Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:27 am BST

PDB ID	:	5V3G
Title	:	PRDM9-allele-C ZnF8-13
Authors	:	Patel, A.; Cheng, X.
Deposited on	:	2017-03-07
Resolution	:	2.42 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 ①) were used in the production of this report:

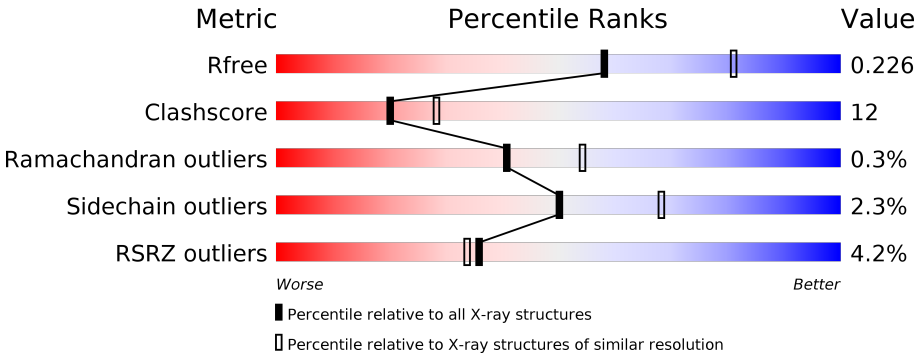
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.42 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 <=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	B	21	10% 57% 33%
1	E	21	14% 57% 29%
2	C	21	10% 62% 29%
2	F	21	19% 48% 33%
3	A	174	2% 76% 16%
3	D	174	5% 68% 26%

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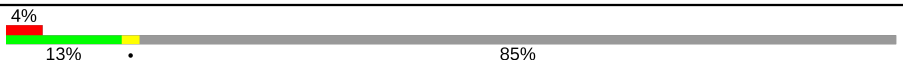
Mol	Chain	Length	Quality of chain
3	G	174	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4712 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(*TP*GP*AP*CP*CP*CP*CP*AP*GP*TP*GP*AP*GP*CP*GP*TP*TP*GP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	21	Total	C	N	O	P	0	0	0
			424	202	77	125	20			
1	B	21	Total	C	N	O	P	0	0	0
			424	202	77	125	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	21	Total	C	N	O	P	0	0	0
			431	204	84	123	20			
2	C	21	Total	C	N	O	P	0	0	0
			431	204	84	123	20			

- Molecule 3 is a protein called PR domain zinc finger protein 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	170	Total	C	N	O	S	0	0	0
			1333	813	272	236	12			
3	A	168	Total	C	N	O	S	0	0	0
			1349	821	277	239	12			
3	G	26	Total	C	N	O	S	0	0	0
			191	117	40	32	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	712	GLY	-	expression tag	UNP D9IWL3
D	713	PRO	-	expression tag	UNP D9IWL3
D	714	GLY	-	expression tag	UNP D9IWL3
D	715	SER	-	expression tag	UNP D9IWL3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	712	GLY	-	expression tag	UNP D9IWL3
A	713	PRO	-	expression tag	UNP D9IWL3
A	714	GLY	-	expression tag	UNP D9IWL3
A	715	SER	-	expression tag	UNP D9IWL3
G	712	GLY	-	expression tag	UNP D9IWL3
G	713	PRO	-	expression tag	UNP D9IWL3
G	714	GLY	-	expression tag	UNP D9IWL3
G	715	SER	-	expression tag	UNP D9IWL3

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Zn 1 1	0	0
4	A	6	Total Zn 6 6	0	0
4	D	6	Total Zn 6 6	0	0

- Molecule 5 is water.

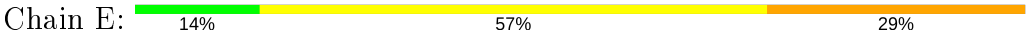
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	16	Total O 16 16	0	0
5	F	15	Total O 15 15	0	0
5	D	30	Total O 30 30	0	0
5	B	21	Total O 21 21	0	0
5	C	11	Total O 11 11	0	0
5	A	19	Total O 19 19	0	0
5	G	4	Total O 4 4	0	0

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 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.

