



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:04 PM UTC

PDB ID : 6ISF / pdb_00006isf
Title : Structure of 9N-I DNA polymerase incorporation with dT in the active site
Authors : Linwu, S.W.; Maestre-Reyna, M.; Tsai, M.D.; Tu, Y.H.; Chang, W.H.
Deposited on : 2018-11-16
Resolution : 2.80 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

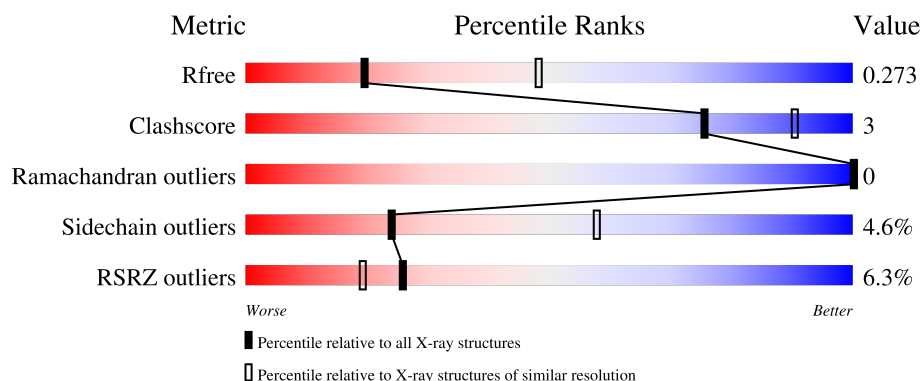
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	783	6% 84% 11% ..
1	B	783	7% 86% 9% ..
2	C	15	87% 13%
2	E	15	100%
3	D	18	11% 100%

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Mol	Chain	Length	Quality of chain
3	F	18	 89% 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13186 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 DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	757	Total	C	N	O	S	0	1	0
			5933	3832	1011	1075	15			
1	B	756	Total	C	N	O	S	0	0	0
			5877	3793	996	1073	15			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ALA	ASP	engineered mutation	UNP Q56366
A	143	ALA	GLU	engineered mutation	UNP Q56366
A	485	LEU	ALA	engineered mutation	UNP Q56366
A	776	LEU	-	expression tag	UNP Q56366
A	777	GLU	-	expression tag	UNP Q56366
A	778	HIS	-	expression tag	UNP Q56366
A	779	HIS	-	expression tag	UNP Q56366
A	780	HIS	-	expression tag	UNP Q56366
A	781	HIS	-	expression tag	UNP Q56366
A	782	HIS	-	expression tag	UNP Q56366
A	783	HIS	-	expression tag	UNP Q56366
B	141	ALA	ASP	engineered mutation	UNP Q56366
B	143	ALA	GLU	engineered mutation	UNP Q56366
B	485	LEU	ALA	engineered mutation	UNP Q56366
B	776	LEU	-	expression tag	UNP Q56366
B	777	GLU	-	expression tag	UNP Q56366
B	778	HIS	-	expression tag	UNP Q56366
B	779	HIS	-	expression tag	UNP Q56366
B	780	HIS	-	expression tag	UNP Q56366
B	781	HIS	-	expression tag	UNP Q56366
B	782	HIS	-	expression tag	UNP Q56366
B	783	HIS	-	expression tag	UNP Q56366

- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*CP*GP*GP*AP*CP*TP*GP*CP*TP*TP*AP*CP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	P	0	0	0
			302	145	53	90	14			
2	E	15	Total	C	N	O	P	0	0	0
			301	145	53	89	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	18	Total	C	N	O	P	0	0	0
			359	170	69	103	17			
3	F	18	Total	C	N	O	P	0	0	0
			359	170	69	103	17			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
4	B	5	Total	Ca	0	0
			5	5		

