



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:25 PM UTC

PDB ID : 7MW8 / pdb_00007mw8
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

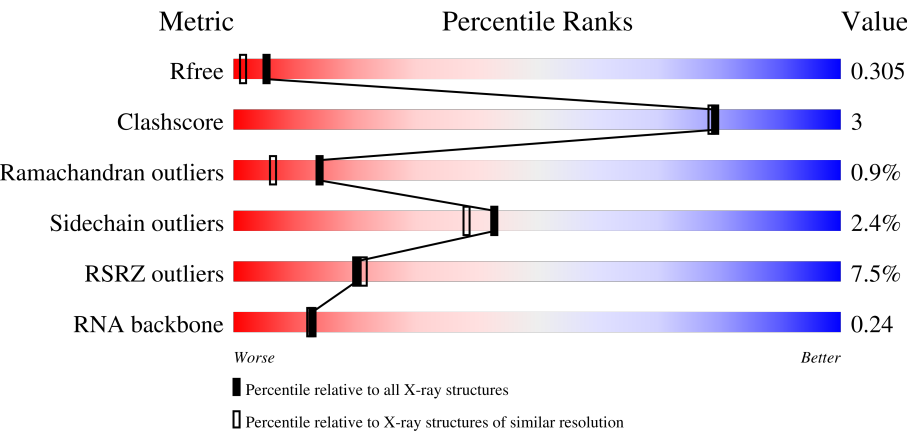
1 Overall quality at a glance i

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)
RNA backbone	3983	1098 (2.30-1.50)

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	5% 81%7%11%
1	B	427	4% 81%8%10%
1	C	427	3% 83%7%10%
1	D	427	10% 83%6%10%

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Mol	Chain	Length	Quality of chain
1	E	427	
1	F	427	
2	J	2	
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	O	2	

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 (CCD ID: 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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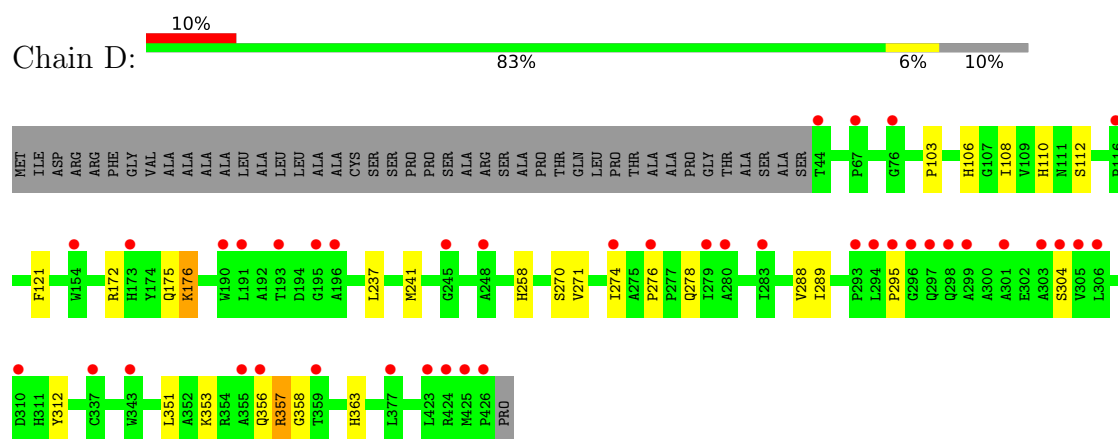
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	2	Total	O	0	0
			2	2		
4	N	1	Total	O	0	0
			1	1		
4	O	1	Total	O	0	0
			1	1		

