



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:05 PM UTC

PDB ID : 5GT0 / pdb_00005gt0
Title : Crystal structure of nucleosome complex with human testis-specific histone variants, Th2a
Authors : Kumarevel, T.; Sivaraman, P.
Deposited on : 2016-08-18
Resolution : 2.82 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

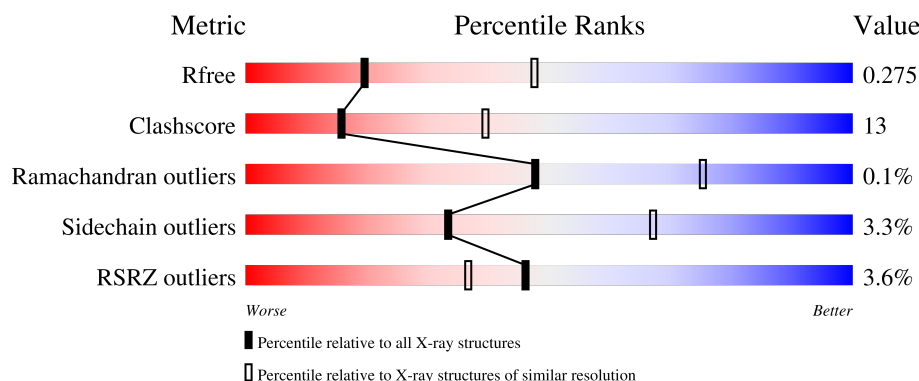
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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.



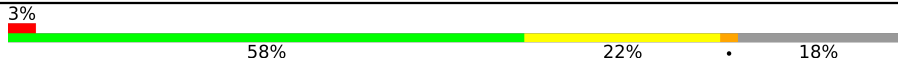
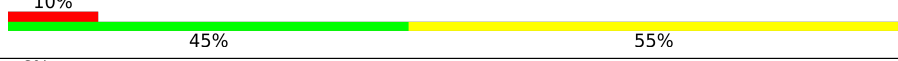
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	A	135	
1	E	135	
2	B	102	
2	F	102	
3	C	130	

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Mol	Chain	Length	Quality of chain
3	G	130	
4	D	125	
4	H	125	
5	I	146	
5	J	146	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12166 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
1	A	99	Total	C	N	O	S	0	0	0
			816	514	158	140	4			
1	E	99	Total	C	N	O	S	0	0	0
			816	514	158	140	4			

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	79	Total	C	N	O	S	0	0	0
			624	394	121	108	1			
2	F	86	Total	C	N	O	S	0	0	0
			694	436	140	117	1			

- Molecule 3 is a protein called Histone H2A type 1-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	106	Total	C	N	O	0	0	0
			814	514	157	143			
3	G	106	Total	C	N	O	0	0	0
			814	514	157	143			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	98	Total	C	N	O	S	0	0	0
			775	485	144	144	2			
4	H	94	Total	C	N	O	S	0	0	0
			735	461	132	140	2			

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

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

- Molecule 6 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total 1	Mn 1	0	0
6	C	1	Total 1	Mn 1	0	0
6	I	6	Total 6	Mn 6	0	0
6	J	6	Total 6	Mn 6	0	0

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total 3	O 3	0	0
8	E	10	Total 10	O 10	0	0
8	F	8	Total 8	O 8	0	0
8	C	14	Total 14	O 14	0	0
8	G	2	Total 2	O 2	0	0
8	D	4	Total 4	O 4	0	0

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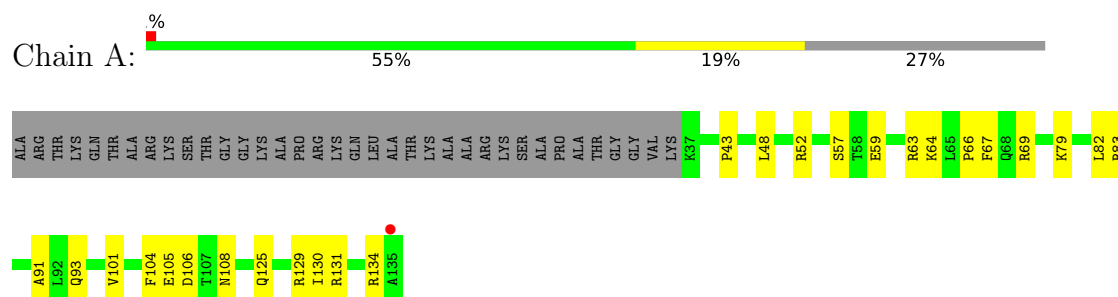
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	1	Total 1	O 1	0	0
8	I	14	Total 14	O 14	0	0
8	J	22	Total 22	O 22	0	0

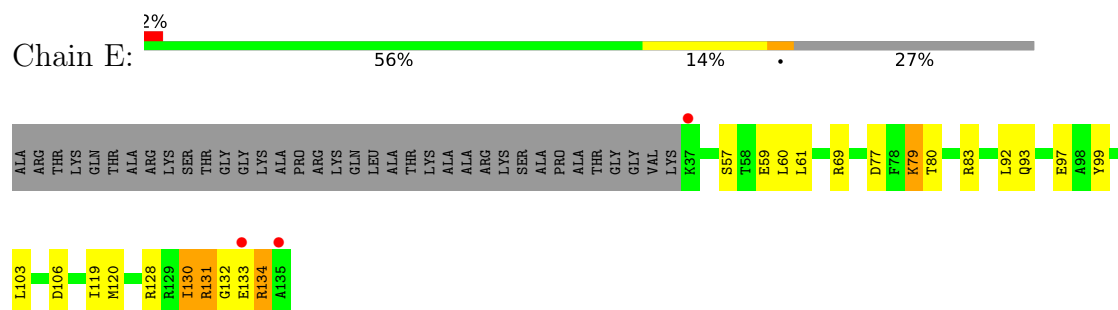
3 Residue-property plots [i](#)

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.