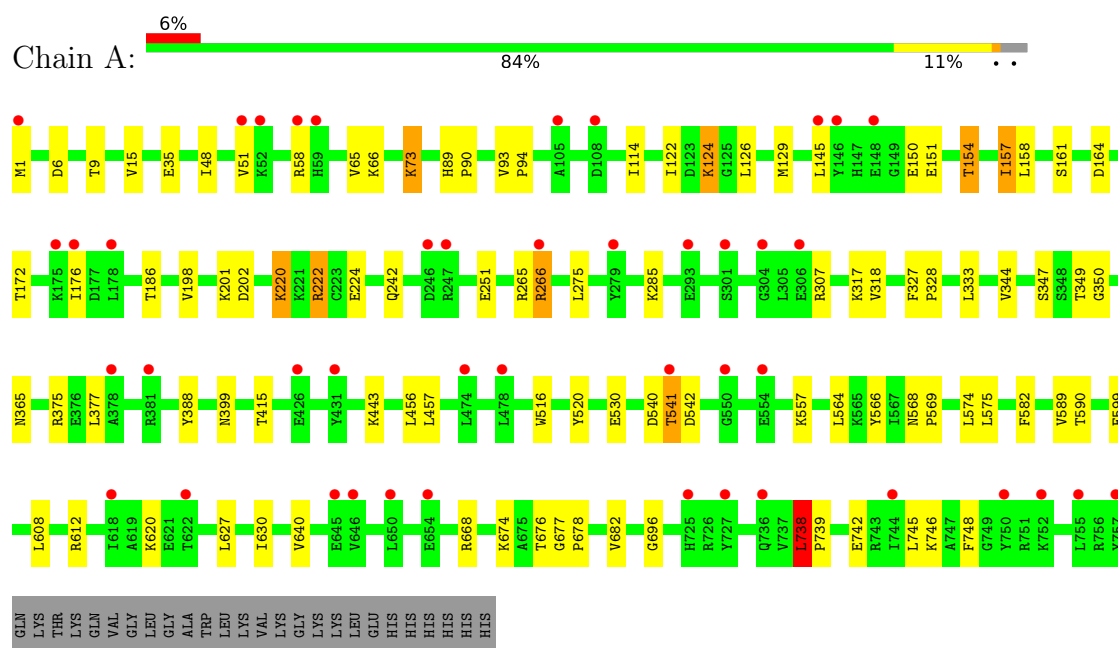
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	28	Total	O	0	0
			28	28		
5	B	19	Total	O	0	0
			19	19		
5	E	1	Total	O	0	0
			1	1		

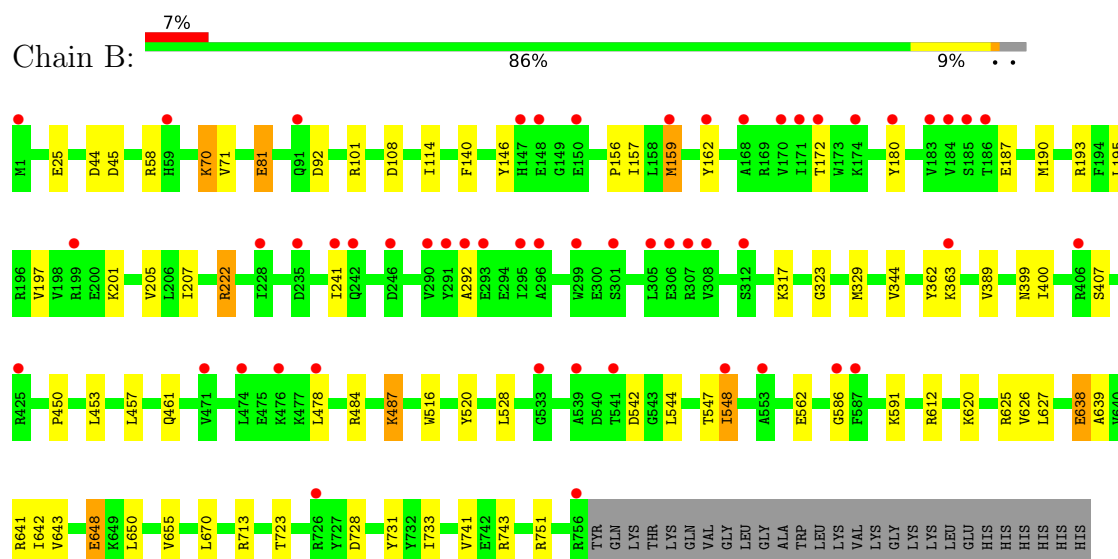
3 Residue-property plots

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: DNA polymerase



• Molecule 1: DNA polymerase

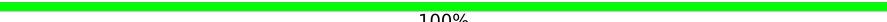


- Molecule 2: DNA (5'-D(P*GP*CP*GP*GP*AP*CP*TP*GP*CP*TP*TP*AP*CP*CP*T)-3')

Chain C:  87% 13%



- Molecule 2: DNA (5'-D(P*GP*CP*GP*GP*AP*CP*TP*GP*CP*TP*TP*AP*CP*CP*T)-3')

Chain E:  100%

There are no outlier residues recorded for this chain.

