



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:21 PM UTC

PDB ID : 2NQB / pdb_00002nqb
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 ⓘ 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

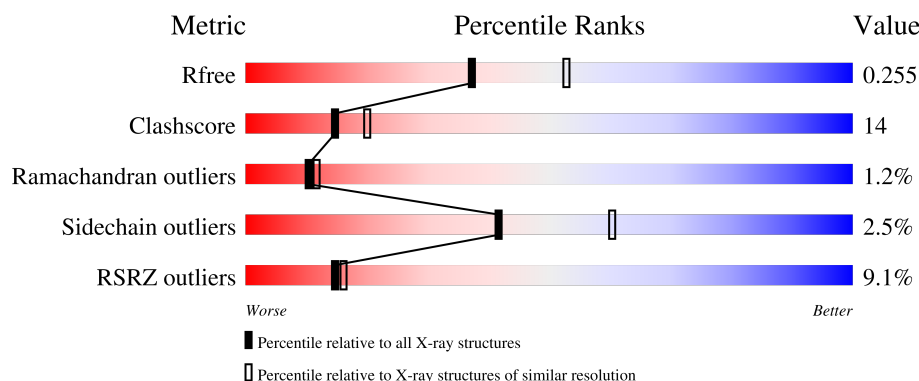
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	19% 49% 50% .
1	J	146	18% 55% 45%
2	A	135	4% 55% 15% . 27%
2	E	135	4% 59% 13% . 27%
3	B	103	3% 64% 11% . 21%

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Mol	Chain	Length	Quality of chain
3	F	103	
4	C	123	
4	G	123	
5	D	123	
5	H	123	

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
1	I	146	Total	C	N	O	P	0	0	0
			2990	1430	541	874	145			
1	J	146	Total	C	N	O	P	0	0	0
			2990	1430	541	874	145			

- Molecule 2 is a protein called Histone H3.

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

- Molecule 3 is a protein called Histone H4.

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

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
4	C	106	Total	C	N	O	S	0	0	0
			812	512	158	141	1			

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

- Molecule 5 is a protein called Histone H2B.

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

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

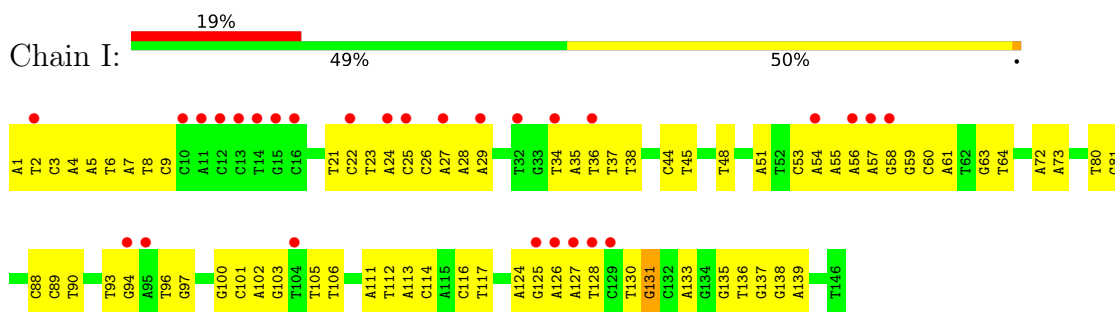
- Molecule 6 is water.

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

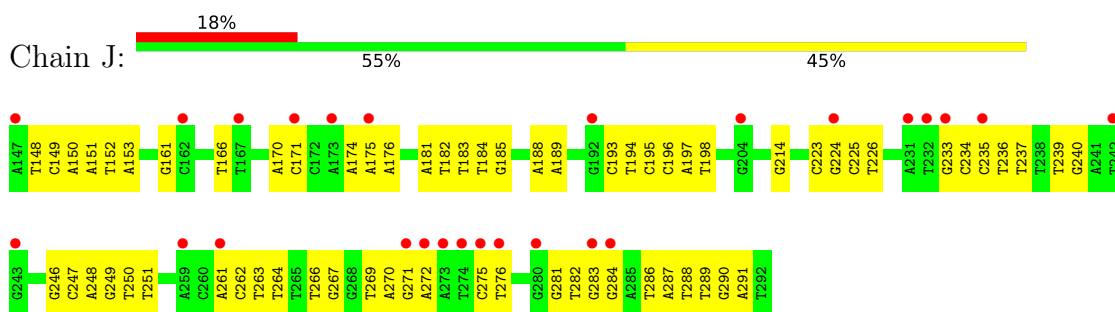
3 Residue-property plots

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.

