Full wwPDB X-ray Structure Validation Report

Feb 19, 2016 – 07:57 PM GMT

PDB ID	:	4WU8
Title	:	Structure of trPtNAP-NCP145
Authors	:	Chua, E.Y.D.; Davey, C.A.
Deposited on	:	2014-10-31
Resolution	:	2.45 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

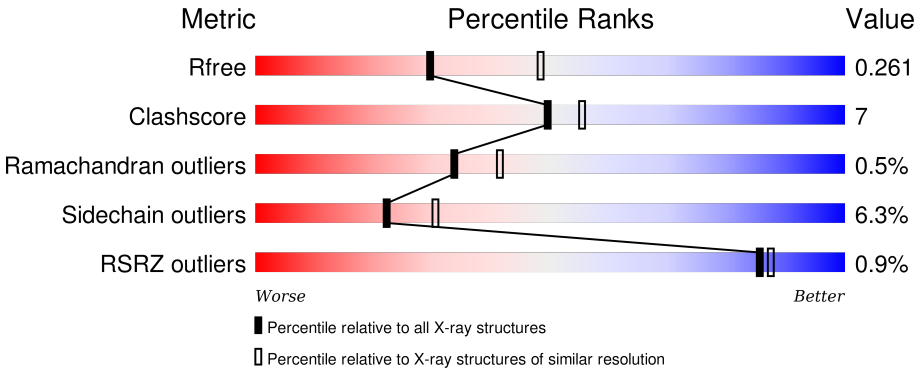
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	I	145	52% 38% 10%
2	J	145	52% 36% 12%
3	A	135	62% 8% 29%
3	E	135	61% 7% 29%
4	B	102	2% 70% 11% 20%

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Mol	Chain	Length	Quality of chain
4	F	102	2% 73% 11% 15%
5	C	129	59% 18% 5% 18%
5	G	129	73% 9% 18%
6	D	125	58% 16% 24%
6	H	125	60% 14% 24%

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	CX3	I	100	-	-	-	X
7	CX3	J	101[A]	-	-	-	X
7	CX3	J	101[B]	-	-	-	X
8	SO4	D	201	-	-	-	X
8	SO4	H	201	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12128 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 DNA (145-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	145	Total	C	N	O	P	0	0	0
			2970	1421	538	867	144			

- Molecule 2 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	145	Total	C	N	O	P	0	0	0
			2969	1421	535	869	144			

- Molecule 3 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	96	Total	C	N	O	S	0	0	0
			791	500	151	137	3			
3	E	96	Total	C	N	O	S	0	0	0
			791	500	151	137	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	engineered mutation	UNP P84233
E	102	ALA	GLY	engineered mutation	UNP P84233

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			
4	F	87	Total	C	N	O	S	0	0	0
			703	442	142	118	1			

- Molecule 5 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	106	Total	C	N	O	0	0	0
			818	516	160	142			
5	G	106	Total	C	N	O	0	0	0
			818	516	160	142			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	engineered mutation	UNP P06897
C	123	SER	ALA	engineered mutation	UNP P06897
G	99	ARG	GLY	engineered mutation	UNP P06897
G	123	SER	ALA	engineered mutation	UNP P06897

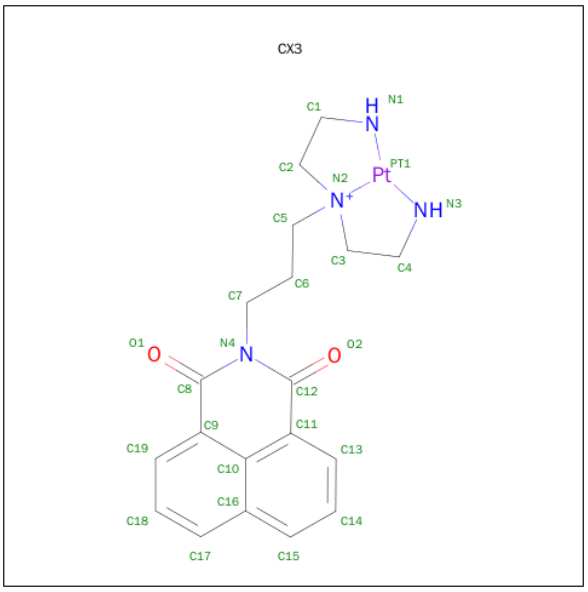
- Molecule 6 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	95	Total	C	N	O	S	0	0	0
			745	469	134	140	2			
6	H	95	Total	C	N	O	S	0	0	0
			745	469	134	140	2			

There are 2 discrepancies between the modelled and reference sequences:

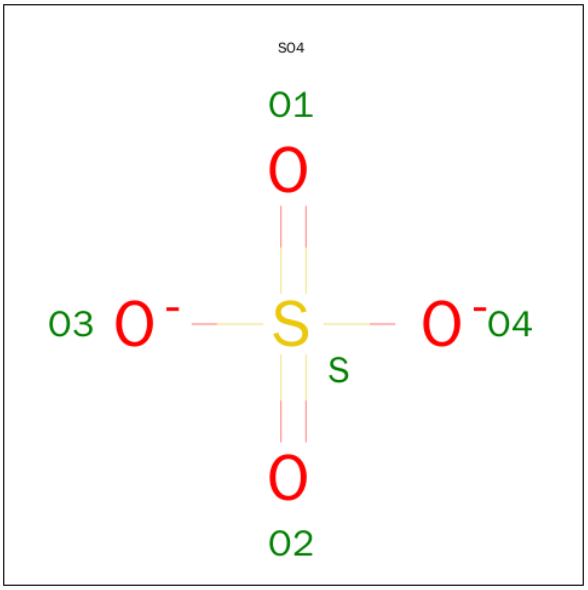
Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	engineered mutation	UNP P02281
H	29	THR	SER	engineered mutation	UNP P02281

- Molecule 7 is [2-(3-{bis[2-(amino-kappaN)ethyl]amino-kappaN}propyl)-1H-benzo[de]isoquinoline-1,3(2H)-dionato(2-)]platinum(1+) (three-letter code: CX3) (formula: $C_{19}H_{22}N_4O_2Pt$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	I	1	Total	C	N	O	Pt	0	0
			26	19	4	2	1		
7	J	1	Total	C	N	O	Pt	0	1
			52	38	8	4	2		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	O	S		0	0
			5	4	1			
8	H	1	Total	O	S		0	0
			5	4	1			

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	1	Total Mg 1 1	0	0

- Molecule 10 is water.