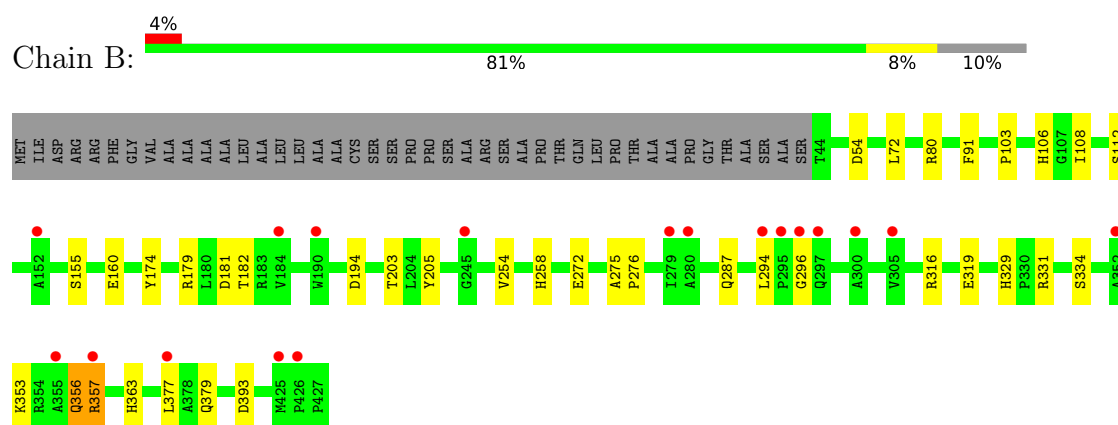
3 Residue-property plots [i](#)

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.

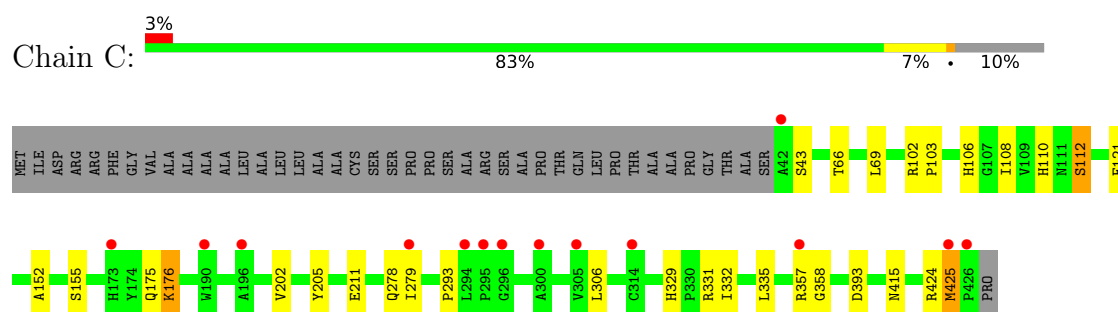
- Molecule 1: Phosphodiesterase-nucleotide pyrophosphatase



