Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:57 pm BST

PDB ID	:	6FHI
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 following versions of software and data (see references ⓘ) were used in the production of this report:

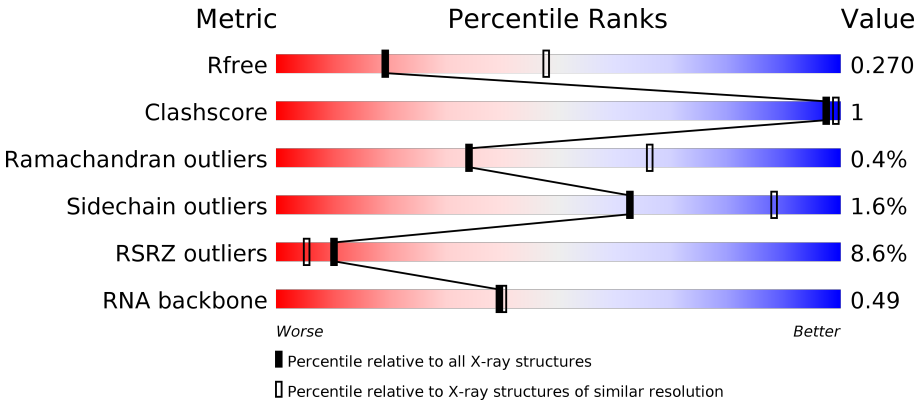
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	738	17% 91%
2	B	776	3% 93%
3	C	809	5% 88% 10%
4	R	18	67% 6% 28%

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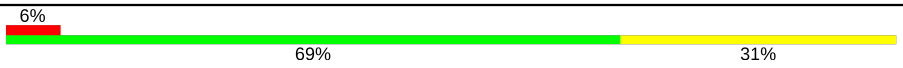
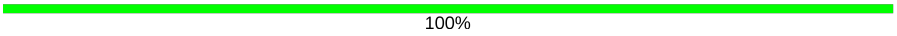
Mol	Chain	Length	Quality of chain
5	V	16	
6	X	19	

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			

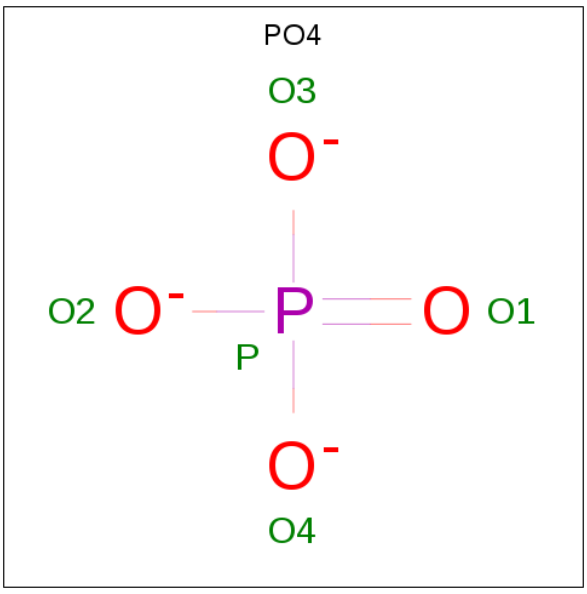
- Molecule 6 is a protein called TYR-SER-PRO-THR-SEP-PRO-SER-TYR-SER-PRO-SER-TYR-SER-PRO-THR-SEP-PRO-SER-TYR.