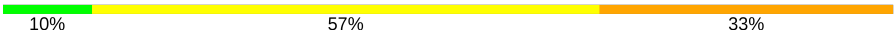
• Molecule 1: DNA (5'-D(*TP*GP*AP*CP*CP*CP*CP*AP*GP*TP*GP*AP*GP*CP*GP*TP*TP*GP*CP*CP*C)-3')

Chain E:



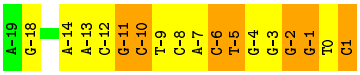
• Molecule 1: DNA (5'-D(*TP*GP*AP*CP*CP*CP*CP*AP*GP*TP*GP*AP*GP*CP*GP*TP*TP*GP*CP*CP*C)-3')

Chain B:



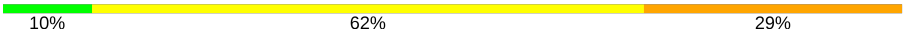
• Molecule 2: DNA (5'-D(*AP*GP*GP*GP*CP*AP*AP*CP*GP*CP*TP*CP*AP*CP*TP*GP*GP*GP*GP*TP*C)-3')

Chain F:



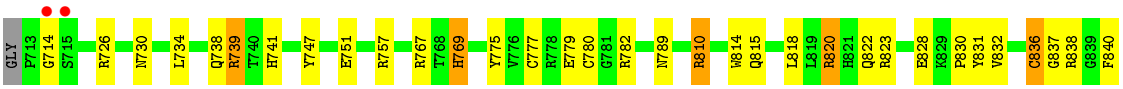
• Molecule 2: DNA (5'-D(*AP*GP*GP*GP*CP*AP*AP*CP*GP*CP*TP*CP*AP*CP*TP*GP*GP*GP*GP*TP*C)-3')

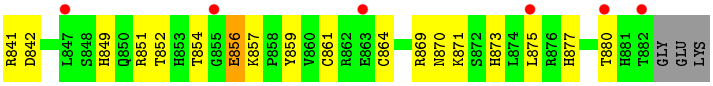
Chain C:



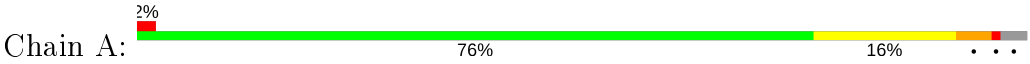
• Molecule 3: PR domain zinc finger protein 9

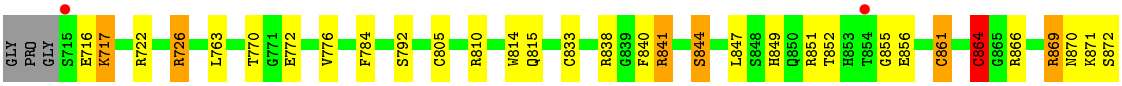
Chain D:

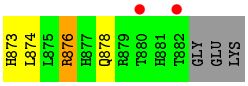




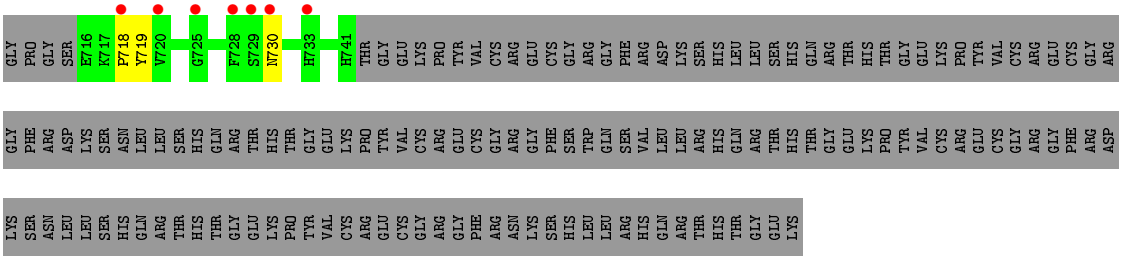
• Molecule 3: PR domain zinc finger protein 9







• Molecule 3: PR domain zinc finger protein 9



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.15Å 123.78Å 70.20Å 90.00° 116.07° 90.00°	Depositor
Resolution (Å)	35.18 – 2.42 35.18 – 2.42	Depositor EDS
% Data completeness (in resolution range)	95.8 (35.18-2.42) 95.8 (35.18-2.42)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.173 , 0.225 0.175 , 0.226	Depositor DCC
R_{free} test set	1775 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	59.6	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 48.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4712	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.67% 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, 0.333 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: ZN