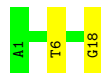
- Molecule 3: DNA (5'-D(*AP*CP*AP*GP*GP*TP*AP*AP*GP*CP*AP*GP*TP*CP*CP*GP*CP*G)-3')

Chain D:  11% 100%



- Molecule 3: DNA (5'-D(*AP*CP*AP*GP*GP*TP*AP*AP*GP*CP*AP*GP*TP*CP*CP*GP*CP*G)-3')

Chain F:  89% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.09Å 107.36Å 255.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.38 – 2.80 46.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.38-2.80) 99.5 (46.38-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.232 , 0.272 0.235 , 0.273	Depositor DCC
R_{free} test set	3143 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13186	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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:
CA

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	1.17	4/6076 (0.1%)	1.54	11/8231 (0.1%)
1	B	1.17	8/6013 (0.1%)	1.55	11/8160 (0.1%)
2	C	0.31	0/337	0.73	0/518
2	E	0.31	0/336	0.75	0/517
3	D	0.35	0/403	0.61	0/620
3	F	0.34	0/403	0.68	0/620
All	All	1.11	12/13568 (0.1%)	1.47	22/18666 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	TYR	C-O	6.32	1.31	1.23
1	B	389	VAL	C-O	6.14	1.30	1.24
1	B	648	GLU	C-O	6.12	1.31	1.24
1	B	626	VAL	C-O	5.76	1.31	1.24
1	B	450	PRO	C-O	-5.62	1.16	1.24
1	B	548	ILE	N-CA	5.37	1.50	1.46
1	A	114	ILE	N-CA	5.35	1.50	1.46
1	B	114	ILE	N-CA	5.33	1.50	1.46
1	A	738	LEU	N-CA	5.30	1.51	1.46
1	B	71	VAL	C-O	5.25	1.29	1.24
1	A	222	ARG	C-O	5.09	1.29	1.24
1	A	456	LEU	C-O	5.02	1.29	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	LEU	CA-C-N	6.41	128.87	120.28
1	A	377	LEU	C-N-CA	6.41	128.87	120.28
1	B	205	VAL	CA-C-O	-6.16	114.27	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	520	TYR	CA-C-O	-6.15	113.97	120.55
1	B	195	LEU	CA-C-N	5.91	128.19	120.28
1	B	195	LEU	C-N-CA	5.91	128.19	120.28
1	A	15	VAL	CA-C-O	-5.86	114.57	120.31
1	A	122	ILE	CA-C-N	5.85	128.70	120.28
1	A	122	ILE	C-N-CA	5.85	128.70	120.28
1	B	317	LYS	CA-C-N	5.70	127.74	120.56
1	B	317	LYS	C-N-CA	5.70	127.74	120.56
1	A	566	TYR	CA-C-O	-5.37	115.16	120.80
1	B	562	GLU	CA-C-O	-5.31	114.92	120.55
1	B	731	TYR	CA-C-O	-5.24	115.32	120.82
1	A	530	GLU	CA-C-O	-5.22	114.44	120.24
1	A	640	VAL	CA-C-O	-5.12	115.63	120.95
1	B	362	TYR	CA-C-O	-5.10	115.14	120.55
1	B	520	TYR	CA-C-O	-5.07	115.48	120.70
1	B	638	GLU	CA-C-N	5.04	127.35	120.54
1	B	638	GLU	C-N-CA	5.04	127.35	120.54
1	A	350	GLY	O-C-N	5.03	127.01	122.18
1	A	161	SER	CA-C-O	-5.01	115.71	121.47