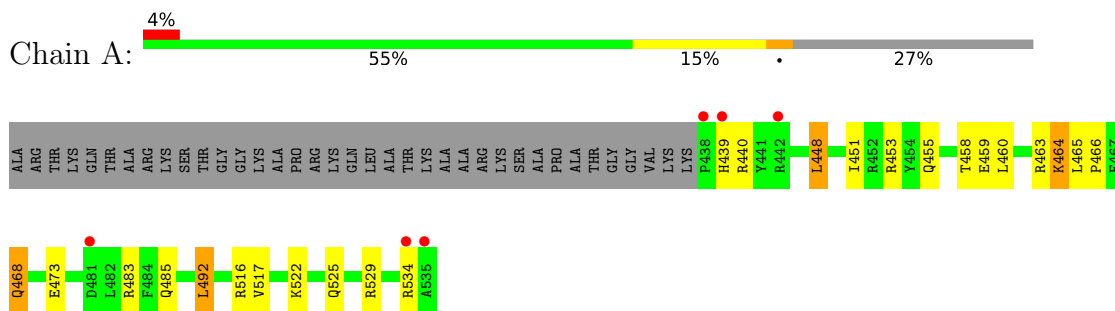
• Molecule 1: alpha-satellite DNA



• Molecule 1: alpha-satellite DNA



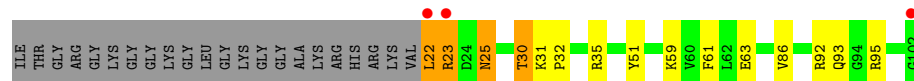
• Molecule 2: Histone H3



• Molecule 2: Histone H3



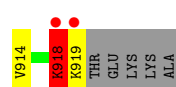
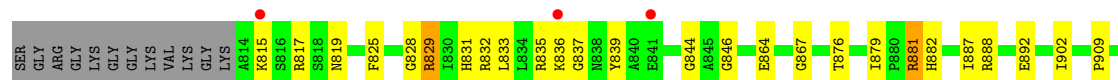
- Molecule 3: Histone H4



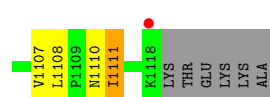
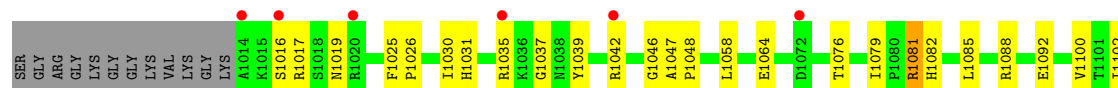
- Molecule 3: Histone H4



- Molecule 4: Histone H2A

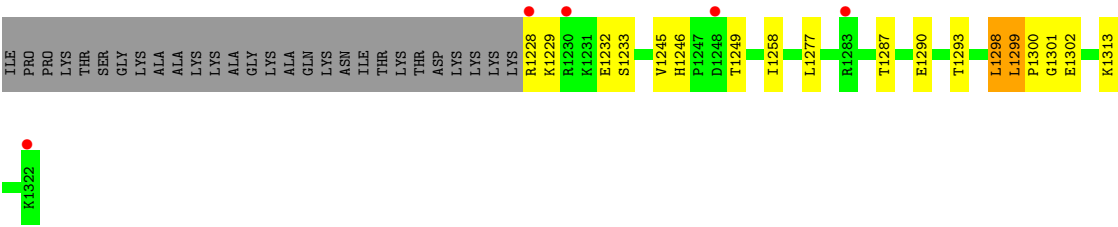


- Molecule 4: Histone H2A

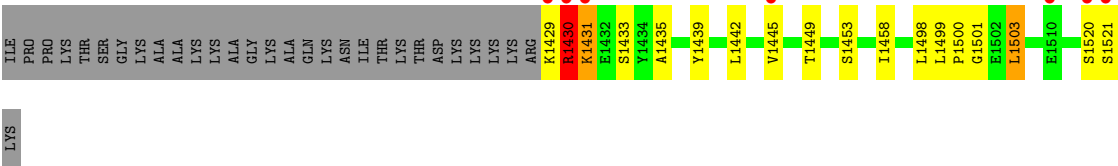


- Molecule 5: Histone H2B





● Molecule 5: Histone H2B



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4 Data and refinement statistics

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 93.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.1 (99.00-2.30) 96.1 (93.88-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.35 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.26	0/3354	0.60	0/5175
1	J	0.27	0/3354	0.61	0/5175
2	A	0.45	0/819	0.90	3/1097 (0.3%)
2	E	0.53	0/819	0.90	3/1097 (0.3%)
3	B	0.48	0/653	0.96	4/873 (0.5%)
3	F	0.54	0/702	1.05	5/937 (0.5%)
4	C	0.50	0/822	0.91	2/1108 (0.2%)
4	G	0.45	0/813	0.90	3/1097 (0.3%)
5	D	0.52	0/762	0.88	2/1023 (0.2%)
5	H	0.46	0/741	0.87	3/998 (0.3%)
All	All	0.39	0/12839	0.76	25/18580 (0.1%)