- Molecule 1: Phosphodiesterase-nucleotide pyrophosphatase

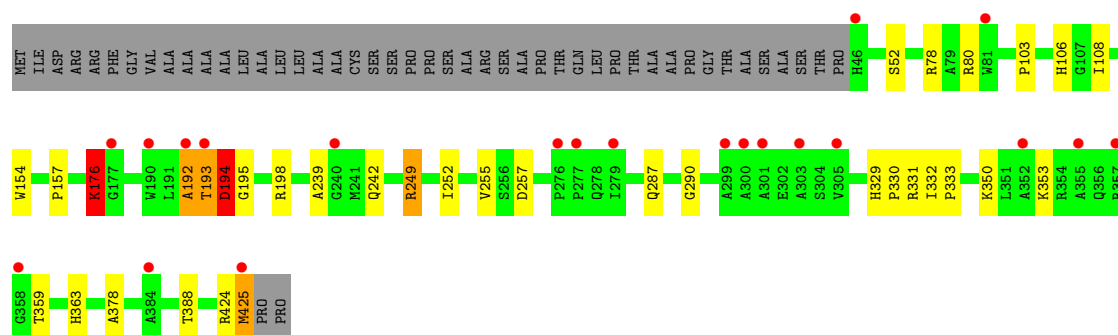


- Molecule 1: Phosphodiesterase-nucleotide pyrophosphatase



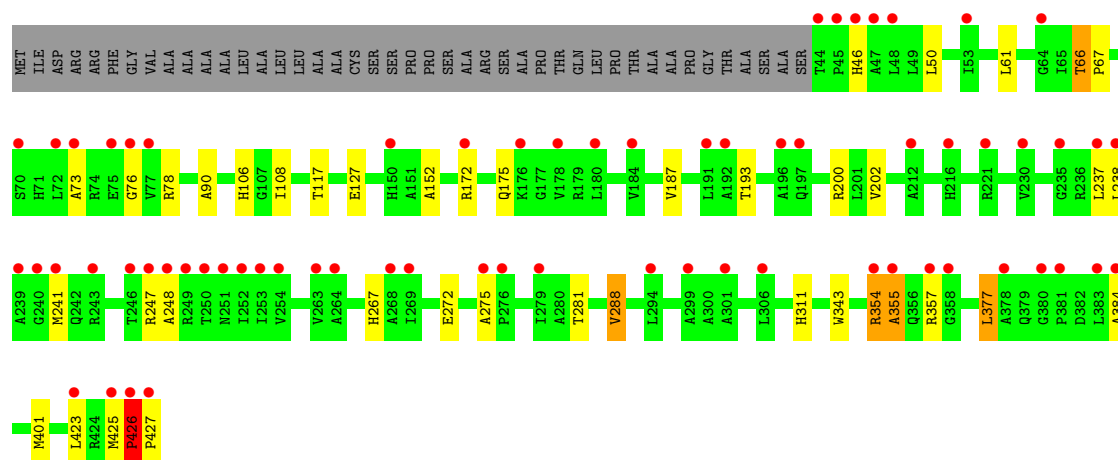
- Molecule 1: Phosphodiesterase-nucleotide pyrophosphatase

Chain A: 



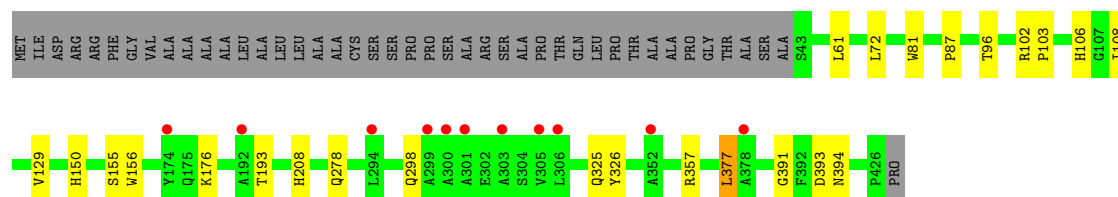
- Molecule 1: Phosphodiesterase-nucleotide pyrophosphatase

Chain E: 



- Molecule 1: Phosphodiesterase-nucleotide pyrophosphatase

Chain F: 



- Molecule 2: pApG

Chain J: 



- 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 30.04 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.04-1.90) 94.5 (30.04-1.90)	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	7597 reflections (4.63%)	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)	0.34 , 26.1	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	0.93	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 [i](#)

5.1 Standard geometry [i](#)

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	0.94	0/2995	1.04	3/4088 (0.1%)
1	B	0.97	2/3030 (0.1%)	1.06	3/4138 (0.1%)
1	C	0.90	0/3029	1.02	4/4136 (0.1%)
1	D	0.86	0/3010	0.99	1/4112 (0.0%)
1	E	0.95	1/3029 (0.0%)	1.05	2/4137 (0.0%)
1	F	0.94	0/3046	1.02	3/4157 (0.1%)
2	J	1.69	0/51	1.61	0/76
2	K	1.78	0/25	1.99	1/35 (2.9%)
2	L	1.65	0/25	2.36	2/35 (5.7%)
2	M	1.35	0/25	2.42	1/35 (2.9%)
2	N	1.80	0/25	2.02	1/35 (2.9%)
2	O	1.65	0/25	1.98	0/35
All	All	0.94	3/18315 (0.0%)	1.04	21/25019 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	THR	N-CA	5.67	1.52	1.45
1	E	426	PRO	CA-C	5.36	1.57	1.52
1	B	112	SER	CA-C	-5.20	1.46	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	90	ALA	N-CA-C	7.05	118.66	110.97
1	A	332	ILE	N-CA-C	-6.80	102.78	108.63
2	N	1	A	OP1-P-OP2	-6.73	99.41	119.60
2	M	1	A	C3'-C2'-C1'	6.39	107.89	101.50
1	C	358	GLY	N-CA-C	6.21	119.07	111.93
1	B	155	SER	N-CA-C	-6.17	98.55	108.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	PHE	O-C-N	6.13	125.22	120.38
1	A	154	TRP	N-CA-C	-5.69	104.72	111.03
1	C	332	ILE	N-CA-C	-5.51	103.89	108.63
1	C	415	ASN	CA-C-N	5.49	125.84	119.47
1	C	415	ASN	C-N-CA	5.49	125.84	119.47
1	D	276	PRO	N-CA-C	5.32	117.20	110.70
1	A	194	ASP	N-CA-C	5.17	121.81	110.80
1	E	288	VAL	CB-CA-C	5.10	118.28	111.19
2	K	1	A	C1'-C2'-O2'	-5.10	104.15	111.80
1	F	150	HIS	N-CA-C	5.06	117.65	109.40
2	L	1	A	C3'-C2'-C1'	5.06	106.56	101.50
2	L	1	A	C3'-C2'-O2'	-5.06	107.01	114.60
1	B	276	PRO	N-CA-C	5.04	116.85	110.70
1	F	394	ASN	N-CA-C	5.04	118.91	112.36
1	F	208	HIS	N-CA-C	5.01	116.82	111.36