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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



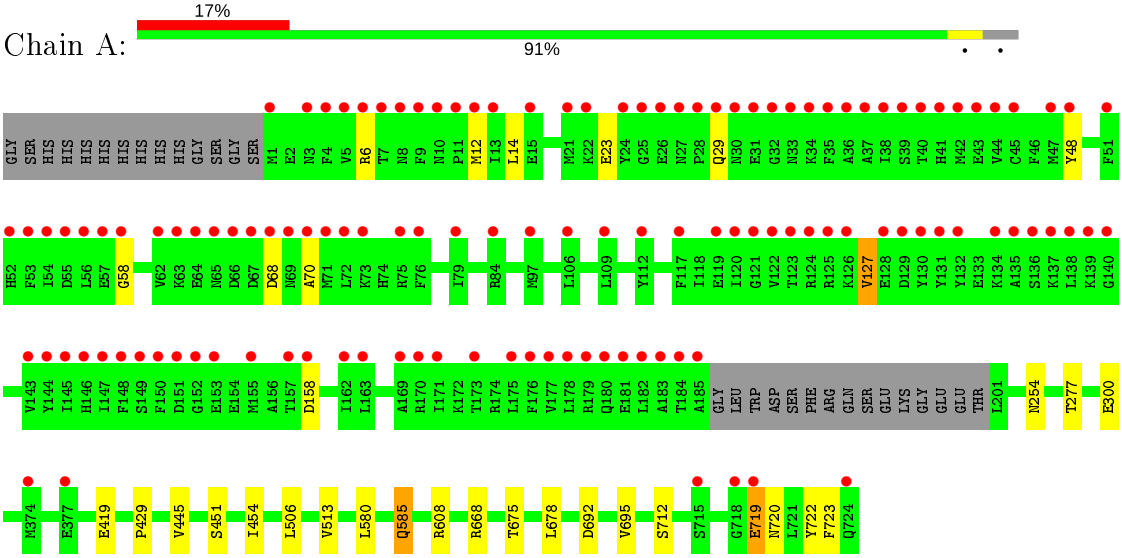
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O P 5 4 1	0	0
8	A	1	Total O P 5 4 1	0	0
8	B	1	Total O P 5 4 1	0	0
8	B	1	Total O P 5 4 1	0	0
8	B	1	Total O P 5 4 1	0	0
8	B	1	Total O P 5 4 1	0	0
8	B	1	Total O P 5 4 1	0	0
8	B	1	Total O P 5 4 1	0	0
8	C	1	Total O P 5 4 1	0	0
8	C	1	Total O P 5 4 1	0	0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

3 Residue-property plots (i)

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

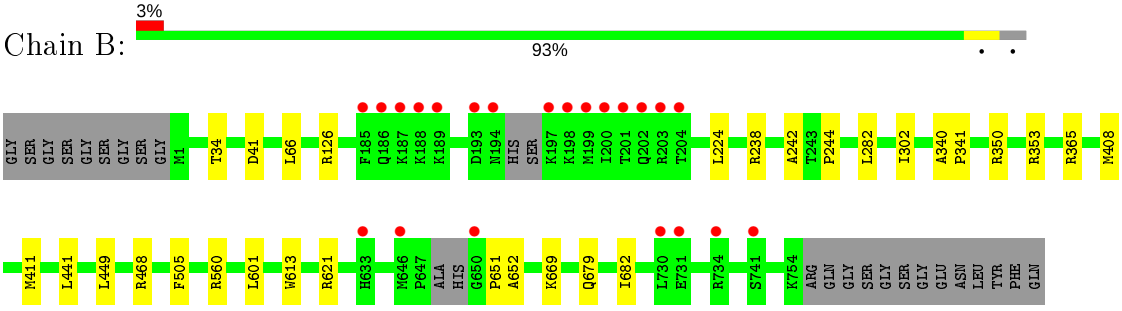
- Molecule 1: Polymerase acidic protein

Chain A:



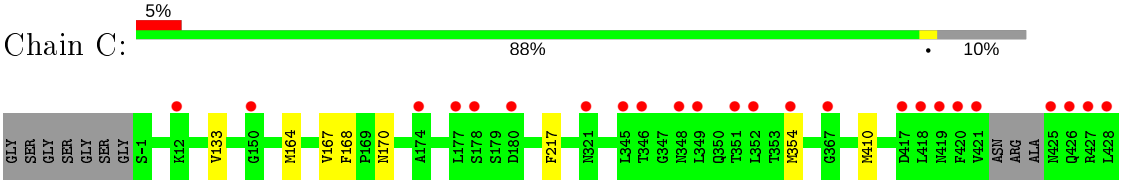
- Molecule 2: RNA-directed RNA polymerase catalytic subunit