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	B	2.23	16/474 (3.4%)	1.82	19/729 (2.6%)
1	E	2.42	16/474 (3.4%)	2.09	24/729 (3.3%)
2	C	2.19	18/484 (3.7%)	1.76	17/746 (2.3%)
2	F	2.23	17/484 (3.5%)	1.97	20/746 (2.7%)
3	A	1.11	6/1383 (0.4%)	1.24	13/1852 (0.7%)
3	D	1.06	2/1368 (0.1%)	1.16	11/1838 (0.6%)
3	G	0.75	0/196	0.81	0/265
All	All	1.65	75/4863 (1.5%)	1.54	104/6905 (1.5%)

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	D	0	1

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	9	DG	N7-C5	14.07	1.47	1.39
1	B	11	DG	N7-C5	10.72	1.45	1.39
1	B	12	DA	C6-N6	-9.68	1.26	1.33
3	A	805	CYS	CB-SG	9.08	1.97	1.82
1	E	4	DC	C3'-O3'	-8.71	1.32	1.44
1	E	10	DT	C5'-C4'	-8.68	1.41	1.51
1	E	11	DG	N3-C4	-8.63	1.29	1.35
1	B	13	DG	N1-C2	8.29	1.44	1.37
1	E	9	DG	N9-C8	7.96	1.43	1.37
2	F	-5	DT	C3'-O3'	-7.91	1.33	1.44
1	E	10	DT	C2-O2	-7.83	1.16	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	19	DG	C3'-O3'	-7.75	1.33	1.44
2	F	-18	DG	C3'-O3'	-7.57	1.34	1.44
2	C	12	DC	C4'-O4'	7.16	1.52	1.45
1	B	6	DC	N3-C4	7.12	1.39	1.33
2	C	6	DA	C3'-O3'	-7.03	1.34	1.44
1	B	10	DT	C5-C7	-6.97	1.45	1.50
2	F	-3	DG	C8-N7	6.74	1.34	1.30
3	A	814	TRP	CE3-CZ3	-6.72	1.27	1.38
1	E	10	DT	C5-C7	-6.71	1.46	1.50
1	B	14	DC	O4'-C1'	-6.57	1.34	1.42
2	C	11	DT	C5-C7	6.47	1.53	1.50
2	C	20	DT	C3'-O3'	-6.39	1.35	1.44
1	B	15	DG	C8-N7	-6.38	1.27	1.30
1	B	11	DG	N9-C8	6.35	1.42	1.37
2	F	1	DC	C3'-O3'	-6.30	1.35	1.44
2	C	2	DG	N7-C5	6.28	1.43	1.39
2	C	11	DT	C5-C6	6.16	1.38	1.34
2	C	16	DG	C8-N7	6.15	1.34	1.30
1	E	5	DC	C2-O2	-6.13	1.19	1.24
2	F	-3	DG	C3'-O3'	-6.12	1.35	1.44
2	C	7	DA	N3-C4	-6.09	1.31	1.34
1	B	9	DG	N7-C5	6.06	1.42	1.39
2	C	17	DG	N9-C8	6.05	1.42	1.37
2	C	17	DG	C5-C4	6.05	1.42	1.38
1	E	2	DG	C6-O6	5.99	1.29	1.24
1	E	15	DG	C4'-C3'	-5.97	1.46	1.52
2	F	0	DT	C4-C5	5.93	1.50	1.45
1	E	7	DC	C1'-N1	-5.89	1.39	1.47
2	F	-10	DC	P-O5'	-5.75	1.53	1.59
2	C	5	DC	C3'-O3'	-5.75	1.36	1.44
1	B	7	DC	C2-N3	5.74	1.40	1.35
2	F	0	DT	C2-O2	-5.74	1.17	1.22
3	A	717	LYS	CD-CE	5.73	1.65	1.51
1	E	14	DC	C3'-O3'	-5.70	1.36	1.44
3	D	775	TYR	CD1-CE1	5.69	1.47	1.39
2	C	13	DA	N9-C4	5.61	1.41	1.37
2	C	7	DA	C3'-O3'	-5.59	1.36	1.44
2	F	-4	DG	O4'-C1'	-5.57	1.35	1.42
1	B	9	DG	N9-C4	-5.56	1.33	1.38
3	A	814	TRP	CE2-CZ2	-5.55	1.30	1.39
1	E	9	DG	C2'-C1'	-5.50	1.46	1.52
1	B	6	DC	C2-N3	5.50	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	17	DG	C8-N7	5.48	1.34	1.30
1	B	9	DG	N9-C8	5.46	1.41	1.37
2	F	-1	DG	C8-N7	5.45	1.34	1.30
2	C	21	DC	C4-N4	5.42	1.38	1.33
1	E	4	DC	C2'-C1'	5.42	1.57	1.52
1	B	11	DG	C8-N7	5.40	1.34	1.30
1	B	6	DC	N1-C6	5.35	1.40	1.37
2	F	-3	DG	C6-O6	-5.32	1.19	1.24
1	B	4	DC	C3'-O3'	-5.28	1.37	1.44
1	E	7	DC	C3'-O3'	-5.28	1.37	1.44
2	F	-10	DC	O5'-C5'	-5.21	1.29	1.42
2	F	-9	DT	C5-C7	5.19	1.53	1.50
3	A	784	PHE	CE1-CZ	5.19	1.47	1.37
2	F	-8	DC	C3'-O3'	-5.13	1.37	1.44
1	E	15	DG	N3-C4	5.12	1.39	1.35
3	A	814	TRP	CG-CD1	5.11	1.44	1.36
2	C	2	DG	C3'-O3'	-5.10	1.37	1.44
2	F	-12	DC	C4'-C3'	5.09	1.58	1.53
3	D	741	HIS	CB-CG	5.08	1.59	1.50
2	F	-9	DT	N1-C2	-5.04	1.34	1.38
2	F	-2	DG	C3'-O3'	-5.02	1.37	1.44
2	C	9	DG	N1-C2	5.01	1.41	1.37