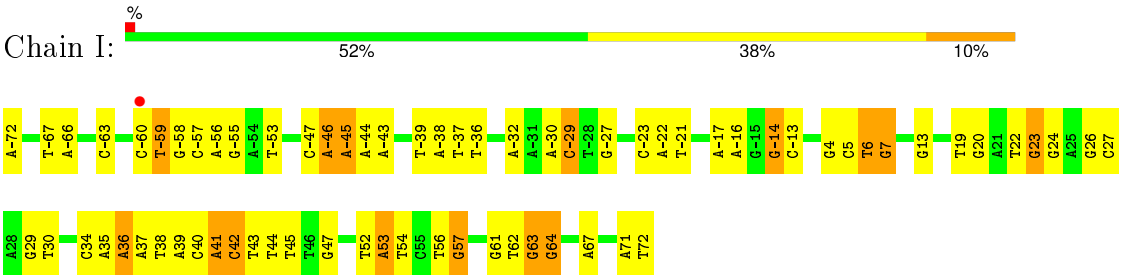
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	J	1	Total O 1 1	0	0
10	A	3	Total O 3 3	0	0
10	B	6	Total O 6 6	0	0
10	C	4	Total O 4 4	0	0
10	D	3	Total O 3 3	0	0
10	E	8	Total O 8 8	0	0
10	F	8	Total O 8 8	0	0
10	G	1	Total O 1 1	0	0
10	H	2	Total O 2 2	0	0

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 errors 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.

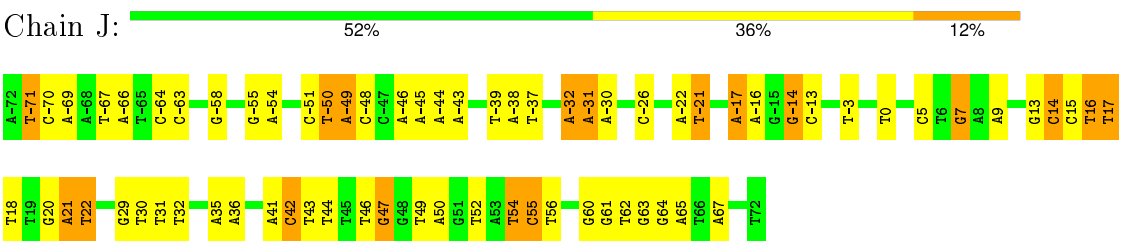
- Molecule 1: DNA (145-MER)

Chain I:



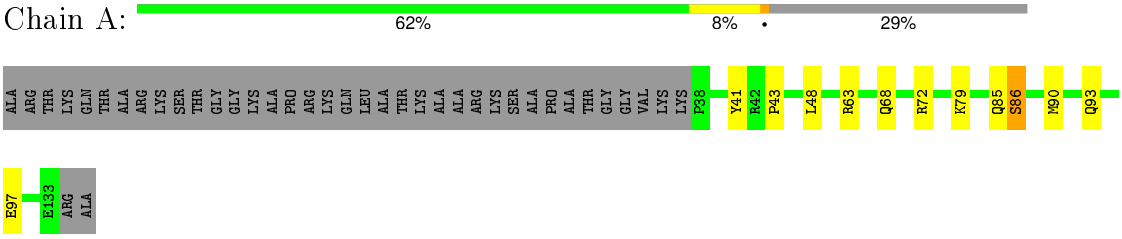
- Molecule 2: DNA (145-MER)

Chain J:



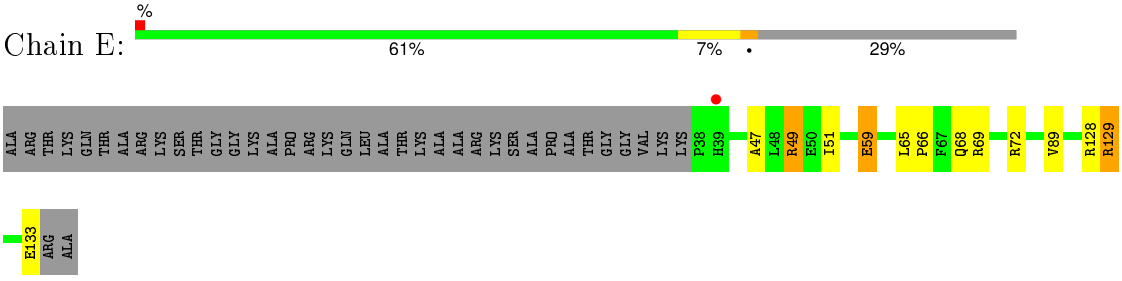
- Molecule 3: Histone H3.2

Chain A:



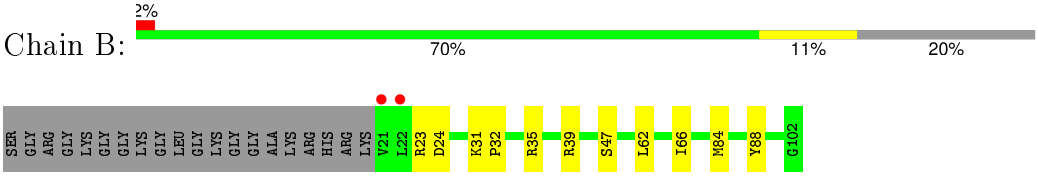
- Molecule 3: Histone H3.2

Chain E:



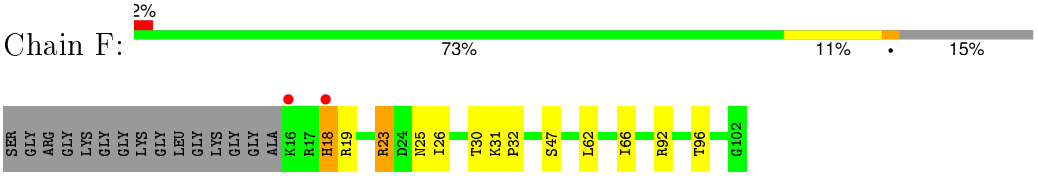
• Molecule 4: Histone H4

Chain B:



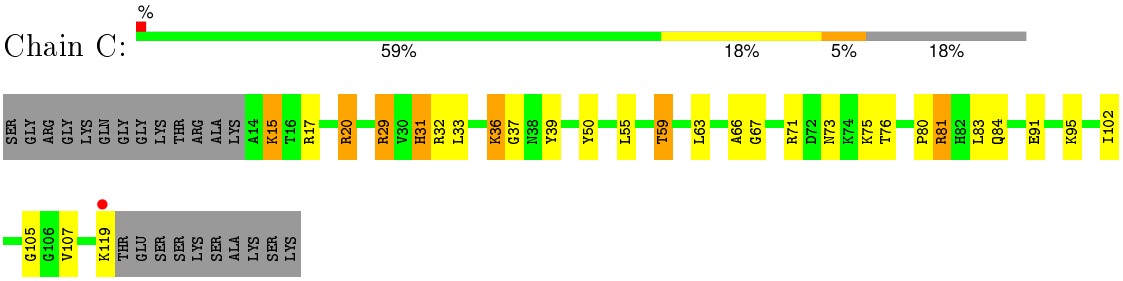
• Molecule 4: Histone H4

Chain F:



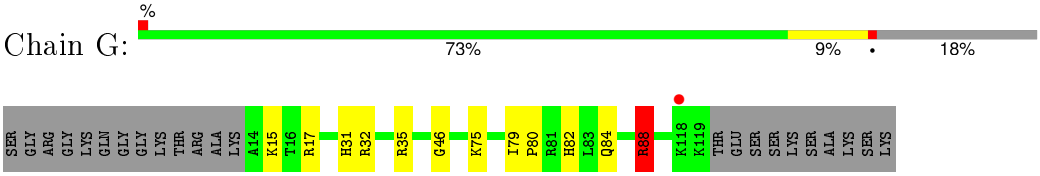
• Molecule 5: Histone H2A type 1

Chain C:



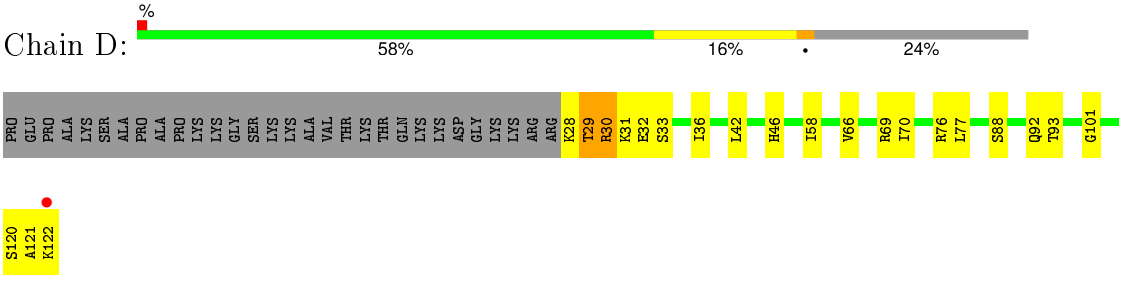
• Molecule 5: Histone H2A type 1

Chain G:



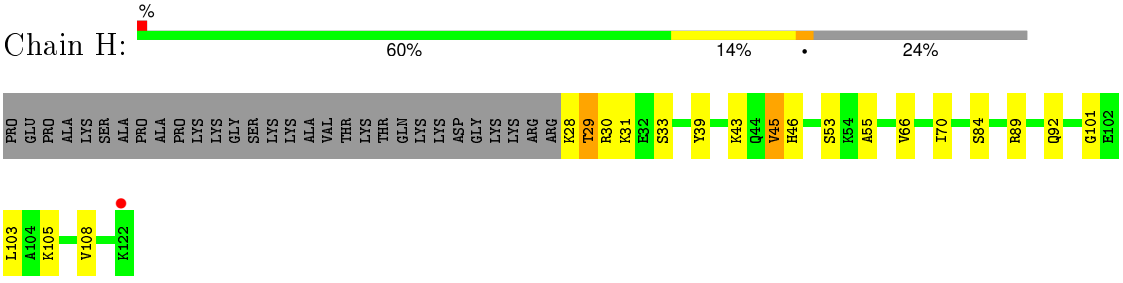
• Molecule 6: Histone H2B 1.1

Chain D:



• Molecule 6: Histone H2B 1.1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.41Å 109.63Å 183.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.05 – 2.45 47.09 – 2.45	Depositor EDS
% Data completeness (in resolution range)	93.1 (94.05-2.45) 93.1 (47.09-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.214 , 0.263 0.213 , 0.261	Depositor DCC
R_{free} test set	1471 reflections (2.03%)	DCC
Wilson B-factor (Å^2)	54.6	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 37.5	EDS
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	1 of 73892 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12128	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, CX3, 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	I	0.49	6/3332 (0.2%)	1.16	40/5141 (0.8%)
2	J	0.57	7/3330 (0.2%)	1.19	47/5138 (0.9%)
3	A	0.49	0/803	0.69	0/1078
3	E	0.64	0/803	0.85	0/1078
4	B	0.54	0/660	0.71	0/883
4	F	0.72	0/711	0.87	2/948 (0.2%)
5	C	0.63	0/828	0.80	1/1117 (0.1%)
5	G	0.51	0/828	0.72	2/1117 (0.2%)
6	D	0.62	0/756	0.82	3/1015 (0.3%)
6	H	0.58	0/756	0.69	0/1015
All	All	0.56	13/12807 (0.1%)	1.02	95/18530 (0.5%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	-14	DG	O3'-P	-16.53	1.41	1.61
1	I	-14	DG	C5-C4	12.42	1.47	1.38
2	J	-14	DG	C5-C4	11.68	1.46	1.38
2	J	-14	DG	N7-C5	-10.17	1.33	1.39
1	I	-14	DG	N7-C5	-8.54	1.34	1.39
2	J	-14	DG	C8-N7	7.82	1.35	1.30
1	I	-14	DG	C5-C6	7.51	1.49	1.42
2	J	-14	DG	C6-N1	-7.24	1.34	1.39
1	I	-14	DG	C6-N1	-6.89	1.34	1.39
1	I	-14	DG	C8-N7	6.24	1.34	1.30
2	J	-14	DG	C5-C6	6.11	1.48	1.42
1	I	-14	DG	C2-N3	5.23	1.36	1.32
2	J	-14	DG	C2-N3	5.18	1.36	1.32

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	-14	DG	N3-C4-C5	-23.41	116.89	128.60
1	I	-14	DG	N3-C4-C5	-21.59	117.81	128.60
2	J	-14	DG	C2-N3-C4	18.01	120.90	111.90
2	J	-14	DG	N3-C4-N9	17.90	136.74	126.00
1	I	-14	DG	C2-N3-C4	17.85	120.83	111.90
1	I	-14	DG	N3-C4-N9	16.16	135.70	126.00
1	I	-14	DG	C4-C5-N7	-15.44	104.62	110.80
1	I	-14	DG	C5-N7-C8	14.16	111.38	104.30
2	J	-14	DG	C5-N7-C8	12.52	110.56	104.30
2	J	-14	DG	C4-C5-N7	-12.43	105.83	110.80
1	I	-14	DG	N7-C8-N9	-10.51	107.84	113.10
2	J	-14	DG	C5-C6-O6	-10.39	122.37	128.60
2	J	-14	DG	O4'-C1'-N9	9.96	114.97	108.00
1	I	-14	DG	C5-C6-N1	9.95	116.47	111.50
1	I	-14	DG	C6-C5-N7	9.90	136.34	130.40
1	I	-14	DG	P-O3'-C3'	9.80	131.46	119.70
2	J	-14	DG	C5-C6-N1	9.65	116.32	111.50
2	J	-14	DG	N7-C8-N9	-9.57	108.31	113.10
2	J	41	DA	P-O3'-C3'	9.38	130.95	119.70
2	J	-31	DA	P-O3'-C3'	9.08	130.60	119.70
2	J	47	DG	P-O3'-C3'	8.53	129.94	119.70
1	I	-63	DC	P-O3'-C3'	8.53	129.93	119.70
2	J	5	DC	P-O3'-C3'	8.38	129.75	119.70
2	J	-50	DT	P-O3'-C3'	8.13	129.46	119.70
5	G	88	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	I	-14	DG	C8-N9-C4	7.97	109.59	106.40
1	I	44	DT	P-O3'-C3'	7.94	129.22	119.70
1	I	-60	DC	P-O3'-C3'	7.79	129.05	119.70
2	J	-32	DA	P-O3'-C3'	7.75	129.00	119.70
1	I	36	DA	P-O3'-C3'	7.68	128.92	119.70
2	J	-58	DG	P-O3'-C3'	7.63	128.85	119.70
1	I	-14	DG	C5-C6-O6	-7.58	124.05	128.60
1	I	45	DT	P-O3'-C3'	7.49	128.69	119.70
1	I	26	DG	P-O3'-C3'	7.46	128.65	119.70
1	I	64	DG	P-O3'-C3'	7.35	128.52	119.70
1	I	-46	DA	P-O3'-C3'	7.21	128.36	119.70