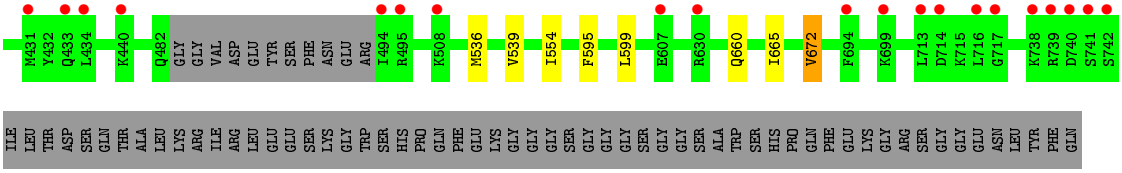
Chain B:



- Molecule 3: Polymerase basic protein 2

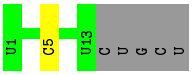
Chain C:





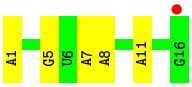
• Molecule 4: RNA (5'-R(*UP*AP*UP*AP*CP*CP*UP*CP*UP*GP*CP*UP*U)-3')

Chain R:



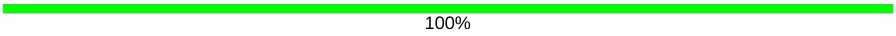
• Molecule 5: RNA (5'-R(P*AP*GP*UP*AP*GP*UP*AP*AP*CP*AP*AP*GP*AP*GP*GP*G)-3')

Chain V:



• Molecule 6: TYR-SER-PRO-THR-SEP-PRO-SER-TYR-SER-PRO-SER-TYR-SER-PRO-THR-SEP-PRO-SER-TYR

Chain X:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

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 49.49 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.1 (50.00-2.80) 96.1 (49.49-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.230 , 0.270 0.230 , 0.270	Depositor DCC
R_{free} test set	3923 reflections (4.84%)	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 , 36.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ZN, 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	0.36	0/5892	0.54	0/7934
2	B	0.36	0/6100	0.57	0/8229
3	C	0.36	0/5894	0.56	0/7955
4	R	0.23	0/273	0.67	0/421
5	V	0.55	1/397 (0.3%)	0.66	0/617
6	X	0.40	0/131	0.47	0/178
All	All	0.36	1/18687 (0.0%)	0.56	0/25334

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	V	1	A	OP3-P	-9.94	1.49	1.61

There are no bond angle outliers.

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	5770	0	5678	15	0
2	B	5986	0	6006	10	0
3	C	5796	0	5923	5	0
4	R	247	0	128	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	V	353	0	175	0	0
6	X	146	0	116	0	0
7	A	1	0	0	0	0
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	28	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 (28) 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: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
1:A:719:GLU:CD	1:A:719:GLU:H	2.14	0.51
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:224:LEU:HD12	2:B:411:MET:HE1	1.97	0.47
2:B:302:ILE:HD12	2:B:449:LEU:HD23	1.97	0.47
3:C:167:VAL:HG23	3:C:168:PHE:CD2	2.51	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
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
1:A:712:SER:O	1:A:720:ASN:ND2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:PRO:HB2	3:C:133:VAL:HG23	2.03	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	705/738 (96%)	660 (94%)	39 (6%)	6 (1%)	17 46
2	B	744/776 (96%)	721 (97%)	21 (3%)	2 (0%)	41 72
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%)	34 66

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%)	53	84
2	B	659/676 (98%)	649 (98%)	10 (2%)	65	89
3	C	647/706 (92%)	638 (99%)	9 (1%)	67	90
6	X	16/17 (94%)	16 (100%)	0	100	100
All	All	1955/2056 (95%)	1923 (98%)	32 (2%)	62	88