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	15	DG	O5'-P-OP2	-14.43	92.71	105.70
2	F	1	DC	O5'-P-OP2	-13.16	93.86	105.70
2	F	-14	DA	O5'-P-OP2	-12.35	94.59	105.70
2	F	-10	DC	O5'-P-OP1	-11.69	95.18	105.70
2	F	-12	DC	OP1-P-OP2	11.45	136.78	119.60
1	E	14	DC	O5'-P-OP2	-11.45	95.40	105.70
1	E	15	DG	OP1-P-OP2	11.45	136.77	119.60
3	A	876	ARG	NE-CZ-NH1	11.38	125.99	120.30
3	A	726	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	B	9	DG	O4'-C4'-C3'	-10.21	99.87	106.00
1	E	11	DG	O5'-P-OP1	-9.69	96.98	105.70
3	D	739	ARG	NE-CZ-NH1	9.57	125.08	120.30
3	A	876	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	E	21	DC	O5'-P-OP2	-9.34	97.29	105.70
1	E	11	DG	OP1-P-OP2	8.83	132.84	119.60
1	B	7	DC	OP1-P-OP2	8.63	132.55	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	-5	DT	O5'-P-OP2	-8.58	97.97	105.70
2	C	17	DG	OP1-P-OP2	-8.52	106.83	119.60
1	E	8	DA	O5'-P-OP1	-8.30	98.23	105.70
2	F	-6	DC	O5'-P-OP2	-8.18	98.34	105.70
2	C	16	DG	O4'-C1'-N9	8.10	113.67	108.00
1	E	14	DC	OP1-P-OP2	7.93	131.49	119.60
1	B	7	DC	O5'-P-OP2	-7.88	98.61	105.70
1	E	13	DG	O5'-P-OP2	-7.78	98.70	105.70
3	A	841	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	E	11	DG	O5'-P-OP2	-7.69	98.78	105.70
1	B	9	DG	OP2-P-O3'	7.61	121.94	105.20
3	D	757	ARG	NE-CZ-NH2	-7.61	116.50	120.30
2	F	-6	DC	OP1-P-OP2	7.38	130.67	119.60
2	F	1	DC	OP1-P-OP2	7.29	130.54	119.60
2	C	19	DG	O5'-P-OP2	-7.29	99.14	105.70
2	F	-11	DG	O5'-P-OP1	-7.19	99.22	105.70
1	E	14	DC	OP1-P-O3'	-7.18	89.40	105.20
2	F	-12	DC	P-O3'-C3'	7.05	128.16	119.70
1	E	8	DA	O4'-C1'-N9	-7.05	103.07	108.00
2	C	3	DG	O4'-C1'-N9	7.00	112.90	108.00
3	D	820	ARG	NE-CZ-NH2	-6.97	116.81	120.30
2	F	-11	DG	OP1-P-OP2	6.90	129.95	119.60
3	D	739	ARG	NE-CZ-NH2	-6.85	116.88	120.30
3	D	726	ARG	NE-CZ-NH1	-6.74	116.93	120.30
3	D	767	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	B	12	DA	OP1-P-OP2	6.68	129.62	119.60
3	A	722	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	B	9	DG	OP1-P-O3'	-6.59	90.71	105.20
3	A	810	ARG	NE-CZ-NH1	-6.55	117.03	120.30
1	E	17	DT	OP1-P-OP2	6.50	129.35	119.60
1	E	14	DC	OP2-P-O3'	6.48	119.45	105.20
1	B	10	DT	OP2-P-O3'	6.46	119.42	105.20
1	E	21	DC	OP1-P-OP2	6.42	129.23	119.60
1	B	2	DG	O5'-P-OP2	-6.38	99.95	105.70
2	C	17	DG	OP2-P-O3'	6.32	119.10	105.20
2	C	17	DG	P-O3'-C3'	6.28	127.24	119.70
