



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:14 am BST

PDB ID : 5FMZ
Title : Crystal structure of Influenza B polymerase with bound 5' vRNA
Authors : Guilligay, D.; Cusack, S.
Deposited on : 2015-11-10
Resolution : 3.40 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
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

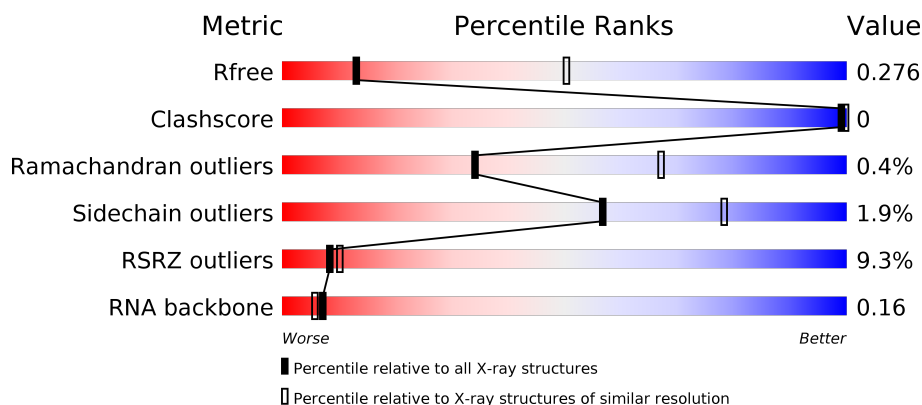
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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 $\leq 5\%$. 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	751	
1	D	751	
2	B	772	
2	E	772	

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Mol	Chain	Length	Quality of chain
3	C	798	<div><div></div><div>11%</div><div>87%</div><div></div><div>11%</div></div>
3	F	798	<div><div></div><div>14%</div><div>85%</div><div></div><div>12%</div></div>
4	H	12	<div><div></div><div>50%</div><div>50%</div><div></div></div>
4	V	12	<div><div></div><div>50%</div><div>50%</div><div></div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 34636 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	712	Total	C	N	O	S	0	0	0
			5717	3634	957	1086	40			
1	D	715	Total	C	N	O	S	0	0	0
			5737	3646	959	1092	40			

There are 50 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

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

- Molecule 2 is a protein called RNA-DIRECTED RNA POLYMERASE CATALYTIC SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	708	Total	C	N	O	S	0	0	0
			5547	3500	953	1042	52			
2	E	733	Total	C	N	O	S	0	0	0
			5755	3633	996	1074	52			

There are 40 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

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

- Molecule 3 is a protein called POLYMERASE BASIC PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	714	Total	C	N	O	S	0	0	0
			5719	3640	999	1040	40			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	703	Total	C	N	O	S	0	0	0
			5637	3591	982	1024	40			

There are 56 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
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
F	-8	GLY	-	expression tag	UNP Q5V8X3
F	-7	SER	-	expression tag	UNP Q5V8X3
F	-6	GLY	-	expression tag	UNP Q5V8X3
F	-5	SER	-	expression tag	UNP Q5V8X3
F	-4	GLY	-	expression tag	UNP Q5V8X3
F	-3	SER	-	expression tag	UNP Q5V8X3
F	-2	GLY	-	expression tag	UNP Q5V8X3
F	-1	SER	-	expression tag	UNP Q5V8X3

