



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:18 AM UTC

PDB ID : 6FHI / pdb_00006fhi
Title : Crystal structure of bat influenza A/H17N10 polymerase with viral RNA promoter bound to a 19-mer serine 5 phosphorylated Pol II CTD peptide with a truncated linker.
Authors : Lukarska, M.; Cusack, S.
Deposited on : 2018-01-14
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
Mogul : 2022.3.0, CSD as543be (2022)
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

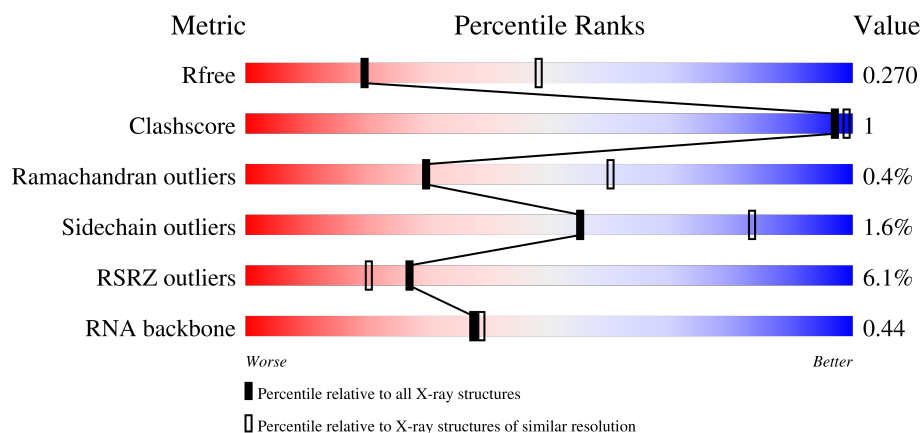
1 Overall quality at a glance

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)
RNA backbone	3983	1114 (3.00-2.60)

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	738	10% 91% • •
2	B	776	4% 93% • •
3	C	809	3% 88% • 10%
4	R	18	67% 6% 28%

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Mol	Chain	Length	Quality of chain
5	V	16	6% 69% 31%
6	X	19	11% 89% 11%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18364 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	709	Total	C	N	O	S	0	0	0
			5770	3665	971	1097	37			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	GLY	-	expression tag	UNP H6QM92
A	-12	SER	-	expression tag	UNP H6QM92
A	-11	HIS	-	expression tag	UNP H6QM92
A	-10	HIS	-	expression tag	UNP H6QM92
A	-9	HIS	-	expression tag	UNP H6QM92
A	-8	HIS	-	expression tag	UNP H6QM92
A	-7	HIS	-	expression tag	UNP H6QM92
A	-6	HIS	-	expression tag	UNP H6QM92
A	-5	HIS	-	expression tag	UNP H6QM92
A	-4	HIS	-	expression tag	UNP H6QM92
A	-3	GLY	-	expression tag	UNP H6QM92
A	-2	SER	-	expression tag	UNP H6QM92
A	-1	GLY	-	expression tag	UNP H6QM92
A	0	SER	-	expression tag	UNP H6QM92
A	714	GLY	-	expression tag	UNP H6QM92
A	715	SER	-	expression tag	UNP H6QM92
A	716	GLY	-	expression tag	UNP H6QM92
A	717	SER	-	expression tag	UNP H6QM92
A	718	GLY	-	expression tag	UNP H6QM92
A	719	GLU	-	expression tag	UNP H6QM92
A	720	ASN	-	expression tag	UNP H6QM92
A	721	LEU	-	expression tag	UNP H6QM92
A	722	TYR	-	expression tag	UNP H6QM92
A	723	PHE	-	expression tag	UNP H6QM92
A	724	GLN	-	expression tag	UNP H6QM92