1	B	2	DG	OP1-P-OP2	6.25	128.97	119.60
3	A	717	LYS	CD-CE-NZ	6.21	125.99	111.70
1	B	11	DG	O5'-P-OP2	-6.19	100.13	105.70
3	A	833	CYS	CA-CB-SG	6.14	125.06	114.00
1	E	3	DA	OP1-P-OP2	-6.10	110.46	119.60
2	F	-13	DA	OP1-P-O3'	-6.07	91.85	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	-13	DA	O5'-P-OP2	-6.06	100.25	105.70
1	E	9	DG	P-O3'-C3'	-6.04	112.45	119.70
2	C	9	DG	O4'-C1'-N9	-6.04	103.77	108.00
1	E	11	DG	O4'-C1'-C2'	-6.00	101.10	105.90
1	B	9	DG	O5'-P-OP2	-5.99	100.31	105.70
2	C	12	DC	O5'-P-OP2	5.98	117.88	110.70
1	B	9	DG	O4'-C1'-N9	5.89	112.12	108.00
2	C	20	DT	N3-C4-O4	5.88	123.43	119.90
2	C	19	DG	OP1-P-OP2	5.78	128.26	119.60
2	C	15	DT	O4'-C1'-N1	-5.75	103.97	108.00
3	D	856	GLU	N-CA-C	5.74	126.49	111.00
1	E	8	DA	OP1-P-OP2	5.68	128.12	119.60
1	E	20	DC	OP2-P-O3'	5.66	117.66	105.20
1	B	3	DA	O5'-P-OP1	5.66	117.49	110.70
3	A	861	CYS	CA-CB-SG	5.59	124.07	114.00
2	F	-5	DT	OP2-P-O3'	5.58	117.48	105.20
2	F	-2	DG	O4'-C1'-N9	-5.57	104.10	108.00
3	A	776	VAL	CA-CB-CG2	-5.56	102.56	110.90
2	C	18	DG	OP2-P-O3'	5.55	117.41	105.20
2	C	6	DA	OP2-P-O3'	5.53	117.36	105.20
1	E	13	DG	OP2-P-O3'	5.51	117.32	105.20
3	D	714	GLY	N-CA-C	5.51	126.87	113.10
2	C	5	DC	OP2-P-O3'	5.50	117.31	105.20
3	D	810	ARG	NE-CZ-NH1	5.50	123.05	120.30
3	D	841	ARG	NE-CZ-NH1	-5.47	117.56	120.30
2	F	-18	DG	OP1-P-O3'	5.42	117.13	105.20
2	F	-5	DT	O4'-C1'-N1	-5.34	104.26	108.00
1	B	9	DG	C5-N7-C8	-5.33	101.64	104.30
1	B	17	DT	OP1-P-OP2	5.29	127.54	119.60
2	C	10	DC	O4'-C1'-N1	-5.29	104.30	108.00
3	D	726	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	B	18	DG	O5'-P-OP2	-5.27	100.95	105.70
2	F	-1	DG	O4'-C1'-N9	5.26	111.68	108.00
2	C	10	DC	P-O3'-C3'	5.26	126.01	119.70
1	E	17	DT	C5-C4-O4	-5.25	121.23	124.90
3	A	864	CYS	CA-CB-SG	-5.23	104.59	114.00
1	B	13	DG	OP2-P-O3'	5.21	116.67	105.20
1	E	17	DT	N3-C4-O4	5.21	123.03	119.90
1	E	12	DA	O4'-C1'-N9	-5.21	104.35	108.00
3	A	864	CYS	CA-C-N	-5.17	105.86	116.20
1	B	7	DC	O5'-P-OP1	-5.15	101.06	105.70
1	B	9	DG	N3-C4-N9	-5.14	122.92	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	763	LEU	CB-CG-CD1	-5.12	102.30	111.00
2	F	0	DT	C4-C5-C7	5.10	122.06	119.00
2	C	11	DT	O4'-C1'-N1	-5.09	104.44	108.00
2	F	1	DC	C4'-C3'-C2'	-5.08	98.53	103.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	769	HIS	Sidechain