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	A	2908	0	2807	22	0
1	B	2943	0	2846	14	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	12	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	95	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 (95) 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: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:E:237:LEU:HG	1:E:241:MET:HE2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:192:ALA:O	1:A:193:THR:C	2.53	0.50
1:E:238:LEU:HA	1:E:241:MET:HE3	1.94	0.50
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
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: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: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:D:356:GLN:O	1:D:357:ARG:CB	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:425:MET:SD	1:A:425:MET:C	3.04	0.40
1:F:155:SER:O	1:F:156:TRP:C	2.64	0.40
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
1:B:287:GLN:N	1:B:287:GLN:CD	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	9	3
1	B	382/427 (90%)	369 (97%)	10 (3%)	3 (1%)	16	8
1	C	383/427 (90%)	367 (96%)	13 (3%)	3 (1%)	16	8
1	D	382/427 (90%)	363 (95%)	15 (4%)	4 (1%)	12	5
1	E	383/427 (90%)	359 (94%)	20 (5%)	4 (1%)	12	5
1	F	383/427 (90%)	372 (97%)	10 (3%)	1 (0%)	36	29
All	All	2292/2562 (90%)	2186 (95%)	86 (4%)	20 (1%)	14	6

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	357	ARG
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%)	282 (97%)	8 (3%)	38	32
1	B	296/326 (91%)	290 (98%)	6 (2%)	48	46
1	C	295/326 (90%)	288 (98%)	7 (2%)	43	38
1	D	291/326 (89%)	287 (99%)	4 (1%)	59	59
1	E	295/326 (90%)	284 (96%)	11 (4%)	30	22
1	F	299/326 (92%)	291 (97%)	8 (3%)	39	34
All	All	1766/1956 (90%)	1722 (98%)	44 (2%)	43	37

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	175	GLN
1	D	176	LYS
1	D	278	GLN
1	D	353	LYS
1	B	80	ARG
1	B	194	ASP
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	279	ILE
1	C	425	MET
1	A	157	PRO
1	A	176	LYS
1	A	249	ARG
1	A	350	LYS
1	A	353	LYS

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Mol	Chain	Res	Type
1	A	359	THR
1	A	424	ARG
1	A	425	MET
1	E	66	THR
1	E	78	ARG
1	E	117	THR
1	E	127	GLU
1	E	172	ARG
1	E	175	GLN
1	E	193	THR
1	E	281	THR
1	E	288	VAL
1	E	377	LEU
1	E	425	MET
1	F	72	LEU
1	F	96	THR
1	F	193	THR
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 (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	106	HIS
1	D	110	HIS
1	D	216	HIS
1	D	278	GLN
1	B	106	HIS
1	B	173	HIS
1	B	329	HIS
1	C	106	HIS
1	C	311	HIS
1	C	329	HIS
1	C	394	ASN
1	A	106	HIS
1	A	173	HIS
1	A	175	GLN
1	A	208	HIS
1	A	216	HIS