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	750	Total	C	N	O	S	0	0	0
			5986	3766	1062	1118	40			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP H6QM91
B	-7	SER	-	expression tag	UNP H6QM91
B	-6	GLY	-	expression tag	UNP H6QM91
B	-5	SER	-	expression tag	UNP H6QM91
B	-4	GLY	-	expression tag	UNP H6QM91
B	-3	SER	-	expression tag	UNP H6QM91
B	-2	GLY	-	expression tag	UNP H6QM91
B	-1	SER	-	expression tag	UNP H6QM91
B	0	GLY	-	expression tag	UNP H6QM91
B	757	GLY	-	expression tag	UNP H6QM91
B	758	SER	-	expression tag	UNP H6QM91
B	759	GLY	-	expression tag	UNP H6QM91
B	760	SER	-	expression tag	UNP H6QM91
B	761	GLY	-	expression tag	UNP H6QM91
B	762	GLU	-	expression tag	UNP H6QM91
B	763	ASN	-	expression tag	UNP H6QM91
B	764	LEU	-	expression tag	UNP H6QM91
B	765	TYR	-	expression tag	UNP H6QM91
B	766	PHE	-	expression tag	UNP H6QM91
B	767	GLN	-	expression tag	UNP H6QM91

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	730	Total	C	N	O	S	0	0	0
			5796	3657	1025	1082	32			

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	expression tag	UNP H6QM90
C	-7	SER	-	expression tag	UNP H6QM90
C	-6	GLY	-	expression tag	UNP H6QM90
C	-5	SER	-	expression tag	UNP H6QM90
C	-4	GLY	-	expression tag	UNP H6QM90
C	-3	SER	-	expression tag	UNP H6QM90
C	-2	GLY	-	expression tag	UNP H6QM90

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP H6QM90
C	0	GLY	-	expression tag	UNP H6QM90
C	761	GLY	-	expression tag	UNP H6QM90
C	762	TRP	-	expression tag	UNP H6QM90
C	763	SER	-	expression tag	UNP H6QM90
C	764	HIS	-	expression tag	UNP H6QM90
C	765	PRO	-	expression tag	UNP H6QM90
C	766	GLN	-	expression tag	UNP H6QM90
C	767	PHE	-	expression tag	UNP H6QM90
C	768	GLU	-	expression tag	UNP H6QM90
C	769	LYS	-	expression tag	UNP H6QM90
C	770	GLY	-	expression tag	UNP H6QM90
C	771	GLY	-	expression tag	UNP H6QM90
C	772	GLY	-	expression tag	UNP H6QM90
C	773	SER	-	expression tag	UNP H6QM90
C	774	GLY	-	expression tag	UNP H6QM90
C	775	GLY	-	expression tag	UNP H6QM90
C	776	GLY	-	expression tag	UNP H6QM90
C	777	SER	-	expression tag	UNP H6QM90
C	778	GLY	-	expression tag	UNP H6QM90
C	779	GLY	-	expression tag	UNP H6QM90
C	780	SER	-	expression tag	UNP H6QM90
C	781	ALA	-	expression tag	UNP H6QM90
C	782	TRP	-	expression tag	UNP H6QM90
C	783	SER	-	expression tag	UNP H6QM90
C	784	HIS	-	expression tag	UNP H6QM90
C	785	PRO	-	expression tag	UNP H6QM90
C	786	GLN	-	expression tag	UNP H6QM90
C	787	PHE	-	expression tag	UNP H6QM90
C	788	GLU	-	expression tag	UNP H6QM90
C	789	LYS	-	expression tag	UNP H6QM90
C	790	GLY	-	expression tag	UNP H6QM90
C	791	ARG	-	expression tag	UNP H6QM90
C	792	SER	-	expression tag	UNP H6QM90
C	793	GLY	-	expression tag	UNP H6QM90
C	794	GLY	-	expression tag	UNP H6QM90
C	795	GLU	-	expression tag	UNP H6QM90
C	796	ASN	-	expression tag	UNP H6QM90
C	797	LEU	-	expression tag	UNP H6QM90
C	798	TYR	-	expression tag	UNP H6QM90
C	799	PHE	-	expression tag	UNP H6QM90
C	800	GLN	-	expression tag	UNP H6QM90

- Molecule 4 is a RNA chain called RNA (5'-R(*UP*AP*UP*AP*CP*CP*UP*CP*UP*GP*CP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	R	13	Total	C	N	O	P	0	0	0
			247	111	37	87	12			

- Molecule 5 is a RNA chain called RNA (5'-R(P*AP*GP*UP*AP*GP*UP*AP*AP*CP*AP*AP*GP*AP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	V	16	Total	C	N	O	P	0	0	0
			353	157	72	108	16			

