.49	0.41
3:F:231:LYS:N	3:F:232:PRO:CD	2.84	0.41
1:I:7:DA:C2	1:J:287:DA:C2	3.09	0.41
1:I:37:DT:H1'	1:I:38:DT:H5'	2.03	0.41
1:J:174:DA:H2"	1:J:175:DA:C5'	2.33	0.41
1:J:223:DC:H2"	1:J:224:DG:N7	2.36	0.41
3:B:31:LYS:HG3	3:B:51:TYR:CE1	2.55	0.41
2:E:729:ARG:HG3	2:E:735:ALA:HA	2.02	0.41
3:F:265:VAL:CB	6:F:531:HOH:O	2.69	0.41
1:I:63:DG:H2"	1:I:64:DT:OP2	2.20	0.41
1:J:248:DA:H2"	1:J:249:DG:H8	1.82	0.41
2:A:439:HIS:ND1	2:A:440:ARG:N	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:832:ARG:NH2	5:D:1232:GLU:OE1	2.50	0.41
4:C:881:ARG:O	4:C:881:ARG:HG3	2.19	0.40
1:I:80:DT:OP1	3:F:247:SER:HB2	2.22	0.40
4:C:888:ARG:HA	4:C:888:ARG:HD3	1.88	0.40
4:G:1046:GLY:N	6:G:518:HOH:O	2.54	0.40
1:I:5:DA:H2"	6:I:402:HOH:O	2.21	0.40
1:J:237:DT:OP1	3:B:23:ARG:NH1	2.44	0.40
2:A:473:GLU:OE1	3:B:25:ASN:HB2	2.21	0.40
4:C:867:GLY:HA3	5:D:1246:HIS:CD2	2.55	0.40
4:C:876:THR:O	5:D:1249:THR:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	96/135 (71%)	95 (99%)	1 (1%)	0	100	100
2	E	96/135 (71%)	95 (99%)	0	1 (1%)	15	17
3	B	79/103 (77%)	77 (98%)	2 (2%)	0	100	100
3	F	84/103 (82%)	79 (94%)	2 (2%)	3 (4%)	3	2
4	C	104/123 (85%)	100 (96%)	3 (3%)	1 (1%)	15	17
4	G	103/123 (84%)	101 (98%)	2 (2%)	0	100	100
5	D	93/123 (76%)	92 (99%)	0	1 (1%)	14	15
5	H	91/123 (74%)	88 (97%)	0	3 (3%)	4	2
All	All	746/968 (77%)	727 (98%)	10 (1%)	9 (1%)	13	14

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	1301	GLY
2	E	734	ARG
3	F	219	ARG
3	F	220	LYS
5	H	1430	ARG
3	F	221	VAL
5	H	1501	GLY
4	C	918	LYS
5	H	1431	LYS

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	
2	A	85/110 (77%)	81 (95%)	4 (5%)	26	37
2	E	85/110 (77%)	85 (100%)	0	100	100
3	B	66/79 (84%)	65 (98%)	1 (2%)	65	79
3	F	71/79 (90%)	70 (99%)	1 (1%)	67	81
4	C	82/93 (88%)	78 (95%)	4 (5%)	25	35
4	G	81/93 (87%)	79 (98%)	2 (2%)	47	65
5	D	82/104 (79%)	81 (99%)	1 (1%)	71	84
5	H	80/104 (77%)	77 (96%)	3 (4%)	33	47
All	All	632/772 (82%)	616 (98%)	16 (2%)	47	65

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	448	LEU
2	A	459	GLU
2	A	468	GLN
2	A	492	LEU
3	B	22	LEU
4	C	829	ARG
4	C	881	ARG

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Mol	Chain	Res	Type
4	C	918	LYS
4	C	919	LYS
5	D	1298	LEU
3	F	252	GLU
4	G	1081	ARG
4	G	1088	ARG
5	H	1433	SER
5	H	1453	SER
5	H	1503	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	819	ASN
4	C	831	HIS
5	D	1292	GLN
2	E	668	GLN
4	G	1019	ASN
4	G	1031	HIS
5	H	1492	GLN

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 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 (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	I	146/146 (100%)	1.34	39 (26%)	0	0	42, 98, 166, 185	0
1	J	146/146 (100%)	1.36	38 (26%)	0	0	49, 102, 158, 200	0
2	A	98/135 (72%)	0.77	3 (3%)	49	56	30, 48, 73, 124	0
2	E	98/135 (72%)	0.86	5 (5%)	28	35	27, 39, 65, 130	0
3	B	81/103 (78%)	0.84	6 (7%)	14	19	31, 44, 71, 161	0
3	F	86/103 (83%)	1.31	15 (17%)	1	1	25, 39, 70, 163	0
4	C	106/123 (86%)	0.81	5 (4%)	31	38	28, 42, 78, 150	0
4	G	105/123 (85%)	0.67	6 (5%)	23	30	35, 48, 89, 138	0
5	D	95/123 (77%)	0.93	10 (10%)	6	8	28, 41, 83, 119	0
5	H	93/123 (75%)	0.93	10 (10%)	5	8	32, 46, 86, 133	0
All	All	1054/1260 (83%)	1.01	137 (12%)	3	4	25, 51, 135, 200	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	273	DA	9.7
2	A	535	ALA	7.8
3	B	23	ARG	7.8
4	G	1014	ALA	7.6
1	J	272	DA	7.3
1	J	274	DT	7.0
3	F	219	ARG	5.8
1	I	115	DA	5.5
1	I	24	DA	5.4
3	B	22	LEU	5.4
2	A	439	HIS	5.2
2	E	735	ALA	5.0
1	I	56	DA	5.0

