



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:07 am BST

PDB ID : 3UTB
Title : Crystal Structure of Nucleosome Core Particle Assembled with the 146b Alpha-Satellite Sequence (NCP146b)
Authors : Chua, E.Y.D.; Vasudevan, D.; Davey, G.E.; Wu, B.; Davey, C.A.
Deposited on : 2011-11-25
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

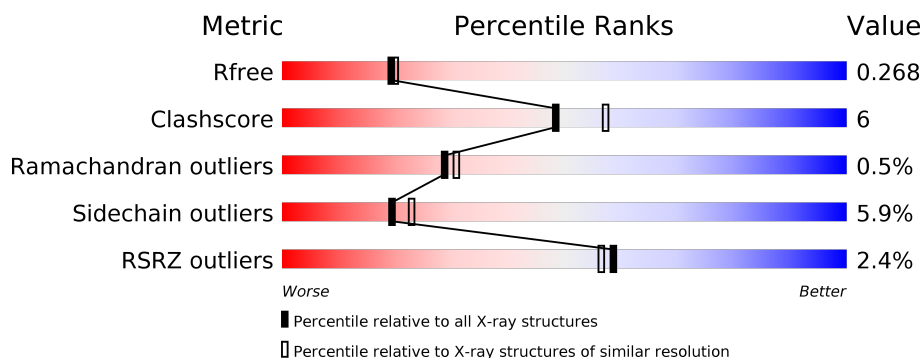
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	<div> <div>2%</div> <div>64% 8% 27%</div> </div>
1	E	135	<div> <div>2%</div> <div>66% 5% 28%</div> </div>
2	B	102	<div> <div>71% 10% 19%</div> </div>
2	F	102	<div> <div>2%</div> <div>67% 9% 24%</div> </div>
3	C	129	<div> <div>3%</div> <div>64% 14% 20%</div> </div>
3	G	129	<div> <div>2%</div> <div>64% 14% 19%</div> </div>

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SO4	G	1103	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12430 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 H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			808	509	156	140	3			
1	E	97	Total	C	N	O	S	0	0	0
			801	504	155	139	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	SEE REMARK 999	UNP P84233
E	102	ALA	GLY	SEE REMARK 999	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			
2	F	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	103	Total	C	N	O		0	0	0
			795	501	155	139				
3	G	105	Total	C	N	O		0	0	0
			809	510	158	141				

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	99	Total	C	N	O	S	0	0	0
			785	493	146	144	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	94	Total	C	N	O	S	0	0	0
			736	463	132	139	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	SEE REMARK 999	UNP P02281
H	29	THR	SER	SEE REMARK 999	UNP P02281

- Molecule 5 is a DNA chain called 146-mer DNA.

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

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	9	Total	Mn	0	0
			9	9		
6	A	1	Total	Mn	0	0
			1	1		
6	D	1	Total	Mn	0	0
			1	1		
6	J	9	Total	Mn	0	0
			9	9		
6	E	1	Total	Mn	0	0
			1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	62	Total	O	0	0
			62	62		
8	B	41	Total	O	0	0
			41	41		
8	C	31	Total	O	0	0
			31	31		
8	D	16	Total	O	0	0
			16	16		
8	E	37	Total	O	0	0
			37	37		
8	F	28	Total	O	0	0
			28	28		
8	G	52	Total	O	0	0
			52	52		
8	H	35	Total	O	0	0
			35	35		
8	I	50	Total	O	0	0
			50	50		

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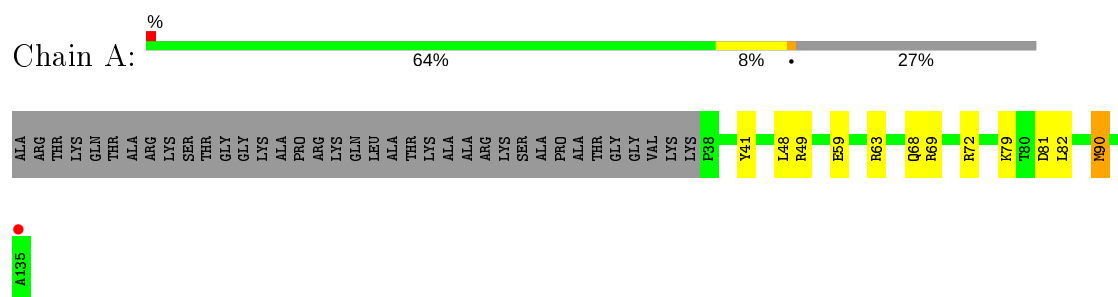
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	47	Total	O	0	0
			47	47		