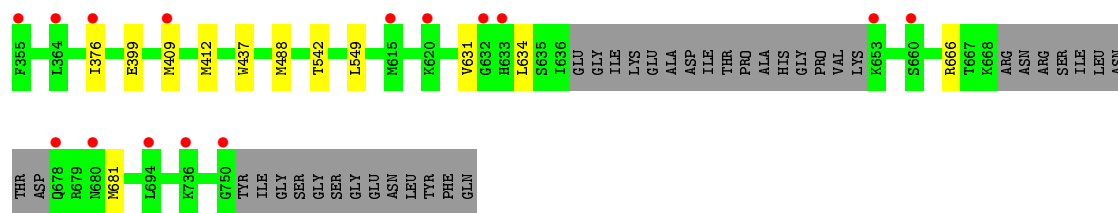
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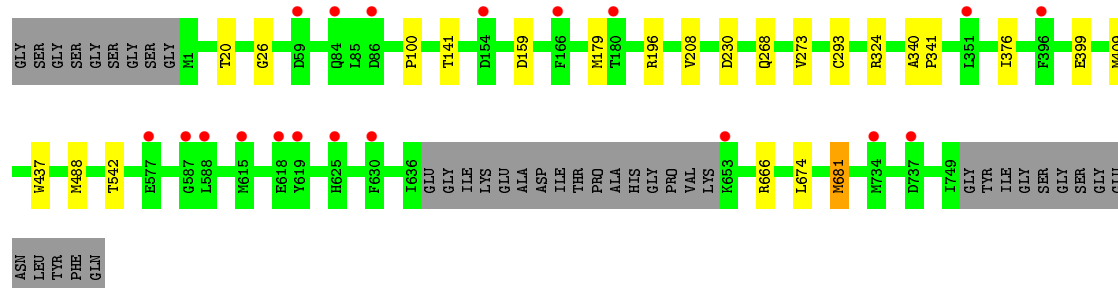
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	GLY	-	expression tag	UNP Q5V8X3
F	771	GLY	-	expression tag	UNP Q5V8X3
F	772	TRP	-	expression tag	UNP Q5V8X3
F	773	SER	-	expression tag	UNP Q5V8X3
F	774	HIS	-	expression tag	UNP Q5V8X3
F	775	PRO	-	expression tag	UNP Q5V8X3
F	776	GLN	-	expression tag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

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

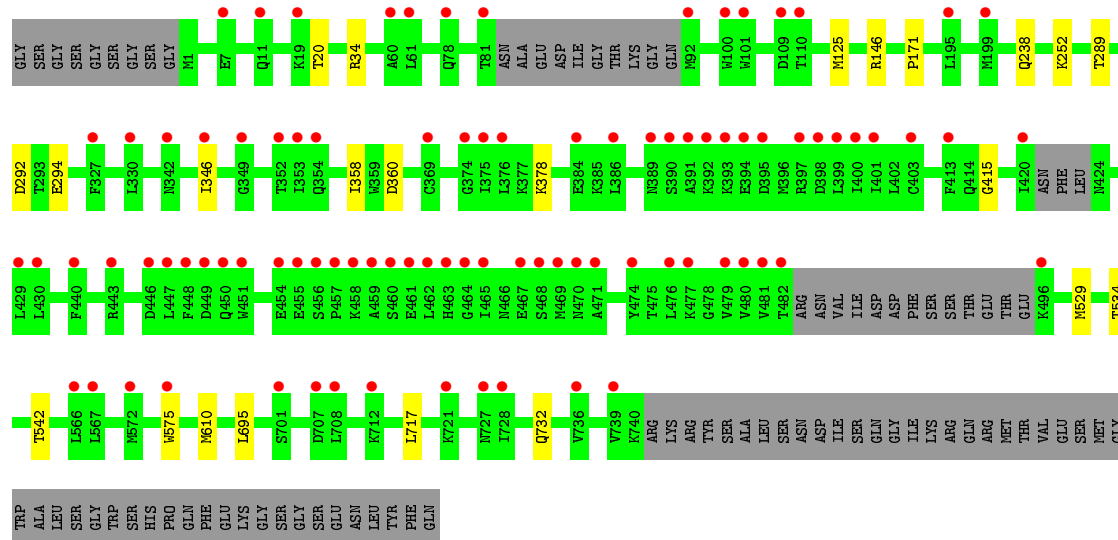
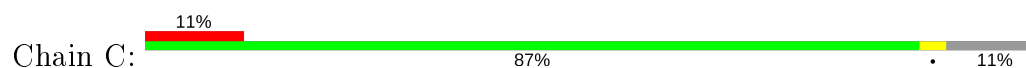
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	12	Total	C	N	O	P	0	0	0
			262	117	52	81	12			
4	V	12	Total	C	N	O	P	0	0	0
			262	117	52	81	12			



