Full wwPDB X-ray Structure Validation Report (i)

Feb 26, 2024 – 06:16 pm GMT

PDB ID	:	5MSG
Title	:	Influenza B polymerase bound to vRNA promoter and capped RNA primer
Authors	:	Cusack, S.; Guilligay, D.
Deposited on	:	2017-01-04
Resolution	:	3.80 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 (i) 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 (i)) were used in the production of this report:

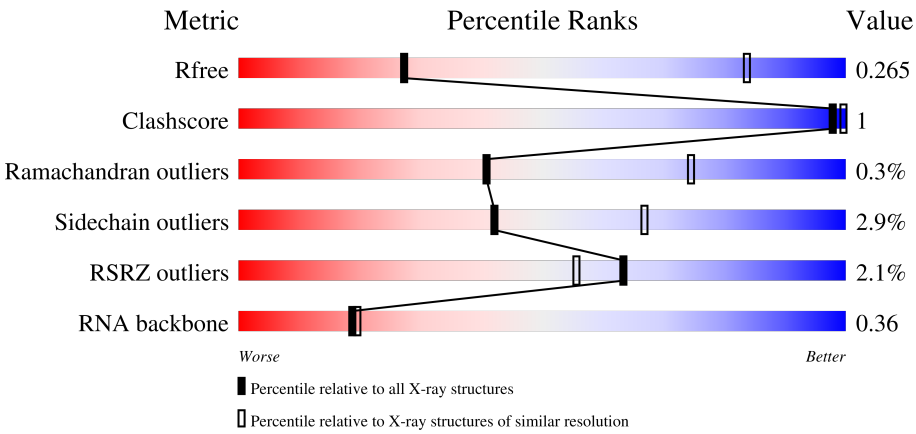
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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 <=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	751	3% 92% • 5%
2	B	772	% 92% • •
3	C	798	2% 86% 6% 8%
4	M	14	7% 14% 21% 64%

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Mol	Chain	Length	Quality of chain
5	R	18	17% 61% 39%
6	V	14	64% 36%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 18236 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
			Total	C	N	O	S			
1	A	717	5755	3657	963	1095	40	0	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	GLY	-	expression tag	UNP Q5V8Z9
A	-12	SER	-	expression tag	UNP Q5V8Z9
A	-11	HIS	-	expression tag	UNP Q5V8Z9
A	-10	HIS	-	expression tag	UNP Q5V8Z9
A	-9	HIS	-	expression tag	UNP Q5V8Z9
A	-8	HIS	-	expression tag	UNP Q5V8Z9
A	-7	HIS	-	expression tag	UNP Q5V8Z9
A	-6	HIS	-	expression tag	UNP Q5V8Z9
A	-5	HIS	-	expression tag	UNP Q5V8Z9
A	-4	HIS	-	expression tag	UNP Q5V8Z9
A	-3	GLY	-	expression tag	UNP Q5V8Z9
A	-2	SER	-	expression tag	UNP Q5V8Z9
A	-1	GLY	-	expression tag	UNP Q5V8Z9
A	0	SER	-	expression tag	UNP Q5V8Z9
A	727	GLY	-	expression tag	UNP Q5V8Z9
A	728	SER	-	expression tag	UNP Q5V8Z9
A	729	GLY	-	expression tag	UNP Q5V8Z9
A	730	SER	-	expression tag	UNP Q5V8Z9
A	731	GLY	-	expression tag	UNP Q5V8Z9
A	732	GLU	-	expression tag	UNP Q5V8Z9
A	733	ASN	-	expression tag	UNP Q5V8Z9
A	734	LEU	-	expression tag	UNP Q5V8Z9
A	735	TYR	-	expression tag	UNP Q5V8Z9
A	736	PHE	-	expression tag	UNP Q5V8Z9
A	737	GLN	-	expression tag	UNP Q5V8Z9