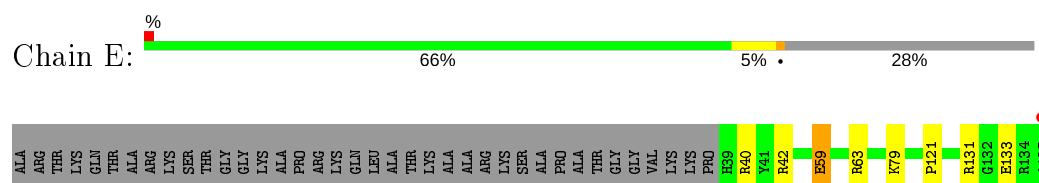
3 Residue-property plots [i](#)

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

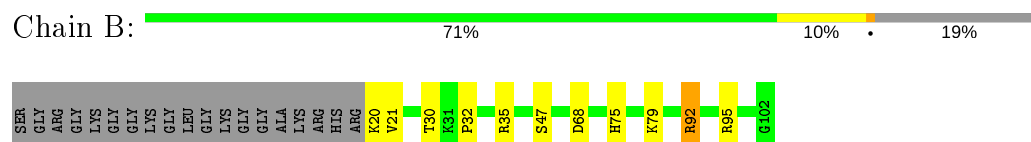
- Molecule 1: Histone H3.2



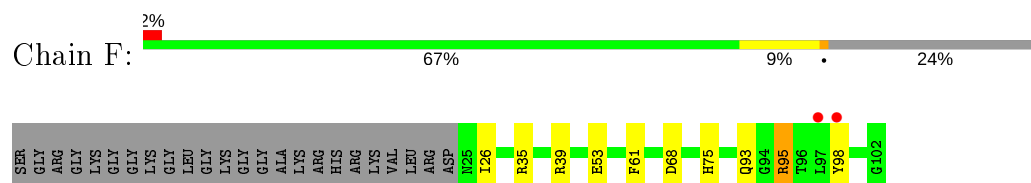
- Molecule 1: Histone H3.2



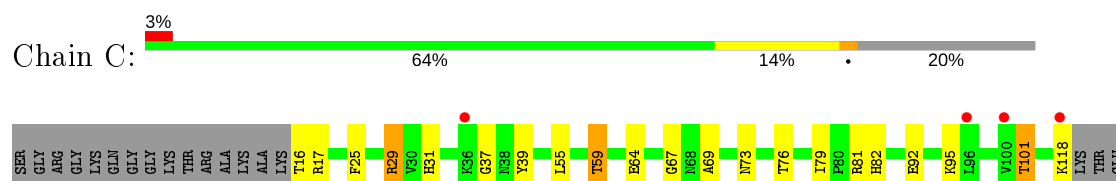
- Molecule 2: Histone H4



- Molecule 2: Histone H4



- Molecule 3: Histone H2A



SER
SER
LYS
SER
ALA
LYS
SER
LYS

• Molecule 3: Histone H2A



SER GLY ARG GLY LYS GLN GLY LYS THR ARG ALA LYS
K14 R17 F25 R51 R38 V42 V43 G44 G45 V54 L55 T59 I62 L63 E64 R71 D72 N73 T76 R77 I78 I79 P80 R81 R82 L83 Q84 R88 I102 K118 LYS THR GLU

SER
SER
LYS
SER
ALA
LYS
SER
LYS

• Molecule 4: Histone H2B 1.1



PRO GLU ALA LYS SER PRO ALA LYS LYS LYS VAL THR THR LYS LYS ASP GLY
R24 R25 R26 R27 R28 T29 R30 K31 E32 S33 Y34 A35 Y39 K43 H46 M56 S61 F67 E73 L77 A78 H79 T87 S88 R89

