



Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2022 – 02:07 PM EDT

PDB ID : 7MW8
Title : Crystal Structure Analysis of Xac Nucleotide Pyrophosphatase/Phosphodiesterase
Authors : Fernandez, D.; Li, L.; Brown, J.A.
Deposited on : 2021-05-15
Resolution : 1.90 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:

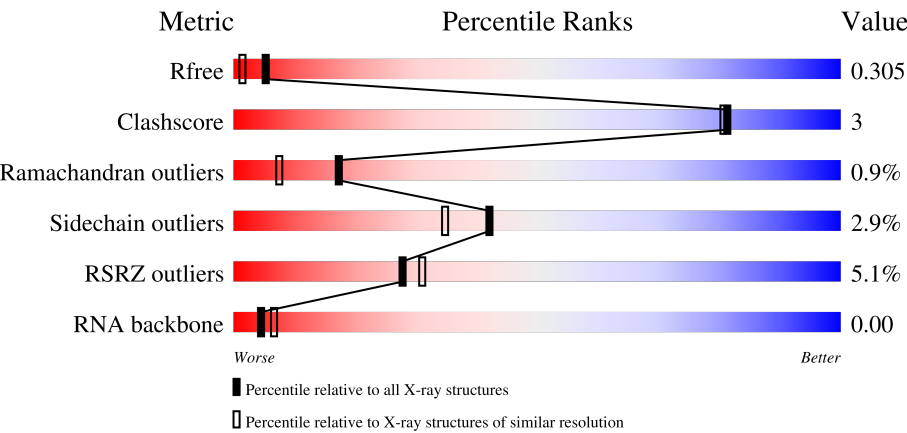
MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.28.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)
RNA backbone	3102	1013 (2.42-1.38)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	427	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>81%7%11%</div></div>
1	B	427	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>81%8%10%</div></div>
1	C	427	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>83%6%10%</div></div>
1	D	427	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>83%7%10%</div></div>

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Mol	Chain	Length	Quality of chain
1	E	427	<div><div></div><div>8%</div><div>79%</div><div>9%</div><div>10%</div></div>
1	F	427	<div><div></div><div>3%</div><div>84%</div><div>6%</div><div>10%</div></div>
2	J	2	<div><div></div><div>50%</div><div>50%</div><div>50%</div></div>
2	K	2	<div><div></div><div>50%</div><div>50%</div></div>
2	L	2	<div><div></div><div>50%</div><div>50%</div></div>
2	M	2	<div><div></div><div>50%</div><div>50%</div></div>
2	N	2	<div><div></div><div>50%</div><div>50%</div></div>
2	O	2	<div><div></div><div>50%</div><div>50%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18189 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 Phosphodiesterase-nucleotide pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	383	Total	C	N	O	S	0	1	0
			2921	1838	543	529	11			
1	B	384	Total	C	N	O	S	0	0	0
			2943	1851	549	532	11			
1	C	385	Total	C	N	O	S	0	0	0
			2943	1850	549	533	11			
1	A	380	Total	C	N	O	S	0	1	0
			2908	1830	542	525	11			
1	E	384	Total	C	N	O	S	0	1	0
			2942	1851	550	530	11			
1	F	384	Total	C	N	O	S	0	1	0
			2960	1858	554	537	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	90	ALA	THR	engineered mutation	UNP A0A0U5FM15
B	90	ALA	THR	engineered mutation	UNP A0A0U5FM15
C	90	ALA	THR	engineered mutation	UNP A0A0U5FM15
A	90	ALA	THR	engineered mutation	UNP A0A0U5FM15
E	90	ALA	THR	engineered mutation	UNP A0A0U5FM15
F	90	ALA	THR	engineered mutation	UNP A0A0U5FM15

- Molecule 2 is a RNA chain called pApG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	2	Total	C	N	O	P	0	0	0
			46	20	10	14	2			
2	K	1	Total	C	N	O	P	0	0	0
			23	10	5	7	1			
2	L	1	Total	C	N	O	P	0	0	0
			23	10	5	7	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	1	Total	C	N	O	P	0	0	0
			23	10	5	7	1			
2	N	1	Total	C	N	O	P	0	0	0
			23	10	5	7	1			
2	O	1	Total	C	N	O	P	0	0	0
			23	10	5	7	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		
3	E	2	Total	Zn	0	0
			2	2		
3	F	2	Total	Zn	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	46	Total	O	0	0
			46	46		
4	B	74	Total	O	0	0
			74	74		
4	C	73	Total	O	0	0
			73	73		
4	A	69	Total	O	0	0
			69	69		
4	E	53	Total	O	0	0
			53	53		
4	F	75	Total	O	0	0
			75	75		
4	J	3	Total	O	0	0
			3	3		
4	L	2	Total	O	0	0
			2	2		