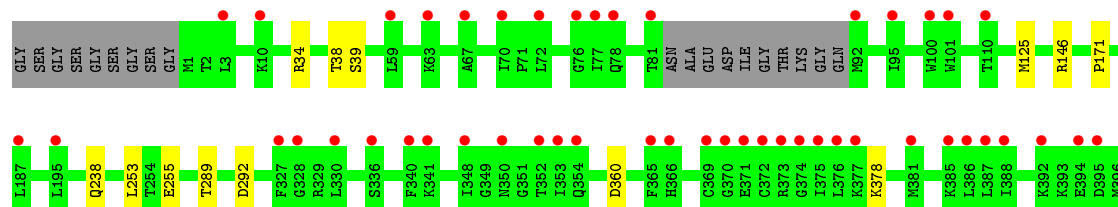
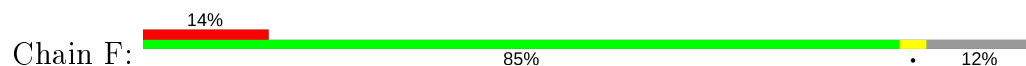
● Molecule 2: RNA-DIRECTED RNA POLYMERASE CATALYTIC SUBUNIT

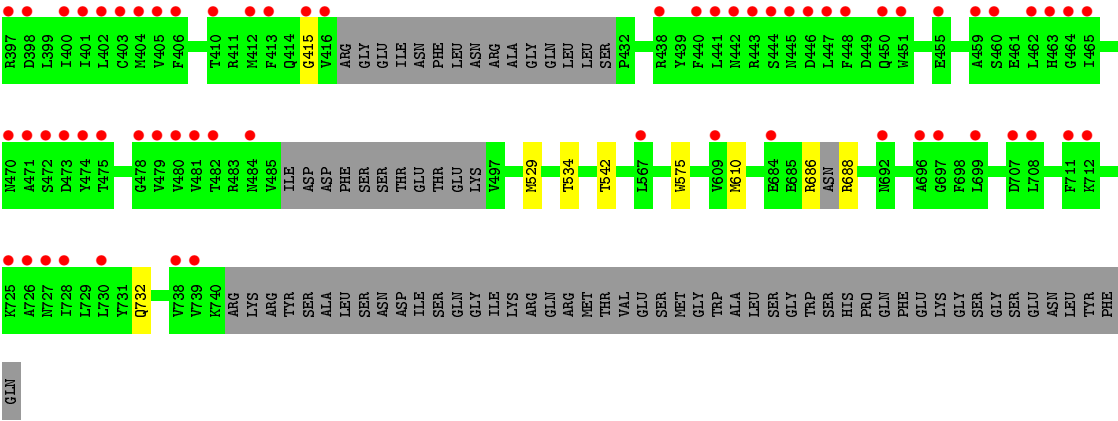


● Molecule 3: POLYMERASE BASIC PROTEIN 2

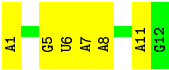


● Molecule 3: POLYMERASE BASIC PROTEIN 2

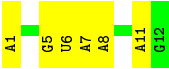




● Molecule 4: 5'-R(*AP*GP*UP*AP*GP*UP*AP*AP*CP*AP*AP*GP)-3'



● Molecule 4: 5'-R(*AP*GP*UP*AP*GP*UP*AP*AP*CP*AP*AP*GP)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	126.57Å 200.54Å 133.13Å 90.00° 107.70° 90.00°	Depositor
Resolution (Å)	126.83 – 3.40 48.98 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (126.83-3.40) 99.8 (48.98-3.40)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.255 , 0.277 0.254 , 0.276	Depositor DCC
R_{free} test set	2595 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	79.7	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	34636	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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](#)

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	0.35	0/5833	0.50	0/7866
1	D	0.35	0/5853	0.51	0/7893
2	B	0.36	0/5655	0.53	0/7623
2	E	0.36	0/5867	0.53	0/7908
3	C	0.36	0/5816	0.54	0/7813
3	F	0.36	0/5733	0.54	0/7701
4	H	0.62	1/294 (0.3%)	0.65	0/455
4	V	0.62	1/294 (0.3%)	0.66	0/455
All	All	0.36	2/35345 (0.0%)	0.53	0/47714

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	A	OP3-P	-10.15	1.49	1.61
4	V	1	A	OP3-P	-10.12	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	5717	0	5693	6	0
1	D	5737	0	5707	4	0
2	B	5547	0	5531	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	5755	0	5772	4	0
3	C	5719	0	5893	2	0
3	F	5637	0	5807	3	0
4	H	262	0	131	0	0
4	V	262	0	131	0	0
All	All	34636	0	34665	18	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 0.