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

Mol	Chain	Res	Type
1	A	12	MET
1	A	29	GLN
1	A	48	TYR
1	A	127	VAL
1	A	158	ASP
1	A	254	ASN
1	A	277	THR
1	A	300	GLU
1	A	419	GLU
1	A	585	GLN
1	A	608	ARG
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	350	ARG
2	B	365	ARG
2	B	468	ARG
2	B	560	ARG
2	B	601	LEU
2	B	669	LYS
3	C	164	MET
3	C	170	ASN
3	C	217	PHE
3	C	354	MET
3	C	410	MET
3	C	536	MET
3	C	539	VAL

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Mol	Chain	Res	Type
3	C	660	GLN
3	C	672	VAL

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

Mol	Chain	Res	Type
1	A	96	ASN
2	B	137	GLN
3	C	13	ASN
3	C	110	HIS
3	C	532	ASN
3	C	632	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	R	11/18 (61%)	1 (9%)	0
5	V	15/16 (93%)	3 (20%)	1 (6%)
All	All	26/34 (76%)	4 (15%)	1 (3%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	R	5	C
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 (i)

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	16	6	8,9,10	0.68	0	8,12,14	1.37	2 (25%)
6	SEP	X	5	6	8,9,10	0.62	0	8,12,14	1.52	1 (12%)

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	16	6	-	3/5/8/10	-
6	SEP	X	5	6	-	2/5/8/10	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	X	5	SEP	OG-CB-CA	3.01	111.08	108.14
6	X	16	SEP	P-OG-CB	2.06	123.97	118.30
6	X	16	SEP	O3P-P-OG	-2.06	101.25	106.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	X	16	SEP	CB-OG-P-O1P
6	X	16	SEP	CB-OG-P-O3P
6	X	5	SEP	N-CA-CB-OG
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 carbohydrates 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	B	803	-	4,4,4	0.85	0	6,6,6	0.44	0
8	PO4	B	804	-	4,4,4	0.93	0	6,6,6	0.51	0
8	PO4	C	905	-	4,4,4	0.93	0	6,6,6	0.43	0
8	PO4	C	904	-	4,4,4	0.90	0	6,6,6	0.54	0
8	PO4	C	903	-	4,4,4	0.86	0	6,6,6	0.45	0
8	PO4	B	806	-	4,4,4	0.91	0	6,6,6	0.46	0
8	PO4	A	802	-	4,4,4	0.91	0	6,6,6	0.48	0
8	PO4	B	802	-	4,4,4	0.89	0	6,6,6	0.40	0
8	PO4	B	805	-	4,4,4	0.92	0	6,6,6	0.48	0
8	PO4	B	801	-	4,4,4	0.87	0	6,6,6	0.52	0
8	PO4	C	901	-	4,4,4	0.89	0	6,6,6	0.52	0
8	PO4	A	803	-	4,4,4	0.90	0	6,6,6	0.42	0
8	PO4	C	902	-	4,4,4	0.92	0	6,6,6	0.42	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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	709/738 (96%)	0.91	125 (17%) 1 1	40, 69, 210, 249	0
2	B	750/776 (96%)	0.16	22 (2%) 51 41	39, 68, 125, 156	0
3	C	730/809 (90%)	0.31	44 (6%) 21 14	43, 78, 124, 148	0
4	R	13/18 (72%)	0.10	0 100 100	52, 63, 96, 97	0
5	V	16/16 (100%)	0.11	1 (6%) 20 12	54, 58, 90, 151	0
6	X	17/19 (89%)	0.20	0 100 100	56, 70, 108, 112	0
All	All	2235/2376 (94%)	0.45	192 (8%) 10 5	39, 72, 184, 249	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	GLY	12.9
1	A	25	GLY	12.0
1	A	27	ASN	11.1
1	A	62	VAL	10.6
1	A	177	VAL	10.0
1	A	122	VAL	9.6
1	A	132	TYR	9.2
1	A	180	GLN	8.0
1	A	145	ILE	8.0
1	A	8	ASN	7.9
1	A	76	PHE	7.8
1	A	148	PHE	7.8
1	A	9	PHE	7.6
1	A	47	MET	7.6
1	A	63	LYS	7.3
1	A	71	MET	7.0
1	A	1	MET	6.9
1	A	30	ASN	6.8
1	A	66	ASP	6.8