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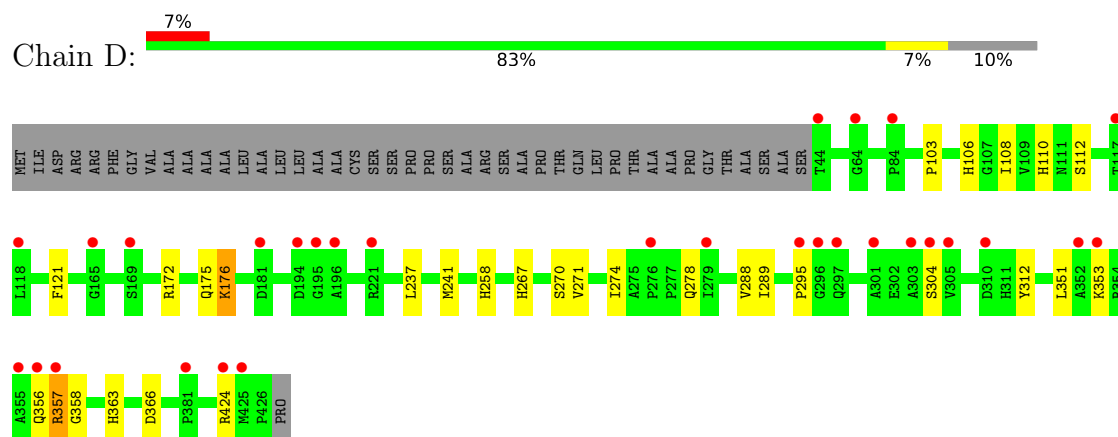
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	2	Total	O	0	0
			2	2		
4	N	1	Total	O	0	0
			1	1		
4	O	1	Total	O	0	0
			1	1		

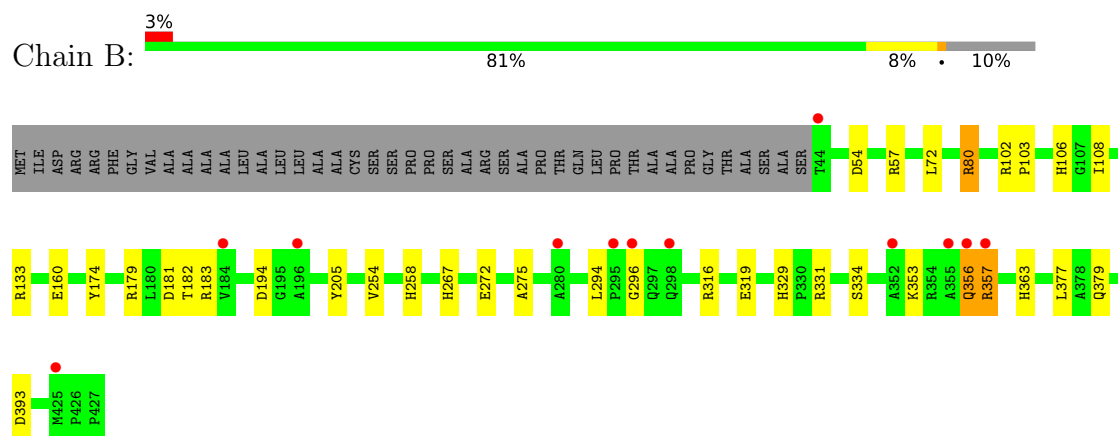
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

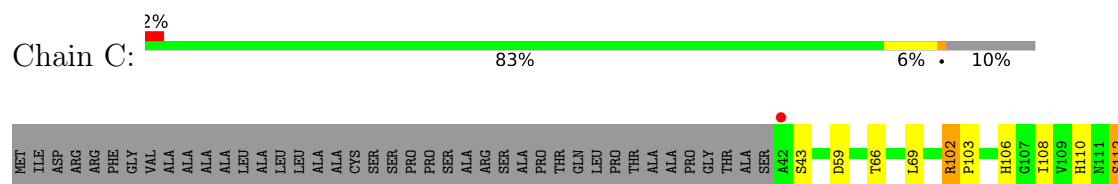
- Molecule 1: Phosphodiesterase-nucleotide pyrophosphatase

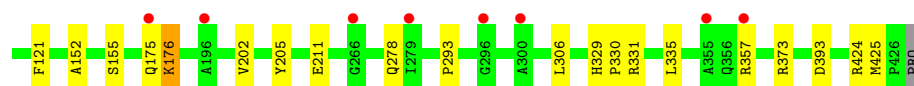


- Molecule 1: Phosphodiesterase-nucleotide pyrophosphatase

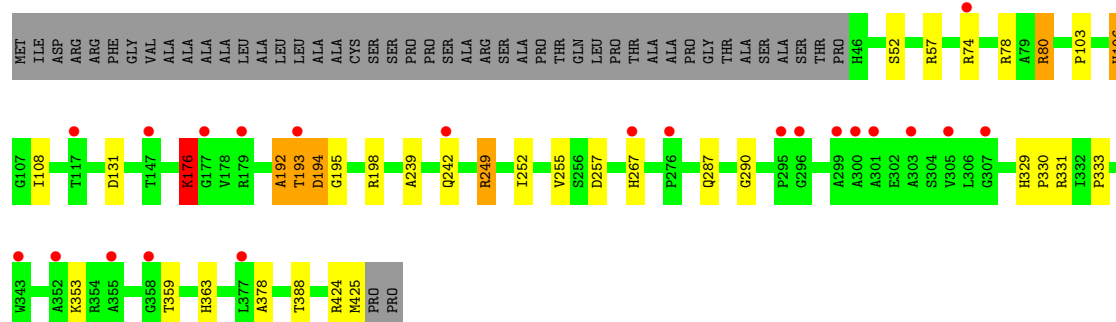
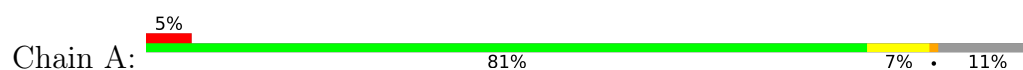