All (18) 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)
2:B:631:VAL:HG12	2:B:634:LEU:HD11	1.82	0.60
1:A:644:TYR:HA	2:B:26:GLY:HA2	1.94	0.50
2:E:681:MET:HG3	3:F:38:THR:HG21	1.96	0.47
1:A:545:PHE:CD1	1:D:245:ARG:HB2	2.49	0.47
3:F:253:LEU:HD23	3:F:255:GLU:HB3	1.97	0.47
1:A:545:PHE:CE1	1:A:550:GLU:HG2	2.51	0.45
2:E:340:ALA:HB3	2:E:341:PRO:HD3	1.99	0.44
2:B:340:ALA:HB3	2:B:341:PRO:HD3	1.99	0.43
1:D:644:TYR:HA	2:E:26:GLY:HA2	2.01	0.42
1:D:582:GLN:HB2	2:E:542:THR:HG21	2.00	0.42
1:A:574:ARG:HB3	2:B:549:LEU:HD22	2.02	0.41
3:C:346:ILE:HD11	3:C:358:ILE:HD11	2.03	0.41
1:A:305:LEU:HD11	1:A:494:ASP:HB3	2.03	0.41
1:A:582:GLN:HB2	2:B:542:THR:HG21	2.02	0.41
3:C:695:LEU:HD11	3:C:717:LEU:HD13	2.03	0.40
3:F:686:ARG:O	3:F:688:ARG:N	2.53	0.40
2:B:244:ALA:HB3	2:B:412:MET:CE	2.52	0.40
1:D:163:ASP:OD2	1:D:165:GLU:HG2	2.21	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	708/751 (94%)	677 (96%)	30 (4%)	1 (0%)	51	82
1	D	711/751 (95%)	679 (96%)	31 (4%)	1 (0%)	51	82
2	B	700/772 (91%)	667 (95%)	30 (4%)	3 (0%)	34	67
2	E	729/772 (94%)	686 (94%)	37 (5%)	6 (1%)	19	51
3	C	706/798 (88%)	666 (94%)	37 (5%)	3 (0%)	34	67
3	F	693/798 (87%)	656 (95%)	33 (5%)	4 (1%)	25	57
All	All	4247/4642 (92%)	4031 (95%)	198 (5%)	18 (0%)	34	67

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	674	LEU
2	B	409	MET
3	C	732	GLN
2	E	409	MET
3	F	39	SER
3	F	732	GLN
3	C	292	ASP
2	E	100	PRO
3	F	292	ASP
1	A	58	GLY
1	D	58	GLY
2	E	196	ARG
3	C	415	GLY
3	F	415	GLY
2	B	208	VAL
2	E	208	VAL
2	B	376	ILE
2	E	376	ILE

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	634/664 (96%)	627 (99%)	7 (1%)	73	86
1	D	635/664 (96%)	629 (99%)	6 (1%)	78	90
2	B	607/657 (92%)	593 (98%)	14 (2%)	50	74
2	E	630/657 (96%)	616 (98%)	14 (2%)	52	75
3	C	625/694 (90%)	609 (97%)	16 (3%)	46	72
3	F	617/694 (89%)	604 (98%)	13 (2%)	53	76
All	All	3748/4030 (93%)	3678 (98%)	70 (2%)	57	78