2	J	42	DC	P-O3'-C3'	7.15	128.28	119.70
1	I	6	DT	P-O3'-C3'	7.12	128.24	119.70
1	I	42	DC	P-O3'-C3'	7.02	128.12	119.70
1	I	-29	DC	P-O3'-C3'	7.00	128.10	119.70
2	J	-71	DT	P-O3'-C3'	6.86	127.93	119.70
2	J	7	DG	P-O3'-C3'	-6.85	111.48	119.70
2	J	49	DT	P-O3'-C3'	6.84	127.91	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	-21	DT	P-O3'-C3'	6.77	127.83	119.70
1	I	23	DG	P-O3'-C3'	6.67	127.70	119.70
2	J	-17	DA	P-O3'-C3'	6.64	127.67	119.70
1	I	7	DG	P-O3'-C3'	6.58	127.59	119.70
1	I	22	DT	P-O3'-C3'	6.57	127.59	119.70
1	I	-32	DA	P-O3'-C3'	6.56	127.57	119.70
1	I	20	DG	P-O3'-C3'	6.48	127.48	119.70
6	D	69	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	I	57	DG	P-O3'-C3'	6.29	127.24	119.70
2	J	-14	DG	C6-C5-N7	6.28	134.17	130.40
1	I	-53	DT	P-O3'-C3'	6.27	127.22	119.70
2	J	-14	DG	C8-N9-C4	6.25	108.90	106.40
1	I	13	DG	P-O3'-C3'	6.24	127.18	119.70
2	J	17	DT	P-O3'-C3'	6.23	127.18	119.70
2	J	-3	DT	P-O3'-C3'	6.14	127.07	119.70
2	J	50	DA	P-O3'-C3'	6.10	127.02	119.70
2	J	56	DT	P-O3'-C3'	6.07	126.99	119.70
2	J	14	DC	P-O3'-C3'	6.05	126.97	119.70
2	J	0	DT	P-O3'-C3'	6.05	126.96	119.70
2	J	60	DG	P-O3'-C3'	6.02	126.92	119.70
2	J	-67	DT	P-O3'-C3'	5.93	126.82	119.70
5	C	81	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	I	-59	DT	P-O3'-C3'	5.91	126.79	119.70
1	I	19	DT	P-O3'-C3'	5.86	126.73	119.70
1	I	52	DT	P-O3'-C3'	5.84	126.71	119.70
2	J	18	DT	P-O3'-C3'	5.83	126.70	119.70
2	J	-37	DT	P-O3'-C3'	5.82	126.68	119.70
2	J	31	DT	P-O3'-C3'	5.72	126.57	119.70
1	I	27	DC	P-O3'-C3'	5.72	126.57	119.70
1	I	53	DA	P-O3'-C3'	5.67	126.50	119.70
1	I	41	DA	P-O3'-C3'	5.59	126.41	119.70
2	J	54	DT	P-O3'-C3'	5.56	126.37	119.70
4	F	23	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	I	63	DG	P-O3'-C3'	5.44	126.22	119.70
6	D	76	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	J	-69	DA	P-O3'-C3'	5.26	126.02	119.70
2	J	21	DA	P-O3'-C3'	5.21	125.95	119.70
2	J	20	DG	P-O3'-C3'	5.14	125.87	119.70
2	J	-49	DA	P-O3'-C3'	5.14	125.87	119.70
1	I	-72	DA	P-O3'-C3'	5.13	125.86	119.70
2	J	16	DT	P-O3'-C3'	5.11	125.83	119.70
1	I	-27	DG	P-O3'-C3'	5.09	125.81	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	32	DT	P-O3'-C3'	5.08	125.80	119.70
2	J	-26	DC	P-O3'-C3'	5.07	125.78	119.70
2	J	-13	DC	OP2-P-O3'	5.06	116.33	105.20
6	D	76	ARG	NE-CZ-NH1	5.06	122.83	120.30
2	J	55	DC	P-O3'-C3'	5.06	125.77	119.70
5	G	88	ARG	NE-CZ-NH2	-5.05	117.77	120.30
2	J	52	DT	P-O3'-C3'	5.05	125.76	119.70
1	I	-45	DA	P-O3'-C3'	5.05	125.76	119.70
2	J	22	DT	P-O3'-C3'	5.01	125.71	119.70
4	F	92	ARG	CB-CA-C	-5.01	100.39	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2970	0	1640	41	0
2	J	2969	0	1641	43	0
3	A	791	0	828	7	0
3	E	791	0	828	12	0
4	B	653	0	696	5	0
4	F	703	0	755	5	0
5	C	818	0	877	23	0
5	G	818	0	877	10	0
6	D	745	0	773	14	0
6	H	745	0	773	9	0
7	I	26	0	20	3	0
7	J	52	0	40	6	0
8	D	5	0	0	1	0
8	H	5	0	0	1	0
9	E	1	0	0	0	0
10	A	3	0	0	0	0
10	B	6	0	0	0	0
10	C	4	0	0	0	0
10	D	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	E	8	0	0	0	0
10	F	8	0	0	1	0
10	G	1	0	0	0	0
10	H	2	0	0	0	0
10	J	1	0	0	0	0
All	All	12128	0	9748	153	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 7.