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 (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	301	GLY	N-CA-C	-9.15	102.69	115.32
2	A	485	GLN	N-CA-C	-7.36	100.12	110.50
4	C	825	PHE	CA-C-N	6.70	128.22	119.84
4	C	825	PHE	C-N-CA	6.70	128.22	119.84
2	A	517	VAL	N-CA-C	-6.69	106.78	113.20
3	F	218	HIS	N-CA-C	6.58	117.27	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	664	LYS	N-CA-C	6.49	118.23	111.03
2	E	717	VAL	N-CA-C	-6.44	107.02	113.20
3	B	23	ARG	N-CA-C	6.42	118.06	107.73
2	E	685	GLN	N-CA-C	-6.40	101.48	110.50
3	F	220	LYS	N-CA-C	-6.33	97.31	110.80
3	B	25	ASN	N-CA-C	6.17	118.52	111.11
2	A	464	LYS	N-CA-C	6.13	118.50	111.02
3	B	93	GLN	N-CA-C	-5.73	106.05	113.16
5	H	1435	ALA	N-CA-C	5.62	117.86	111.11
3	B	30	THR	N-CA-C	5.61	118.12	110.55
4	G	1100	VAL	N-CA-C	5.61	117.07	108.71
4	G	1025	PHE	CA-C-N	5.59	126.83	119.84
4	G	1025	PHE	C-N-CA	5.59	126.83	119.84
5	H	1430	ARG	N-CA-C	5.48	122.47	110.80
5	H	1498	LEU	N-CA-C	5.44	120.02	112.90
3	F	230	THR	N-CA-C	5.33	117.57	110.53
3	F	228	GLY	N-CA-C	-5.22	107.85	114.16
5	D	1299	LEU	CA-C-N	5.08	125.48	119.99
5	D	1299	LEU	C-N-CA	5.08	125.48	119.99

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 ⓘ

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	14	0
3	B	646	0	687	17	0
3	F	694	0	742	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	812	0	866	32	0
4	G	803	0	853	27	0
5	D	751	0	779	17	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	2	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	301	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 (301) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:262:LEU:C	6:F:531:HOH:O	2.29	0.72
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:C:844:GLY:C	6:C:499:HOH:O	2.38	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:G:1110:ASN:C	4:G:1111:ILE:HD12	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:220:LYS:O	3:F:221:VAL:C	2.55	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
3:F:230:THR:HB	3:F:232:PRO:HD2	1.95	0.49
1:J:261:DA:H1'	1:J:262:DC:H5''	1.94	0.48
2:E:664:LYS:NZ	2:E:690:MET:HE1	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:297:LEU:O	3:F:302:GLY:C	2.58	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:D:1313:LYS:NZ	6:D:495:HOH:O	2.52	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	96/135 (71%)	95 (99%)	1 (1%)	0	100	100
2	E	96/135 (71%)	95 (99%)	0	1 (1%)	12	15
3	B	79/103 (77%)	77 (98%)	2 (2%)	0	100	100
3	F	84/103 (82%)	79 (94%)	2 (2%)	3 (4%)	2	1
4	C	104/123 (85%)	100 (96%)	3 (3%)	1 (1%)	12	15
4	G	103/123 (84%)	101 (98%)	2 (2%)	0	100	100
5	D	93/123 (76%)	92 (99%)	0	1 (1%)	11	13
5	H	91/123 (74%)	88 (97%)	0	3 (3%)	3	2
All	All	746/968 (77%)	727 (98%)	10 (1%)	9 (1%)	10	12

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

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%)	23	35
2	E	85/110 (77%)	85 (100%)	0	100	100
3	B	66/79 (84%)	65 (98%)	1 (2%)	57	75
3	F	71/79 (90%)	70 (99%)	1 (1%)	59	76
4	C	82/93 (88%)	79 (96%)	3 (4%)	30	45
4	G	81/93 (87%)	78 (96%)	3 (4%)	30	45
5	D	82/104 (79%)	81 (99%)	1 (1%)	63	79
5	H	80/104 (77%)	77 (96%)	3 (4%)	29	44
All	All	632/772 (82%)	616 (98%)	16 (2%)	42	60

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
4	C	918	LYS
5	D	1298	LEU
3	F	252	GLU
4	G	1081	ARG
4	G	1088	ARG
4	G	1111	ILE
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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	476	GLN
4	C	819	ASN
4	C	831	HIS
5	D	1292	GLN