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	B	424	0	235	11	0
1	E	424	0	237	9	0
2	C	431	0	236	11	0
2	F	431	0	236	8	0
3	A	1349	0	1261	32	0
3	D	1333	0	1226	42	0
3	G	191	0	159	1	0
4	A	6	0	0	0	0
4	D	6	0	0	0	0
4	G	1	0	0	0	0
5	A	19	0	0	1	1
5	B	21	0	0	1	0
5	C	11	0	0	0	0
5	D	30	0	0	2	1
5	E	16	0	0	0	0
5	F	15	0	0	0	0
5	G	4	0	0	0	0
All	All	4712	0	3590	102	1

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 12.

All (102) 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:A:815:GLN:HG3	5:A:1112:HOH:O	1.36	1.23
3:D:854:THR:O	3:D:869:ARG:NH2	1.92	1.02
3:A:864:CYS:HB3	3:A:866:ARG:H	1.24	1.01
3:D:851:ARG:O	3:D:854:THR:HG22	1.68	0.92
2:C:4:DG:H2"	2:C:5:DC:H5'	1.53	0.91
1:E:10:DT:OP2	3:D:815:GLN:NE2	2.03	0.91
1:B:8:DA:H2"	1:B:9:DG:H5"	1.58	0.86
3:A:852:THR:HA	3:A:869:ARG:HH21	1.41	0.86
3:D:815:GLN:NE2	5:D:1101:HOH:O	2.10	0.84
2:C:2:DG:N7	3:A:876:ARG:NH2	2.26	0.82
3:A:851:ARG:HH21	3:A:870:ASN:HD21	1.32	0.77
3:D:851:ARG:O	3:D:854:THR:CG2	2.37	0.73
3:D:854:THR:C	3:D:869:ARG:HH22	1.93	0.72
3:D:810:ARG:HG2	3:D:810:ARG:HH11	1.54	0.71
1:B:9:DG:H2"	1:B:10:DT:H5'	1.74	0.69
2:F:-11:DG:H2"	2:F:-10:DC:H5"	1.75	0.68
5:B:114:HOH:O	3:A:844:SER:HB2	1.92	0.68
2:F:-10:DC:H5'	3:D:814:TRP:CH2	2.29	0.67
1:E:9:DG:H2"	1:E:10:DT:H5"	1.76	0.67
1:B:8:DA:C2'	1:B:9:DG:H5"	2.24	0.67
3:D:840:PHE:CE2	3:D:849:HIS:CD2	2.83	0.67
3:A:851:ARG:HH21	3:A:870:ASN:ND2	1.93	0.66
1:E:6:DC:H2"	1:E:7:DC:H5'	1.78	0.66
3:D:851:ARG:HB2	3:D:851:ARG:CZ	2.26	0.66
1:E:4:DC:OP2	3:D:747:TYR:OH	2.08	0.66
2:F:-7:DA:H62	3:D:789:ASN:HD21	1.45	0.65
3:A:874:LEU:O	3:A:878:GLN:HG2	1.98	0.64
3:D:871:LYS:HG2	3:D:875:LEU:CD1	2.28	0.64
3:D:871:LYS:O	3:D:875:LEU:HD12	1.97	0.63
2:F:-11:DG:H2"	2:F:-10:DC:C5'	2.30	0.62
3:A:855:GLY:HA2	3:A:869:ARG:HH12	1.64	0.62
1:E:8:DA:H2"	1:E:9:DG:O5'	1.99	0.61
3:A:770:THR:CG2	3:A:772:GLU:HG3	2.31	0.60
3:A:873:HIS:CD2	3:A:876:ARG:HH11	2.19	0.60
3:A:855:GLY:HA2	3:A:869:ARG:HH22	1.67	0.60
1:B:19:DC:H2"	1:B:20:DC:H5'	1.83	0.59
1:B:16:DT:OP1	3:A:871:LYS:HE3	2.03	0.59
3:D:857:LYS:HA	3:D:869:ARG:HA	1.85	0.59
3:D:854:THR:HG23	3:D:869:ARG:HH21	1.68	0.58
3:D:854:THR:HG23	3:D:869:ARG:NH2	2.17	0.58
3:D:840:PHE:HE2	3:D:849:HIS:CD2	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:871:LYS:HG2	3:D:875:LEU:HD11	1.86	0.57
3:D:856:GLU:O	3:D:857:LYS:C	2.38	0.57
2:F:-11:DG:C2'	2:F:-10:DC:H5"	2.35	0.57
3:A:856:GLU:OE2	3:A:856:GLU:N	2.37	0.57