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Mol	Chain	Res	Type	RSRZ
2	B	734	ARG	6.8
1	A	173	THR	6.7
1	A	64	GLU	6.6
2	B	188	LYS	6.6
1	A	136	SER	6.5
1	A	54	ILE	6.3
3	C	349	LEU	6.3
1	A	48	TYR	6.2
1	A	184	THR	6.1
1	A	38	ILE	5.9
1	A	51	PHE	5.9
1	A	26	GLU	5.8
1	A	40	THR	5.8
1	A	21	MET	5.7
1	A	42	MET	5.6
1	A	75	ARG	5.6
1	A	126	LYS	5.5
1	A	120	ILE	5.5
1	A	4	PHE	5.5
1	A	36	ALA	5.4
1	A	178	LEU	5.4
1	A	124	ARG	5.4
1	A	24	TYR	5.4
1	A	70	ALA	5.4
1	A	157	THR	5.4
1	A	162	ILE	5.2
1	A	144	TYR	5.1
3	C	420	PHE	5.1
1	A	155	MET	5.1
1	A	138	LEU	5.1
1	A	147	ILE	5.0
1	A	151	ASP	5.0
1	A	67	ASP	4.9
1	A	123	THR	4.9
2	B	203	ARG	4.9
1	A	65	ASN	4.8
1	A	163	LEU	4.8
1	A	185	ALA	4.8
1	A	7	THR	4.8
1	A	139	LYS	4.7
1	A	125	ARG	4.7
2	B	199	MET	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	183	ALA	4.7
1	A	35	PHE	4.7
1	A	117	PHE	4.6
3	C	177	LEU	4.6
2	B	197	LYS	4.6
1	A	182	LEU	4.6
1	A	130	TYR	4.5
2	B	200	ILE	4.5
1	A	179	ARG	4.5
3	C	428	LEU	4.4
1	A	13	ILE	4.4
1	A	28	PRO	4.4
3	C	351	THR	4.3
1	A	11	PRO	4.3
1	A	34	LYS	4.3
3	C	354	MET	4.3
1	A	146	HIS	4.2
5	V	16	G	4.1
1	A	72	LEU	4.0
1	A	31	GLU	4.0
2	B	194	ASN	4.0
1	A	106	LEU	3.8
1	A	29	GLN	3.8
2	B	186	GLN	3.7
3	C	348	ASN	3.7
1	A	152	GLY	3.7
3	C	741	SER	3.7
1	A	134	LYS	3.7
1	A	15	GLU	3.6
3	C	418	LEU	3.6
1	A	128	GLU	3.6
1	A	158	ASP	3.6
1	A	718	GLY	3.6
1	A	129	ASP	3.6
3	C	345	LEU	3.6
1	A	377	GLU	3.6
1	A	58	GLY	3.5
3	C	417	ASP	3.5
3	C	419	ASN	3.5
1	A	73	LYS	3.5
1	A	181	GLU	3.5
1	A	39	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	5	VAL	3.4
1	A	140	GLY	3.4
2	B	198	LYS	3.4
3	C	494	ILE	3.4
3	C	421	VAL	3.4
1	A	719	GLU	3.4
3	C	742	SER	3.3
1	A	137	LYS	3.3
3	C	740	ASP	3.3
1	A	32	GLY	3.2
1	A	10	ASN	3.2
2	B	187	LYS	3.2
1	A	131	TYR	3.2
1	A	37	ALA	3.2
1	A	52	HIS	3.1
1	A	53	PHE	3.1
1	A	57	GLU	3.1
1	A	112	TYR	3.1
3	C	495	ARG	3.0
1	A	84	ARG	3.0
1	A	170	ARG	3.0
1	A	176	PHE	3.0
3	C	433	GLN	3.0
3	C	699	LYS	2.9
3	C	174	ALA	2.9
2	B	650	GLY	2.9
3	C	713	LEU	2.9
1	A	55	ASP	2.9