- Molecule 1: Phosphodiesterase-nucleotide pyrophosphatase

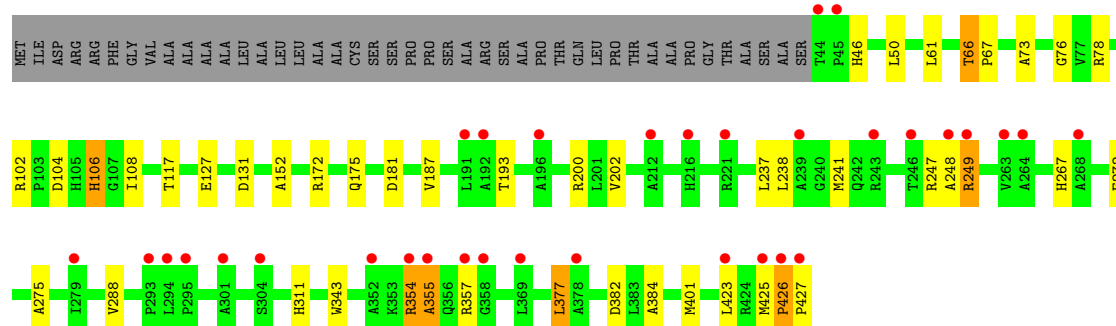
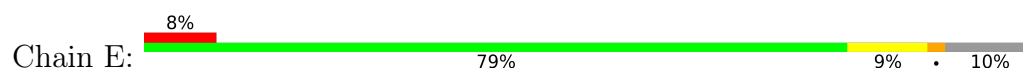




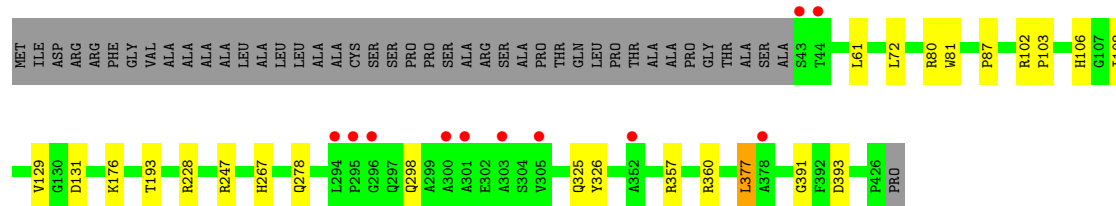
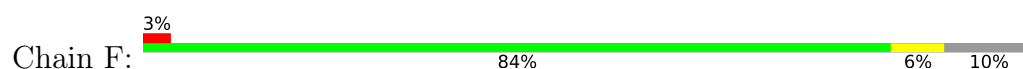
- Molecule 1: Phosphodiesterase-nucleotide pyrophosphatase



- Molecule 1: Phosphodiesterase-nucleotide pyrophosphatase



- Molecule 1: Phosphodiesterase-nucleotide pyrophosphatase



- Molecule 2: pApG



● Molecule 2: pApG

Chain K:  50% 50% A1 G

● Molecule 2: pApG

Chain L:  50% 50% A1 G

● Molecule 2: pApG

Chain M:  50% 50% A1 G

● Molecule 2: pApG

Chain N:  50% 50% A1 G

● Molecule 2: pApG

Chain O:  50% 50% A1 G

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	130.42Å 66.72Å 134.96Å 90.00° 116.25° 90.00°	Depositor
Resolution (Å)	30.04 – 1.90 38.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.04-1.90) 94.5 (38.99-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.243 , 0.303 0.249 , 0.305	Depositor DCC
R_{free} test set	7565 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.761	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.036 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18189	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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 50.81 % 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 6.1311e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	A	0.67	0/2995	0.83	2/4088 (0.0%)
1	B	0.70	0/3030	0.88	6/4138 (0.1%)
1	C	0.65	0/3029	0.84	3/4136 (0.1%)
1	D	0.61	0/3010	0.80	1/4112 (0.0%)
1	E	0.67	0/3029	0.86	4/4137 (0.1%)
1	F	0.67	0/3046	0.84	4/4157 (0.1%)
2	J	4.31	12/51 (23.5%)	6.32	20/76 (26.3%)
2	K	4.34	7/25 (28.0%)	6.26	11/35 (31.4%)
2	L	3.89	4/25 (16.0%)	6.88	12/35 (34.3%)
2	M	3.68	5/25 (20.0%)	7.13	13/35 (37.1%)
2	N	4.34	6/25 (24.0%)	6.73	10/35 (28.6%)
2	O	4.65	7/25 (28.0%)	5.88	9/35 (25.7%)
All	All	0.78	41/18315 (0.2%)	1.06	95/25019 (0.4%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1	A	C5-C4	13.30	1.48	1.38
2	J	2	G	C5-C4	13.02	1.47	1.38
2	K	1	A	C5-C4	11.03	1.46	1.38
2	N	1	A	N7-C5	-10.70	1.32	1.39
2	J	1	A	C5-C4	10.34	1.46	1.38
2	L	1	A	C5-C4	10.25	1.46	1.38
2	O	1	A	N9-C4	-9.58	1.32	1.37
2	O	1	A	N7-C5	-9.45	1.33	1.39
2	N	1	A	C5-C4	9.41	1.45	1.38
2	J	1	A	OP3-P	-9.08	1.50	1.61
2	K	1	A	OP3-P	-8.93	1.50	1.61
2	M	1	A	C5-C4	8.90	1.45	1.38
2	L	1	A	C5-C6	8.83	1.49	1.41
2	J	2	G	C8-N7	8.59	1.36	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	2	G	N7-C5	-8.46	1.34	1.39
2	L	1	A	OP3-P	-8.45	1.51	1.61
2	K	1	A	N7-C5	-8.44	1.34	1.39
2	M	1	A	OP3-P	-8.41	1.51	1.61
2	J	1	A	N7-C5	-7.91	1.34	1.39
2	J	1	A	N9-C4	-7.79	1.33	1.37
2	N	1	A	OP3-P	-7.71	1.51	1.61
2	O	1	A	OP3-P	-7.56	1.52	1.61
2	K	1	A	N9-C4	-7.14	1.33	1.37
2	M	1	A	N9-C4	-6.88	1.33	1.37
2	J	1	A	C5-C6	6.75	1.47	1.41
2	N	1	A	N9-C8	-6.72	1.32	1.37
2	N	1	A	N9-C4	-6.71	1.33	1.37
2	M	1	A	C5-C6	6.31	1.46	1.41
2	J	1	A	N9-C8	-6.26	1.32	1.37
2	J	2	G	C5-C6	6.25	1.48	1.42
2	K	1	A	N9-C8	-6.06	1.32	1.37
2	O	1	A	C5-C6	6.05	1.46	1.41
2	K	1	A	C5-C6	6.00	1.46	1.41
2	K	1	A	P-OP2	5.69	1.58	1.49
2	O	1	A	C8-N7	5.65	1.35	1.31
2	O	1	A	N9-C8	-5.54	1.33	1.37
2	M	1	A	N7-C5	-5.51	1.35	1.39
2	L	1	A	N9-C4	-5.26	1.34	1.37
2	J	2	G	N9-C4	-5.18	1.33	1.38
2	J	2	G	C6-N1	-5.17	1.35	1.39
2	N	1	A	C5-C6	5.08	1.45	1.41