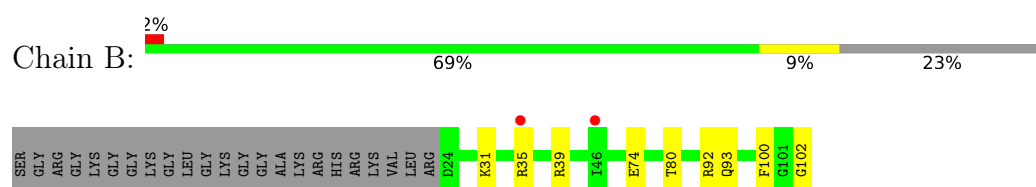
- Molecule 1: Histone H3.1



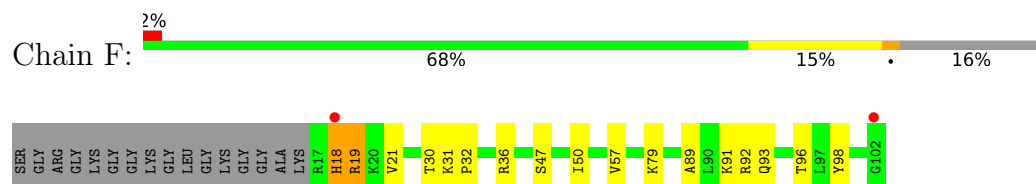
- Molecule 1: Histone H3.1



- Molecule 2: Histone H4



- Molecule 2: Histone H4

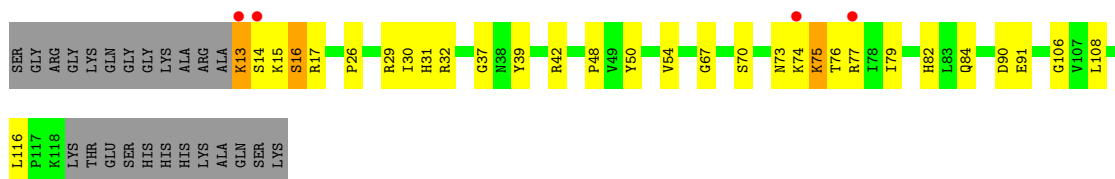


- Molecule 3: Histone H2A type 1-A

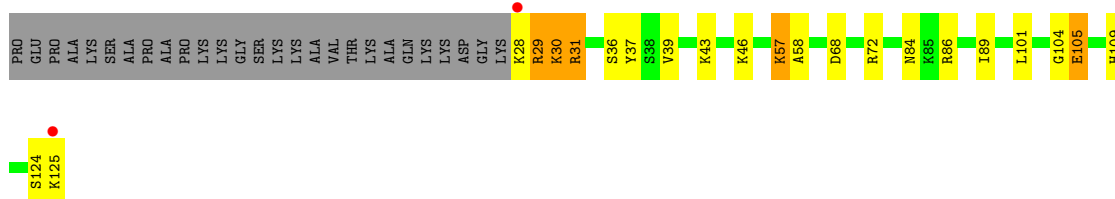




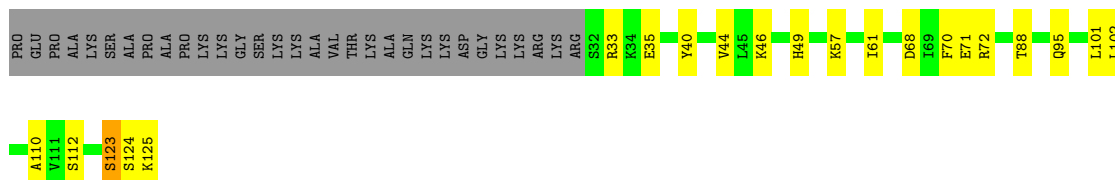
- Molecule 3: Histone H2A type 1-A



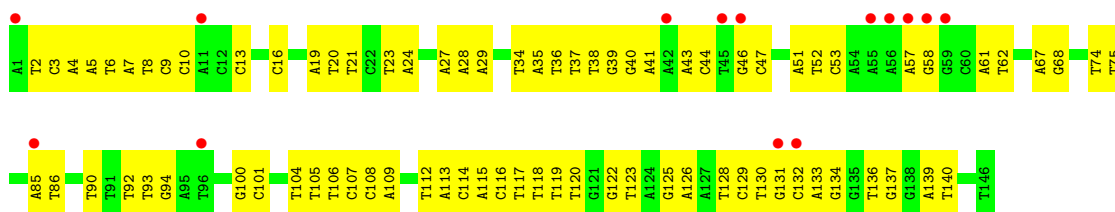
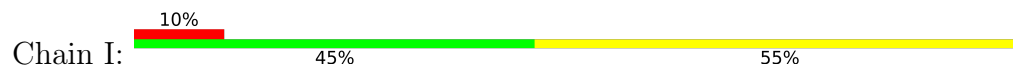
- Molecule 4: Histone H2B type 1-J



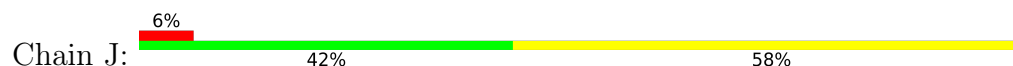
- Molecule 4: Histone H2B type 1-J

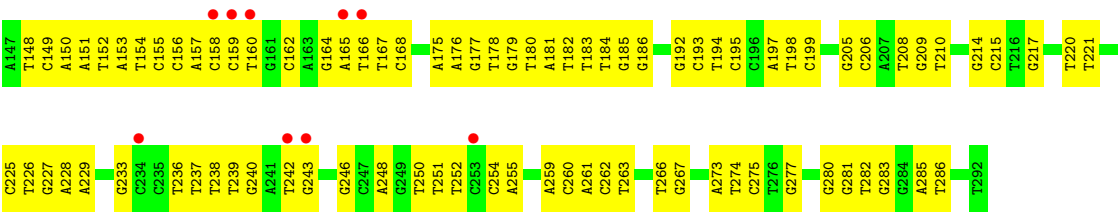


- Molecule 5: DNA (146-MER)



