Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2016 – 04:52 PM EDT

PDB ID	:	5EEA
Title	:	Structure of HOXB13-DNA(CAA) complex
Authors	:	Morgunova, E.; Yin, Y.; Jolma, A.; Popov, A.; Taipale, J.
Deposited on	:	2015-10-22
Resolution	:	2.19 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 ⓘ symbol.

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

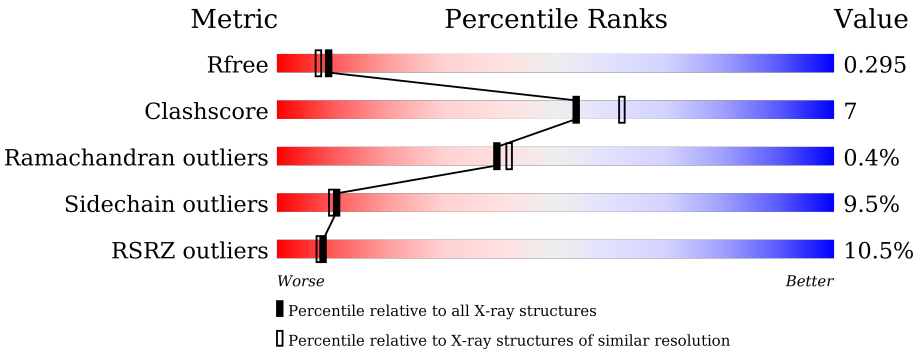
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.19 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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. 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	C	18	6%, 94%, 6%
1	D	18	17%, 89%, 6%, 6%
1	H	18	11%, 94%, 6%
1	K	18	6%, 89%, 6%, 6%
2	E	18	11%, 67%, 28%, 6%
2	F	18	11%, 78%, 22%

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Mol	Chain	Length	Quality of chain
2	I	18	11% 72% 28%
2	L	18	11% 78% 22%
3	A	63	11% 78% 16% 5%
3	B	63	10% 78% 16%
3	G	63	14% 81% 14% 5%
3	J	63	6% 75% 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5585 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 (5'-D(P*TP*TP*GP*TP*GP*TP*TP*TP*TP*AP*TP*TP*GP*GP*GP*TP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	18	Total	C	N	O	P	0	0	0
			369	178	56	117	18			
1	C	18	Total	C	N	O	P	0	0	0
			369	178	56	117	18			
1	H	18	Total	C	N	O	P	0	0	0
			369	178	56	117	18			
1	K	18	Total	C	N	O	P	0	0	0
			369	178	56	117	18			

- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*GP*AP*CP*CP*CP*AP*AP*TP*AP*AP*AP*AP*CP*AP*CP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			369	175	77	99	18			
2	F	18	Total	C	N	O	P	0	0	0
			369	175	77	99	18			
2	I	18	Total	C	N	O	P	0	0	0
			366	175	77	97	17			
2	L	18	Total	C	N	O	P	0	0	0
			369	175	77	99	18			

- Molecule 3 is a protein called Homeobox protein Hox-B13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	61	Total	C	N	O	0	2	0
			536	340	108	88			
3	A	62	Total	C	N	O	0	0	0
			528	334	106	88			
3	G	63	Total	C	N	O	0	0	0
			533	337	107	89			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	61	Total	C	N	O	0	0	0
			521	329	105	87			

- Molecule 4 is water.

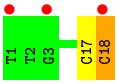
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	36	Total	O	0	0
			36	36		
4	E	55	Total	O	0	0
			55	55		
4	C	32	Total	O	0	0
			32	32		
4	F	42	Total	O	0	0
			42	42		
4	H	34	Total	O	0	0
			34	34		
4	I	37	Total	O	0	0
			37	37		
4	K	35	Total	O	0	0
			35	35		
4	L	45	Total	O	0	0
			45	45		
4	B	50	Total	O	0	0
			50	50		
4	A	55	Total	O	0	0
			55	55		
4	G	46	Total	O	0	0
			46	46		
4	J	51	Total	O	0	0
			51	51		

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.