All (153) 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:E:49:ARG:HG3	3:E:49:ARG:HH11	1.35	0.92
5:G:17:ARG:HH12	5:G:31:HIS:HD2	1.02	0.92
5:G:17:ARG:HH12	5:G:31:HIS:CD2	1.91	0.87
1:I:62:DT:H2"	1:I:63:DG:O5'	1.81	0.81
2:J:-51:DC:H2"	2:J:-50:DT:H5'	1.63	0.80
5:C:55:LEU:O	5:C:59:THR:HG23	1.83	0.78
7:J:101[B]:CX3:H9	7:J:101[B]:CX3:O2	1.83	0.77
1:I:71:DA:H2"	1:I:72:DT:H5'	1.69	0.75
2:J:-17:DA:H2"	2:J:-16:DA:N7	2.02	0.74
7:J:101[B]:CX3:H9	7:J:101[B]:CX3:H15	1.75	0.69
2:J:-46:DA:H2"	2:J:-45:DA:C8	2.28	0.69
3:A:68:GLN:HE21	3:A:72:ARG:HH21	1.39	0.68
2:J:-45:DA:H4'	2:J:-44:DA:OP1	1.94	0.68
1:I:35:DA:H2"	1:I:36:DA:OP2	1.95	0.67
2:J:61:DG:H2"	2:J:62:DT:H5'	1.76	0.66
6:D:121:ALA:O	6:D:122:LYS:HB2	1.96	0.66
5:G:84:GLN:OE1	5:G:88:ARG:HD2	1.96	0.65
1:I:-66:DA:C2	2:J:67:DA:C2	2.85	0.65
3:E:59:GLU:O	3:E:59:GLU:HG2	1.95	0.64
7:I:100:CX3:H9	7:I:100:CX3:O1	1.97	0.64
5:G:17:ARG:NH1	5:G:31:HIS:HD2	1.85	0.63
5:C:17:ARG:HH22	5:C:31:HIS:CD2	2.16	0.63
1:I:62:DT:C2'	1:I:63:DG:O5'	2.48	0.62
2:J:54:DT:H2"	2:J:55:DC:OP2	1.98	0.62
2:J:30:DT:OP1	6:H:28:LYS:HD3	1.99	0.62
1:I:-57:DC:H2"	1:I:-56:DA:N7	2.14	0.61
2:J:61:DG:H2"	2:J:62:DT:C5'	2.31	0.60
2:J:-17:DA:H4'	2:J:-16:DA:OP1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:-17:DA:H2"	1:I:-16:DA:OP2	2.02	0.60
5:C:55:LEU:O	5:C:59:THR:CG2	2.50	0.60
2:J:-55:DG:H2"	2:J:-54:DA:OP2	2.02	0.60
1:I:47:DG:H21	6:H:30:ARG:HH22	1.50	0.60
2:J:-14:DG:O6	7:J:101[A]:CX3:N3	2.34	0.59
2:J:7:DG:H5'	4:B:47:SER:HA	1.83	0.59
5:C:17:ARG:HH22	5:C:31:HIS:HD2	1.49	0.59
1:I:56:DT:H2"	1:I:57:DG:N7	2.19	0.58
5:C:81:ARG:HG3	5:C:81:ARG:O	2.03	0.57
2:J:15:DC:H2"	2:J:16:DT:OP2	2.03	0.57
1:I:63:DG:H2"	1:I:64:DG:OP2	2.03	0.57
1:I:35:DA:H1'	1:I:36:DA:H5'	1.86	0.57
1:I:41:DA:H1'	1:I:42:DC:H5'	1.87	0.56
5:G:79:ILE:HG12	5:G:82:HIS:CE1	2.40	0.56
2:J:-44:DA:H2"	2:J:-43:DA:C8	2.42	0.55
2:J:-49:DA:H1'	2:J:-48:DC:O5'	2.06	0.55
3:E:128:ARG:HD2	3:E:133:GLU:OE1	2.06	0.55
7:I:100:CX3:H3	2:J:15:DC:O2	2.07	0.55
1:I:23:DG:H2"	1:I:24:DG:OP2	2.07	0.55
6:D:77:LEU:HD21	6:D:93:THR:HB	1.88	0.54
1:I:-14:DG:O6	7:I:100:CX3:N3	2.41	0.54
2:J:-43:DA:OP2	5:G:32:ARG:HD3	2.07	0.54
1:I:-67:DT:H2"	1:I:-66:DA:OP2	2.08	0.54
1:I:-56:DA:H4'	1:I:-55:DG:OP1	2.07	0.54
4:F:30:THR:HB	4:F:32:PRO:HD2	1.89	0.54
1:I:-44:DA:H2"	1:I:-43:DA:C8	2.42	0.54
3:E:49:ARG:CG	3:E:49:ARG:HH11	2.12	0.53
2:J:14:DC:H4'	2:J:15:DC:OP1	2.08	0.53
1:I:29:DG:H2"	1:I:30:DT:O5'	2.08	0.53
5:G:46:GLY:N	8:H:201:SO4:O2	2.30	0.53
2:J:17:DT:H4'	3:A:63:ARG:CZ	2.38	0.53
6:H:39:TYR:CE2	6:H:43:LYS:HE3	2.44	0.52
5:C:15:LYS:HB2	5:C:20:ARG:NH2	2.25	0.52
1:I:53:DA:C2	1:I:54:DT:C2	2.98	0.51
5:C:102:ILE:HG23	6:D:58:ILE:HD13	1.91	0.51
1:I:41:DA:H2"	1:I:42:DC:OP2	2.11	0.51
5:C:33:LEU:HD23	5:C:36:LYS:HD3	1.91	0.51
7:J:101[B]:CX3:C6	7:J:101[B]:CX3:O2	2.58	0.51
1:I:4:DG:H2"	1:I:5:DC:OP2	2.11	0.51
2:J:-51:DC:C2'	2:J:-50:DT:H5'	2.37	0.50
5:C:32:ARG:HH22	6:D:32:GLU:CD	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:-66:DA:H5'	3:A:41:TYR:OH	2.11	0.49
5:C:50:TYR:OH	6:D:92:GLN:NE2	2.30	0.49
5:G:31:HIS:O	5:G:35:ARG:HG3	2.13	0.49
2:J:64:DG:H2"	2:J:65:DA:OP2	2.13	0.49
3:E:65:LEU:HB3	3:E:66:PRO:HD3	1.95	0.49
3:E:49:ARG:HG3	3:E:49:ARG:NH1	2.14	0.49
5:C:81:ARG:NH2	5:C:107:VAL:O	2.34	0.49
4:F:96:THR:HA	10:F:206:HOH:O	2.13	0.48
3:E:129:ARG:HD2	3:E:129:ARG:C	2.34	0.48
1:I:-14:DG:H2"	1:I:-13:DC:O5'	2.12	0.48
2:J:42:DC:H2"	2:J:43:DT:OP2	2.12	0.48
5:C:67:GLY:HA3	6:D:46:HIS:CD2	2.49	0.48
5:C:84:GLN:HG2	5:C:105:GLY:O	2.14	0.48
5:C:15:LYS:HB2	5:C:20:ARG:HH21	1.78	0.48
1:I:-47:DC:H2"	1:I:-46:DA:N7	2.28	0.48
1:I:-30:DA:H2"	1:I:-29:DC:OP2	2.14	0.47
2:J:-39:DT:H2"	2:J:-38:DA:OP2	2.14	0.47
2:J:62:DT:H2"	2:J:63:DG:H5'	1.96	0.47
1:I:67:DA:C2	2:J:-66:DA:C2	3.02	0.47