- Molecule 5: DNA (146-MER)





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.79Å 108.97Å 170.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.80 – 2.82 36.80 – 2.82	Depositor EDS
% Data completeness (in resolution range)	98.5 (36.80-2.82) 93.9 (36.80-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.210 , 0.280 0.211 , 0.275	Depositor DCC
R_{free} test set	2721 reflections (6.04%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 23.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12166	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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

5.1 Standard geometry

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

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	0.64	0/828	1.00	1/1109 (0.1%)
1	E	1.00	2/828 (0.2%)	1.25	8/1109 (0.7%)
2	B	0.69	0/631	0.95	0/844
2	F	0.94	0/702	1.00	0/937
3	C	0.75	0/824	0.96	0/1110
3	G	0.93	2/824 (0.2%)	1.11	7/1110 (0.6%)
4	D	0.83	0/786	1.14	2/1051 (0.2%)
4	H	0.89	1/746 (0.1%)	0.95	1/1001 (0.1%)
5	I	0.46	0/3354	0.67	0/5175
5	J	0.46	0/3354	0.69	0/5175
All	All	0.67	5/12877 (0.0%)	0.87	19/18621 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	125	LYS	C-OXT	-15.47	0.92	1.23
1	E	131	ARG	CA-C	-7.52	1.43	1.53
3	G	90	ASP	C-O	-6.03	1.16	1.24
3	G	108	LEU	CA-C	-5.15	1.46	1.53
1	E	131	ARG	C-O	-5.01	1.17	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	134	ARG	N-CA-C	13.72	133.19	114.12
4	D	104	GLY	N-CA-C	12.10	129.37	113.27
1	E	130	ILE	N-CA-C	-11.33	97.70	110.05
1	E	134	ARG	N-CA-CB	-9.19	98.20	110.88
4	D	105	GLU	N-CA-C	-8.09	101.74	111.69
3	G	16	SER	N-CA-C	7.69	120.93	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	131	ARG	N-CA-C	-7.56	101.54	111.74
3	G	116	LEU	CA-C-N	7.14	127.56	119.92
3	G	116	LEU	C-N-CA	7.14	127.56	119.92
3	G	14	SER	N-CA-C	-6.99	104.57	113.23
3	G	91	GLU	N-CA-C	6.95	118.85	111.28
1	E	130	ILE	CA-C-N	-6.49	113.04	122.19
1	E	130	ILE	C-N-CA	-6.49	113.04	122.19
1	E	131	ARG	CB-CA-C	-6.18	102.95	111.73
1	E	134	ARG	CB-CA-C	-5.58	100.00	109.38
3	G	75	LYS	N-CA-C	-5.40	100.23	109.24
1	A	64	LYS	N-CA-C	5.16	116.59	111.07
4	H	123	SER	CB-CA-C	-5.03	102.31	110.85
3	G	108	LEU	N-CA-C	-5.01	102.93	110.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	816	0	856	22	0
1	E	816	0	856	35	0
2	B	624	0	661	9	0
2	F	694	0	742	10	0
3	C	814	0	871	13	0
3	G	814	0	871	35	0
4	D	775	0	808	27	0
4	H	735	0	756	13	0
5	I	2990	0	1652	86	0
5	J	2990	0	1652	87	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	I	6	0	0	0	0
6	J	6	0	0	0	0
7	E	1	0	0	1	0
7	I	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	J	1	0	0	1	0
8	A	3	0	0	0	0
8	C	14	0	0	0	0
8	D	4	0	0	0	0
8	E	10	0	0	1	0
8	F	8	0	0	0	0
8	G	2	0	0	0	0
8	H	1	0	0	0	0
8	I	14	0	0	2	0
8	J	22	0	0	2	0
All	All	12166	0	9725	283	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 13.