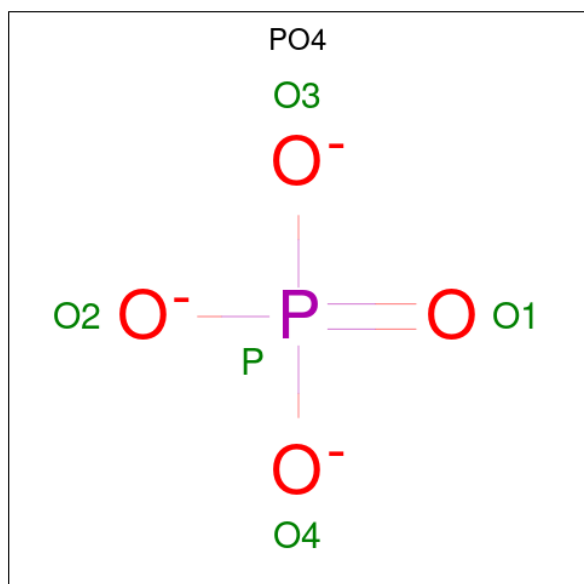
- Molecule 6 is a protein called TYR-SER-PRO-THR-SEP-PRO-SER-TYR-SER-PRO-SER-TYR-SER-PRO-THR-SEP-PRO-SER-TYR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	X	19	Total	C	N	O	P	0	0	0
			146	87	19	38	2			

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

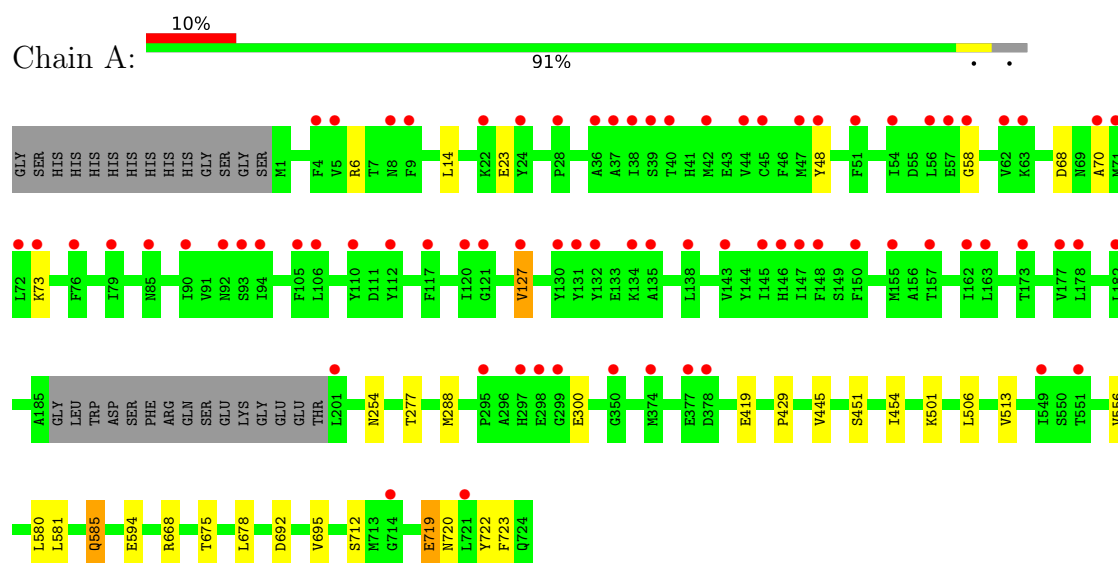


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	P	0	0
			5	4	1		
8	A	1	Total	O	P	0	0
			5	4	1		
8	B	1	Total	O	P	0	0
			5	4	1		
8	B	1	Total	O	P	0	0
			5	4	1		
8	B	1	Total	O	P	0	0
			5	4	1		
8	B	1	Total	O	P	0	0
			5	4	1		
8	B	1	Total	O	P	0	0
			5	4	1		
8	B	1	Total	O	P	0	0
			5	4	1		
8	C	1	Total	O	P	0	0
			5	4	1		
8	C	1	Total	O	P	0	0
			5	4	1		
8	C	1	Total	O	P	0	0
			5	4	1		
8	C	1	Total	O	P	0	0
			5	4	1		