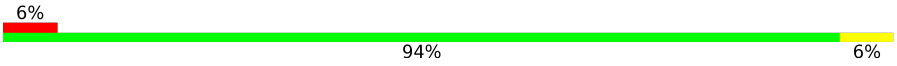
• Molecule 1: DNA (5'-D(P*TP*TP*GP*TP*GP*TP*TP*TP*TP*AP*TP*TP*GP*GP*GP*TP*CP*C)-3')

Chain D:



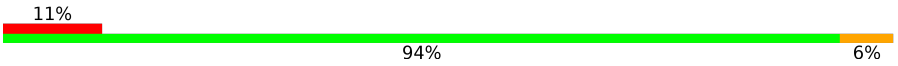
• Molecule 1: DNA (5'-D(P*TP*TP*GP*TP*GP*TP*TP*TP*TP*AP*TP*TP*GP*GP*GP*TP*CP*C)-3')

Chain C:



• Molecule 1: DNA (5'-D(P*TP*TP*GP*TP*GP*TP*TP*TP*TP*AP*TP*TP*GP*GP*GP*TP*CP*C)-3')

Chain H:



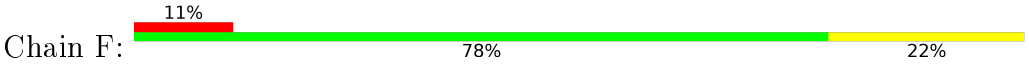
• Molecule 1: DNA (5'-D(P*TP*TP*GP*TP*GP*TP*TP*TP*TP*AP*TP*TP*GP*GP*GP*TP*CP*C)-3')

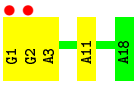
Chain K:

• Molecule 2: DNA (5'-D(P*GP*GP*AP*CP*CP*CP*AP*AP*TP*AP*AP*AP*AP*CP*AP*CP*AP*A)-3')

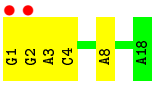
Chain E:

• Molecule 2: DNA (5'-D(P*GP*GP*AP*CP*CP*CP*AP*AP*TP*AP*AP*AP*AP*CP*AP*C P*AP*A)-3')

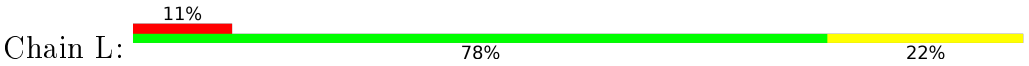


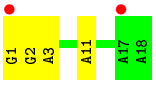


• Molecule 2: DNA (5'-D(P*GP*GP*AP*CP*CP*CP*AP*AP*TP*AP*AP*AP*AP*CP*AP*C P*AP*A)-3')

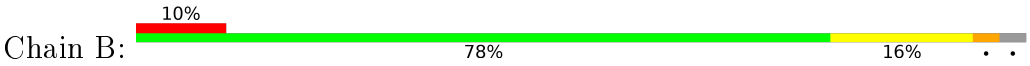


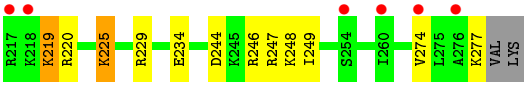
• Molecule 2: DNA (5'-D(P*GP*GP*AP*CP*CP*CP*AP*AP*TP*AP*AP*AP*AP*CP*AP*C P*AP*A)-3')