All (283) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:ILE:O	1:E:131:ARG:HB3	1.50	1.10
1:E:131:ARG:HH21	1:E:134:ARG:NH2	1.56	1.02
5:I:36:DT:H2''	5:I:37:DT:H5''	1.43	1.01
1:E:131:ARG:NH2	1:E:134:ARG:HH22	1.60	0.97
1:E:131:ARG:HH21	1:E:134:ARG:HH22	0.99	0.96
1:E:131:ARG:N	8:E:301:HOH:O	1.65	0.94
4:D:29:ARG:HG3	4:D:29:ARG:HH11	1.33	0.91
1:A:125:GLN:HA	1:A:134:ARG:HH21	1.39	0.87
4:D:28:LYS:HD2	4:D:28:LYS:N	1.92	0.85
5:J:194:DT:H2''	5:J:195:DC:H5'	1.59	0.85
1:E:131:ARG:O	1:E:131:ARG:HG2	1.76	0.84
5:I:128:DT:H2''	5:I:129:DC:H5''	1.61	0.80
4:D:30:LYS:HD3	5:I:104:DT:OP1	1.84	0.78
4:D:29:ARG:HD3	4:D:29:ARG:N	1.98	0.77
4:D:30:LYS:CD	5:I:104:DT:OP1	2.32	0.77
5:I:27:DA:OP2	8:I:301:HOH:O	2.02	0.77
1:E:131:ARG:O	1:E:131:ARG:CG	2.29	0.77
1:A:79:LYS:HB3	1:A:82:LEU:HD11	1.68	0.75
5:J:217:DG:N7	7:J:307:CL:CL	2.57	0.75
1:A:79:LYS:HD3	1:A:82:LEU:HD21	1.69	0.75
3:C:32:ARG:NH1	5:I:29:DA:OP1	2.19	0.74
3:G:13:LYS:HG3	3:G:16:SER:HA	1.67	0.73
5:I:108:DC:H2''	5:I:109:DA:N7	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:233:DG:N3	8:J:401:HOH:O	2.22	0.73
5:I:40:DG:H2''	5:I:41:DA:C8	2.24	0.72
4:D:29:ARG:HD3	4:D:29:ARG:H	1.54	0.71
4:D:29:ARG:HG3	4:D:29:ARG:NH1	2.04	0.71
1:A:63:ARG:HG3	1:A:66:PRO:HG2	1.71	0.70
5:J:240:DG:N2	8:J:402:HOH:O	2.23	0.70
5:J:183:DT:H2''	5:J:184:DT:H5'	1.74	0.69
2:B:92:ARG:HH21	4:D:101:LEU:HD23	1.56	0.69
5:J:166:DT:H1'	5:J:167:DT:H5'	1.75	0.69
5:J:192:DG:H2''	5:J:193:DC:H5''	1.75	0.68
5:I:35:DA:H2''	5:I:36:DT:H5''	1.73	0.68
5:J:181:DA:H2''	5:J:182:DT:H5''	1.73	0.68
5:J:277:DG:H8	5:J:277:DG:H5''	1.58	0.68
5:I:51:DA:H2''	5:I:52:DT:H5''	1.76	0.68
5:I:134:DG:H1	5:J:159:DC:H42	1.41	0.68
5:J:205:DG:H1'	5:J:206:DC:H5'	1.75	0.68
5:I:101:DC:H5''	5:I:101:DC:H6	1.60	0.67
5:J:209:DG:H1'	5:J:210:DT:H5'	1.76	0.67
5:I:57:DA:H2''	5:I:58:DG:C8	2.28	0.67
5:I:43:DA:H2''	5:I:44:DC:H5''	1.75	0.67
5:I:5:DA:H2''	5:I:6:DT:H5''	1.75	0.67
5:J:277:DG:H5''	5:J:277:DG:C8	2.30	0.67
5:I:125:DG:H2''	5:I:126:DA:C8	2.31	0.66
1:E:130:ILE:O	1:E:131:ARG:CB	2.26	0.65
5:J:198:DT:H2''	5:J:199:DC:H5'	1.78	0.65
5:I:13:DC:H42	5:J:280:DG:H1	1.43	0.64
2:B:92:ARG:NH2	4:D:101:LEU:HD23	2.12	0.64
5:I:2:DT:H2''	5:I:3:DC:H5''	1.79	0.64
4:H:123:SER:OG	4:H:124:SER:N	2.30	0.64
5:J:274:DT:H2''	5:J:275:DC:H5''	1.80	0.63
3:C:80:PRO:HG2	4:D:57:LYS:HE3	1.79	0.63
3:G:13:LYS:HD2	3:G:15:LYS:O	1.99	0.63
4:D:31:ARG:HH12	5:J:194:DT:P	2.23	0.62
3:C:17:ARG:HH22	3:C:31:HIS:CD2	2.18	0.62
1:E:131:ARG:O	1:E:133:GLU:N	2.29	0.62
1:A:59:GLU:CD	1:A:59:GLU:H	2.07	0.62
3:G:13:LYS:HZ3	5:J:177:DG:H3'	1.63	0.62
1:E:103:LEU:HD13	1:E:134:ARG:HH12	1.64	0.61
3:G:13:LYS:HD3	5:J:178:DT:OP1	2.00	0.61
5:J:194:DT:C2'	5:J:195:DC:H5'	2.31	0.61
1:A:57:SER:HB2	1:A:59:GLU:OE2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:262:DC:H1'	5:J:263:DT:H5'	1.84	0.60
1:A:125:GLN:HA	1:A:134:ARG:NH2	2.12	0.60
5:I:112:DT:H1'	5:I:113:DA:H5'	1.83	0.60
5:I:108:DC:H2''	5:I:109:DA:C5	2.36	0.60
5:I:139:DA:H2''	5:I:140:DT:H5'	1.85	0.59
5:J:185:DG:H1'	5:J:186:DG:H5'	1.85	0.59
3:G:84:GLN:NE2	3:G:106:GLY:O	2.34	0.58
3:G:13:LYS:CG	3:G:16:SER:HA	2.33	0.58