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	746	5855	3695	1014	1094	52	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP Q5V8Y6
B	-7	SER	-	expression tag	UNP Q5V8Y6
B	-6	GLY	-	expression tag	UNP Q5V8Y6
B	-5	SER	-	expression tag	UNP Q5V8Y6
B	-4	GLY	-	expression tag	UNP Q5V8Y6
B	-3	SER	-	expression tag	UNP Q5V8Y6
B	-2	GLY	-	expression tag	UNP Q5V8Y6
B	-1	SER	-	expression tag	UNP Q5V8Y6
B	0	GLY	-	expression tag	UNP Q5V8Y6
B	753	GLY	-	expression tag	UNP Q5V8Y6
B	754	SER	-	expression tag	UNP Q5V8Y6
B	755	GLY	-	expression tag	UNP Q5V8Y6
B	756	SER	-	expression tag	UNP Q5V8Y6
B	757	GLY	-	expression tag	UNP Q5V8Y6
B	758	GLU	-	expression tag	UNP Q5V8Y6
B	759	ASN	-	expression tag	UNP Q5V8Y6
B	760	LEU	-	expression tag	UNP Q5V8Y6
B	761	TYR	-	expression tag	UNP Q5V8Y6
B	762	PHE	-	expression tag	UNP Q5V8Y6
B	763	GLN	-	expression tag	UNP Q5V8Y6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	731	5847	3717	1024	1066	40	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	expression tag	UNP Q5V8X3
C	-7	SER	-	expression tag	UNP Q5V8X3
C	-6	GLY	-	expression tag	UNP Q5V8X3
C	-5	SER	-	expression tag	UNP Q5V8X3
C	-4	GLY	-	expression tag	UNP Q5V8X3
C	-3	SER	-	expression tag	UNP Q5V8X3
C	-2	GLY	-	expression tag	UNP Q5V8X3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP Q5V8X3
C	0	GLY	-	expression tag	UNP Q5V8X3
C	771	GLY	-	expression tag	UNP Q5V8X3
C	772	TRP	-	expression tag	UNP Q5V8X3
C	773	SER	-	expression tag	UNP Q5V8X3
C	774	HIS	-	expression tag	UNP Q5V8X3
C	775	PRO	-	expression tag	UNP Q5V8X3
C	776	GLN	-	expression tag	UNP Q5V8X3
C	777	PHE	-	expression tag	UNP Q5V8X3
C	778	GLU	-	expression tag	UNP Q5V8X3
C	779	LYS	-	expression tag	UNP Q5V8X3
C	780	GLY	-	expression tag	UNP Q5V8X3
C	781	SER	-	expression tag	UNP Q5V8X3
C	782	GLY	-	expression tag	UNP Q5V8X3
C	783	SER	-	expression tag	UNP Q5V8X3
C	784	GLU	-	expression tag	UNP Q5V8X3
C	785	ASN	-	expression tag	UNP Q5V8X3
C	786	LEU	-	expression tag	UNP Q5V8X3
C	787	TYR	-	expression tag	UNP Q5V8X3
C	788	PHE	-	expression tag	UNP Q5V8X3
C	789	GLN	-	expression tag	UNP Q5V8X3

- Molecule 4 is a RNA chain called RNA (5'-D(*(GDM))-R(P*AP*AP*UP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	M	5	113	49	20	38	6	0	0	0

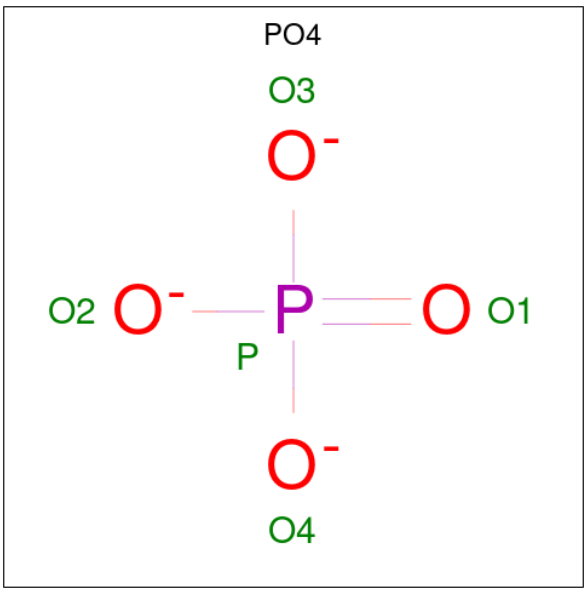
- Molecule 5 is a RNA chain called RNA (5'-R(*UP*AP*UP*AP*CP*CP*UP*CP*UP*GP*CP*UP*UP*CP*UP*GP*CP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	R	18	349	156	52	124	17	0	0	0

- Molecule 6 is a RNA chain called RNA (5'-R(P*AP*GP*UP*AP*GP*UP*AP*AP*CP*AP*AP*GP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	V	14	307	137	62	94	14	0	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