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1	A	C2-N3-C4	26.20	123.70	110.60
2	L	1	A	C2-N3-C4	24.63	122.92	110.60
2	K	1	A	C2-N3-C4	22.16	121.68	110.60
2	N	1	A	C2-N3-C4	20.78	120.99	110.60
2	O	1	A	C2-N3-C4	20.73	120.97	110.60
2	J	1	A	C2-N3-C4	19.98	120.59	110.60
2	J	2	G	N3-C4-C5	-18.67	119.27	128.60
2	J	2	G	C2-N3-C4	18.36	121.08	111.90
2	M	1	A	N1-C2-N3	-16.86	120.87	129.30
2	L	1	A	N1-C2-N3	-16.50	121.05	129.30
2	K	1	A	N1-C2-N3	-15.88	121.36	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	A	N1-C2-N3	-15.71	121.45	129.30
2	J	1	A	N1-C2-N3	-15.33	121.63	129.30
2	J	2	G	N3-C4-N9	14.56	134.74	126.00
2	N	1	A	OP1-P-OP2	-13.46	99.41	119.60
2	M	1	A	N3-C4-C5	-13.27	117.51	126.80
2	J	2	G	C5-C6-O6	-13.12	120.72	128.60
2	N	1	A	N3-C4-N9	12.92	137.74	127.40
2	N	1	A	N1-C2-N3	-12.40	123.10	129.30
2	N	1	A	N3-C4-C5	-12.31	118.18	126.80
2	J	2	G	C5-C6-N1	12.27	117.63	111.50
2	M	1	A	N3-C4-N9	11.58	136.66	127.40
2	J	1	A	N3-C4-C5	-10.83	119.22	126.80
2	K	1	A	N3-C4-C5	-10.81	119.23	126.80
2	L	1	A	N3-C4-C5	-10.80	119.24	126.80
2	J	1	A	N3-C4-N9	10.71	135.97	127.40
2	J	2	G	C4-C5-N7	-10.56	106.58	110.80
2	K	1	A	N3-C4-N9	10.49	135.79	127.40
2	L	1	A	N3-C4-N9	10.45	135.76	127.40
2	N	1	A	C8-N9-C4	10.37	109.95	105.80
2	L	1	A	OP1-P-OP2	-9.91	104.74	119.60
2	O	1	A	N3-C4-C5	-9.88	119.89	126.80
2	N	1	A	C5-C6-N6	-9.83	115.84	123.70
2	J	2	G	C6-C5-N7	9.65	136.19	130.40
2	N	1	A	N1-C6-N6	9.36	124.22	118.60
2	J	1	A	C6-N1-C2	9.36	124.21	118.60
2	J	1	A	N1-C6-N6	9.33	124.19	118.60
2	J	1	A	C8-N9-C4	9.11	109.44	105.80
2	L	1	A	C8-N9-C4	8.95	109.38	105.80
2	O	1	A	N3-C4-N9	8.67	134.34	127.40
2	O	1	A	OP1-P-OP2	-8.57	106.75	119.60
2	O	1	A	C6-N1-C2	8.25	123.55	118.60
2	K	1	A	C6-N1-C2	8.18	123.51	118.60
2	M	1	A	OP1-P-OP2	-8.05	107.52	119.60
2	M	1	A	C3'-C2'-C1'	7.99	107.89	101.50
2	K	1	A	N1-C6-N6	7.92	123.35	118.60
2	J	2	G	OP1-P-OP2	-7.81	107.89	119.60
2	M	1	A	C8-N9-C4	7.77	108.91	105.80
2	J	2	G	C5-N7-C8	7.46	108.03	104.30
2	K	1	A	C8-N9-C4	7.33	108.73	105.80
2	L	1	A	C6-C5-N7	7.12	137.29	132.30
2	M	1	A	C4-C5-N7	-7.03	107.19	110.70
1	F	131	ASP	CB-CG-OD1	6.89	124.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	A	C4-C5-N7	-6.89	107.26	110.70
2	M	1	A	C5-C6-N6	-6.48	118.51	123.70
1	B	80	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	J	2	G	C8-N9-C4	6.34	108.94	106.40
2	L	1	A	C3'-C2'-C1'	6.32	106.56	101.50
2	K	1	A	OP1-P-OP2	-6.26	110.20	119.60
2	N	1	A	N7-C8-N9	-6.20	110.70	113.80
2	L	1	A	O4'-C1'-N9	6.17	113.14	108.20
2	N	1	A	C5-N7-C8	6.13	106.96	103.90
2	O	1	A	C4-C5-N7	-6.08	107.66	110.70
2	J	1	A	C5-C6-N6	-6.06	118.85	123.70
1	C	59	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	102	ARG	NE-CZ-NH2	-5.89	117.36	120.30
2	J	1	A	C4-C5-N7	-5.86	107.77	110.70
2	K	1	A	C3'-C2'-C1'	5.82	106.16	101.50
1	E	131	ASP	CB-CG-OD1	5.78	123.50	118.30
2	O	1	A	N1-C6-N6	5.73	122.04	118.60
2	L	1	A	C6-N1-C2	5.73	122.04	118.60
2	M	1	A	C5-N7-C8	5.71	106.76	103.90
2	M	1	A	C6-C5-N7	5.67	136.27	132.30
1	F	247	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	F	360	ARG	NE-CZ-NH2	-5.63	117.48	120.30
2	O	1	A	C8-N9-C4	5.58	108.03	105.80
2	L	1	A	C5-C6-N6	-5.52	119.28	123.70
2	M	1	A	N1-C6-N6	5.50	121.90	118.60
1	D	366	ASP	CB-CG-OD1	5.43	123.19	118.30
2	K	1	A	C4-C5-N7	-5.43	107.99	110.70
1	A	57	ARG	NE-CZ-NH1	5.37	122.99	120.30
2	M	1	A	C6-N1-C2	5.33	121.80	118.60
2	J	2	G	N7-C8-N9	-5.30	110.45	113.10
1	F	80	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	183	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	131	ASP	CB-CG-OD1	5.24	123.02	118.30
1	C	373	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	102	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	K	1	A	C5-C6-N6	-5.21	119.53	123.70
1	E	102	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	57	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	80	ARG	CG-CD-NE	-5.12	101.05	111.80
1	E	249	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	E	104	ASP	CB-CG-OD1	5.11	122.89	118.30
1	B	133	ARG	NE-CZ-NH2	-5.08	117.76	120.30