T93 R96 L97 L98 P100 G101 E102 L103 A104 S109 V115 T119 K122

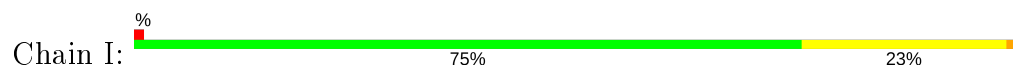
• Molecule 4: Histone H2B 1.1



PRO GLU ALA LYS SER PRO ALA LYS LYS LYS VAL THR THR LYS LYS ASP GLY
T29 R30 Y34 A35 V38 V45 H46 M56 S57 I58 M59 N60 S61 F62 E68 N81 K82 R83 S84 T85 T93 A94

V95 G101 A104 V108 S120 A121 K122

• Molecule 5: 146-mer DNA

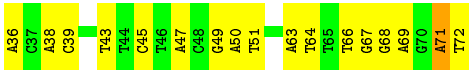
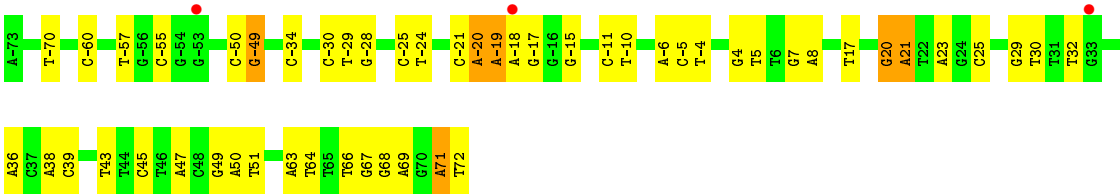


A-72 C-67 A-66 A-62 A-51 A-46 A-43 G-35 C-29 T-28 G-27 T-23 A-22 T-21 C-20 A-19 A-18 G-14 A-13 A-12 G-2 T1 T2 C3 A4 A10 G11 C17 A22 G25 G30 T33 G34 C38 A39 C40 C46 T47 C53 C54

G55 C56 A57 G71 A72 T73

• Molecule 5: 146-mer DNA





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.46Å 109.28Å 175.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.46 – 2.20 57.46 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (57.46-2.20) 98.1 (57.46-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.232 , 0.275 0.227 , 0.268	Depositor DCC
R_{free} test set	2034 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.594	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12430	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: MN, SO4