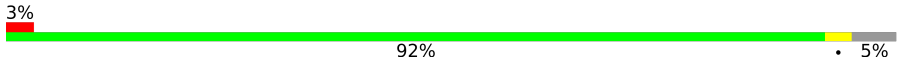
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O P 5 4 1	0	0
7	B	1	Total O P 5 4 1	0	0

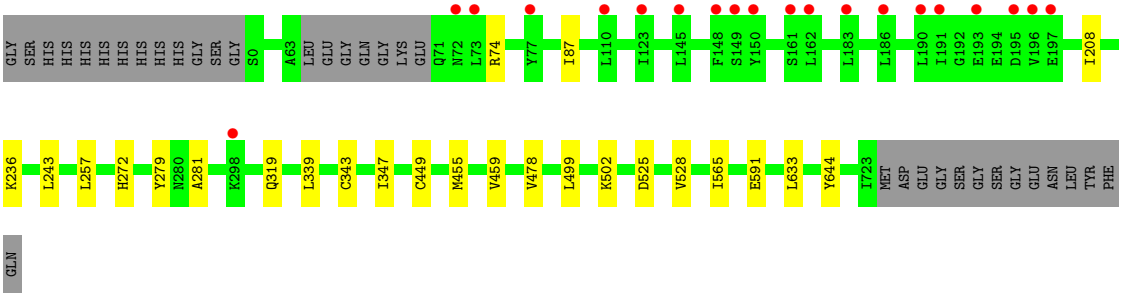
3 Residue-property plots (i)

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: Polymerase acidic protein

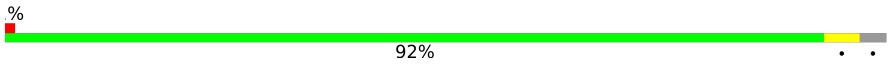
Chain A:

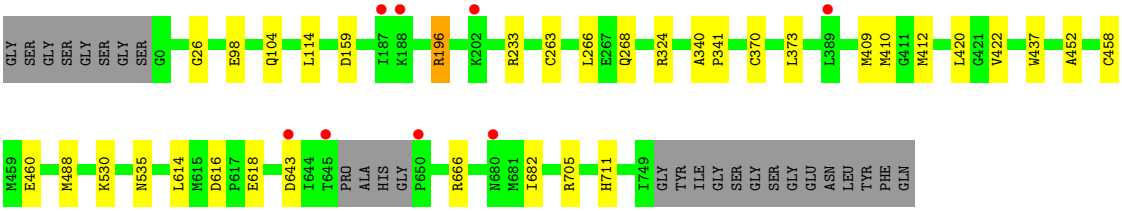




• Molecule 2: RNA-directed RNA polymerase catalytic subunit

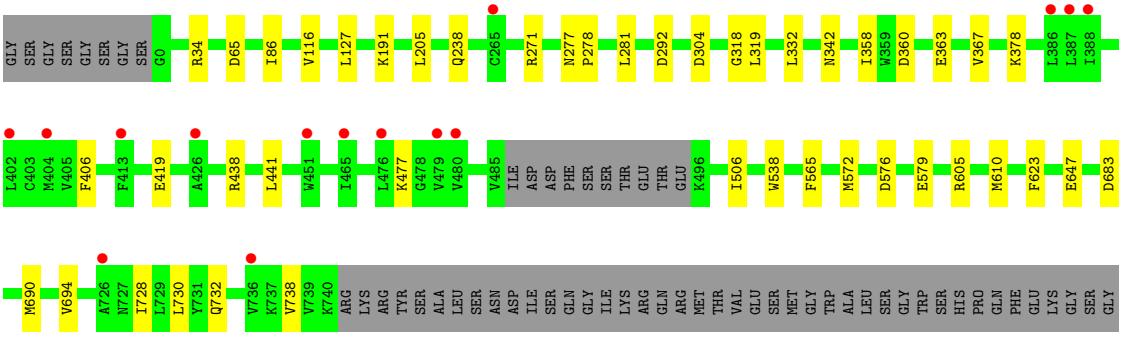
Chain B:





• Molecule 3: Polymerase basic protein 2

Chain C:

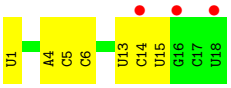


• Molecule 4: RNA (5'-D(*(GDM))-R(P*AP*AP*UP*C)-3')

Chain M:

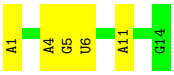
• Molecule 5: RNA (5'-R(*UP*AP*UP*AP*CP*CP*UP*CP*UP*GP*CP*UP*UP*CP*UP*GP*CP*U)-3')

Chain R:



• Molecule 6: RNA (5'-R(P*AP*GP*UP*AP*GP*UP*AP*AP*CP*AP*AP*GP*AP*G)-3')

Chain V:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	200.41Å 200.41Å 254.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	173.56 – 3.80 49.16 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (173.56-3.80) 100.0 (49.16-3.80)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.235 , 0.267 0.236 , 0.265	Depositor DCC
R_{free} test set	2785 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	139.8	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 120.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18236	wwPDB-VP
Average B, all atoms (Å^2)	176.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: M7G, PO4

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	0.37	0/5871	0.53	0/7918
2	B	0.37	0/5968	0.55	0/8042
3	C	0.37	0/5947	0.55	0/7992
4	M	0.21	0/93	0.66	0/142
5	R	0.25	0/386	0.71	0/598
6	V	0.58	1/345 (0.3%)	0.65	0/535
All	All	0.37	1/18610 (0.0%)	0.55	0/25227

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	1	A	OP3-P	-10.17	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 (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	5755	0	5730	8	0
2	B	5855	0	5882	8	0
3	C	5847	0	6018	11	0
4	M	113	0	60	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	349	0	177	0	0
6	V	307	0	153	0	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
All	All	18236	0	18020	24	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 (24) 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)
3:C:406:PHE:CE1	4:M:0:M7G:H82	2.38	0.58
3:C:728:ILE:HD13	3:C:738:VAL:HB	1.88	0.55
1:A:347:ILE:HD13	1:A:499:LEU:HD13	1.88	0.54
3:C:116:VAL:HG13	3:C:205:LEU:HD23	1.90	0.52
3:C:342:ASN:O	3:C:358:ILE:N	2.41	0.52
1:A:644:TYR:HA	2:B:26:GLY:HA2	1.91	0.52
2:B:370:CYS:HA	2:B:373:LEU:HD13	1.91	0.50
1:A:347:ILE:HD11	1:A:478:VAL:HG11	1.94	0.49
2:B:266:LEU:HD13	2:B:422:VAL:HG11	1.96	0.48
3:C:332:LEU:CD2	3:C:367:VAL:HG12	2.45	0.46
2:B:682:ILE:HG23	3:C:86:ILE:HG23	1.98	0.45
3:C:363:GLU:OE2	4:M:0:M7G:N2	2.49	0.45
1:A:455:MET:O	1:A:459:VAL:HG23	2.18	0.43
1:A:525:ASP:HB3	1:A:528:VAL:HG23	2.01	0.43
3:C:565:PHE:O	3:C:605:ARG:NH1	2.53	0.42
3:C:277:ASN:N	3:C:278:PRO:HD3	2.34	0.42
3:C:318:GLY:O	3:C:319:LEU:HB2	2.20	0.42
1:A:87:ILE:HD11	2:B:711:HIS:CD2	2.55	0.41
1:A:279:TYR:CE1	1:A:281:ALA:HB3	2.56	0.41
3:C:579:GLU:HG2	3:C:623:PHE:CZ	2.56	0.41
1:A:343:CYS:O	1:A:347:ILE:HD12	2.20	0.41
2:B:268:GLN:CG	2:B:422:VAL:HG13	2.51	0.41
2:B:340:ALA:HB3	2:B:341:PRO:HD3	2.03	0.41
2:B:452:ALA:HB3	2:B:458:CYS:SG	2.61	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	713/751 (95%)	673 (94%)	39 (6%)	1 (0%)	51	83
2	B	742/772 (96%)	699 (94%)	42 (6%)	1 (0%)	51	83
3	C	727/798 (91%)	670 (92%)	52 (7%)	5 (1%)	22	60
All	All	2182/2321 (94%)	2042 (94%)	133 (6%)	7 (0%)	41	74

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	292	ASP
3	C	477	LYS
2	B	196	ARG
3	C	419	GLU
3	C	730	LEU
3	C	538	TRP
1	A	236	LYS

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	638/664 (96%)	626 (98%)	12 (2%)	57	76
2	B	641/657 (98%)	618 (96%)	23 (4%)	35	63
3	C	638/694 (92%)	617 (97%)	21 (3%)	38	65
All	All	1917/2015 (95%)	1861 (97%)	56 (3%)	42	67