1:E:9:DG:H2"	1:E:10:DT:C5'	2.34	0.56
3:D:780:CYS:SG	3:D:782:ARG:HG3	2.48	0.54
3:A:844:SER:HA	3:A:847:LEU:HD12	1.89	0.54
2:C:20:DT:H2"	2:C:21:DC:C6	2.43	0.53
2:C:3:DG:H2"	2:C:4:DG:O5'	2.08	0.53
3:A:770:THR:HG22	3:A:772:GLU:HG3	1.91	0.52
2:C:5:DC:OP1	3:A:849:HIS:CE1	2.63	0.52
3:D:820:ARG:HD2	3:D:842:ASP:OD1	2.10	0.51
3:D:870:ASN:OD1	3:D:873:HIS:N	2.41	0.51
3:A:852:THR:HA	3:A:869:ARG:NH2	2.17	0.51
3:A:864:CYS:HB3	3:A:866:ARG:N	2.08	0.50
3:D:877:HIS:O	3:D:880:THR:HB	2.11	0.50
2:C:2:DG:C8	3:A:876:ARG:NH2	2.79	0.49
2:F:-2:DG:H2'	2:F:-1:DG:C8	2.48	0.49
3:D:851:ARG:NH1	3:D:851:ARG:HB2	2.27	0.49
3:D:871:LYS:HZ3	3:D:871:LYS:HB2	1.77	0.49
3:D:751:GLU:HB2	3:D:769:HIS:CD2	2.47	0.49
1:E:6:DC:H2"	1:E:7:DC:C5'	2.40	0.49
3:D:840:PHE:CZ	3:D:849:HIS:CG	3.00	0.48
1:B:1:DT:H2"	1:B:2:DG:C8	2.47	0.48
1:B:9:DG:H2"	1:B:10:DT:C5'	2.42	0.48
3:D:823:ARG:HD2	3:D:828:GLU:HB3	1.95	0.48
1:E:1:DT:H2"	1:E:2:DG:H5'	1.96	0.48
3:A:855:GLY:HA2	3:A:869:ARG:NH1	2.28	0.48
3:D:734:LEU:O	3:D:738:GLN:HG3	2.14	0.48
3:D:849:HIS:O	3:D:852:THR:HB	2.14	0.48
2:F:-6:DC:H2"	2:F:-5:DT:O5'	2.14	0.47
3:A:855:GLY:HA2	3:A:869:ARG:NH2	2.30	0.47
1:B:8:DA:H2"	1:B:9:DG:C5'	2.39	0.47
2:C:5:DC:OP1	3:A:838:ARG:NH2	2.47	0.47
2:C:7:DA:H2"	2:C:8:DC:H5'	1.97	0.47
1:B:14:DC:H2"	1:B:15:DG:O5'	2.15	0.46
3:A:770:THR:O	3:A:770:THR:HG22	2.15	0.46
3:D:832:VAL:HG13	3:D:837:GLY:O	2.16	0.46
1:B:10:DT:H2"	1:B:11:DG:C8	2.51	0.46
2:C:7:DA:H2'	2:C:8:DC:C6	2.51	0.46
3:D:836:CYS:SG	3:D:838:ARG:HB2	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:DG:OP2	3:D:739:ARG:NH2	2.50	0.45
2:C:4:DG:H2"	2:C:5:DC:C5'	2.35	0.45
1:B:17:DT:H71	3:A:872:SER:OG	2.18	0.44
2:F:1:DC:H5'	2:F:1:DC:H2'	1.69	0.44
3:A:770:THR:HG21	3:A:772:GLU:HG3	1.99	0.44
3:D:871:LYS:HG2	3:D:875:LEU:HD12	2.00	0.43
3:D:777:CYS:C	3:D:779:GLU:H	2.21	0.43
3:A:716:GLU:OE1	3:A:716:GLU:HA	2.19	0.43
3:D:818:LEU:O	3:D:822:GLN:HG3	2.18	0.43
3:A:855:GLY:CA	3:A:869:ARG:HH12	2.31	0.42
3:D:859:TYR:CD1	3:D:859:TYR:N	2.87	0.42
3:D:861:CYS:HB3	3:D:864:CYS:SG	2.59	0.42
3:G:718:PRO:HG2	3:G:719:TYR:CD2	2.53	0.42
3:A:726:ARG:HH11	3:A:726:ARG:HG3	1.83	0.42
3:A:716:GLU:O	3:A:717:LYS:HE2	2.20	0.42
3:D:830:PRO:HG2	3:D:831:TYR:CE1	2.55	0.41
2:C:7:DA:OP2	3:A:841:ARG:HD2	2.19	0.41
3:A:840:PHE:CZ	3:A:849:HIS:CD2	3.08	0.41
3:D:730:ASN:HB2	5:D:1116:HOH:O	2.21	0.41
3:D:854:THR:C	3:D:869:ARG:NH2	2.62	0.41