6:D:66:VAL:HG12	6:D:70:ILE:HD12	1.97	0.46
2:J:21:DA:H2"	2:J:22:DT:OP2	2.16	0.46
4:B:31:LYS:HB3	4:B:32:PRO:HD3	1.98	0.46
1:I:53:DA:H1'	1:I:54:DT:O5'	2.15	0.46
1:I:-39:DT:C2'	1:I:-38:DA:O5'	2.64	0.46
5:C:37:GLY:HA3	5:C:39:TYR:CE1	2.50	0.46
7:J:101[B]:CX3:H13	7:J:101[B]:CX3:H10	1.64	0.46
2:J:46:DT:H2"	2:J:47:DG:C8	2.51	0.46
2:J:9:DA:H5'	3:A:43:PRO:HA	1.98	0.45
3:E:47:ALA:O	3:E:51:ILE:HG13	2.17	0.45
5:C:63:LEU:HD13	6:D:42:LEU:HB2	1.99	0.45
6:H:92:GLN:NE2	6:H:108:VAL:HG13	2.32	0.45
6:D:30:ARG:H	6:D:30:ARG:HG3	1.53	0.45
5:G:84:GLN:O	5:G:88:ARG:HG2	2.15	0.45
2:J:43:DT:H2"	2:J:44:DT:OP2	2.15	0.45
6:H:45:VAL:HG12	6:H:46:HIS:HD2	1.82	0.45
5:C:73:ASN:O	5:C:75:LYS:HG2	2.17	0.44
2:J:-71:DT:H4'	2:J:-70:DC:OP1	2.16	0.44
1:I:61:DG:H3'	1:I:62:DT:H72	2.00	0.44
5:C:66:ALA:HB2	5:C:83:LEU:HD23	1.99	0.44
5:C:66:ALA:CB	5:C:83:LEU:HD23	2.47	0.44
2:J:-31:DA:H2"	2:J:-30:DA:O5'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:13:DG:H2"	2:J:14:DC:C6	2.52	0.44
2:J:29:DG:OP1	6:H:29:THR:HB	2.18	0.44
7:J:101[B]:CX3:H9	7:J:101[B]:CX3:C1	2.39	0.44
4:F:62:LEU:O	4:F:66:ILE:HD12	2.18	0.44
3:E:68:GLN:NE2	3:E:72:ARG:HH21	2.16	0.43
6:H:66:VAL:HG12	6:H:70:ILE:HD12	2.00	0.43
4:B:35:ARG:O	4:B:39:ARG:HG2	2.17	0.43
5:C:17:ARG:NH2	5:C:31:HIS:HD2	2.14	0.43
5:G:80:PRO:HD3	6:H:55:ALA:HB2	1.98	0.43
5:C:17:ARG:HH12	5:C:31:HIS:CD2	2.36	0.43
1:I:53:DA:H2"	1:I:54:DT:OP2	2.17	0.43
1:I:64:DG:N2	2:J:-64:DC:O2	2.40	0.43
2:J:-17:DA:H2"	2:J:-16:DA:C8	2.53	0.42
6:H:43:LYS:HA	6:H:43:LYS:HD3	1.71	0.42
3:E:68:GLN:HG3	3:E:89:VAL:HG11	2.02	0.42
1:I:-22:DA:H1'	1:I:-21:DT:H5'	2.02	0.42
1:I:42:DC:H2"	1:I:43:DT:OP2	2.20	0.42
1:I:-37:DT:H2"	1:I:-36:DT:OP2	2.19	0.42
1:I:39:DA:H2"	1:I:40:DC:O5'	2.18	0.42
3:E:129:ARG:CD	3:E:129:ARG:C	2.88	0.42
2:J:13:DG:H2"	2:J:14:DC:C5	2.55	0.42
5:C:29:ARG:NH2	6:D:33:SER:O	2.53	0.42
1:I:37:DA:H2'	1:I:38:DT:C6	2.55	0.42
2:J:-64:DC:H2'	2:J:-63:DC:C6	2.54	0.42
1:I:29:DG:OP1	6:D:29:THR:HG22	2.19	0.41
3:A:86:SER:O	3:A:90:MET:HG2	2.20	0.41
1:I:-23:DC:OP1	3:A:85:GLN:HG2	2.19	0.41
1:I:6:DT:H2"	1:I:7:DG:C8	2.54	0.41
3:E:69:ARG:HD2	4:F:25:ASN:OD1	2.20	0.41
3:A:93:GLN:O	3:A:97:GLU:HG3	2.20	0.41
6:D:88:SER:N	8:D:201:SO4:O3	2.45	0.41
6:D:36:ILE:HD13	6:D:36:ILE:HG21	1.80	0.41
2:J:-22:DA:H1'	2:J:-21:DT:H5'	2.02	0.41
1:I:-45:DA:H4'	1:I:-44:DA:OP1	2.21	0.41
5:C:80:PRO:HB3	6:D:58:ILE:CD1	2.50	0.41
1:I:-59:DT:H2"	1:I:-58:DG:OP2	2.20	0.41
4:F:31:LYS:HB3	4:F:32:PRO:HD3	2.03	0.41
2:J:35:DA:H2"	2:J:36:DA:OP2	2.21	0.41
1:I:34:DC:H4'	1:I:35:DA:OP1	2.21	0.41
4:B:84:MET:HE3	4:B:88:TYR:CZ	2.56	0.40
2:J:-49:DA:H2"	2:J:-48:DC:OP2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:-32:DA:H2"	2:J:-31:DA:OP2	2.20	0.40
4:B:62:LEU:HB3	4:B:66:ILE:HD12	2.04	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
3	A	94/135 (70%)	92 (98%)	2 (2%)	0	100 100
3	E	94/135 (70%)	93 (99%)	1 (1%)	0	100 100
4	B	80/102 (78%)	79 (99%)	1 (1%)	0	100 100
4	F	85/102 (83%)	81 (95%)	2 (2%)	2 (2%)	7 4
5	C	104/129 (81%)	100 (96%)	4 (4%)	0	100 100
5	G	104/129 (81%)	100 (96%)	4 (4%)	0	100 100
6	D	93/125 (74%)	89 (96%)	3 (3%)	1 (1%)	17 19
6	H	93/125 (74%)	89 (96%)	3 (3%)	1 (1%)	17 19
All	All	747/982 (76%)	723 (97%)	20 (3%)	4 (0%)	34 41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	18	HIS
6	D	101	GLY
6	H	101	GLY
4	F	26	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	84/110 (76%)	81 (96%)	3 (4%)	42 58
3	E	84/110 (76%)	81 (96%)	3 (4%)	42 58
4	B	67/78 (86%)	65 (97%)	2 (3%)	48 65
4	F	72/78 (92%)	68 (94%)	4 (6%)	26 36
5	C	84/101 (83%)	73 (87%)	11 (13%)	5 4
5	G	84/101 (83%)	81 (96%)	3 (4%)	42 58
6	D	81/105 (77%)	76 (94%)	5 (6%)	23 31
6	H	81/105 (77%)	72 (89%)	9 (11%)	8 8
All	All	637/788 (81%)	597 (94%)	40 (6%)	22 30