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Mol	Chain	Res	Type
1	A	329	HIS
1	A	385	GLN
1	E	106	HIS
1	E	173	HIS
1	E	214	HIS
1	E	242	GLN
1	E	267	HIS
1	E	385	GLN
1	F	106	HIS
1	F	150	HIS
1	F	278	GLN
1	F	325	GLN
1	F	338	GLN
1	F	385	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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	380/427 (88%)	0.75	21 (5%)	30	32	19, 36, 59, 74	1 (0%)
1	B	384/427 (89%)	0.38	18 (4%)	36	39	18, 31, 58, 78	0
1	C	385/427 (90%)	0.41	14 (3%)	46	49	19, 33, 59, 72	0
1	D	383/427 (89%)	0.95	41 (10%)	11	11	28, 42, 68, 84	1 (0%)
1	E	384/427 (89%)	1.04	67 (17%)	4	4	19, 40, 64, 82	1 (0%)
1	F	384/427 (89%)	0.37	11 (2%)	53	57	13, 32, 53, 65	1 (0%)
2	J	2/2 (100%)	0.61	0	100	100	31, 31, 31, 62	0
2	K	1/2 (50%)	-0.09	0	100	100	37, 37, 37, 37	0
2	L	1/2 (50%)	-0.40	0	100	100	25, 25, 25, 25	0
2	M	1/2 (50%)	-0.78	0	100	100	27, 27, 27, 27	0
2	N	1/2 (50%)	-0.17	0	100	100	35, 35, 35, 35	0
2	O	1/2 (50%)	0.09	0	100	100	34, 34, 34, 34	0
All	All	2307/2574 (89%)	0.65	172 (7%)	20	21	13, 35, 61, 84	4 (0%)