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Mol	Chain	Res	Type
4	G	1019	ASN
4	G	1024	GLN
4	G	1031	HIS
4	G	1068	ASN
5	H	1444	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 oligosaccharides 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, 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%)	1.17	28 (19%) 3 3	42, 98, 166, 185	0
1	J	146/146 (100%)	1.26	26 (17%) 4 4	49, 102, 158, 200	0
2	A	98/135 (72%)	0.38	6 (6%) 27 29	30, 48, 73, 124	0
2	E	98/135 (72%)	0.05	5 (5%) 33 35	27, 39, 65, 130	0
3	B	81/103 (78%)	0.18	3 (3%) 45 48	31, 44, 71, 161	0
3	F	86/103 (83%)	0.20	4 (4%) 36 38	25, 39, 70, 163	0
4	C	106/123 (86%)	0.11	5 (4%) 36 38	28, 42, 78, 150	0
4	G	105/123 (85%)	0.38	7 (6%) 24 26	35, 48, 89, 138	0
5	D	95/123 (77%)	0.24	5 (5%) 32 34	28, 41, 83, 119	0
5	H	93/123 (75%)	0.40	7 (7%) 20 22	32, 46, 86, 133	0
All	All	1054/1260 (83%)	0.51	96 (9%) 15 16	25, 51, 135, 200	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	535	ALA	6.8
3	F	302	GLY	6.7
2	A	438	PRO	6.5
3	F	219	ARG	4.6
5	H	1520	SER	4.2
5	H	1521	SER	3.7
2	E	638	PRO	3.5
3	F	220	LYS	3.4
1	J	271	DG	3.4
2	E	735	ALA	3.4
1	J	173	DA	3.3
3	B	23	ARG	3.3
1	J	274	DT	3.3

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Mol	Chain	Res	Type	RSRZ
5	D	1230	ARG	3.3
2	A	439	HIS	3.2
1	J	204	DG	3.2
1	J	273	DA	3.2
5	D	1248	ASP	3.2
1	I	15	DG	3.1
3	B	22	LEU	3.1
1	J	232	DT	3.1
1	I	11	DA	3.1
1	J	233	DG	3.1
5	D	1322	LYS	3.0
1	I	10	DC	3.0
3	B	102	GLY	3.0
4	G	1072	ASP	2.9
2	A	481	ASP	2.9
1	I	125	DG	2.9
1	J	243	DG	2.8
1	I	54	DA	2.8
1	J	275	DC	2.8
4	G	1035	ARG	2.8
1	I	57	DA	2.7
2	A	442	ARG	2.7
4	G	1014	ALA	2.6
1	I	58	DG	2.6
2	A	534	ARG	2.6
4	C	919	LYS	2.6
1	J	175	DA	2.6
2	E	639	HIS	2.6
1	J	283	DG	2.5
1	I	13	DC	2.5
5	D	1283	ARG	2.5
1	J	242	DT	2.5
4	C	918	LYS	2.5
5	H	1429	LYS	2.5
1	I	27	DA	2.5
1	J	261	DA	2.5
5	H	1430	ARG	2.4
1	I	126	DA	2.4
5	H	1445	VAL	2.4
4	C	836	LYS	2.4
1	J	162	DC	2.4
1	I	24	DA	2.4

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Mol	Chain	Res	Type	RSRZ
4	G	1020	ARG	2.4
4	C	815	LYS	2.4
1	I	12	DC	2.4
2	E	734	ARG	2.4
3	F	217	ARG	2.4
4	G	1042	ARG	2.4
5	D	1228	ARG	2.4
1	J	224	DG	2.3
1	J	272	DA	2.3
1	I	14	DT	2.3
4	G	1016	SER	2.3
1	J	280	DG	2.3
1	J	284	DG	2.3
2	E	678	PHE	2.3
1	I	29	DA	2.3
1	J	231	DA	2.3
1	I	16	DC	2.2
1	I	127	DA	2.2
5	H	1510	GLU	2.2
1	I	104	DT	2.2
1	I	94	DG	2.2
4	C	841	GLU	2.2
1	I	34	DT	2.2
5	H	1431	LYS	2.2
1	I	36	DT	2.1
1	I	128	DT	2.1
1	J	192	DG	2.1
1	I	2	DT	2.1
1	J	167	DT	2.1
1	J	171	DC	2.1
1	J	276	DT	2.1
1	I	95	DA	2.1
1	J	147	DA	2.1
1	J	259	DA	2.1
1	I	129	DC	2.1
1	J	235	DC	2.1
1	I	56	DA	2.0
1	I	22	DC	2.0
1	I	25	DC	2.0
4	G	1118	LYS	2.0
1	I	32	DT	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 oligosaccharides 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.