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	0.67	0/820	0.66	0/1099
1	E	0.54	0/812	0.65	0/1088
2	B	0.73	0/669	0.73	0/894
2	F	0.58	0/626	0.67	0/837
3	C	0.52	0/805	0.62	0/1088
3	G	0.62	0/819	0.71	0/1106
4	D	0.58	0/796	0.67	1/1065 (0.1%)
4	H	0.62	0/747	0.68	0/1004
5	I	0.73	0/3354	1.34	16/5175 (0.3%)
5	J	0.72	0/3354	1.37	25/5175 (0.5%)
All	All	0.67	0/12802	1.10	42/18531 (0.2%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	-30	DC	O4'-C1'-N1	7.85	113.49	108.00
5	I	-14	DG	P-O3'-C3'	7.76	129.01	119.70
5	I	-35	DG	O4'-C1'-N9	-7.47	102.77	108.00
5	J	-19	DA	O4'-C1'-N9	7.44	113.21	108.00
5	J	23	DA	P-O3'-C3'	7.09	128.21	119.70
5	J	21	DA	P-O3'-C3'	6.98	128.07	119.70
5	J	45	DC	P-O3'-C3'	6.93	128.01	119.70
5	J	20	DG	P-O3'-C3'	6.72	127.76	119.70
5	J	-18	DA	P-O3'-C3'	6.68	127.72	119.70
5	I	53	DC	P-O3'-C3'	6.67	127.71	119.70
5	J	21	DA	O4'-C1'-N9	6.66	112.66	108.00
5	I	10	DA	O4'-C1'-N9	6.33	112.43	108.00
5	I	-51	DA	P-O3'-C3'	6.20	127.14	119.70
5	J	-17	DG	P-O3'-C3'	6.20	127.14	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	-29	DC	P-O3'-C3'	6.16	127.09	119.70
5	I	38	DC	O4'-C1'-N1	6.10	112.27	108.00
5	I	-12	DA	P-O3'-C3'	6.09	127.01	119.70
5	J	4	DG	P-O3'-C3'	6.08	127.00	119.70
5	J	30	DT	O4'-C1'-N1	6.03	112.22	108.00
5	J	-15	DG	O4'-C1'-N9	6.03	112.22	108.00
5	I	40	DC	P-O3'-C3'	6.01	126.92	119.70
5	J	-49	DG	P-O3'-C3'	5.96	126.85	119.70
5	I	25	DG	O4'-C1'-N9	5.86	112.10	108.00
5	I	57	DA	P-O3'-C3'	5.79	126.65	119.70
5	J	71	DA	P-O3'-C3'	5.64	126.47	119.70
5	J	32	DT	O4'-C1'-N1	5.62	111.93	108.00
5	J	-60	DC	P-O3'-C3'	5.60	126.42	119.70
5	I	1	DT	O4'-C1'-N1	5.50	111.85	108.00
5	J	29	DG	O4'-C1'-N9	5.49	111.84	108.00
5	I	-21	DT	O4'-C1'-N1	5.46	111.82	108.00
4	D	77	LEU	CA-CB-CG	5.37	127.64	115.30
5	J	-6	DA	O4'-C1'-N9	-5.30	104.29	108.00
5	J	25	DC	O4'-C1'-N1	5.30	111.71	108.00
5	I	-2	DG	O4'-C1'-N9	5.26	111.68	108.00
5	J	-20	DA	P-O3'-C3'	5.17	125.90	119.70
5	J	5	DT	O4'-C1'-N1	-5.13	104.41	108.00
5	I	-35	DG	P-O3'-C3'	5.10	125.83	119.70
5	I	-18	DA	P-O3'-C3'	5.09	125.81	119.70
5	J	64	DT	P-O3'-C3'	5.07	125.79	119.70
5	J	-11	DC	P-O3'-C3'	5.06	125.78	119.70
5	J	51	DT	P-O3'-C3'	5.03	125.73	119.70
5	J	43	DT	O4'-C1'-N1	5.00	111.50	108.00

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	808	0	846	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	801	0	838	4	0
2	B	662	0	709	10	0
2	F	619	0	659	9	0
3	C	795	0	846	16	0
3	G	809	0	864	28	0
4	D	785	0	825	24	0
4	H	736	0	760	25	0
5	I	2990	0	1651	21	0
5	J	2990	0	1651	32	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	I	9	0	0	0	0
6	J	9	0	0	0	0
7	C	5	0	0	1	0
7	D	5	0	0	0	0
7	G	5	0	0	3	0
8	A	62	0	0	2	0
8	B	41	0	0	1	0
8	C	31	0	0	0	0
8	D	16	0	0	3	0
8	E	37	0	0	0	0
8	F	28	0	0	2	0
8	G	52	0	0	4	0
8	H	35	0	0	0	0
8	I	50	0	0	0	0
8	J	47	0	0	1	0
All	All	12430	0	9649	130	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 6.