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	2908	0	2807	21	0
1	B	2943	0	2846	13	0
1	C	2943	0	2843	13	0
1	D	2921	0	2809	13	0
1	E	2942	0	2844	21	0
1	F	2960	0	2864	11	0
2	J	46	0	23	1	0
2	K	23	0	12	1	0
2	L	23	0	12	0	0
2	M	23	0	12	0	0
2	N	23	0	12	0	0
2	O	23	0	12	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	69	0	0	0	0
4	B	74	0	0	0	0
4	C	73	0	0	0	0
4	D	46	0	0	1	0
4	E	53	0	0	0	0
4	F	75	0	0	0	0
4	J	3	0	0	0	0
4	L	2	0	0	0	0
4	M	2	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	1	0
All	All	18189	0	17096	92	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 3.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80[B]:ARG:HG3	1:A:80[B]:ARG:NH1	1.59	1.03
1:A:80[B]:ARG:HG3	1:A:80[B]:ARG:HH11	0.91	1.03
1:A:80[B]:ARG:HH11	1:A:80[B]:ARG:CG	1.73	1.02
1:E:106:HIS:HD2	1:E:108:ILE:H	1.39	0.70
1:E:187:VAL:HG13	1:E:202:VAL:HG11	1.79	0.65
1:C:106:HIS:HD2	1:C:108:ILE:H	1.45	0.64
1:E:384:ALA:HB2	1:E:423:LEU:O	1.99	0.62
1:A:194:ASP:OD2	1:A:198:ARG:NH1	2.34	0.61
1:E:237:LEU:HG	1:E:241:MET:HE2	1.81	0.61
1:F:106:HIS:HD2	1:F:108:ILE:H	1.49	0.60
1:B:106:HIS:HD2	1:B:108:ILE:H	1.49	0.60
1:D:106:HIS:HD2	1:D:108:ILE:H	1.51	0.58
1:A:329:HIS:HD2	1:A:331:ARG:H	1.52	0.57
1:C:424:ARG:O	1:C:425:MET:HG2	2.04	0.56
1:E:355:ALA:O	1:E:357:ARG:N	2.39	0.56
1:D:237:LEU:O	1:D:241:MET:HG3	2.06	0.56
1:A:193:THR:O	1:A:194:ASP:HB2	2.06	0.56
1:C:102:ARG:NH2	1:C:393:ASP:OD1	2.32	0.55
1:A:239:ALA:O	1:A:242:GLN:HB3	2.09	0.53
1:A:193:THR:O	1:A:194:ASP:CB	2.57	0.52
1:E:238:LEU:HA	1:E:241:MET:HE3	1.92	0.52
1:C:155:SER:OG	1:C:205:TYR:HB3	2.10	0.51
1:D:176:LYS:NZ	2:K:1:A:O2'	2.35	0.51
1:E:272:GLU:HA	1:E:275:ALA:O	2.12	0.50
1:F:102:ARG:HE	1:F:325:GLN:HE21	1.60	0.50
1:F:129:VAL:HG11	4:O:101:HOH:O	2.11	0.49
1:D:112:SER:HA	1:D:121:PHE:O	2.13	0.49
1:D:258:HIS:CE1	1:D:363:HIS:CD2	3.01	0.49
1:B:181:ASP:OD1	1:B:182:THR:N	2.47	0.48
1:E:66:THR:N	1:E:67:PRO:CD	2.76	0.48
1:F:87:PRO:HD3	1:F:326:TYR:CE2	2.49	0.48
1:A:290:GLY:HA3	1:A:333:PRO:HG2	1.95	0.47
1:F:103:PRO:HA	1:F:106:HIS:NE2	2.29	0.47
1:A:257:ASP:OD1	1:A:257:ASP:N	2.47	0.47
1:E:426:PRO:HB2	1:E:427:PRO:HD3	1.96	0.47
1:B:316:ARG:NH1	1:B:319:GLU:OE1	2.44	0.47
1:E:73:ALA:O	1:E:76:GLY:O	2.31	0.47
1:C:306:LEU:HD21	1:C:335:LEU:HD22	1.96	0.47
1:A:106:HIS:HD2	1:A:108:ILE:H	1.63	0.47
1:A:103:PRO:HA	1:A:106:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:HIS:HD2	1:B:331:ARG:H	1.63	0.46
1:C:66:THR:HB	1:C:69:LEU:HB2	1.97	0.46
1:A:192:ALA:O	1:A:193:THR:C	2.53	0.46