1:E:131:ARG:C	1:E:133:GLU:H	2.11	0.58
5:I:9:DC:H2''	5:I:10:DC:H5'	1.86	0.58
5:I:51:DA:C2'	5:I:52:DT:H5''	2.34	0.58
3:G:17:ARG:HH12	3:G:31:HIS:HD2	1.52	0.57
5:I:29:DA:H8	5:I:29:DA:H5''	1.68	0.57
1:E:131:ARG:HE	1:E:134:ARG:NH2	2.03	0.56
5:J:155:DC:H2''	5:J:156:DC:H5'	1.85	0.56
4:D:124:SER:O	4:D:125:LYS:HB2	2.05	0.56
1:E:131:ARG:NH2	1:E:134:ARG:NH2	2.32	0.56
1:E:69:ARG:NH2	5:I:90:DT:OP2	2.34	0.56
5:I:5:DA:C2'	5:I:6:DT:H5''	2.35	0.56
5:J:250:DT:H1'	5:J:251:DT:H5''	1.87	0.56
5:J:157:DA:C8	5:J:157:DA:H5'	2.41	0.56
5:J:157:DA:H5'	5:J:157:DA:H8	1.70	0.56
1:E:128:ARG:HG2	1:E:134:ARG:NH1	2.20	0.55
5:I:119:DT:H1'	5:I:120:DT:H5'	1.87	0.55
1:A:129:ARG:NH1	1:E:106:ASP:OD1	2.36	0.55
1:E:131:ARG:CZ	1:E:134:ARG:HH22	2.19	0.55
4:H:40:TYR:O	4:H:44:VAL:HG23	2.06	0.55
5:I:93:DT:H1'	5:I:94:DG:H5'	1.88	0.55
5:I:101:DC:H5''	5:I:101:DC:C6	2.42	0.55
5:J:183:DT:C2'	5:J:184:DT:H5'	2.37	0.55
1:A:106:ASP:OD2	1:A:131:ARG:NH1	2.37	0.55
3:G:13:LYS:HG2	5:J:177:DG:C3'	2.37	0.55
5:I:29:DA:H5''	5:I:29:DA:C8	2.43	0.54
1:E:130:ILE:O	1:E:131:ARG:C	2.48	0.54
3:G:13:LYS:NZ	5:J:177:DG:H3'	2.23	0.54
3:G:17:ARG:HH22	3:G:31:HIS:CD2	2.25	0.54
2:F:30:THR:HB	2:F:32:PRO:HD2	1.90	0.54
5:J:150:DA:H1'	5:J:151:DA:H5'	1.90	0.54
5:J:164:DG:H2''	5:J:165:DA:H5''	1.90	0.54
5:J:175:DA:H2''	5:J:176:DA:C8	2.44	0.53
5:I:132:DC:H2''	5:I:133:DA:N7	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:251:DT:H1'	5:J:252:DT:H5'	1.90	0.53
5:I:7:DA:H1'	5:I:8:DT:H5'	1.91	0.53
5:I:139:DA:H5'	8:I:302:HOH:O	2.08	0.53
4:D:29:ARG:NH1	4:D:29:ARG:CG	2.67	0.53
1:A:63:ARG:O	1:A:66:PRO:HD2	2.09	0.52
3:G:13:LYS:HG2	5:J:177:DG:O3'	2.09	0.52
5:J:192:DG:C2'	5:J:193:DC:H5''	2.40	0.52
5:I:104:DT:H1'	5:I:105:DT:H5''	1.91	0.52
5:I:128:DT:C2'	5:I:129:DC:H5''	2.33	0.52
3:G:13:LYS:CD	3:G:16:SER:HA	2.40	0.52
5:I:131:DG:H2''	5:I:132:DC:C6	2.44	0.52
5:I:67:DA:H2''	5:I:68:DG:C8	2.45	0.51
4:D:30:LYS:HD2	5:I:104:DT:OP1	2.10	0.51
5:I:43:DA:C2'	5:I:44:DC:H5''	2.40	0.51
1:E:99:TYR:CE1	1:E:134:ARG:NH2	2.78	0.51
5:J:214:DG:H2''	5:J:215:DC:C6	2.45	0.51
4:D:68:ASP:O	4:D:72:ARG:HG3	2.11	0.51
5:I:113:DA:H2''	5:I:114:DC:H5''	1.92	0.51
3:G:31:HIS:CG	3:G:48:PRO:HG3	2.46	0.51
3:G:30:ILE:HG23	4:H:70:PHE:HE1	1.76	0.51
3:G:73:ASN:OD1	3:G:73:ASN:O	2.30	0.50
3:G:54:VAL:HG13	4:H:110:ALA:HB1	1.93	0.50
5:J:197:DA:H2''	5:J:198:DT:H5''	1.94	0.50
3:G:70:SER:HB3	3:G:75:LYS:O	2.11	0.50
5:J:155:DC:C2'	5:J:156:DC:H5'	2.42	0.50
3:C:15:LYS:HE3	3:C:20:ARG:HG3	1.94	0.50
3:C:80:PRO:HD3	4:D:58:ALA:HB2	1.93	0.50
1:E:83:ARG:NH1	5:I:100:DG:OP1	2.44	0.49
5:I:74:DT:H1'	5:I:75:DT:H5'	1.94	0.49
1:A:67:PHE:CZ	1:A:93:GLN:HA	2.47	0.49
4:D:31:ARG:NH1	5:J:194:DT:O5'	2.45	0.49
5:J:152:DT:H2''	5:J:153:DA:H5'	1.94	0.49
5:I:105:DT:H1'	5:I:106:DT:H5'	1.94	0.49
5:J:259:DA:H1'	5:J:260:DC:H5''	1.93	0.49
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.47	0.49
4:H:33:ARG:HG2	5:I:122:DG:H4'	1.94	0.49
5:I:9:DC:C2'	5:I:10:DC:H5'	2.42	0.49
5:I:52:DT:H2''	5:I:53:DC:H5'	1.92	0.49
1:A:91:ALA:HB2	2:B:100:PHE:CD2	2.47	0.49
1:E:99:TYR:HE1	1:E:134:ARG:NH2	2.10	0.49
5:I:6:DT:H2''	5:I:7:DA:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:280:DG:H1'	5:J:281:DG:H5'	1.94	0.49