All (130) 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)
2:B:75:HIS:CD2	4:D:93:THR:HG21	1.80	1.17
2:F:75:HIS:CD2	4:H:93:THR:HG21	1.85	1.10
2:B:75:HIS:HD2	4:D:93:THR:HG21	1.18	0.98
2:B:95:ARG:HD2	8:B:502:HOH:O	1.69	0.92
2:F:75:HIS:HD2	4:H:93:THR:HG21	1.28	0.90
3:C:55:LEU:O	3:C:59:THR:HG23	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:55:LEU:O	3:G:59:THR:HG23	1.75	0.87
3:G:102:ILE:HG23	4:H:58:ILE:HD13	1.56	0.85
2:B:75:HIS:HD2	4:D:93:THR:CG2	1.92	0.83
2:B:75:HIS:CD2	4:D:93:THR:CG2	2.62	0.82
2:F:75:HIS:CD2	4:H:93:THR:CG2	2.62	0.82
4:D:30:ARG:HG3	5:J:49:DG:H4'	1.63	0.81
4:D:79:HIS:HE1	3:G:38:ASN:HD22	1.28	0.81
4:H:35:ALA:HA	4:H:56:MET:CE	2.11	0.80
4:D:98:LEU:HB2	8:D:503:HOH:O	1.82	0.79
3:G:44:GLY:HA3	7:G:1103:SO4:O3	1.84	0.78
4:H:35:ALA:HA	4:H:56:MET:HE1	1.67	0.77
3:G:46:GLY:N	7:G:1103:SO4:O1	2.17	0.74
4:H:34:TYR:H	4:H:60:ASN:ND2	1.87	0.73
3:C:29:ARG:NH2	4:D:33:SER:O	2.22	0.72
4:D:79:HIS:CE1	3:G:38:ASN:HD22	2.09	0.71
5:J:67:DG:H2''	5:J:68:DG:H5''	1.73	0.70
2:F:75:HIS:HD2	4:H:93:THR:CG2	1.99	0.70
4:H:85:THR:HG23	5:J:-34:DC:OP1	1.93	0.69
3:G:62:ILE:HD11	4:H:62:PHE:CZ	2.27	0.68
1:A:69:ARG:NH2	5:J:17:DT:OP2	2.28	0.67
5:J:68:DG:H2''	5:J:69:DA:C8	2.30	0.67
1:A:69:ARG:NH2	5:J:17:DT:P	2.70	0.65
3:C:17:ARG:HH12	3:C:31:HIS:CD2	2.16	0.64
4:D:35:ALA:HA	4:D:56:MET:HE1	1.82	0.62
4:H:34:TYR:H	4:H:60:ASN:HD21	1.49	0.61
1:A:90:MET:HE1	8:A:404:HOH:O	2.02	0.60
3:G:71:ARG:NH1	8:G:137:HOH:O	2.35	0.59
3:G:42:ARG:HB2	4:H:85:THR:HB	1.83	0.59
3:G:84:GLN:NE2	3:G:88:ARG:HD2	2.18	0.58
3:G:84:GLN:O	3:G:88:ARG:HG2	2.04	0.58
1:E:63:ARG:HE	5:I:17:DC:H5''	1.69	0.57
3:C:16:THR:HA	5:I:-43:DA:H5''	1.87	0.57
5:I:-46:DA:H2	5:J:47:DA:H2	1.54	0.55
2:B:20:LYS:HG3	2:B:21:VAL:N	2.20	0.54
3:G:64:GLU:O	4:H:46:HIS:HE1	1.90	0.54
5:J:-21:DC:H2''	5:J:-20:DA:O5'	2.07	0.54
3:G:44:GLY:CA	7:G:1103:SO4:O3	2.55	0.54
3:G:17:ARG:HH12	3:G:31:HIS:CD2	2.26	0.54
5:I:46:DC:H2''	5:I:47:DT:H71	1.90	0.53
1:A:69:ARG:HH22	5:J:17:DT:P	2.31	0.53
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:63:LEU:HD11	4:H:38:VAL:HG13	1.91	0.53
2:B:68:ASP:OD2	2:B:92:ARG:NH1	2.40	0.53
3:C:55:LEU:O	3:C:59:THR:CG2	2.53	0.53