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	426	PRO	5.4
1	C	279	ILE	4.6
1	D	426	PRO	4.6
1	E	378	ALA	4.5
1	E	301	ALA	4.3
1	E	44	THR	4.2
1	E	196	ALA	3.9
1	A	299	ALA	3.9
1	A	193	THR	3.8
1	E	358	GLY	3.8
1	E	279	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	358	GLY	3.7
1	C	296	GLY	3.7
1	E	427	PRO	3.7
1	C	42	ALA	3.7
1	D	296	GLY	3.7
1	E	264	ALA	3.6
1	C	426	PRO	3.6
1	A	425	MET	3.6
1	E	248	ALA	3.5
1	B	296	GLY	3.5
1	E	230	VAL	3.5
1	E	250	THR	3.4
1	D	276	PRO	3.4
1	A	352	ALA	3.3
1	B	279	ILE	3.2
1	D	355	ALA	3.2
1	D	295	PRO	3.2
1	E	355	ALA	3.2
1	E	246	THR	3.2
1	C	196	ALA	3.1
1	A	301	ALA	3.1
1	B	425	MET	3.1
1	A	192	ALA	3.1
1	E	239	ALA	3.1
1	A	177	GLY	3.0
1	A	240	GLY	3.0
1	D	297	GLN	3.0
1	B	355	ALA	3.0
1	E	294	LEU	3.0
1	D	305	VAL	3.0
1	D	44	THR	3.0
1	B	295	PRO	3.0
1	D	294	LEU	2.9
1	E	249	ARG	2.9
1	F	300	ALA	2.9
1	D	279	ILE	2.9
1	E	212	ALA	2.8
1	D	193	THR	2.8
1	B	305	VAL	2.8
1	E	45	PRO	2.8
1	C	300	ALA	2.8
1	E	192	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	245	GLY	2.8
1	E	237	LEU	2.8
1	E	306	LEU	2.8
1	D	425	MET	2.8
1	E	384	ALA	2.7
1	F	303	ALA	2.7
1	F	378	ALA	2.7
1	E	77	VAL	2.7
1	E	76	GLY	2.7
1	E	425	MET	2.7
1	B	357	ARG	2.7
1	D	274	ILE	2.7
1	E	235	GLY	2.6
1	E	423	LEU	2.6
1	E	380	GLY	2.6
1	A	277	PRO	2.6
1	E	197	GLN	2.6
1	A	305	VAL	2.6
1	D	154	TRP	2.6
1	D	195	GLY	2.6
1	D	424	ARG	2.5
1	B	280	ALA	2.5
1	E	73	ALA	2.5
1	C	294	LEU	2.5
1	E	240	GLY	2.5
1	A	384	ALA	2.5
1	E	46	HIS	2.5
1	E	252	ILE	2.5
1	D	303	ALA	2.5
1	B	300	ALA	2.5
1	A	300	ALA	2.5
1	B	294	LEU	2.4
1	E	48	LEU	2.4
1	E	238	LEU	2.4
1	D	196	ALA	2.4
1	A	276	PRO	2.4
1	E	357	ARG	2.4
1	D	280	ALA	2.4
1	B	152	ALA	2.4
1	B	184	VAL	2.4
1	D	337	CYS	2.4
1	E	176	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	174	TYR	2.4
1	A	279	ILE	2.4
1	A	357	ARG	2.4
1	D	116	PRO	2.4
1	B	190	TRP	2.4
1	D	377	LEU	2.3
1	E	191	LEU	2.3
1	F	306	LEU	2.3
1	E	383	LEU	2.3
1	D	299	ALA	2.3
1	F	299	ALA	2.3
1	C	295	PRO	2.3
1	E	47	ALA	2.3
1	E	276	PRO	2.3
1	F	192	ALA	2.3
1	E	178	VAL	2.3
1	E	184	VAL	2.3
1	B	377	LEU	2.3
1	B	426	PRO	2.2
1	A	355	ALA	2.2
1	F	294	LEU	2.2
1	E	64	GLY	2.2
1	D	310	ASP	2.2
1	B	352	ALA	2.2
1	E	268	ALA	2.2
1	E	299	ALA	2.2
1	D	173	HIS	2.2
1	A	46	HIS	2.2
1	C	425	MET	2.2
1	D	359	THR	2.2
1	D	304	SER	2.2
1	E	253	ILE	2.2
1	C	190	TRP	2.2
1	E	216	HIS	2.2
1	E	241	MET	2.2
1	D	423	LEU	2.2
1	E	72	LEU	2.2
1	A	81	TRP	2.1
1	F	305	VAL	2.1
1	E	180	LEU	2.1
1	E	221	ARG	2.1
1	E	381	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	303	ALA	2.1
1	B	297	GLN	2.1
1	D	306	LEU	2.1
1	D	298	GLN	2.1
1	F	301	ALA	2.1
1	D	76	GLY	2.1
1	C	173	HIS	2.1
1	C	305	VAL	2.1
1	E	263	VAL	2.1
1	D	293	PRO	2.1
1	D	356	GLN	2.1
1	D	191	LEU	2.1
1	D	248	ALA	2.1
1	D	301	ALA	2.1
1	E	275	ALA	2.1
1	F	352	ALA	2.1
1	E	243	ARG	2.1
1	E	354	ARG	2.1
1	D	283	ILE	2.0
1	E	53	ILE	2.0
1	E	75	GLU	2.0
1	D	245	GLY	2.0
1	E	251	ASN	2.0
1	E	254	VAL	2.0
1	D	190	TRP	2.0
1	D	343	TRP	2.0
1	C	314	CYS	2.0
1	A	190	TRP	2.0
1	C	357	ARG	2.0
1	E	247	ARG	2.0
1	E	70	SER	2.0
1	E	150	HIS	2.0
1	E	269	ILE	2.0
1	D	67	PRO	2.0
1	E	172	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	E	502	1/1	0.97	0.03	33,33,33,33	0
3	ZN	E	501	1/1	0.98	0.03	37,37,37,37	0
3	ZN	A	502	1/1	0.98	0.04	26,26,26,26	0
3	ZN	A	501	1/1	0.99	0.03	26,26,26,26	0
3	ZN	D	501	1/1	0.99	0.03	29,29,29,29	0
3	ZN	D	502	1/1	0.99	0.03	32,32,32,32	0
3	ZN	B	502	1/1	0.99	0.02	24,24,24,24	0
3	ZN	F	502	1/1	0.99	0.02	28,28,28,28	0
3	ZN	C	502	1/1	1.00	0.02	24,24,24,24	0
3	ZN	B	501	1/1	1.00	0.01	21,21,21,21	0
3	ZN	F	501	1/1	1.00	0.01	26,26,26,26	0
3	ZN	C	501	1/1	1.00	0.01	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.