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	5933	0	5682	45	0
1	B	5877	0	5611	30	0
2	C	302	0	171	2	0
2	E	301	0	168	0	0
3	D	359	0	197	0	0
3	F	359	0	197	2	0
4	A	2	0	0	0	0
4	B	5	0	0	0	0
5	A	28	0	0	0	0
5	B	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1	0	0	0	0
All	All	13186	0	12026	76	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 (76) 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:B:146:TYR:CB	1:B:292:ALA:HB1	1.84	1.06
1:A:220:LYS:O	1:A:224:GLU:HG3	1.72	0.89
1:A:266[A]:ARG:NH1	1:A:347:SER:O	2.07	0.87
1:B:146:TYR:CB	1:B:292:ALA:CB	2.57	0.81
1:A:265:ARG:NH2	1:A:696:GLY:O	2.12	0.81
1:A:388:TYR:O	1:A:540:ASP:O	2.07	0.71
1:B:643:VAL:HG21	1:B:741:VAL:HG21	1.75	0.69
1:B:713:ARG:NH1	1:B:728:ASP:OD2	2.32	0.62
1:A:151:GLU:O	1:A:154:THR:CG2	2.49	0.61
1:A:93:VAL:HB	1:A:94:PRO:HD3	1.84	0.58
1:B:157:ILE:O	1:B:190:MET:HE1	2.04	0.57
1:B:544:LEU:O	1:B:544:LEU:HD12	2.05	0.57
1:B:457:LEU:O	1:B:461:GLN:HG3	2.05	0.56
1:A:35:GLU:OE1	1:A:66:LYS:HE2	2.05	0.55
1:A:541:THR:O	1:A:542:ASP:OD1	2.24	0.55
1:B:639:ALA:HA	1:B:642:ILE:HD12	1.90	0.54
1:A:630:ILE:HD13	1:A:748:PHE:CE2	2.43	0.54
1:A:157:ILE:HG13	1:A:222:ARG:HG3	1.90	0.53
1:A:145:LEU:HB2	1:A:158:LEU:HD21	1.90	0.52
1:B:45:ASP:OD2	1:B:70:LYS:NZ	2.24	0.52
1:B:58:ARG:NH2	1:B:92:ASP:OD1	2.41	0.52
1:A:415:THR:O	1:A:443:LYS:NZ	2.42	0.51
1:B:544:LEU:HD12	1:B:544:LEU:C	2.36	0.51
1:B:407:SER:OG	1:B:487:LYS:NZ	2.43	0.50
1:A:220:LYS:O	1:A:224:GLU:CG	2.53	0.49
1:A:742:GLU:O	1:A:746:LYS:N	2.44	0.49
1:A:151:GLU:O	1:A:154:THR:HG22	2.11	0.49
1:B:643:VAL:CG2	1:B:741:VAL:HG21	2.42	0.48
1:A:48:ILE:O	1:A:51:VAL:HG22	2.14	0.48
1:B:591:LYS:HD3	3:F:6:DT:H5''	1.95	0.47
1:A:674:LYS:NZ	2:C:-4:DC:OP1	2.47	0.47
1:B:650:LEU:HD13	1:B:655:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HG3	1:A:129:MET:HA	1.98	0.47
1:B:193:ARG:O	1:B:197:VAL:HG23	2.15	0.46
3:F:18:DG:OP2	3:F:18:DG:H4'	2.14	0.46
1:A:172:THR:HG21	1:A:176:ILE:HD12	1.97	0.46
1:A:242:GLN:NE2	1:A:251:GLU:OE2	2.48	0.46