1:E:121:PRO:HB3	2:F:53:GLU:HG3	1.91	0.52
8:G:545:HOH:O	4:H:68:GLU:HG3	2.09	0.52
4:D:96:ARG:NH1	8:D:470:HOH:O	2.39	0.51
5:J:-20:DA:H2"	5:J:-19:DA:OP2	2.10	0.51
5:J:66:DT:OP1	8:J:517:HOH:O	2.18	0.51
4:H:85:THR:CG2	5:J:-34:DC:OP1	2.58	0.51
1:A:63:ARG:HH12	2:B:30:THR:CG2	2.25	0.50
4:H:35:ALA:HA	4:H:56:MET:HE2	1.92	0.50
3:C:101:THR:CG2	8:F:105:HOH:O	2.59	0.50
5:I:-28:DT:H2"	5:I:-27:DG:C8	2.47	0.49
3:G:55:LEU:O	3:G:59:THR:CG2	2.55	0.49
3:G:84:GLN:HE21	3:G:84:GLN:HA	1.77	0.49
4:D:35:ALA:HA	4:D:56:MET:CE	2.43	0.49
5:J:-29:DT:H2"	5:J:-28:DG:C8	2.49	0.48
5:J:-5:DC:H2"	5:J:-4:DT:H72	1.96	0.47
4:D:39:TYR:CE2	4:D:43:LYS:HE2	2.49	0.47
3:C:25:PHE:CZ	3:C:59:THR:HG21	2.49	0.47
5:J:-50:DC:H2"	5:J:-49:DG:C8	2.49	0.47
4:D:115:VAL:O	4:D:119:THR:HG23	2.15	0.46
5:I:33:DT:H2"	5:I:34:DG:C8	2.50	0.46
4:D:67:PHE:C	4:D:67:PHE:CD2	2.89	0.46
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.50	0.46
5:J:20:DG:H2"	5:J:21:DA:OP2	2.15	0.46
4:H:81:ASN:O	4:H:83:ARG:NH1	2.48	0.45
1:A:41:TYR:HA	5:I:71:DG:H5"	1.98	0.45
5:I:-67:DC:H2'	5:I:-66:DA:C8	2.52	0.45
5:I:71:DG:N2	5:J:-70:DT:O2	2.50	0.45
1:E:131:ARG:HD3	1:E:133:GLU:OE2	2.16	0.45
5:I:-29:DC:H2"	5:I:-28:DT:OP2	2.15	0.45
3:G:64:GLU:HB2	4:H:45:VAL:HG11	1.98	0.45
4:H:121:ALA:O	4:H:122:LYS:HB2	2.16	0.44
4:H:104:ALA:O	4:H:108:VAL:HG23	2.17	0.44
5:I:57:DA:H61	5:J:-57:DT:H3	1.64	0.44
3:G:62:ILE:HD11	4:H:62:PHE:CE1	2.52	0.44
3:C:69:ALA:O	3:C:73:ASN:ND2	2.50	0.44
5:J:49:DG:H2'	5:J:50:DA:C8	2.53	0.44
5:I:-62:DA:C2	5:J:63:DA:C2	3.06	0.44
5:J:-25:DC:H2"	5:J:-24:DT:H72	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:GLY:HA3	4:D:46:HIS:CE1	2.53	0.44
3:C:64:GLU:O	4:D:46:HIS:HE1	2.00	0.44
4:D:29:THR:HB	5:I:30:DG:OP1	2.18	0.43
3:C:37:GLY:HA3	3:C:39:TYR:CE1	2.53	0.43
5:J:71:DA:H2"	5:J:72:DT:OP2	2.18	0.43
4:D:89:ARG:O	4:D:93:THR:HG22	2.19	0.43
5:J:7:DG:H2"	5:J:8:DA:OP2	2.18	0.43
2:B:35:ARG:HH22	5:J:8:DA:P	2.40	0.43
3:C:17:ARG:HH22	3:C:31:HIS:HD2	1.67	0.43
4:D:25:LYS:HA	4:D:25:LYS:HE3	2.00	0.43
1:A:72:ARG:HH22	5:I:-23:DT:P	2.42	0.42
5:I:46:DA:H2	5:J:47:DA:C2	2.35	0.42
3:G:77:ARG:NE	5:J:-55:DC:H4'	2.35	0.42