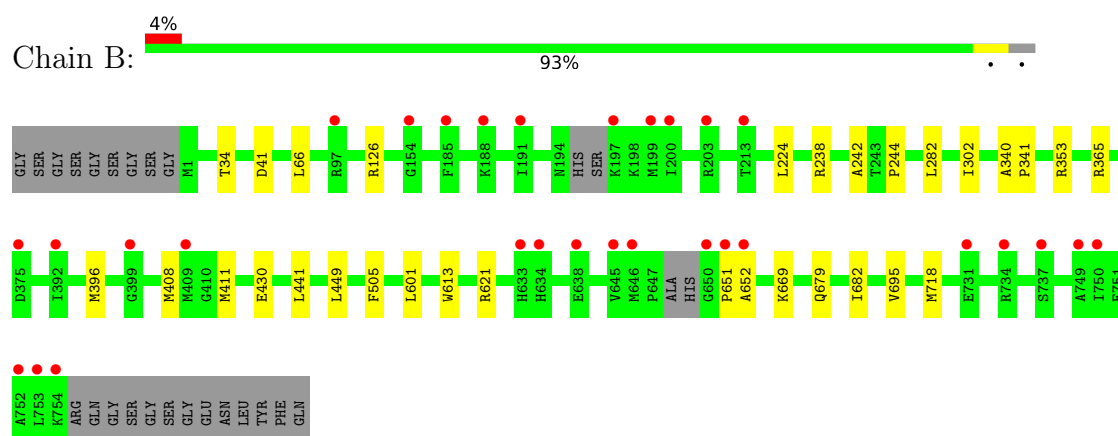
3 Residue-property plots

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.

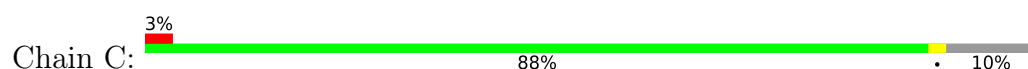
- Molecule 1: Polymerase acidic protein

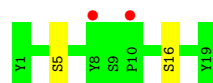


- Molecule 2: RNA-directed RNA polymerase catalytic subunit



- Molecule 3: Polymerase basic protein 2





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	268.74Å 147.52Å 88.54Å 90.00° 96.63° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.1 (50.00-2.80) 96.1 (50.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.230 , 0.270 0.232 , 0.270	Depositor DCC
R_{free} test set	3923 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18364	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: ZN, PO4, SEP

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	0.52	0/5892	0.77	0/7934
2	B	0.53	0/6100	0.79	0/8229
3	C	0.54	0/5894	0.76	0/7955
4	R	0.35	0/273	0.69	0/421
5	V	0.37	0/397	0.65	0/617
6	X	0.52	0/131	0.82	0/178
All	All	0.52	0/18687	0.77	0/25334

There are no bond length outliers.

There are no bond angle outliers.

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	5770	0	5678	16	0
2	B	5986	0	6006	13	0
3	C	5796	0	5923	6	0
4	R	247	0	128	0	0
5	V	353	0	175	0	0
6	X	146	0	116	0	0
7	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	10	0	0	0	0
8	B	30	0	0	0	0
8	C	25	0	0	0	0
All	All	18364	0	18026	33	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 1.