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	48	LEU
3	A	79	LYS
3	A	86	SER
4	B	23	ARG
4	B	24	ASP
5	C	15	LYS
5	C	20	ARG
5	C	29	ARG
5	C	31	HIS
5	C	36	LYS
5	C	59	THR
5	C	71	ARG
5	C	76	THR
5	C	91	GLU
5	C	95	LYS
5	C	119	LYS
6	D	28	LYS
6	D	29	THR
6	D	30	ARG

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Mol	Chain	Res	Type
6	D	31	LYS
6	D	120	SER
3	E	49	ARG
3	E	59	GLU
3	E	129	ARG
4	F	18	HIS
4	F	19	ARG
4	F	23	ARG
4	F	47	SER
5	G	15	LYS
5	G	75	LYS
5	G	88	ARG
6	H	29	THR
6	H	31	LYS
6	H	33	SER
6	H	45	VAL
6	H	53	SER
6	H	84	SER
6	H	89	ARG
6	H	103	LEU
6	H	105	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	68	GLN
5	C	31	HIS
6	D	92	GLN
3	E	68	GLN
4	F	18	HIS
5	G	31	HIS
6	H	46	HIS
6	H	92	GLN

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 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\#\|Z\| > 2$
8	SO4	D	201	-	4,4,4	0.71	0	6,6,6	0.58	0
8	SO4	H	201	-	4,4,4	0.74	0	6,6,6	0.71	0
7	CX3	I	100	1	22,30,30	2.07	4 (18%)	20,45,45	2.47	3 (15%)
7	CX3	J	101[A]	2	22,30,30	1.90	4 (18%)	20,45,45	1.83	3 (15%)
7	CX3	J	101[B]	-	22,30,30	1.84	4 (18%)	20,45,45	1.76	2 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SO4	D	201	-	-	0/0/0/0	0/0/0/0
8	SO4	H	201	-	-	0/0/0/0	0/0/0/0
7	CX3	I	100	1	-	1/4/27/27	0/3/5/5
7	CX3	J	101[A]	2	-	0/4/27/27	0/3/5/5
7	CX3	J	101[B]	-	-	0/4/27/27	0/3/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	101[B]	CX3	C12-N4	2.25	1.41	1.38
7	J	101[A]	CX3	C12-N4	2.37	1.41	1.38
7	J	101[A]	CX3	C8-N4	2.52	1.42	1.38
7	J	101[B]	CX3	C8-N4	2.54	1.42	1.38
7	I	100	CX3	C12-N4	3.12	1.42	1.38
7	I	100	CX3	C8-N4	3.47	1.43	1.38
7	J	101[B]	CX3	C12-C11	4.82	1.49	1.41
7	J	101[B]	CX3	C8-C9	4.99	1.49	1.41
7	J	101[A]	CX3	C12-C11	5.01	1.49	1.41
7	J	101[A]	CX3	C8-C9	5.24	1.50	1.41
7	I	100	CX3	C8-C9	5.33	1.50	1.41
7	I	100	CX3	C12-C11	5.46	1.50	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	J	101[A]	CX3	C7-N4-C8	2.04	121.10	119.10
7	J	101[B]	CX3	C11-C12-N4	4.39	119.72	116.09
7	J	101[B]	CX3	C9-C8-N4	4.74	120.00	116.09
7	J	101[A]	CX3	C9-C8-N4	4.77	120.03	116.09
7	J	101[A]	CX3	C11-C12-N4	5.25	120.43	116.09
7	I	100	CX3	C7-N4-C8	5.77	124.77	119.10
7	I	100	CX3	C9-C8-N4	5.82	120.89	116.09
7	I	100	CX3	C11-C12-N4	6.46	121.42	116.09

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	100	CX3	C6-C7-N4-C12

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	201	SO4	1	0
8	H	201	SO4	1	0
7	I	100	CX3	3	0
7	J	101[A]	CX3	1	0
7	J	101[B]	CX3	5	0

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, 95^{th} 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	145/145 (100%)	-0.27	1 (0%) 89 90	41, 94, 136, 165	0
2	J	145/145 (100%)	-0.29	0 100 100	49, 95, 140, 168	0
3	A	96/135 (71%)	-0.17	0 100 100	30, 47, 70, 121	0
3	E	96/135 (71%)	-0.22	1 (1%) 84 86	24, 35, 55, 107	0
4	B	82/102 (80%)	-0.13	2 (2%) 62 65	31, 43, 68, 124	0
4	F	87/102 (85%)	0.07	2 (2%) 64 66	24, 33, 57, 164	0
5	C	106/129 (82%)	-0.16	1 (0%) 85 87	24, 40, 67, 119	0
5	G	106/129 (82%)	-0.17	1 (0%) 85 87	33, 48, 83, 107	0
6	D	95/125 (76%)	-0.06	1 (1%) 82 84	30, 42, 75, 118	0
6	H	95/125 (76%)	0.02	1 (1%) 82 84	31, 47, 92, 132	0
All	All	1053/1272 (82%)	-0.15	10 (0%) 85 87	24, 48, 122, 168	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	16	LYS	9.5
5	C	119	LYS	6.0
6	H	122	LYS	5.4
6	D	122	LYS	4.0
4	B	21	VAL	3.9
5	G	118	LYS	3.5
4	F	18	HIS	3.2
4	B	22	LEU	2.5
1	I	-60	DC	2.3
3	E	39	HIS	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
7	CX3	J	101[A]	26/26	0.86	0.40	24.50	96,100,107,108	26
8	SO4	D	201	5/5	0.96	0.24	6.46	59,60,66,72	0
7	CX3	J	101[B]	26/26	0.86	0.40	5.82	112,125,157,159	26
8	SO4	H	201	5/5	0.97	0.19	2.47	57,58,63,76	0
7	CX3	I	100	26/26	0.88	0.27	2.39	134,148,186,194	0
9	MG	E	201	1/1	0.98	0.12	-0.57	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.