1	A	150	PHE	2.9
1	A	45	CYS	2.9
1	A	3	ASN	2.8
3	C	739	ARG	2.8
3	C	716	LEU	2.8
2	B	185	PHE	2.7
2	B	202	GLN	2.7
3	C	352	LEU	2.7
1	A	135	ALA	2.6
3	C	346	THR	2.6
2	B	189	LYS	2.6
3	C	426	GLN	2.6
1	A	12	MET	2.6
2	B	201	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	97	MET	2.5
1	A	153	GLU	2.5
3	C	321	ASN	2.5
3	C	607	GLU	2.5
1	A	171	ILE	2.5
3	C	427	ARG	2.5
3	C	508	LYS	2.5
3	C	150	GLY	2.5
1	A	175	LEU	2.5
2	B	646	MET	2.5
1	A	169	ALA	2.5
3	C	738	LYS	2.5
3	C	434	LEU	2.5
1	A	143	VAL	2.5
3	C	367	GLY	2.4
1	A	374	MET	2.4
1	A	43	GLU	2.4
1	A	56	LEU	2.4
3	C	12	LYS	2.4
2	B	633	HIS	2.3
1	A	68	ASP	2.3
1	A	6	ARG	2.3
3	C	431	MET	2.3
3	C	180	ASP	2.3
2	B	204	THR	2.3
1	A	715	SER	2.3
1	A	44	VAL	2.3
3	C	440	LYS	2.3
1	A	119	GLU	2.2
3	C	178	SER	2.2
3	C	694	PHE	2.2
1	A	109	LEU	2.2
1	A	41	HIS	2.2
2	B	730	LEU	2.2
1	A	22	LYS	2.2
2	B	731	GLU	2.2
1	A	724	GLN	2.1
3	C	425	ASN	2.1
1	A	79	ILE	2.1
1	A	69	ASN	2.1
2	B	193	ASP	2.1
1	A	33	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	149	SER	2.0
3	C	714	ASP	2.0
3	C	630	ARG	2.0
3	C	717	GLY	2.0
2	B	741	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SEP	X	5	10/11	0.94	0.12	71,76,85,85	0
6	SEP	X	16	10/11	0.98	0.17	55,55,57,57	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	PO4	B	804	5/5	0.69	0.32	109,112,115,120	0
8	PO4	C	901	5/5	0.79	0.24	120,120,123,124	0
8	PO4	A	803	5/5	0.83	0.29	123,123,125,127	0
8	PO4	C	903	5/5	0.84	0.18	96,97,101,101	0
8	PO4	A	802	5/5	0.85	0.34	110,110,113,118	0
8	PO4	B	801	5/5	0.88	0.19	99,101,103,104	0
8	PO4	C	904	5/5	0.88	0.24	92,95,97,97	0
8	PO4	C	905	5/5	0.89	0.15	104,104,106,108	0
8	PO4	B	805	5/5	0.89	0.27	93,96,97,98	0
8	PO4	B	803	5/5	0.91	0.14	93,95,97,99	0
8	PO4	B	802	5/5	0.93	0.15	88,90,90,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	PO4	C	902	5/5	0.94	0.18	116,116,117,118	0
8	PO4	B	806	5/5	0.95	0.15	75,75,77,78	0
7	ZN	A	801	1/1	0.97	0.18	72,72,72,72	0

6.5 Other polymers (i)

There are no such residues in this entry.