All (33) 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:719:GLU:N	1:A:719:GLU:OE2	2.20	0.73
1:A:506:LEU:HD11	1:A:513:VAL:CG2	2.24	0.67
2:B:224:LEU:HD22	2:B:244:PRO:HA	1.86	0.57
1:A:719:GLU:H	1:A:719:GLU:CD	2.14	0.55
1:A:445:VAL:HG13	1:A:580:LEU:HD22	1.89	0.55
1:A:445:VAL:CG1	1:A:580:LEU:HD22	2.37	0.54
2:B:34:THR:HG22	2:B:353:ARG:HB2	1.94	0.50
1:A:585:GLN:HG2	2:B:505:PHE:CD2	2.48	0.49
3:C:554:ILE:HD12	3:C:672:VAL:HG13	1.95	0.49
1:A:720:ASN:O	1:A:720:ASN:ND2	2.47	0.48
2:B:242:ALA:HB2	2:B:408:MET:HE3	1.95	0.47
2:B:302:ILE:HD12	2:B:449:LEU:HD23	1.97	0.47
2:B:408:MET:HB3	2:B:411:MET:HE3	1.96	0.46
2:B:408:MET:CB	2:B:411:MET:HE3	2.45	0.46
3:C:167:VAL:HG23	3:C:168:PHE:CD2	2.51	0.46
1:A:288:MET:HE1	1:A:556:VAL:HG13	1.98	0.46
2:B:613:TRP:CZ2	2:B:621:ARG:HD3	2.51	0.46
1:A:692:ASP:HB3	1:A:695:VAL:HG12	1.98	0.45
2:B:679:GLN:HB3	2:B:682:ILE:HD12	1.98	0.44
2:B:695:VAL:HG13	2:B:718:MET:HE1	2.00	0.44
1:A:6:ARG:HA	1:A:14:LEU:HD21	2.00	0.44
1:A:720:ASN:ND2	1:A:722:TYR:O	2.50	0.44
2:B:282:LEU:HG	2:B:441:LEU:HD22	2.01	0.42
3:C:595:PHE:CE2	3:C:599:LEU:HD11	2.54	0.42
2:B:340:ALA:HB3	2:B:341:PRO:HD3	2.01	0.42
1:A:675:THR:HG21	1:A:678:LEU:HD13	2.01	0.42
3:C:554:ILE:HD11	3:C:665:ILE:HD12	2.00	0.42
1:A:506:LEU:HD11	1:A:513:VAL:HG23	2.02	0.42
1:A:451:SER:HA	1:A:454:ILE:HD12	2.02	0.41
2:B:224:LEU:HD12	2:B:411:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:399:ILE:HD13	3:C:402:MET:HE2	2.02	0.41
1:A:712:SER:O	1:A:720:ASN:ND2	2.49	0.40
1:A:429:PRO:HB2	3:C:133:VAL:HG23	2.03	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	705/738 (96%)	660 (94%)	39 (6%)	6 (1%)	14	41
2	B	744/776 (96%)	721 (97%)	21 (3%)	2 (0%)	36	66
3	C	724/809 (90%)	698 (96%)	26 (4%)	0	100	100
6	X	15/19 (79%)	13 (87%)	2 (13%)	0	100	100
All	All	2188/2342 (93%)	2092 (96%)	88 (4%)	8 (0%)	30	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	GLY
1	A	127	VAL
2	B	651	PRO
2	B	652	ALA
1	A	68	ASP
1	A	723	PHE
1	A	23	GLU
1	A	70	ALA

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	633/657 (96%)	620 (98%)	13 (2%)	47	79
2	B	659/676 (98%)	650 (99%)	9 (1%)	59	85
3	C	647/706 (92%)	637 (98%)	10 (2%)	57	84
6	X	16/17 (94%)	16 (100%)	0	100	100
All	All	1955/2056 (95%)	1923 (98%)	32 (2%)	55	83

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	TYR
1	A	73	LYS
1	A	127	VAL
1	A	254	ASN
1	A	277	THR
1	A	300	GLU
1	A	419	GLU
1	A	501	LYS
1	A	581	LEU
1	A	585	GLN
1	A	594	GLU
1	A	668	ARG
1	A	719	GLU
2	B	41	ASP
2	B	66	LEU
2	B	126	ARG
2	B	238	ARG
2	B	365	ARG
2	B	396	MET
2	B	430	GLU
2	B	601	LEU
2	B	669	LYS
3	C	164	MET
3	C	170	ASN

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Mol	Chain	Res	Type
3	C	354	MET
3	C	395	LEU
3	C	410	MET
3	C	431	MET
3	C	536	MET
3	C	539	VAL
3	C	660	GLN
3	C	672	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	69	ASN
1	A	96	ASN
1	A	100	ASN
1	A	115	ASN
1	A	354	ASN
1	A	476	GLN
1	A	582	GLN
2	B	137	GLN
2	B	153	ASN
2	B	186	GLN
2	B	202	GLN
2	B	216	ASN
2	B	268	GLN
2	B	394	HIS
2	B	425	ASN
2	B	485	ASN
2	B	537	ASN
2	B	549	GLN
2	B	679	GLN
3	C	110	HIS
3	C	182	GLN
3	C	320	ASN
3	C	321	ASN
3	C	329	ASN
3	C	379	GLN
3	C	419	ASN
3	C	532	ASN
3	C	548	ASN
3	C	581	GLN

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Mol	Chain	Res	Type
3	C	723	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	R	11/18 (61%)	1 (9%)	0
5	V	15/16 (93%)	5 (33%)	1 (6%)
All	All	26/34 (76%)	6 (23%)	1 (3%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	R	5	C
5	V	5	G
5	V	6	U
5	V	7	A
5	V	8	A
5	V	11	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	V	5	G