3:G:32:ARG:HH11	5:J:176:DA:P	2.35	0.49
2:F:98:TYR:CE2	3:C:100:VAL:HG11	2.47	0.49
3:G:13:LYS:CE	5:J:177:DG:H3'	2.43	0.49
1:A:43:PRO:HA	5:J:229:DA:H5''	1.95	0.49
5:I:85:DA:H2''	5:I:86:DT:H5'	1.95	0.49
5:I:136:DT:H2''	5:I:137:DG:H5'	1.95	0.49
5:J:148:DT:H2''	5:J:149:DC:H5''	1.94	0.49
5:I:130:DT:H2''	5:I:131:DG:N7	2.29	0.48
5:I:61:DA:H2''	5:I:62:DT:H5'	1.95	0.48
3:G:13:LYS:N	5:J:177:DG:O3'	2.46	0.48
5:J:238:DT:H1'	5:J:239:DT:H5'	1.95	0.48
5:J:261:DA:H1'	5:J:262:DC:H5''	1.96	0.48
1:E:128:ARG:HG2	1:E:134:ARG:HH11	1.78	0.48
3:G:26:PRO:HB2	3:G:29:ARG:HB3	1.94	0.48
3:G:73:ASN:O	3:G:73:ASN:CG	2.56	0.48
5:I:131:DG:C8	5:I:131:DG:H5''	2.49	0.48
5:J:197:DA:C2'	5:J:198:DT:H5''	2.44	0.48
5:J:237:DT:H1'	5:J:238:DT:H5''	1.96	0.48
1:E:60:LEU:HD13	1:E:93:GLN:CD	2.39	0.47
2:F:31:LYS:HB3	2:F:32:PRO:HD3	1.95	0.47
3:G:37:GLY:HA3	3:G:39:TYR:CE1	2.49	0.47
3:C:29:ARG:NH1	4:D:36:SER:O	2.48	0.47
5:I:115:DA:H2''	5:I:116:DC:H5''	1.96	0.47
5:J:153:DA:H1'	5:J:154:DT:H5'	1.95	0.47
5:J:254:DC:H2''	5:J:255:DA:N7	2.30	0.47
1:E:106:ASP:OD2	1:E:131:ARG:NH1	2.47	0.47
5:I:92:DT:H2''	5:I:93:DT:H5'	1.97	0.47
5:I:117:DT:H1'	5:I:118:DT:H5''	1.97	0.47
4:D:84:ASN:HB3	4:D:86:ARG:NH1	2.30	0.47
3:G:32:ARG:HD3	5:J:176:DA:OP2	2.15	0.46
5:J:226:DT:H2''	5:J:227:DG:C8	2.50	0.46
1:E:119:ILE:HG13	2:F:50:ILE:HG13	1.97	0.46
5:I:133:DA:C6	5:I:134:DG:C6	3.03	0.46
2:B:80:THR:HB	5:J:248:DA:H5'	1.97	0.46
5:I:5:DA:H2''	5:I:6:DT:C5'	2.46	0.46
5:J:285:DA:H2''	5:J:286:DT:H5'	1.98	0.46
2:B:100:PHE:C	2:B:102:GLY:H	2.24	0.46
5:J:165:DA:H2''	5:J:166:DT:H5'	1.97	0.46
5:I:36:DT:C2'	5:I:37:DT:H5''	2.30	0.46
3:G:50:TYR:OH	4:H:95:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:114:DC:H2''	5:I:115:DA:C8	2.51	0.45
2:F:92:ARG:HH21	4:H:101:LEU:HD23	1.81	0.45
5:I:108:DC:H2''	5:I:109:DA:C8	2.52	0.45
5:I:132:DC:N4	5:J:160:DT:O4	2.50	0.45
5:J:282:DT:H2''	5:J:283:DG:H5'	1.99	0.45
1:E:120:MET:HG2	2:F:47:SER:HB2	1.99	0.45
1:E:57:SER:HB2	1:E:59:GLU:HG2	1.97	0.45
5:J:220:DT:H1'	5:J:221:DT:H5'	1.99	0.45
3:G:67:GLY:HA3	4:H:49:HIS:ND1	2.31	0.45
5:I:37:DT:H2''	5:I:38:DT:H5'	1.99	0.45
5:J:158:DC:H1'	5:J:159:DC:H5''	1.99	0.45
1:A:63:ARG:HG3	1:A:66:PRO:CG	2.43	0.44
5:J:227:DG:H2''	5:J:228:DA:OP2	2.17	0.44
5:I:2:DT:C2'	5:I:3:DC:H5''	2.46	0.44
2:B:92:ARG:HH21	4:D:101:LEU:CD2	2.27	0.44
3:G:77:ARG:HH21	5:J:166:DT:H4'	1.82	0.44
5:I:37:DT:H2''	5:I:38:DT:C6	2.52	0.44
5:I:68:DG:H1	5:J:225:DC:H42	1.66	0.44
5:J:179:DG:H2''	5:J:180:DT:H5''	1.99	0.44
5:J:273:DA:H2''	5:J:274:DT:OP2	2.17	0.44
1:A:83:ARG:NH2	5:J:246:DG:H4'	2.33	0.44
5:I:19:DA:H2''	5:I:20:DT:H5'	2.00	0.44
5:I:23:DT:H2''	5:I:24:DA:C8	2.53	0.44
3:G:42:ARG:HB2	4:H:88:THR:HG23	2.00	0.44
5:I:3:DC:H2''	5:I:4:DA:N7	2.33	0.44
5:I:39:DG:H2''	5:I:40:DG:H5''	1.98	0.44
1:A:48:LEU:HB3	1:A:52:ARG:NH1	2.33	0.43
3:C:20:ARG:HD3	4:D:125:LYS:HB2	2.00	0.43
5:I:34:DT:H2''	5:I:35:DA:C8	2.53	0.43
5:I:37:DT:H2'	5:I:38:DT:H71	1.99	0.43
2:F:18:HIS:ND1	2:F:19:ARG:N	2.66	0.43
3:C:88:ARG:HA	3:C:88:ARG:HD3	1.84	0.43
5:I:8:DT:H2''	5:I:9:DC:H5''	2.01	0.43
5:I:133:DA:C5	5:I:134:DG:C6	3.06	0.43