All (1) 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)
5:D:1122:HOH:O	5:A:1109:HOH:O[1_655]	2.04	0.16

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	166/174 (95%)	163 (98%)	2 (1%)	1 (1%)	25 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	D	168/174 (97%)	167 (99%)	1 (1%)	0	100 100
3	G	24/174 (14%)	21 (88%)	3 (12%)	0	100 100
All	All	358/522 (69%)	351 (98%)	6 (2%)	1 (0%)	41 54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	864	CYS

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	143/154 (93%)	138 (96%)	5 (4%)	36 53
3	D	139/154 (90%)	138 (99%)	1 (1%)	84 92
3	G	18/154 (12%)	17 (94%)	1 (6%)	21 32
All	All	300/462 (65%)	293 (98%)	7 (2%)	50 68

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	836	CYS
3	A	792	SER
3	A	844	SER
3	A	861	CYS
3	A	864	CYS
3	A	869	ARG
3	G	730	ASN

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

Mol	Chain	Res	Type
3	D	789	ASN

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Mol	Chain	Res	Type
3	D	794	GLN
3	D	873	HIS
3	A	738	GLN
3	A	815	GLN
3	A	849	HIS
3	A	870	ASN
3	A	873	HIS

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

Of 13 ligands modelled in this entry, 13 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, 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	B	21/21 (100%)	-0.58	0 100 100	47, 63, 92, 109	0
1	E	21/21 (100%)	-0.52	0 100 100	51, 64, 82, 92	0
2	C	21/21 (100%)	-0.47	0 100 100	46, 55, 86, 98	0
2	F	21/21 (100%)	-0.47	0 100 100	48, 56, 79, 82	0
3	A	168/174 (96%)	0.09	4 (2%) 59 56	39, 63, 102, 136	0
3	D	170/174 (97%)	0.08	8 (4%) 31 29	42, 66, 105, 125	0
3	G	26/174 (14%)	1.21	7 (26%) 0 0	85, 99, 113, 117	0
All	All	448/606 (73%)	0.04	19 (4%) 36 34	39, 65, 105, 136	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	714	GLY	7.2
3	A	715	SER	6.6
3	A	882	THR	5.8
3	G	733	HIS	3.5
3	D	715	SER	3.5
3	G	720	VAL	3.4
3	G	729	SER	3.1
3	G	730	ASN	3.1
3	D	882	THR	3.0
3	D	875	LEU	2.8
3	D	855	GLY	2.7
3	G	728	PHE	2.6
3	A	880	THR	2.6
3	G	725	GLY	2.5
3	D	880	THR	2.3
3	G	718	PRO	2.3
3	A	854	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	847	LEU	2.1
3	D	863	GLU	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. 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	B-factors(Å^2)	Q<0.9
4	ZN	A	1006	1/1	0.97	0.05	89,89,89,89	0
4	ZN	A	1005	1/1	0.98	0.10	82,82,82,82	0
4	ZN	A	1002	1/1	0.98	0.09	63,63,63,63	0
4	ZN	G	1001	1/1	0.98	0.07	92,92,92,92	0
4	ZN	D	1006	1/1	0.98	0.04	88,88,88,88	0
4	ZN	D	1003	1/1	0.98	0.09	65,65,65,65	0
4	ZN	D	1004	1/1	0.99	0.14	51,51,51,51	0
4	ZN	D	1001	1/1	0.99	0.12	55,55,55,55	0
4	ZN	A	1003	1/1	0.99	0.13	55,55,55,55	0
4	ZN	D	1005	1/1	0.99	0.09	80,80,80,80	0
4	ZN	A	1004	1/1	1.00	0.14	48,48,48,48	0
4	ZN	D	1002	1/1	1.00	0.07	59,59,59,59	0
4	ZN	A	1001	1/1	1.00	0.15	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.