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	GLU
1	A	198	LYS
1	A	300	LYS
1	A	317	ARG
1	A	320	THR
1	A	449	CYS
1	A	575	ARG
2	B	141	THR
2	B	159	ASP
2	B	179	MET
2	B	230	ASP
2	B	267	GLU
2	B	268	GLN
2	B	273	VAL
2	B	293	CYS
2	B	324	ARG
2	B	399	GLU
2	B	437	TRP
2	B	488	MET
2	B	666	ARG
2	B	681	MET
3	C	20	THR
3	C	34	ARG
3	C	125	MET
3	C	146	ARG
3	C	171	PRO
3	C	238	GLN
3	C	252	LYS
3	C	289	THR
3	C	294	GLU

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Mol	Chain	Res	Type
3	C	360	ASP
3	C	378	LYS
3	C	529	MET
3	C	534	THR
3	C	542	THR
3	C	575	TRP
3	C	610	MET
1	D	81	GLU
1	D	198	LYS
1	D	317	ARG
1	D	320	THR
1	D	449	CYS
1	D	575	ARG
2	E	20	THR
2	E	141	THR
2	E	159	ASP
2	E	179	MET
2	E	230	ASP
2	E	268	GLN
2	E	273	VAL
2	E	293	CYS
2	E	324	ARG
2	E	399	GLU
2	E	437	TRP
2	E	488	MET
2	E	666	ARG
2	E	681	MET
3	F	34	ARG
3	F	125	MET
3	F	146	ARG
3	F	171	PRO
3	F	238	GLN
3	F	289	THR
3	F	360	ASP
3	F	378	LYS
3	F	529	MET
3	F	534	THR
3	F	542	THR
3	F	575	TRP
3	F	610	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	H	11/12 (91%)	4 (36%)	1 (9%)
4	V	11/12 (91%)	4 (36%)	1 (9%)
All	All	22/24 (91%)	8 (36%)	2 (9%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	H	6	U
4	H	7	A
4	H	8	A
4	H	11	A
4	V	6	U
4	V	7	A
4	V	8	A
4	V	11	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	H	5	G
4	V	5	G

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	712/751 (94%)	0.42	45 (6%) 20 21	62, 93, 175, 202	0
1	D	715/751 (95%)	0.73	112 (15%) 2 2	57, 90, 218, 239	0
2	B	708/772 (91%)	0.29	22 (3%) 49 48	57, 99, 133, 155	0
2	E	733/772 (94%)	0.39	19 (2%) 56 54	61, 104, 153, 189	0
3	C	714/798 (89%)	0.67	91 (12%) 3 4	67, 113, 187, 223	0
3	F	703/798 (88%)	0.88	111 (15%) 2 2	70, 124, 197, 229	0
4	H	12/12 (100%)	-0.10	0 100 100	69, 72, 81, 87	0
4	V	12/12 (100%)	-0.10	0 100 100	70, 78, 92, 105	0
All	All	4309/4666 (92%)	0.56	400 (9%) 8 10	57, 102, 190, 239	0