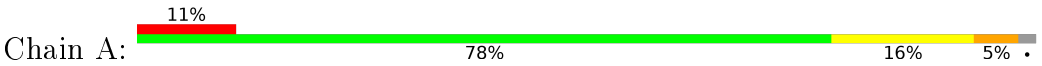


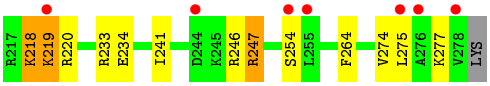
• Molecule 3: Homeobox protein Hox-B13



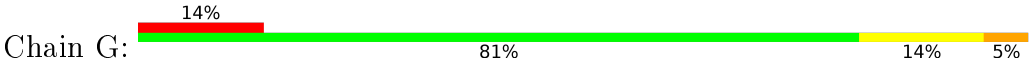


• Molecule 3: Homeobox protein Hox-B13



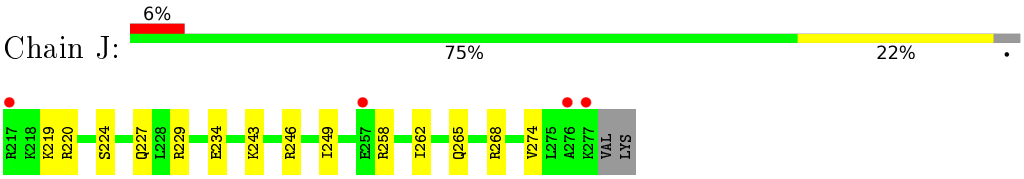


• Molecule 3: Homeobox protein Hox-B13



• Molecule 3: Homeobox protein Hox-B13

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	77.36Å 57.92Å 101.28Å 90.00° 101.57° 90.00°	Depositor
Resolution (Å)	45.95 – 2.19 46.02 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.0 (45.95-2.19) 97.4 (46.02-2.19)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.251 , 0.296 0.254 , 0.295	Depositor DCC
R_{free} test set	1260 reflections (2.87%)	DCC
Wilson B-factor (Å^2)	35.9	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 36.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5585	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.12 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0388e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	C	0.57	0/410	1.06	0/632
1	D	0.59	0/410	1.16	1/632 (0.2%)
1	H	0.56	0/410	1.11	1/632 (0.2%)
1	K	0.56	0/410	1.16	3/632 (0.5%)
2	E	0.53	0/416	0.86	1/638 (0.2%)
2	F	0.52	0/416	0.83	0/638
2	I	0.47	0/413	0.79	0/634
2	L	0.53	0/416	0.81	0/638
3	A	0.90	0/534	1.05	2/707 (0.3%)
3	B	0.84	0/545	1.01	2/719 (0.3%)
3	G	0.88	0/539	1.03	2/714 (0.3%)
3	J	0.89	0/527	1.02	4/697 (0.6%)
All	All	0.69	0/5446	1.00	16/7913 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	G	0	1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	220	ARG	NE-CZ-NH2	-8.93	115.83	120.30
1	K	18	DC	O4'-C4'-C3'	-7.52	101.49	106.00
3	G	220	ARG	NE-CZ-NH2	-7.39	116.60	120.30
3	A	220	ARG	NE-CZ-NH2	-7.28	116.66	120.30
3	A	246	ARG	NE-CZ-NH1	6.76	123.68	120.30
3	G	246	ARG	NE-CZ-NH1	6.70	123.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	246	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	K	18	DC	C1'-O4'-C4'	-6.29	103.81	110.10
1	H	18	DC	O4'-C1'-N1	6.13	112.29	108.00
3	J	220	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	D	18	DC	O4'-C1'-N1	6.08	112.26	108.00
3	J	246	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	E	1	DG	O5'-P-OP1	5.50	117.31	110.70
1	K	18	DC	O4'-C1'-N1	5.39	111.77	108.00
3	J	268	ARG	NE-CZ-NH1	5.21	122.90	120.30
3	J	246	ARG	NE-CZ-NH2	-5.17	117.71	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	275	LEU	Peptide

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	C	369	0	209	1	0
1	D	369	0	208	4	0
1	H	369	0	209	2	0
1	K	369	0	209	2	11
2	E	369	0	199	18	0
2	F	369	0	200	3	0
2	I	366	0	201	5	11
2	L	369	0	200	4	0
3	A	528	0	577	4	0
3	B	536	0	593	7	0
3	G	533	0	579	4	0
3	J	521	0	568	8	0
4	A	55	0	0	2	0
4	B	50	0	0	4	0
4	C	32	0	0	1	0
4	D	36	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	55	0	0	7	0
4	F	42	0	0	2	0
4	G	46	0	0	1	0
4	H	34	0	0	1	0
4	I	37	0	0	1	0
4	J	51	0	0	6	0
4	K	35	0	0	1	0
4	L	45	0	0	3	0
All	All	5585	0	3952	58	11