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SEP	X	5	6	8,9,10	0.64	0	7,12,14	1.56	1 (14%)
6	SEP	X	16	6	8,9,10	0.70	0	7,12,14	1.24	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SEP	X	5	6	-	2/6/8/10	-
6	SEP	X	16	6	-	3/6/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	5	SEP	OG-CB-CA	3.01	111.08	108.14
6	X	16	SEP	O3P-P-OG	-2.08	101.25	106.67

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	X	5	SEP	N-CA-CB-OG
6	X	16	SEP	CB-OG-P-O1P
6	X	16	SEP	CB-OG-P-O3P
6	X	5	SEP	CA-CB-OG-P
6	X	16	SEP	CB-OG-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	PO4	C	901	-	4,4,4	0.94	0	6,6,6	0.55	0
8	PO4	B	802	-	4,4,4	0.94	0	6,6,6	0.44	0
8	PO4	A	802	-	4,4,4	0.95	0	6,6,6	0.51	0
8	PO4	B	803	-	4,4,4	0.89	0	6,6,6	0.47	0
8	PO4	B	805	-	4,4,4	0.96	0	6,6,6	0.52	0
8	PO4	C	904	-	4,4,4	0.95	0	6,6,6	0.57	0
8	PO4	B	804	-	4,4,4	0.97	0	6,6,6	0.54	0
8	PO4	B	801	-	4,4,4	0.91	0	6,6,6	0.55	0
8	PO4	A	803	-	4,4,4	0.94	0	6,6,6	0.46	0
8	PO4	C	903	-	4,4,4	0.90	0	6,6,6	0.48	0
8	PO4	B	806	-	4,4,4	0.96	0	6,6,6	0.49	0
8	PO4	C	902	-	4,4,4	0.96	0	6,6,6	0.46	0
8	PO4	C	905	-	4,4,4	0.98	0	6,6,6	0.46	0