1:B:207:ILE:HD13	1:B:323:GLY:HA3	1.98	0.46
1:B:156:PRO:HA	1:B:222:ARG:HE	1.81	0.46
1:B:157:ILE:N	1:B:187:GLU:OE2	2.47	0.46
1:B:650:LEU:HD23	1:B:733:ILE:HG13	1.98	0.46
1:A:399:ASN:HA	1:A:582:PHE:CZ	2.50	0.46
1:B:101:ARG:NH1	1:B:108:ASP:OD1	2.49	0.46
1:A:73:LYS:HE2	1:A:365:ASN:OD1	2.17	0.45
1:A:6:ASP:C	1:A:6:ASP:OD1	2.60	0.45
1:A:738:LEU:HB2	1:A:739:PRO:HD3	2.00	0.44
1:A:677:GLY:O	1:A:678:PRO:C	2.59	0.43
1:A:333:LEU:HG	1:A:344:VAL:HG11	1.99	0.43
1:A:678:PRO:O	1:A:682:VAL:HG23	2.18	0.43
1:A:612:ARG:NH2	2:C:-1:DA:O4'	2.52	0.43
1:A:164:ASP:OD2	1:A:201:LYS:NZ	2.52	0.43
1:B:399:ASN:O	1:B:547:THR:OG1	2.32	0.43
1:A:333:LEU:HG	1:A:344:VAL:CG1	2.48	0.43
1:A:124:LYS:HB3	1:A:126:LEU:HG	2.01	0.43
1:A:612:ARG:O	1:A:620:LYS:HD3	2.18	0.43
1:A:568:ASN:N	1:A:569:PRO:CD	2.82	0.42
1:B:159:MET:HG3	1:B:172:THR:HB	2.02	0.42
1:A:327:PHE:N	1:A:328:PRO:CD	2.82	0.42
1:B:70:LYS:HE2	1:B:81:GLU:HG2	2.02	0.42
1:A:150:GLU:HG2	1:A:154:THR:HG23	2.02	0.42
1:B:612:ARG:O	1:B:620:LYS:HD3	2.20	0.42
1:B:625:ARG:NH2	1:B:642:ILE:HG23	2.35	0.42
1:A:541:THR:O	1:A:542:ASP:CG	2.62	0.41
1:A:198:VAL:O	1:A:202:ASP:N	2.52	0.41
1:A:589:VAL:HG12	1:A:590:THR:HG23	2.02	0.41
1:B:400:ILE:CD1	1:B:586:GLY:HA3	2.50	0.41
1:A:89:HIS:CG	1:A:90:PRO:HD2	2.56	0.41
1:B:70:LYS:HE2	1:B:81:GLU:CG	2.51	0.41
1:A:557:LYS:NZ	1:A:599:GLU:OE1	2.41	0.41
1:A:58:ARG:O	1:A:58:ARG:CG	2.68	0.40
1:A:275:LEU:HD23	1:A:275:LEU:HA	1.96	0.40
1:B:528:LEU:HD12	1:B:528:LEU:HA	1.96	0.40
1:A:589:VAL:HG21	1:A:608:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:GLU:C	1:A:154:THR:HG22	2.46	0.40
1:A:399:ASN:HA	1:A:582:PHE:CE1	2.57	0.40
1:B:638:GLU:HA	1:B:641:ARG:NH1	2.35	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	756/783 (97%)	717 (95%)	39 (5%)	0	100	100
1	B	754/783 (96%)	714 (95%)	40 (5%)	0	100	100
All	All	1510/1566 (96%)	1431 (95%)	79 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	563/675 (83%)	536 (95%)	27 (5%)	23	56
1	B	562/675 (83%)	536 (95%)	26 (5%)	24	58
All	All	1125/1350 (83%)	1072 (95%)	53 (5%)	24	57