All (400) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	404	MET	8.3
3	F	481	VAL	8.2
1	D	73	LEU	7.9
1	A	191	ILE	7.7
3	F	401	ILE	7.4
3	F	376	LEU	7.2
3	C	482	THR	7.1
1	D	36	PHE	7.0
1	D	187	TRP	7.0
3	F	370	GLY	6.7
3	F	374	GLY	6.5
1	D	183	LEU	6.1
3	C	462	LEU	5.8
1	D	190	LEU	5.8
3	C	395	ASP	5.8
1	D	186	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
3	C	457	PRO	5.6
1	D	125	LYS	5.6
1	D	62	THR	5.6
3	F	440	PHE	5.5
1	A	73	LEU	5.5
3	C	394	GLU	5.5
3	C	463	HIS	5.5
1	D	152	GLN	5.4
1	D	123	ILE	5.3
1	D	174	LEU	5.3
3	F	100	TRP	5.2
1	D	72	ASN	5.2
3	C	447	LEU	5.1
1	A	150	TYR	5.1
3	C	446	ASP	5.0
1	D	4	PHE	5.0
1	D	9	PHE	5.0
1	D	8	ASN	4.9
3	F	92	MET	4.9
1	D	161	SER	4.9
3	F	465	ILE	4.9
1	D	122	GLY	4.8
1	D	150	TYR	4.7
1	D	162	LEU	4.7
3	C	481	VAL	4.7
1	D	51	MET	4.7
3	F	480	VAL	4.7
1	A	7	ARG	4.7
1	D	189	VAL	4.6
1	D	191	ILE	4.6
3	F	354	GLN	4.6
1	D	99	HIS	4.5
1	D	63	ALA	4.4
1	D	196	VAL	4.4
2	B	653	LYS	4.4
3	F	403	CYS	4.4
1	D	32	PRO	4.4
1	D	170	VAL	4.4
3	F	70	ILE	4.4
3	F	395	ASP	4.4
1	D	37	ASN	4.3
3	F	394	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
3	C	392	LYS	4.3
3	C	461	GLU	4.2
3	F	442	ASN	4.2
1	D	7	ARG	4.2
3	F	373	ARG	4.2
3	F	447	LEU	4.2
3	C	460	SER	4.2
3	C	479	VAL	4.2
3	C	476	LEU	4.2
3	F	451	TRP	4.1
1	D	195	ASP	4.1
1	D	193	GLU	4.1
1	D	143	MET	4.1
1	A	186	LEU	4.1
1	A	195	ASP	4.0
1	D	58	GLY	4.0
3	F	725	LYS	4.0
1	D	77	TYR	4.0
3	F	443	ARG	4.0
3	F	328	GLY	4.0
3	F	707	ASP	3.9
3	F	482	THR	3.9
3	F	726	ALA	3.9
3	F	371	GLU	3.9
3	F	398	ASP	3.8
1	D	33	ALA	3.8
1	A	381	ILE	3.8
3	C	469	MET	3.8
1	D	61	TYR	3.8
2	E	180	THR	3.8
3	C	430	LEU	3.8
3	F	101	TRP	3.8
1	D	149	SER	3.8
1	D	138	LYS	3.8
3	C	440	PHE	3.8
3	F	415	GLY	3.8
1	D	160	SER	3.8
1	D	43	GLU	3.8
3	C	477	LYS	3.8
1	A	122	GLY	3.8
1	D	1	MET	3.7
3	F	63	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
3	F	72	LEU	3.7
3	C	450	GLN	3.7
1	D	13	ILE	3.6
1	A	192	GLY	3.6
1	D	11	THR	3.6
3	F	473	ASP	3.6
1	D	48	ILE	3.6
3	C	390	SER	3.6
3	F	327	PHE	3.6
3	F	479	VAL	3.5
3	C	567	LEU	3.5
3	F	478	GLY	3.5
3	C	78	GLN	3.5
1	A	193	GLU	3.5
3	F	67	ALA	3.5
1	D	5	ILE	3.5
1	D	177	LEU	3.5
1	A	164	GLU	3.5
1	D	156	LEU	3.4
3	F	81	THR	3.4
1	A	188	GLN	3.4
1	D	57	GLU	3.4
3	C	480	VAL	3.4
3	F	692	ASN	3.4
3	F	386	LEU	3.4
3	F	405	VAL	3.4
3	F	446	ASP	3.4
3	F	385	LYS	3.4
1	D	151	ASN	3.4
3	C	374	GLY	3.4
1	A	187	TRP	3.4
3	F	350	ASN	3.4
3	C	471	ALA	3.4