1:A:68:GLN:HE21	1:A:72:ARG:HE	1.67	0.42
5:I:3:DC:H2"	5:I:4:DA:N7	2.35	0.42
3:G:73:ASN:ND2	8:G:136:HOH:O	2.44	0.42
1:A:49:ARG:NH2	8:A:137:HOH:O	2.48	0.42
3:C:101:THR:HG22	8:F:105:HOH:O	2.19	0.42
1:A:79:LYS:HB3	1:A:82:LEU:HD11	2.02	0.42
5:I:11:DG:N2	5:J:-10:DT:C2	2.88	0.42
2:B:30:THR:HB	2:B:32:PRO:HD2	2.02	0.42
5:I:-20:DC:H2"	5:I:-19:DA:C8	2.55	0.42
5:I:54:DC:H2"	5:I:55:DG:N7	2.35	0.42
7:C:1102:SO4:O3	4:D:87:THR:HB	2.20	0.41
3:C:95:LYS:HE3	3:C:95:LYS:HB2	1.85	0.41
1:E:59:GLU:HG3	1:E:59:GLU:H	1.41	0.41
5:I:-35:DG:N2	5:J:36:DA:C2	2.88	0.41
3:C:92:GLU:HB3	4:D:103:LEU:HD22	2.01	0.41
3:G:77:ARG:CZ	5:J:-55:DC:H4'	2.50	0.41
2:F:68:ASP:OD2	2:F:93:GLN:NE2	2.53	0.41
2:F:61:PHE:HE1	2:F:95:ARG:HD2	1.85	0.41
3:G:25:PHE:CZ	3:G:59:THR:HG21	2.55	0.41
3:G:64:GLU:OE2	4:H:45:VAL:CG1	2.68	0.41
4:D:73:GLU:HG3	8:D:503:HOH:O	2.20	0.41
3:G:54:VAL:HG21	4:H:95:VAL:HG21	2.03	0.41
4:D:61:SER:HB3	2:F:98:TYR:CD1	2.56	0.41
5:J:38:DA:H2"	5:J:39:DC:OP2	2.21	0.41
3:G:62:ILE:HD11	4:H:62:PHE:CE2	2.56	0.41
3:G:81:ARG:HD3	8:G:145:HOH:O	2.22	0.40
5:I:-46:DA:C2	5:J:47:DA:H2	2.35	0.40
2:F:35:ARG:O	2:F:39:ARG:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:71:DA:H1'	5:J:72:DT:H5'	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	96/135 (71%)	96 (100%)	0	0	100	100
1	E	95/135 (70%)	94 (99%)	1 (1%)	0	100	100
2	B	81/102 (79%)	81 (100%)	0	0	100	100
2	F	76/102 (74%)	75 (99%)	1 (1%)	0	100	100
3	C	101/129 (78%)	98 (97%)	3 (3%)	0	100	100
3	G	103/129 (80%)	100 (97%)	3 (3%)	0	100	100
4	D	97/125 (78%)	95 (98%)	0	2 (2%)	7	4
4	H	92/125 (74%)	90 (98%)	0	2 (2%)	6	4
All	All	741/982 (76%)	729 (98%)	8 (1%)	4 (0%)	29	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	101	GLY
4	H	101	GLY
4	H	120	SER
4	D	25	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	
1	A	85/110 (77%)	81 (95%)	4 (5%)	26	33
1	E	84/110 (76%)	80 (95%)	4 (5%)	25	32
2	B	68/78 (87%)	65 (96%)	3 (4%)	28	35
2	F	63/78 (81%)	61 (97%)	2 (3%)	39	50
3	C	82/101 (81%)	76 (93%)	6 (7%)	14	15
3	G	83/101 (82%)	77 (93%)	6 (7%)	14	15
4	D	85/105 (81%)	80 (94%)	5 (6%)	19	23
4	H	80/105 (76%)	73 (91%)	7 (9%)	10	10
All	All	630/788 (80%)	593 (94%)	37 (6%)	19	23