5:I:122:DG:H1'	5:I:123:DT:H5'	2.00	0.43
3:G:32:ARG:NH2	4:H:35:GLU:OE2	2.46	0.43
1:A:79:LYS:HD2	2:B:74:GLU:HG2	2.01	0.43
4:D:30:LYS:H	4:D:30:LYS:HG3	1.32	0.43
1:E:61:LEU:HD22	2:F:36:ARG:HD2	2.01	0.43
3:G:13:LYS:HD2	3:G:16:SER:HA	2.01	0.43
4:H:57:LYS:O	4:H:61:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:32:ARG:NH1	5:J:176:DA:OP1	2.52	0.43
5:J:162:DC:H6	5:J:162:DC:H2'	1.70	0.43
5:J:175:DA:H2''	5:J:176:DA:H8	1.84	0.43
5:I:106:DT:H1'	5:I:107:DC:H5'	2.00	0.42
5:I:115:DA:C2'	5:I:116:DC:H5''	2.49	0.42
5:J:266:DT:H2''	5:J:267:DG:C8	2.54	0.42
5:I:20:DT:H1'	5:I:21:DT:H5'	2.00	0.42
5:I:125:DG:H2''	5:I:126:DA:H8	1.80	0.42
2:F:89:ALA:O	2:F:93:GLN:HG3	2.19	0.42
5:J:194:DT:H2''	5:J:195:DC:C6	2.54	0.42
1:E:131:ARG:NE	1:E:134:ARG:NH2	2.68	0.42
3:C:30:ILE:HD12	3:C:52:ALA:HB2	2.00	0.42
4:H:68:ASP:O	4:H:72:ARG:HG3	2.19	0.42
4:D:31:ARG:NH1	5:J:194:DT:P	2.91	0.42
1:E:77:ASP:OD1	7:E:202:CL:CL	2.75	0.42
4:D:36:SER:OG	4:D:37:TYR:N	2.53	0.42
5:I:131:DG:H5''	5:I:131:DG:H8	1.84	0.42
5:J:208:DT:H2''	5:J:209:DG:C8	2.54	0.42
3:C:40:ALA:HB2	4:D:89:ILE:HG13	2.01	0.42
2:F:91:LYS:HD3	2:F:96:THR:HG23	2.02	0.42
3:C:17:ARG:HH22	3:C:31:HIS:HD2	1.65	0.42
5:J:242:DT:H1'	5:J:243:DG:H5''	2.02	0.42
5:I:16:DC:H6	5:I:16:DC:H2'	1.64	0.42
4:H:101:LEU:C	4:H:102:LEU:HD23	2.45	0.41
5:J:193:DC:H2''	5:J:194:DT:C7	2.50	0.41
1:A:129:ARG:HA	1:A:134:ARG:HB2	2.01	0.41
5:I:27:DA:H2''	5:I:28:DA:C8	2.55	0.41
5:J:198:DT:C2'	5:J:199:DC:H5'	2.47	0.41
5:J:154:DT:H1'	5:J:155:DC:H5''	2.02	0.41
1:A:130:ILE:HG22	1:E:131:ARG:HB2	2.02	0.41
1:E:61:LEU:H	1:E:97:GLU:CD	2.28	0.41
5:I:139:DA:C2'	5:I:140:DT:H5'	2.50	0.41
1:A:104:PHE:O	1:A:108:ASN:HB2	2.21	0.41
4:D:39:VAL:O	4:D:43:LYS:HG3	2.20	0.41
5:I:68:DG:O6	7:I:207:CL:CL	2.76	0.41
3:C:73:ASN:O	3:C:75:LYS:HG2	2.21	0.41
1:E:79:LYS:HD3	1:E:80:THR:N	2.36	0.41
1:E:92:LEU:HA	1:E:92:LEU:HD23	1.88	0.41
2:B:31:LYS:NZ	2:B:35:ARG:HH21	2.19	0.41
5:I:40:DG:H2''	5:I:41:DA:N7	2.34	0.41
5:J:236:DT:H1'	5:J:237:DT:H5'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:ARG:O	2:B:39:ARG:HG2	2.21	0.40
3:G:13:LYS:HG2	5:J:177:DG:C4'	2.52	0.40
5:J:193:DC:H2''	5:J:194:DT:H71	2.02	0.40
1:A:63:ARG:HB2	5:J:238:DT:OP1	2.22	0.40
1:A:101:VAL:O	1:A:105:GLU:HG3	2.21	0.40
1:E:99:TYR:CE1	1:E:134:ARG:CZ	3.04	0.40
4:D:105:GLU:O	4:D:109:HIS:ND1	2.55	0.40
5:I:38:DT:H2''	5:I:39:DG:N7	2.36	0.40
5:I:46:DG:H2''	5:I:47:DC:H5''	2.03	0.40
5:J:167:DT:H1'	5:J:168:DC:H5'	2.04	0.40
3:G:13:LYS:NZ	5:J:178:DT:OP2	2.53	0.40
3:G:31:HIS:CD2	3:G:48:PRO:HG3	2.55	0.40
5:J:155:DC:H1'	5:J:156:DC:H5'	2.03	0.40
5:J:179:DG:C2'	5:J:180:DT:H5''	2.51	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	
1	A	97/135 (72%)	97 (100%)	0	0	100	100
1	E	97/135 (72%)	96 (99%)	0	1 (1%)	12	36
2	B	77/102 (76%)	76 (99%)	1 (1%)	0	100	100
2	F	84/102 (82%)	82 (98%)	2 (2%)	0	100	100
3	C	104/130 (80%)	101 (97%)	3 (3%)	0	100	100
3	G	104/130 (80%)	102 (98%)	2 (2%)	0	100	100
4	D	96/125 (77%)	95 (99%)	1 (1%)	0	100	100
4	H	92/125 (74%)	91 (99%)	1 (1%)	0	100	100
All	All	751/984 (76%)	740 (98%)	10 (1%)	1 (0%)	48	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	132	GLY