3	C	7	GLU	3.3
3	F	110	THR	3.3
3	F	463	HIS	3.3
3	C	376	LEU	3.3
3	C	386	LEU	3.3
3	C	398	ASP	3.3
3	C	449	ASP	3.3
3	C	459	ALA	3.3
3	F	739	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
3	F	475	THR	3.3
1	D	126	GLY	3.3
1	A	183	LEU	3.3
3	C	727	ASN	3.3
1	A	162	LEU	3.2
1	A	137	GLU	3.2
1	A	133	TRP	3.2
1	D	121	VAL	3.2
2	B	678	GLN	3.2
2	B	633	HIS	3.2
3	C	369	CYS	3.2
2	E	630	PHE	3.2
3	F	460	SER	3.2
1	D	146	MET	3.2
3	F	474	TYR	3.2
1	D	181	LEU	3.2
3	C	451	TRP	3.2
3	C	342	ASN	3.2
1	D	29	GLU	3.1
1	D	172	SER	3.1
1	D	182	SER	3.1
1	D	163	ASP	3.1
3	F	375	ILE	3.1
1	D	197	GLU	3.1
3	F	387	LEU	3.1
1	D	120	GLU	3.1
3	C	397	ARG	3.1
1	D	375	ILE	3.1
3	F	462	LEU	3.1
3	C	474	TYR	3.1
3	C	391	ALA	3.0
1	D	374	LYS	3.0
3	C	353	ILE	3.0
3	F	402	LEU	3.0
1	D	175	THR	3.0
1	A	138	LYS	3.0
3	F	59	LEU	3.0
1	D	28	PRO	3.0
2	E	734	MET	3.0
1	A	114	LYS	3.0
3	F	708	LEU	3.0
1	D	180	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	448	PHE	3.0
1	D	26	GLU	3.0
1	D	76	GLN	3.0
3	F	372	CYS	2.9
2	E	615	MET	2.9
3	C	375	ILE	2.9
1	A	61	TYR	2.9
3	C	458	LYS	2.9
1	D	0	SER	2.9
1	D	35	LEU	2.9
3	F	445	ASN	2.9
3	C	465	ILE	2.9
3	F	352	THR	2.9
2	E	625	HIS	2.9
3	F	381	MET	2.8
1	D	31	GLN	2.8
1	D	110	LEU	2.8
1	D	2	ASP	2.8
3	F	609	VAL	2.8
1	D	178	GLN	2.8
3	F	464	GLY	2.8
3	C	199	MET	2.8
3	F	388	ILE	2.8
3	F	438	ARG	2.8
2	B	187	ILE	2.8
3	C	464	GLY	2.8
1	D	147	ILE	2.8
3	F	400	ILE	2.8
3	F	336	SER	2.8
3	C	384	GLU	2.8
2	E	588	LEU	2.7
1	D	39	CYS	2.7
3	F	727	ASN	2.7
3	C	352	THR	2.7
1	D	145	LEU	2.7
1	A	118	PHE	2.7
1	D	30	LEU	2.7
3	F	406	PHE	2.7
3	F	471	ALA	2.7
1	A	148	PHE	2.7
3	F	412	MET	2.7
1	D	297	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
3	F	728	ILE	2.7
1	D	129	ASP	2.6
3	F	348	ILE	2.6
1	D	45	CYS	2.6
3	F	341	LYS	2.6
3	F	369	CYS	2.6
3	C	467	GLU	2.6
3	F	76	GLY	2.6
3	F	78	GLN	2.6
1	A	171	LEU	2.6
1	D	21	MET	2.6
3	F	696	ALA	2.6
3	C	468	SER	2.6
1	A	121	VAL	2.6
1	A	159	GLU	2.6
1	D	18	LYS	2.6
3	F	10	LYS	2.6
3	F	195	LEU	2.6
2	B	680	ASN	2.6
1	D	185	ASN	2.6
3	C	728	ILE	2.6
3	F	416	VAL	2.5
1	A	181	LEU	2.5
1	A	123	ILE	2.5
3	C	454	GLU	2.5
3	C	420	ILE	2.5
3	F	738	VAL	2.5
2	E	166	PHE	2.5
1	D	188	GLN	2.5
3	C	195	LEU	2.5
1	D	115	THR	2.5
3	C	413	PHE	2.5
1	A	386	MET	2.5
2	E	653	LYS	2.5
1	D	164	GLU	2.5
3	C	443	ARG	2.5
3	C	61	LEU	2.5
3	C	399	LEU	2.5
3	C	354	GLN	2.5
3	F	3	LEU	2.5
3	F	567	LEU	2.5