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	709/738 (96%)	0.64	76 (10%) 11 8	40, 69, 210, 249	0
2	B	750/776 (96%)	0.38	30 (4%) 42 33	39, 68, 125, 156	0
3	C	730/809 (90%)	0.50	28 (3%) 44 35	43, 78, 124, 148	0
4	R	13/18 (72%)	0.16	0 100 100	52, 63, 96, 97	0
5	V	16/16 (100%)	-0.01	1 (6%) 26 19	54, 58, 90, 151	0
6	X	17/19 (89%)	0.39	2 (11%) 9 7	56, 70, 108, 112	0
All	All	2235/2376 (94%)	0.50	137 (6%) 27 20	39, 72, 184, 249	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	THR	4.7
1	A	120	ILE	4.4
1	A	177	VAL	4.2
1	A	178	LEU	4.1
1	A	121	GLY	4.1
2	B	197	LYS	4.1
1	A	182	LEU	4.0
1	A	36	ALA	4.0
1	A	48	TYR	4.0
1	A	106	LEU	3.9
1	A	147	ILE	3.9
1	A	56	LEU	3.8
2	B	633	HIS	3.7
3	C	-1	SER	3.7
3	C	354	MET	3.6
1	A	38	ILE	3.6
1	A	8	ASN	3.6
1	A	94	ILE	3.5
1	A	117	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
3	C	521	ALA	3.4
1	A	201	LEU	3.3
1	A	295	PRO	3.3
1	A	54	ILE	3.3
1	A	145	ILE	3.3
1	A	148	PHE	3.3
2	B	200	ILE	3.3
1	A	73	LYS	3.2
1	A	71	MET	3.2
3	C	494	ILE	3.2
1	A	112	TYR	3.1
2	B	753	LEU	3.1
1	A	42	MET	3.1
1	A	4	PHE	3.0
1	A	297	HIS	3.0
1	A	44	VAL	3.0
3	C	420	PHE	3.0
1	A	377	GLU	3.0
1	A	85	ASN	3.0
2	B	651	PRO	3.0
1	A	39	SER	3.0
2	B	199	MET	2.9
1	A	162	ILE	2.9
2	B	646	MET	2.9
3	C	446	LEU	2.9
3	C	138	GLN	2.9
1	A	28	PRO	2.8
1	A	135	ALA	2.8
3	C	421	VAL	2.8
2	B	203	ARG	2.8
2	B	645	VAL	2.8
3	C	654	GLN	2.8
3	C	352	LEU	2.8
2	B	213	THR	2.8
1	A	138	LEU	2.8
1	A	45	CYS	2.7
1	A	105	PHE	2.7
1	A	37	ALA	2.7
1	A	76	PHE	2.7
3	C	349	LEU	2.7
1	A	47	MET	2.7
2	B	638	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	346	THR	2.6
3	C	428	LEU	2.6
2	B	191	ILE	2.6
2	B	392	ILE	2.6
1	A	93	SER	2.6
2	B	737	SER	2.6
1	A	92	ASN	2.6
1	A	134	LYS	2.6
6	X	10	PRO	2.6
2	B	754	LYS	2.6
1	A	90	ILE	2.6
1	A	127	VAL	2.6
3	C	8	MET	2.6
1	A	22	LYS	2.5
1	A	58	GLY	2.5
2	B	154	GLY	2.5
2	B	749	ALA	2.5
2	B	375	ASP	2.5
1	A	79	ILE	2.5
1	A	299	GLY	2.5
1	A	5	VAL	2.5
1	A	157	THR	2.5
2	B	185	PHE	2.4
3	C	651	GLY	2.4
1	A	132	TYR	2.4
3	C	655	VAL	2.4
1	A	298	GLU	2.4
1	A	350	GLY	2.4
5	V	16	G	2.4
1	A	72	LEU	2.4
1	A	62	VAL	2.3
2	B	650	GLY	2.3
1	A	378	ASP	2.3
3	C	29	ALA	2.3
2	B	97	ARG	2.3
1	A	155	MET	2.3
3	C	345	LEU	2.3
1	A	173	THR	2.3
2	B	409	MET	2.3
1	A	549	ILE	2.2
1	A	9	PHE	2.2
3	C	344	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	399	GLY	2.2
3	C	431	MET	2.2
1	A	51	PHE	2.2
1	A	150	PHE	2.2
2	B	188	LYS	2.2
1	A	130	TYR	2.2
1	A	70	ALA	2.2
2	B	731	GLU	2.2
3	C	28	MET	2.2
1	A	24	TYR	2.2
1	A	131	TYR	2.2
2	B	652	ALA	2.2
2	B	750	ILE	2.1
3	C	321	ASN	2.1
1	A	714	GLY	2.1
3	C	351	THR	2.1
3	C	390	THR	2.1
1	A	721	LEU	2.1
1	A	146	HIS	2.1
1	A	374	MET	2.1
3	C	137	ASN	2.1
3	C	418	LEU	2.1
2	B	734	ARG	2.1
2	B	752	ALA	2.0
1	A	110	TYR	2.0
3	C	12	LYS	2.0
1	A	143	VAL	2.0
2	B	634	HIS	2.0
1	A	163	LEU	2.0
1	A	551	THR	2.0
3	C	343	ALA	2.0
1	A	57	GLU	2.0
1	A	63	LYS	2.0
6	X	8	TYR	2.0

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

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
6	SEP	X	5	10/11	0.90	0.10	71,76,85,85	0
6	SEP	X	16	10/11	0.96	0.06	55,55,57,57	0

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
8	PO4	A	803	5/5	0.74	0.11	123,123,125,127	0
8	PO4	B	804	5/5	0.79	0.14	109,112,115,120	0
8	PO4	C	903	5/5	0.80	0.16	96,97,101,101	0
8	PO4	B	801	5/5	0.81	0.13	99,101,103,104	0
8	PO4	C	901	5/5	0.82	0.14	120,120,123,124	0
8	PO4	B	803	5/5	0.84	0.12	93,95,97,99	0
8	PO4	A	802	5/5	0.85	0.26	110,110,113,118	0
8	PO4	C	902	5/5	0.86	0.10	116,116,117,118	0
8	PO4	C	905	5/5	0.86	0.14	104,104,106,108	0
8	PO4	C	904	5/5	0.88	0.20	92,95,97,97	0
8	PO4	B	805	5/5	0.92	0.19	93,96,97,98	0
8	PO4	B	802	5/5	0.92	0.16	88,90,90,96	0
8	PO4	B	806	5/5	0.93	0.07	75,75,77,78	0
7	ZN	A	801	1/1	0.98	0.05	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.