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 (58) 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:E:1:DG:H5"	4:E:106:HOH:O	1.22	1.28
3:J:224:SER:OG	4:J:301:HOH:O	1.64	1.13
2:E:1:DG:H2'	2:E:2:DG:C4	1.88	1.07
1:H:18:DC:N4	2:I:1:DG:O6	1.97	0.97
2:E:1:DG:C5'	4:E:106:HOH:O	1.94	0.81
2:L:1:DG:N2	4:L:102:HOH:O	2.16	0.78
1:D:18:DC:O2	2:E:1:DG:N2	2.16	0.76
3:B:229:ARG:NH1	4:B:301:HOH:O	2.17	0.75
3:J:265:GLN:NE2	4:J:303:HOH:O	2.19	0.73
3:J:227:GLN:N	4:J:301:HOH:O	2.08	0.69
2:L:3:DA:N7	4:L:103:HOH:O	2.26	0.68
2:E:1:DG:C2'	2:E:2:DG:C4	2.74	0.67
1:C:18:DC:N3	4:C:101:HOH:O	2.27	0.67
2:E:11:DA:OP2	4:E:102:HOH:O	2.13	0.67
3:B:234:GLU:HG2	3:B:249:ILE:HD11	1.77	0.66
1:H:18:DC:OP2	4:H:101:HOH:O	2.14	0.65
2:L:11:DA:OP2	4:L:101:HOH:O	2.15	0.65
2:F:11:DA:OP2	4:F:101:HOH:O	2.15	0.64
3:A:247:ARG:N	4:A:301:HOH:O	2.32	0.61
3:J:234:GLU:HG2	3:J:249:ILE:HD11	1.84	0.59
3:J:234:GLU:HG3	4:J:327:HOH:O	2.03	0.57
2:E:1:DG:H2'	2:E:2:DG:N3	2.18	0.56
2:E:1:DG:O3'	2:E:2:DG:O4'	2.23	0.55
3:G:255:LEU:HB2	3:G:260:ILE:HD11	1.88	0.55
2:E:12:DA:OP2	4:E:103:HOH:O	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:243:LYS:O	4:J:302:HOH:O	2.18	0.52
2:E:6:DC:H1'	4:E:104:HOH:O	2.09	0.52
3:B:244:ASP:OD1	3:B:247:ARG:NH2	2.42	0.52
3:B:219:LYS:NZ	4:B:304:HOH:O	2.43	0.52
2:E:8:DA:N6	4:E:107:HOH:O	2.43	0.51
3:J:262:ILE:HG12	4:J:303:HOH:O	2.11	0.51
2:I:2:DG:N2	2:I:3:DA:C2	2.79	0.50
1:K:7:DT:OP2	4:K:101:HOH:O	2.20	0.49
2:E:1:DG:OP1	2:E:2:DG:OP1	2.31	0.49
1:D:17:DC:H3'	1:D:18:DC:H5"	1.93	0.49
2:F:2:DG:H2"	2:F:3:DA:C8	2.48	0.49
2:I:4:DC:OP1	3:G:243:LYS:NZ	2.44	0.49
2:E:1:DG:H2'	2:E:2:DG:C5	2.42	0.48
2:L:1:DG:H1'	2:L:2:DG:C8	2.49	0.48
3:A:218:LYS:N	3:A:219:LYS:HA	2.29	0.48
2:E:1:DG:C2'	2:E:2:DG:N3	2.77	0.47
2:E:1:DG:O3'	2:E:1:DG:P	2.73	0.47
2:I:8:DA:N6	4:I:102:HOH:O	2.48	0.46
1:D:18:DC:C2	2:E:1:DG:N2	2.83	0.46
2:F:1:DG:C3'	2:F:2:DG:H4'	2.46	0.45
3:B:234:GLU:HG3	4:B:315:HOH:O	2.16	0.45
3:B:277:LYS:NZ	4:B:305:HOH:O	2.50	0.45
3:A:241:ILE:HD13	3:A:264:PHE:CZ	2.51	0.45
3:J:258:ARG:NE	3:J:262:ILE:HD11	2.32	0.45
3:G:277:LYS:HE2	3:G:277:LYS:HA	1.99	0.45
1:K:18:DC:OP1	1:K:18:DC:H4'	2.16	0.44
2:E:2:DG:C8	2:E:2:DG:OP2	2.70	0.44
3:G:246:ARG:NH2	4:G:303:HOH:O	2.50	0.43
2:I:1:DG:C6	2:I:2:DG:C6	3.06	0.43
3:A:234:GLU:HG3	4:A:328:HOH:O	2.19	0.42
2:E:1:DG:N2	4:E:110:HOH:O	2.53	0.42
1:D:17:DC:H3'	1:D:18:DC:C5'	2.50	0.42
4:F:138:HOH:O	3:B:225:LYS:HG2	2.18	0.42

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1:DG:O4'	1:K:18:DC:O4'[2_545]	0.71	1.49
2:I:1:DG:N3	1:K:18:DC:C2'[2_545]	1.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1:DG:C1'	1:K:18:DC:C3'[2_545]	1.72	0.48
2:I:1:DG:O4'	1:K:18:DC:C4'[2_545]	1.73	0.47
2:I:1:DG:C1'	1:K:18:DC:O4'[2_545]	1.79	0.41
2:I:1:DG:O4'	1:K:18:DC:C1'[2_545]	1.89	0.31
2:I:1:DG:C4'	1:K:18:DC:O4'[2_545]	2.01	0.19
2:I:1:DG:C1'	1:K:18:DC:C4'[2_545]	2.05	0.15
2:I:1:DG:C8	1:K:18:DC:C6[2_545]	2.06	0.14
2:I:1:DG:C1'	1:K:18:DC:C2'[2_545]	2.15	0.05
2:I:1:DG:C4	1:K:18:DC:C2'[2_545]	2.17	0.03