1:D:103:PRO:HA	1:D:106:HIS:CE1	2.51	0.46
1:E:267:HIS:HA	1:E:343:TRP:CZ3	2.51	0.46
1:D:356:GLN:O	1:D:357:ARG:CB	2.64	0.45
1:E:241:MET:HB2	1:E:247:ARG:HB2	1.98	0.45
1:C:103:PRO:HA	1:C:106:HIS:CE1	2.50	0.45
1:A:176:LYS:HE2	2:J:1:A:O2'	2.16	0.45
1:A:252:ILE:O	1:A:378:ALA:HA	2.17	0.45
1:D:172:ARG:CB	4:D:632:HOH:O	2.64	0.45
1:D:274:ILE:HG23	1:D:312:TYR:CE2	2.52	0.45
1:D:103:PRO:HA	1:D:106:HIS:NE2	2.32	0.45
1:F:61:LEU:HD11	1:F:377:LEU:HD21	1.99	0.45
1:F:176:LYS:NZ	2:O:1:A:O2'	2.50	0.45
1:B:72:LEU:HD11	1:B:379:GLN:HB3	1.99	0.44
1:A:194:ASP:OD2	1:A:249:ARG:NH1	2.50	0.44
1:B:160:GLU:OE2	1:B:174:TYR:N	2.44	0.44
1:D:270:SER:HB2	1:D:351:LEU:HD22	1.99	0.44
1:A:194:ASP:HA	1:A:198:ARG:HD3	1.99	0.44
1:B:272:GLU:HA	1:B:275:ALA:O	2.17	0.44
1:C:329:HIS:HD2	1:C:331:ARG:H	1.64	0.44
1:E:354:ARG:O	1:E:355:ALA:HB2	2.19	0.43
1:B:258:HIS:CE1	1:B:363:HIS:CD2	3.07	0.43
1:F:102:ARG:NE	1:F:325:GLN:HE21	2.17	0.43
1:A:78:ARG:O	1:A:388:THR:HA	2.18	0.43
1:E:50:LEU:HD22	1:E:401:MET:SD	2.59	0.43
1:E:311:HIS:NE2	1:E:343:TRP:CZ2	2.87	0.42
1:C:106:HIS:CD2	1:C:108:ILE:H	2.31	0.42
1:B:179:ARG:NH2	1:B:181:ASP:OD2	2.53	0.42
1:F:102:ARG:HE	1:F:325:GLN:NE2	2.17	0.42
1:B:254:VAL:HB	1:B:377:LEU:CD1	2.50	0.42
1:C:103:PRO:HA	1:C:106:HIS:NE2	2.34	0.42
1:E:61:LEU:HD11	1:E:377:LEU:HD23	2.01	0.42
1:E:152:ALA:O	1:E:202:VAL:HA	2.19	0.42
1:C:110:HIS:HB3	1:C:112:SER:O	2.20	0.42
1:A:52:SER:HA	1:A:255:VAL:O	2.20	0.42
1:E:66:THR:N	1:E:67:PRO:HD3	2.34	0.42
1:D:271:VAL:HG12	1:D:289:ILE:HG21	2.02	0.42
1:A:287:GLN:HG2	1:A:363:HIS:O	2.19	0.41
1:F:81:TRP:CE2	1:F:391:GLY:HA3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:PRO:HA	1:F:106:HIS:CD2	2.56	0.41
1:B:356:GLN:O	1:B:357:ARG:CB	2.68	0.41
1:E:241:MET:CB	1:E:247:ARG:HB2	2.50	0.41
1:D:110:HIS:HE1	1:D:288:VAL:O	2.02	0.41
1:E:354:ARG:O	1:E:355:ALA:CB	2.68	0.41
1:B:54:ASP:HB2	1:B:205:TYR:CE1	2.56	0.41
1:C:152:ALA:O	1:C:202:VAL:HA	2.21	0.41
1:A:329:HIS:CD2	1:A:330:PRO:HD2	2.55	0.41
1:C:176:LYS:HE2	1:C:211:GLU:OE2	2.21	0.40
1:E:46:HIS:O	1:E:200:ARG:NE	2.54	0.40
1:B:103:PRO:HA	1:B:106:HIS:NE2	2.37	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	379/427 (89%)	356 (94%)	18 (5%)	5 (1%)	12	4
1	B	382/427 (90%)	369 (97%)	10 (3%)	3 (1%)	19	9
1	C	383/427 (90%)	367 (96%)	13 (3%)	3 (1%)	19	9
1	D	382/427 (90%)	363 (95%)	15 (4%)	4 (1%)	15	6
1	E	383/427 (90%)	359 (94%)	20 (5%)	4 (1%)	15	6
1	F	383/427 (90%)	372 (97%)	10 (3%)	1 (0%)	41	31
All	All	2292/2562 (90%)	2186 (95%)	86 (4%)	20 (1%)	17	7