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	
1	A	86/110 (78%)	85 (99%)	1 (1%)	63	86
1	E	86/110 (78%)	85 (99%)	1 (1%)	63	86
2	B	63/78 (81%)	62 (98%)	1 (2%)	55	82
2	F	71/78 (91%)	66 (93%)	5 (7%)	14	39
3	C	84/101 (83%)	82 (98%)	2 (2%)	43	75
3	G	84/101 (83%)	81 (96%)	3 (4%)	31	64
4	D	85/105 (81%)	80 (94%)	5 (6%)	18	46
4	H	81/105 (77%)	78 (96%)	3 (4%)	30	63
All	All	640/788 (81%)	619 (97%)	21 (3%)	33	67

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ARG
1	E	79	LYS
2	B	93	GLN
2	F	18	HIS
2	F	19	ARG
2	F	21	VAL
2	F	57	VAL
2	F	79	LYS
3	C	16	SER
3	C	118	LYS
3	G	13	LYS
3	G	74	LYS
3	G	76	THR

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Mol	Chain	Res	Type
4	D	29	ARG
4	D	30	LYS
4	D	31	ARG
4	D	46	LYS
4	D	57	LYS
4	H	46	LYS
4	H	71	GLU
4	H	112	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	E	85	GLN
2	B	25	ASN
2	B	93	GLN
3	C	24	GLN
3	C	31	HIS
3	C	104	GLN
3	G	31	HIS
3	G	38	ASN
3	G	89	ASN
3	G	104	GLN
3	G	110	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 20 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	99/135 (73%)	0.19	1 (1%) 79 72	26, 42, 67, 91	0
1	E	99/135 (73%)	-0.18	3 (3%) 52 42	12, 24, 49, 75	0
2	B	79/102 (77%)	0.17	2 (2%) 58 48	24, 35, 55, 68	0
2	F	86/102 (84%)	-0.32	2 (2%) 61 51	15, 23, 32, 82	0
3	C	106/130 (81%)	-0.21	1 (0%) 81 74	14, 23, 44, 88	0
3	G	106/130 (81%)	0.11	4 (3%) 44 35	16, 34, 70, 92	0
4	D	98/125 (78%)	0.01	2 (2%) 65 55	12, 24, 68, 86	0
4	H	94/125 (75%)	0.02	0 100 100	15, 30, 53, 74	0
5	I	146/146 (100%)	0.71	14 (9%) 13 10	33, 68, 116, 128	0
5	J	146/146 (100%)	0.64	9 (6%) 26 19	33, 64, 115, 130	0
All	All	1059/1276 (82%)	0.17	38 (3%) 46 37	12, 35, 100, 130	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	56	DA	5.7
2	B	35	ARG	4.1
4	D	28	LYS	3.8
5	J	159	DC	3.7
1	E	133	GLU	3.4
3	G	13	LYS	3.2
3	G	14	SER	3.2
5	I	57	DA	3.1
2	F	102	GLY	3.1
1	E	37	LYS	3.1
5	I	11	DA	3.0
5	J	158	DC	3.0
5	I	55	DA	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	18	HIS	2.5
5	J	165	DA	2.5
5	I	58	DG	2.5
5	I	45	DT	2.5
1	A	135	ALA	2.4
5	I	42	DA	2.4
5	J	243	DG	2.4
5	J	242	DT	2.3
3	C	18	SER	2.3
4	D	125	LYS	2.3
5	I	59	DG	2.3
5	I	132	DC	2.3
5	J	160	DT	2.3
3	G	74	LYS	2.3
1	E	135	ALA	2.2
5	I	46	DG	2.2
2	B	46	ILE	2.2
5	I	96	DT	2.2
5	J	234	DC	2.2
5	J	253	DC	2.2
5	J	166	DT	2.2
5	I	131	DG	2.2
5	I	1	DA	2.1
5	I	85	DA	2.1
3	G	77	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
6	MN	I	204	1/1	0.76	0.13	106,106,106,106	0
6	MN	I	203	1/1	0.88	0.16	87,87,87,87	0
6	MN	J	305	1/1	0.88	0.11	75,75,75,75	0
6	MN	J	303	1/1	0.90	0.10	70,70,70,70	0
6	MN	E	201	1/1	0.90	0.11	42,42,42,42	0
7	CL	I	210	1/1	0.90	0.20	68,68,68,68	0
7	CL	I	207	1/1	0.92	0.22	57,57,57,57	0
6	MN	I	206	1/1	0.92	0.06	87,87,87,87	0
7	CL	I	209	1/1	0.93	0.26	61,61,61,61	0
6	MN	I	202	1/1	0.93	0.06	77,77,77,77	0
7	CL	I	208	1/1	0.94	0.22	73,73,73,73	0
6	MN	J	302	1/1	0.95	0.05	49,49,49,49	0
6	MN	J	306	1/1	0.95	0.20	73,73,73,73	0
6	MN	I	205	1/1	0.95	0.05	66,66,66,66	0
7	CL	J	307	1/1	0.95	0.10	37,37,37,37	0
6	MN	J	304	1/1	0.96	0.07	53,53,53,53	0
7	CL	E	202	1/1	0.97	0.15	37,37,37,37	0
6	MN	C	201	1/1	0.97	0.06	48,48,48,48	0
6	MN	I	201	1/1	0.97	0.12	54,54,54,54	0
6	MN	J	301	1/1	0.98	0.07	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.