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

Mol	Chain	Res	Type
1	A	9	THR
1	A	65	VAL
1	A	73	LYS
1	A	124	LYS
1	A	154	THR
1	A	157	ILE
1	A	186	THR
1	A	220	LYS
1	A	266[A]	ARG
1	A	266[B]	ARG
1	A	285	LYS
1	A	307	ARG
1	A	317	LYS
1	A	318	VAL
1	A	349	THR
1	A	375	ARG
1	A	457	LEU
1	A	516	TRP
1	A	541	THR
1	A	564	LEU
1	A	574	LEU
1	A	575	LEU
1	A	627	LEU
1	A	668	ARG
1	A	676	THR
1	A	738	LEU
1	A	745	LEU
1	B	25	GLU
1	B	44	ASP
1	B	70	LYS
1	B	81	GLU
1	B	140	PHE
1	B	159	MET
1	B	180	TYR
1	B	201	LYS
1	B	222	ARG
1	B	241	ILE
1	B	329	MET
1	B	344	VAL
1	B	363	LYS
1	B	453	LEU
1	B	478	LEU
1	B	484	ARG

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Mol	Chain	Res	Type
1	B	487	LYS
1	B	516	TRP
1	B	542	ASP
1	B	548	ILE
1	B	627	LEU
1	B	648	GLU
1	B	670	LEU
1	B	723	THR
1	B	743	ARG
1	B	751	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	ASN
1	A	424	ASN
1	A	491	ASN
1	B	91	GLN
1	B	461	GLN
1	B	491	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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	757/783 (96%)	0.60	44 (5%) 29 22	33, 62, 96, 119	4 (0%)
1	B	756/783 (96%)	0.60	53 (7%) 22 16	36, 62, 104, 141	1 (0%)
2	C	15/15 (100%)	-0.41	0 100 100	33, 47, 60, 66	0
2	E	15/15 (100%)	-0.33	0 100 100	34, 40, 58, 60	0
3	D	18/18 (100%)	0.64	2 (11%) 10 7	34, 46, 80, 88	2 (11%)
3	F	18/18 (100%)	-0.02	0 100 100	34, 48, 67, 89	0
All	All	1579/1632 (96%)	0.58	99 (6%) 26 19	33, 61, 100, 141	7 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	18	DG	6.0
3	D	1	DA	5.3
1	A	725	HIS	5.1
1	A	757	TYR	5.0
1	B	241	ILE	4.2
1	A	381	ARG	4.1
1	A	279	TYR	3.7
1	B	299	TRP	3.5
1	A	148	GLU	3.5
1	A	431	TYR	3.4
1	A	59	HIS	3.4
1	B	292	ALA	3.4
1	B	290	VAL	3.3
1	A	646	VAL	3.3
1	A	541	THR	3.2
1	B	162	TYR	3.2
1	B	533	GLY	3.2
1	B	183	VAL	3.1
1	B	148	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	246	ASP	3.0
1	B	726	ARG	3.0
1	B	185	SER	3.0
1	B	406	ARG	3.0
1	A	654	GLU	2.9
1	B	296	ALA	2.9
1	A	301	SER	2.9
1	A	108	ASP	2.9
1	B	180	TYR	2.9
1	A	247	ARG	2.8
1	A	52	LYS	2.8
1	B	301	SER	2.8
1	B	756	ARG	2.8
1	B	174	LYS	2.8
1	A	306	GLU	2.8
1	B	147	HIS	2.8
1	B	293	GLU	2.7
1	B	305	LEU	2.7
1	B	553	ALA	2.7
1	A	750	TYR	2.7
1	A	622	THR	2.7
1	A	474	LEU	2.7
1	B	308	VAL	2.7
1	B	171	ILE	2.6
1	B	587	PHE	2.6
1	A	146	TYR	2.6
1	A	1	MET	2.6
1	A	293	GLU	2.6
1	A	752	LYS	2.6
1	A	105	ALA	2.6
1	B	476	LYS	2.5
1	A	650	LEU	2.5
1	A	178	LEU	2.5
1	B	478	LEU	2.5
1	B	586	GLY	2.5
1	B	170	VAL	2.5
1	A	175	LYS	2.5
1	A	176	ILE	2.5
1	A	618	ILE	2.5
1	B	312	SER	2.5
1	B	541	THR	2.5
1	B	159	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	554	GLU	2.4
1	B	307	ARG	2.4
1	B	91	GLN	2.4
1	A	266[A]	ARG	2.4
1	B	291	TYR	2.4
1	B	474	LEU	2.4
1	B	295	ILE	2.4
1	A	51	VAL	2.4
1	A	645	GLU	2.4
1	B	199	ARG	2.4
1	A	246	ASP	2.3
1	B	228	ILE	2.3
1	A	378	ALA	2.3
1	B	306	GLU	2.3
1	A	426	GLU	2.2
1	A	736	GLN	2.2
1	B	172	THR	2.2
1	B	363	LYS	2.2
1	B	242	GLN	2.2
1	A	58	ARG	2.2
1	B	1	MET	2.2
1	A	145	LEU	2.2
1	A	478	LEU	2.2
1	B	150	GLU	2.2
1	B	235	ASP	2.2
1	A	550	GLY	2.2
1	A	755	LEU	2.2
1	B	539	ALA	2.2
1	B	425	ARG	2.1
1	B	471	VAL	2.1
1	A	744	ILE	2.1
1	B	184	VAL	2.1
1	B	168	ALA	2.1
1	B	186	THR	2.1
1	A	727	TYR	2.1
1	A	304	GLY	2.1
1	B	59	HIS	2.0
1	B	548	ILE	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($\text{\AA}^2$)	Q<0.9
4	CA	B	802	1/1	0.85	0.17	104,104,104,104	0
4	CA	B	801	1/1	0.92	0.14	85,85,85,85	0
4	CA	B	804	1/1	0.92	0.07	90,90,90,90	0
4	CA	B	805	1/1	0.92	0.17	75,75,75,75	0
4	CA	A	801	1/1	0.95	0.06	80,80,80,80	0
4	CA	A	802	1/1	0.96	0.24	101,101,101,101	0
4	CA	B	803	1/1	0.97	0.04	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.