2	B	206	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	175	THR	2.5
3	F	410	THR	2.5
2	B	736	LYS	2.4
3	C	330	LEU	2.4
3	C	708	LEU	2.4
3	C	400	ILE	2.4
1	A	143	MET	2.4
1	A	167	LYS	2.4
3	F	377	LYS	2.4
3	F	450	GLN	2.4
3	F	697	GLY	2.4
1	D	46	TYR	2.4
1	D	118	PHE	2.4
3	F	470	ASN	2.4
2	E	577	GLU	2.4
2	E	396	PHE	2.4
3	C	393	LYS	2.4
3	C	721	LYS	2.4
1	A	160	SER	2.4
3	F	340	PHE	2.4
3	C	455	GLU	2.4
3	C	401	ILE	2.4
2	B	185	LYS	2.4
1	D	84	PRO	2.4
2	E	619	TYR	2.4
3	F	397	ARG	2.4
1	D	44	VAL	2.4
1	D	106	TYR	2.4
3	F	699	LEU	2.4
2	B	208	VAL	2.4
2	E	84	GLN	2.4
3	F	95	ILE	2.4
1	D	59	LYS	2.3
1	D	119	ILE	2.3
1	D	15	GLN	2.3
3	C	701	SER	2.3
3	F	711	PHE	2.3
1	D	116	LYS	2.3
1	D	3	THR	2.3
1	D	12	THR	2.3
1	D	54	LEU	2.3
3	F	441	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	739	VAL	2.3
1	D	159	GLU	2.3
1	D	154	TYR	2.3
2	E	618	GLU	2.3
3	C	101	TRP	2.3
3	F	484	ASN	2.3
2	E	154	ASP	2.3
2	B	620	LYS	2.3
3	C	403	CYS	2.3
1	D	127	LEU	2.3
3	C	566	LEU	2.3
3	C	456	SER	2.3
3	F	353	ILE	2.3
3	C	100	TRP	2.3
1	A	190	LEU	2.3
3	C	92	MET	2.3
1	A	57	GLU	2.2
2	B	750	GLY	2.2
2	E	737	ASP	2.2
1	D	114	LYS	2.2
1	A	385	THR	2.2
1	D	130	ASP	2.2
2	B	409	MET	2.2
3	C	575	TRP	2.2
3	F	366	HIS	2.2
2	B	364	LEU	2.2
1	A	8	ASN	2.2
1	D	616	SER	2.2
2	B	694	LEU	2.2
1	A	147	ILE	2.2
2	B	376	ILE	2.2
1	A	377	LYS	2.2
1	A	149	SER	2.2
2	B	207	LYS	2.2
2	B	186	ASN	2.2
1	D	179	ALA	2.2
3	F	459	ALA	2.2
2	B	355	PHE	2.2
3	F	77	ILE	2.2
3	F	455	GLU	2.2
1	D	192	GLY	2.2
3	C	349	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	201	ASP	2.2
1	A	14	ILE	2.2
3	C	11	GLN	2.2
3	C	109	ASP	2.2
1	A	1	MET	2.2
2	B	632	GLY	2.2
3	C	470	ASN	2.1
1	D	184	LYS	2.1
1	D	381	ILE	2.1
3	C	712	LYS	2.1
3	F	330	LEU	2.1
3	F	365	PHE	2.1
3	C	429	LEU	2.1
3	F	730	LEU	2.1
3	C	81	THR	2.1
3	F	413	PHE	2.1
2	E	587	GLY	2.1
3	C	572	MET	2.1
3	C	707	ASP	2.1
3	F	448	PHE	2.1
3	C	736	VAL	2.1
3	F	187	LEU	2.1
1	A	151	ASN	2.1
1	D	24	PHE	2.1
2	E	59	ASP	2.1
3	C	110	THR	2.1
1	D	148	PHE	2.1
3	F	444	SER	2.1
3	F	472	SER	2.1
3	F	684	GLU	2.1
3	C	496	LYS	2.1
3	F	392	LYS	2.1
3	F	712	LYS	2.1
3	C	346	ILE	2.1
1	A	504	GLN	2.1
2	B	615	MET	2.1
3	C	327	PHE	2.1
1	D	171	LEU	2.1
2	E	86	ASP	2.1
3	C	60	ALA	2.0
3	C	389	ASN	2.0
2	B	205	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	95	LEU	2.0
2	E	351	LEU	2.0
3	C	19	LYS	2.0
1	D	117	ARG	2.0
2	B	660	SER	2.0
1	A	373	GLN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.