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	59	GLU
1	A	81	ASP
1	A	90	MET
2	B	47	SER
2	B	79	LYS
2	B	92	ARG
3	C	29	ARG
3	C	59	THR
3	C	76	THR
3	C	81	ARG
3	C	101	THR
3	C	118	LYS
4	D	25	LYS
4	D	77	LEU
4	D	93	THR
4	D	103	LEU
4	D	109	SER
1	E	40	ARG

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Mol	Chain	Res	Type
1	E	42	ARG
1	E	59	GLU
1	E	79	LYS
2	F	26	ILE
2	F	95	ARG
3	G	42	ARG
3	G	59	THR
3	G	76	THR
3	G	81	ARG
3	G	84	GLN
3	G	88	ARG
4	H	30	ARG
4	H	68	GLU
4	H	82	LYS
4	H	83	ARG
4	H	85	THR
4	H	93	THR
4	H	120	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	68	GLN
2	B	75	HIS
3	C	31	HIS
4	D	46	HIS
4	D	79	HIS
2	F	75	HIS
3	G	31	HIS
3	G	84	GLN
4	H	46	HIS
4	H	60	ASN
4	H	92	GLN
4	H	106	HIS

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 21 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	SO4	D	1101	-	4,4,4	0.13	0	6,6,6	0.07	0
7	SO4	C	1102	-	4,4,4	0.24	0	6,6,6	0.36	0
7	SO4	G	1103	-	4,4,4	0.35	0	6,6,6	0.21	0

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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1102	SO4	1	0
7	G	1103	SO4	3	0

5.7 Other polymers [i](#)

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	98/135 (72%)	0.22	1 (1%) 82 81	27, 40, 60, 69	0
1	E	97/135 (71%)	0.20	1 (1%) 82 81	36, 48, 62, 70	0
2	B	83/102 (81%)	0.25	0 100 100	27, 38, 47, 54	0
2	F	78/102 (76%)	0.41	2 (2%) 56 53	37, 44, 55, 59	0
3	C	103/129 (79%)	0.47	4 (3%) 39 37	36, 50, 64, 75	0
3	G	105/129 (81%)	0.39	2 (1%) 66 65	28, 43, 60, 73	0
4	D	99/125 (79%)	0.69	9 (9%) 9 8	39, 52, 87, 100	0
4	H	94/125 (75%)	0.58	2 (2%) 63 61	32, 44, 67, 79	0
5	I	146/146 (100%)	0.15	1 (0%) 87 86	48, 95, 144, 155	0
5	J	146/146 (100%)	0.08	3 (2%) 63 61	52, 93, 129, 142	0
All	All	1049/1274 (82%)	0.32	25 (2%) 59 56	27, 50, 118, 155	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	24	LYS	8.5
1	A	135	ALA	6.4
3	C	118	LYS	6.3
4	H	122	LYS	3.7
5	J	-18	DA	3.3
4	D	122	LYS	3.0
3	G	118	LYS	2.9
3	C	100	VAL	2.7
5	J	33	DG	2.7
3	G	14	ALA	2.6
4	D	25	LYS	2.6
5	I	22	DA	2.5
4	D	27	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	97	LEU	2.4
1	E	135	ALA	2.3
4	D	98	LEU	2.2
5	J	-53	DG	2.2
4	D	39	TYR	2.1
3	C	36	LYS	2.1
4	D	104	ALA	2.1
4	H	45	VAL	2.1
4	D	99	LEU	2.1
4	D	31	LYS	2.0
2	F	98	TYR	2.0
3	C	96	LEU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MN	I	1013	1/1	-0.57	0.19	176,176,176,176	0
6	MN	J	1010	1/1	0.05	0.38	188,188,188,188	0
6	MN	J	1009	1/1	0.46	0.12	120,120,120,120	0
6	MN	J	1018	1/1	0.53	0.15	115,115,115,115	0
6	MN	I	1017	1/1	0.61	0.12	125,125,125,125	0
6	MN	J	1011	1/1	0.66	0.18	124,124,124,124	0
6	MN	J	1015	1/1	0.70	0.10	124,124,124,124	0
6	MN	D	1007	1/1	0.72	0.17	130,130,130,130	0
6	MN	I	1021	1/1	0.74	0.19	134,134,134,134	0
6	MN	J	1012	1/1	0.79	0.09	121,121,121,121	0
7	SO4	D	1101	5/5	0.79	0.40	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MN	J	1020	1/1	0.79	0.18	150,150,150,150	0
6	MN	I	1004	1/1	0.80	0.13	127,127,127,127	0
6	MN	I	1005	1/1	0.87	0.14	83,83,83,83	0
6	MN	J	1016	1/1	0.87	0.19	102,102,102,102	0
6	MN	I	1006	1/1	0.92	0.12	83,83,83,83	0
7	SO4	C	1102	5/5	0.93	0.22	45,48,49,51	5
6	MN	I	1019	1/1	0.95	0.23	118,118,118,118	0
6	MN	I	1014	1/1	0.95	0.13	108,108,108,108	0
6	MN	I	1003	1/1	0.95	0.22	77,77,77,77	0
6	MN	E	1002	1/1	0.96	0.20	94,94,94,94	0
7	SO4	G	1103	5/5	0.97	0.30	32,37,40,41	5
6	MN	J	1008	1/1	0.98	0.05	147,147,147,147	0
6	MN	A	1001	1/1	1.00	0.18	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.