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Mol	Chain	Res	Type	RSRZ
3	F	302	GLY	4.9
1	I	15	DG	4.8
1	J	271	DG	4.6
1	J	275	DC	4.6
1	I	116	DC	4.5
1	I	14	DT	4.4
1	I	125	DG	4.4
1	I	127	DA	4.4
1	J	270	DA	4.3
1	J	233	DG	4.1
1	I	25	DC	3.9
4	C	918	LYS	3.8
1	I	128	DT	3.8
1	J	285	DA	3.8
2	E	734	ARG	3.8
4	C	919	LYS	3.8
1	I	126	DA	3.7
1	J	179	DG	3.7
5	D	1228	ARG	3.7
1	I	104	DT	3.7
1	J	171	DC	3.7
5	D	1229	LYS	3.6
1	J	168	DC	3.6
1	I	36	DT	3.6
1	I	57	DA	3.6
1	J	253	DC	3.5
4	G	1015	LYS	3.5
1	I	45	DT	3.4
1	J	241	DA	3.4
1	I	129	DC	3.4
1	I	3	DC	3.3
1	I	23	DT	3.3
1	I	22	DC	3.3
1	I	26	DC	3.3
5	D	1230	ARG	3.2
1	I	21	DT	3.2
5	H	1429	LYS	3.2
1	I	97	DG	3.1
1	I	16	DC	3.1
5	H	1520	SER	3.1
2	A	534	ARG	3.1
3	F	289	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	290	LEU	2.9
3	F	217	ARG	2.9
1	I	34	DT	2.9
1	J	167	DT	2.9
1	J	161	DG	2.8
1	J	261	DA	2.8
1	J	284	DG	2.8
4	C	833	LEU	2.8
1	I	13	DC	2.8
1	J	204	DG	2.8
5	D	1267	PHE	2.8
3	F	287	VAL	2.8
1	J	180	DT	2.8
1	I	96	DT	2.8
5	H	1480	TYR	2.7
1	J	262	DC	2.7
1	I	1	DA	2.7
3	B	94	GLY	2.7
1	I	43	DA	2.6
1	J	232	DT	2.6
3	F	291	LYS	2.6
5	H	1472	ALA	2.6
1	I	54	DA	2.5
1	J	178	DT	2.5
3	F	288	TYR	2.5
1	I	55	DA	2.5
4	G	1102	ILE	2.5
5	H	1467	PHE	2.5
4	G	1118	LYS	2.5
2	E	695	ALA	2.5
1	I	95	DA	2.5
1	J	283	DG	2.4
5	D	1262	PHE	2.4
1	J	231	DA	2.4
5	D	1263	VAL	2.4
5	D	1283	ARG	2.4
1	I	33	DG	2.4
1	I	98	DG	2.4
5	D	1266	ILE	2.4
2	E	700	LEU	2.3
1	J	193	DC	2.3
1	I	11	DA	2.3

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Mol	Chain	Res	Type	RSRZ
3	B	98	TYR	2.3
3	F	293	GLN	2.3
3	F	265	VAL	2.3
3	F	286	VAL	2.3
1	J	191	DT	2.3
5	H	1474	ALA	2.3
1	I	117	DT	2.2
5	D	1322	LYS	2.2
2	E	688	ALA	2.2
4	G	1016	SER	2.2
5	H	1471	ALA	2.2
1	I	105	DT	2.2
1	I	27	DA	2.2
3	F	262	LEU	2.2
1	I	12	DC	2.2
5	H	1478	ALA	2.2
1	J	268	DG	2.2
5	H	1430	ARG	2.1
1	J	190	DC	2.1
3	F	261	PHE	2.1
5	D	1272	ALA	2.1
1	J	177	DG	2.1
1	J	173	DA	2.1
1	J	188	DA	2.1
1	J	234	DC	2.1
3	B	88	TYR	2.1
1	I	32	DT	2.1
1	J	192	DG	2.1
1	J	259	DA	2.1
4	C	836	LYS	2.1
4	G	1039	TYR	2.1
1	J	252	DT	2.1
4	C	900	VAL	2.1
1	J	149	DC	2.0
5	H	1477	LEU	2.0
1	J	242	DT	2.0
1	J	181	DA	2.0
3	F	295	ARG	2.0
3	F	298	TYR	2.0
3	B	24	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.