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	357	ARG

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Mol	Chain	Res	Type
1	A	176	LYS
1	A	194	ASP
1	E	248	ALA
1	E	354	ARG
1	E	355	ALA
1	E	426	PRO
1	D	304	SER
1	D	358	GLY
1	C	43	SER
1	A	193	THR
1	F	357	ARG
1	B	356	GLN
1	B	357	ARG
1	C	357	ARG
1	C	293	PRO
1	A	192	ALA
1	A	195	GLY
1	B	296	GLY
1	D	295	PRO

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	290/326 (89%)	279 (96%)	11 (4%)	33	24
1	B	296/326 (91%)	289 (98%)	7 (2%)	49	43
1	C	295/326 (90%)	289 (98%)	6 (2%)	55	51
1	D	291/326 (89%)	285 (98%)	6 (2%)	53	48
1	E	295/326 (90%)	281 (95%)	14 (5%)	26	16
1	F	299/326 (92%)	290 (97%)	9 (3%)	41	33
All	All	1766/1956 (90%)	1713 (97%)	53 (3%)	42	33

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	175	GLN
1	D	176	LYS
1	D	267	HIS
1	D	278	GLN
1	D	353	LYS
1	D	424	ARG
1	B	80	ARG
1	B	194	ASP
1	B	267	HIS
1	B	294	LEU
1	B	334	SER
1	B	353	LYS
1	B	393	ASP
1	C	112	SER
1	C	121	PHE
1	C	175	GLN
1	C	176	LYS
1	C	278	GLN
1	C	330	PRO
1	A	74	ARG
1	A	80[A]	ARG
1	A	80[B]	ARG
1	A	106	HIS
1	A	176	LYS
1	A	249	ARG
1	A	267	HIS
1	A	353	LYS
1	A	359	THR
1	A	424	ARG
1	A	425	MET
1	E	66	THR
1	E	78	ARG
1	E	106	HIS
1	E	117	THR
1	E	127	GLU
1	E	172	ARG
1	E	175	GLN
1	E	181	ASP
1	E	193	THR
1	E	249	ARG
1	E	288	VAL
1	E	377	LEU
1	E	382	ASP