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	60/63 (95%)	57 (95%)	3 (5%)	0	100 100
3	B	61/63 (97%)	61 (100%)	0	0	100 100
3	G	61/63 (97%)	59 (97%)	1 (2%)	1 (2%)	12 8
3	J	59/63 (94%)	57 (97%)	2 (3%)	0	100 100
All	All	241/252 (96%)	234 (97%)	6 (2%)	1 (0%)	39 42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	275	LEU

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	56/57 (98%)	48 (86%)	8 (14%)	4 3
3	B	57/57 (100%)	53 (93%)	4 (7%)	19 19
3	G	56/57 (98%)	50 (89%)	6 (11%)	8 7
3	J	55/57 (96%)	52 (94%)	3 (6%)	27 30
All	All	224/228 (98%)	203 (91%)	21 (9%)	11 10

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

Mol	Chain	Res	Type
3	B	219	LYS
3	B	225	LYS
3	B	248	LYS
3	B	274	VAL
3	A	218	LYS
3	A	219	LYS
3	A	233	ARG
3	A	247	ARG
3	A	254	SER
3	A	274	VAL
3	A	275	LEU
3	A	277	LYS
3	G	219	LYS
3	G	229	ARG
3	G	242	THR
3	G	265	GLN
3	G	274	VAL
3	G	277	LYS
3	J	219	LYS
3	J	229	ARG
3	J	274	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	266	ASN
3	A	266	ASN
3	G	266	ASN
3	J	266	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	C	18/18 (100%)	0.72	1 (5%) 28 27	24, 38, 69, 83	0
1	D	18/18 (100%)	0.84	3 (16%) 2 2	23, 38, 75, 89	0
1	H	18/18 (100%)	0.71	2 (11%) 7 7	24, 38, 67, 80	0
1	K	18/18 (100%)	0.96	1 (5%) 28 27	25, 39, 69, 86	0
2	E	18/18 (100%)	1.04	2 (11%) 7 7	27, 37, 66, 75	0
2	F	18/18 (100%)	0.93	2 (11%) 7 7	25, 41, 69, 97	0
2	I	18/18 (100%)	0.98	2 (11%) 7 7	27, 40, 63, 82	0
2	L	18/18 (100%)	0.77	2 (11%) 7 7	26, 41, 59, 69	0
3	A	62/63 (98%)	0.91	7 (11%) 7 6	22, 32, 68, 99	0
3	B	61/63 (96%)	0.92	6 (9%) 10 8	20, 31, 65, 116	0
3	G	63/63 (100%)	1.04	9 (14%) 4 3	22, 34, 88, 108	0
3	J	61/63 (96%)	0.92	4 (6%) 22 21	23, 30, 67, 122	0
All	All	391/396 (98%)	0.92	41 (10%) 8 7	20, 36, 80, 122	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	217	ARG	8.7
3	A	278	VAL	8.2
2	I	1	DG	8.1
2	F	1	DG	6.7
3	G	217	ARG	6.3
2	E	1	DG	6.1
3	G	278	VAL	5.7
3	G	274	VAL	5.7
3	B	274	VAL	5.5
3	B	217	ARG	5.4
3	J	276	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	K	18	DC	5.4
2	L	1	DG	5.1
2	E	2	DG	5.1
3	J	277	LYS	4.6
3	A	219	LYS	4.5
3	G	279	LYS	3.7
1	H	18	DC	3.6
1	D	1	DT	3.6
3	A	276	ALA	3.5
3	G	219	LYS	3.5
3	G	218	LYS	3.3
1	C	18	DC	3.3
2	I	2	DG	3.1
3	A	275	LEU	3.1
3	B	218	LYS	2.9
1	D	18	DC	2.9
1	H	1	DT	2.7
3	B	254	SER	2.7
3	G	277	LYS	2.6
2	F	2	DG	2.5
3	A	255	LEU	2.4
3	A	244	ASP	2.3
3	B	276	ALA	2.3
1	D	3	DG	2.2
3	G	247	ARG	2.2
3	B	260	ILE	2.1
3	G	221	ILE	2.1
3	J	257	GLU	2.1
2	L	17	DA	2.1
3	A	254	SER	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.