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ARG
1	A	208	ILE
1	A	243	LEU
1	A	257	LEU
1	A	272	HIS
1	A	319	GLN
1	A	339	LEU
1	A	449	CYS
1	A	502	LYS
1	A	565	ILE
1	A	591	GLU
1	A	633	LEU
2	B	98	GLU
2	B	104	GLN
2	B	114	LEU
2	B	159	ASP
2	B	196	ARG
2	B	233	ARG
2	B	263	CYS
2	B	324	ARG
2	B	409	MET
2	B	410	MET
2	B	412	MET
2	B	420	LEU
2	B	437	TRP
2	B	460	GLU
2	B	488	MET
2	B	530	LYS
2	B	535	ASN
2	B	614	LEU
2	B	616	ASP
2	B	618	GLU
2	B	643	ASP
2	B	666	ARG
2	B	705	ARG
3	C	34	ARG
3	C	65	ASP
3	C	127	LEU
3	C	191	LYS
3	C	238	GLN
3	C	271	ARG
3	C	281	LEU

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Mol	Chain	Res	Type
3	C	304	ASP
3	C	360	ASP
3	C	378	LYS
3	C	438	ARG
3	C	441	LEU
3	C	506	ILE
3	C	572	MET
3	C	576	ASP
3	C	610	MET
3	C	647	GLU
3	C	683	ASP
3	C	690	MET
3	C	694	VAL
3	C	732	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	265	ASN
2	B	346	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	M	3/14 (21%)	2 (66%)	0
5	R	16/18 (88%)	6 (37%)	3 (18%)
6	V	13/14 (92%)	4 (30%)	1 (7%)
All	All	32/46 (69%)	12 (37%)	4 (12%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	M	2	A
4	M	3	U
5	R	4	A
5	R	5	C
5	R	6	C
5	R	13	U
5	R	14	C
5	R	15	U

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Mol	Chain	Res	Type
6	V	4	A
6	V	5	G
6	V	6	U
6	V	11	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	R	1	U
5	R	4	A
5	R	5	C
6	V	5	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\| > 2$
7	PO4	A	801	-	4,4,4	0.91	0	6,6,6	0.48	0
7	PO4	B	801	-	4,4,4	0.92	0	6,6,6	0.40	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	717/751 (95%)	0.05	20 (2%)	53	43	109, 163, 264, 323	0
2	B	746/772 (96%)	0.01	8 (1%)	80	74	118, 164, 202, 239	0
3	C	731/798 (91%)	0.11	15 (2%)	63	55	124, 175, 251, 286	0
4	M	4/14 (28%)	0.86	1 (25%)	0	0	222, 224, 256, 273	0
5	R	18/18 (100%)	0.92	3 (16%)	1	2	135, 165, 254, 258	0
6	V	14/14 (100%)	-0.15	0	100	100	131, 142, 149, 157	0
All	All	2230/2367 (94%)	0.06	47 (2%)	63	55	109, 167, 254, 323	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	R	18	U	6.3
1	A	190	LEU	5.4
1	A	148	PHE	5.1
2	B	650	PRO	5.0
3	C	479	VAL	4.0
2	B	188	LYS	3.8
1	A	77	TYR	3.5
3	C	451	TRP	3.4
1	A	145	LEU	3.2
1	A	186	LEU	3.1
1	A	191	ILE	3.0
3	C	386	LEU	3.0
1	A	150	TYR	3.0
1	A	196	VAL	3.0
5	R	14	C	2.9
3	C	402	LEU	2.9
1	A	73	LEU	2.8
1	A	195	ASP	2.8
1	A	123	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	183	LEU	2.6
3	C	426	ALA	2.4
2	B	643	ASP	2.4
3	C	476	LEU	2.4
5	R	16	G	2.4
3	C	726	ALA	2.4
4	M	1	A	2.4
1	A	149	SER	2.3
3	C	388	ILE	2.3
3	C	387	LEU	2.3
3	C	480	VAL	2.2
1	A	197	GLU	2.2
1	A	110	LEU	2.2
1	A	161	SER	2.2
3	C	413	PHE	2.2
1	A	298	LYS	2.2
2	B	202	LYS	2.1
3	C	736	VAL	2.1
1	A	193	GLU	2.1
1	A	162	LEU	2.1
3	C	265	CYS	2.1
2	B	187	ILE	2.1
3	C	465	ILE	2.1
2	B	645	THR	2.1
2	B	389	LEU	2.1
1	A	72	ASN	2.1
2	B	680	ASN	2.0
3	C	404	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PO4	A	801	5/5	0.76	0.17	204,205,207,207	0
7	PO4	B	801	5/5	0.81	0.86	189,190,192,192	0

6.5 Other polymers (i)

There are no such residues in this entry.