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Mol	Chain	Res	Type
1	E	425	MET
1	F	72	LEU
1	F	193	THR
1	F	228	ARG
1	F	267	HIS
1	F	278	GLN
1	F	298	GLN
1	F	377	LEU
1	F	393[A]	ASP
1	F	393[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	106	HIS
1	D	110	HIS
1	D	175	GLN
1	D	216	HIS
1	B	106	HIS
1	B	173	HIS
1	B	267	HIS
1	B	329	HIS
1	C	106	HIS
1	C	242	GLN
1	C	267	HIS
1	C	329	HIS
1	A	106	HIS
1	A	175	GLN
1	A	329	HIS
1	E	106	HIS
1	E	242	GLN
1	E	267	HIS
1	E	329	HIS
1	F	106	HIS
1	F	278	GLN
1	F	298	GLN
1	F	325	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	J	1/2 (50%)	0	0
2	K	0/2	-	-
2	L	0/2	-	-
2	M	0/2	-	-
2	N	0/2	-	-
2	O	0/2	-	-
All	All	1/12 (8%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	380/427 (88%)	0.55	22 (5%) 23 25	22, 36, 59, 74	0
1	B	384/427 (89%)	0.16	12 (3%) 49 51	18, 31, 58, 78	0
1	C	385/427 (90%)	0.16	9 (2%) 60 63	19, 33, 59, 72	0
1	D	383/427 (89%)	0.64	30 (7%) 13 14	28, 42, 68, 84	0
1	E	384/427 (89%)	0.70	33 (8%) 10 12	21, 40, 64, 82	0
1	F	384/427 (89%)	0.24	11 (2%) 51 54	21, 32, 53, 65	0
2	J	2/2 (100%)	0.95	1 (50%) 0 0	31, 31, 31, 62	0
2	K	1/2 (50%)	-0.58	0 100 100	37, 37, 37, 37	0
2	L	1/2 (50%)	-0.60	0 100 100	25, 25, 25, 25	0
2	M	1/2 (50%)	-0.44	0 100 100	27, 27, 27, 27	0
2	N	1/2 (50%)	-0.27	0 100 100	35, 35, 35, 35	0
2	O	1/2 (50%)	-0.14	0 100 100	34, 34, 34, 34	0
All	All	2307/2574 (89%)	0.41	118 (5%) 28 31	18, 35, 61, 84	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	299	ALA	6.1
1	F	303	ALA	6.1
1	E	301	ALA	5.9
1	A	177	GLY	5.8
1	E	358	GLY	5.7
1	B	355	ALA	5.7
1	E	294	LEU	5.4
1	E	44	THR	5.1
1	A	303	ALA	5.1
1	B	425	MET	4.9
1	A	296	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	355	ALA	4.7
1	D	295	PRO	4.5
1	E	378	ALA	4.3
1	A	301	ALA	4.2
1	C	42	ALA	4.2
1	E	196	ALA	4.0
1	D	304	SER	4.0
1	A	358	GLY	3.9
1	D	425	MET	3.9
1	C	355	ALA	3.7
1	D	296	GLY	3.7
1	D	276	PRO	3.6
1	D	195	GLY	3.3
1	E	354	ARG	3.3
1	D	357	ARG	3.3
1	E	426	PRO	3.2
1	E	427	PRO	3.2
1	A	193	THR	3.2
1	F	43	SER	3.2
1	A	305	VAL	3.1
1	B	296	GLY	3.1
1	A	307	GLY	3.1
1	E	279	ILE	3.1
1	B	196	ALA	3.1
1	D	64	GLY	3.1
1	C	196	ALA	3.0
1	D	305	VAL	3.0
1	A	300	ALA	3.0
1	F	295	PRO	3.0
1	C	279	ILE	3.0
1	D	356	GLN	2.9
1	D	221	ARG	2.9
1	B	357	ARG	2.9
1	C	300	ALA	2.9
1	D	352	ALA	2.8
1	D	117	THR	2.8
1	A	352	ALA	2.8
1	F	44	THR	2.8
1	E	264	ALA	2.7
1	C	296	GLY	2.7
1	A	267	HIS	2.7
1	E	216	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	355	ALA	2.7
1	A	74	ARG	2.7
1	A	242	GLN	2.6
1	A	147	THR	2.6
1	E	221	ARG	2.6
1	D	194	ASP	2.6
1	A	295	PRO	2.6
1	B	295	PRO	2.6
1	E	191	LEU	2.6
1	D	301	ALA	2.6
1	F	301	ALA	2.5
1	E	295	PRO	2.5
1	E	268	ALA	2.5
1	D	196	ALA	2.5
1	B	352	ALA	2.5
1	E	45	PRO	2.5
1	A	179	ARG	2.5
1	E	425	MET	2.4
1	D	118	LEU	2.4
1	F	352	ALA	2.4
1	B	298	GLN	2.4
1	B	184	VAL	2.4
1	E	369	LEU	2.4
1	E	293	PRO	2.4
1	E	352	ALA	2.4
1	D	424	ARG	2.4
1	E	357	ARG	2.4
1	D	279	ILE	2.4
1	B	356	GLN	2.3
1	D	181	ASP	2.3
1	D	84	PRO	2.3
1	C	357	ARG	2.3
1	E	212	ALA	2.3
1	E	248	ALA	2.3
1	D	165	GLY	2.2
1	F	305	VAL	2.2
1	A	343	TRP	2.2
1	D	303	ALA	2.2
1	F	296	GLY	2.2
2	J	2	G	2.2
1	F	294	LEU	2.2
1	B	44	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	300	ALA	2.2
1	D	310	ASP	2.2
1	D	297	GLN	2.2
1	E	263	VAL	2.2
1	D	381	PRO	2.2
1	E	304	SER	2.2
1	D	353	LYS	2.1
1	B	280	ALA	2.1
1	E	239	ALA	2.1
1	C	175	GLN	2.1
1	D	44	THR	2.1
1	C	266	GLY	2.1
1	A	117	THR	2.1
1	E	423	LEU	2.1
1	E	192	ALA	2.1
1	E	243	ARG	2.1
1	F	378	ALA	2.1
1	A	276	PRO	2.1
1	E	246	THR	2.0
1	A	355	ALA	2.0
1	A	377	LEU	2.0
1	D	169	SER	2.0
1	E	249	ARG	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 monosaccharides 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	A	502	1/1	0.98	0.04	26,26,26,26	0
3	ZN	E	501	1/1	0.98	0.06	37,37,37,37	0
3	ZN	A	501	1/1	0.99	0.04	26,26,26,26	0
3	ZN	D	502	1/1	0.99	0.05	32,32,32,32	0
3	ZN	B	502	1/1	0.99	0.06	24,24,24,24	0
3	ZN	E	502	1/1	0.99	0.04	33,33,33,33	0
3	ZN	B	501	1/1	1.00	0.05	21,21,21,21	0
3	ZN	D	501	1/1	1.00	0.04	29,29,29,29	0
3	ZN	C	501	1/1	1.00	0.04	24,24,24,24	0
3	ZN	C	502	1/1	1.00	0.06	24,24,24,24	0
3	ZN	F	501	1/1	1.00	0.07	26,26,26,26	0
3	ZN	F	502	1/1	1.00	0.05	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.