



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:52 AM UTC

PDB ID : 4A8O / pdb_00004a8o
Title : Non-Catalytic Ions Direct the RNA-Dependent RNA Polymerase of Bacterial dsRNA virus phi6 from De Novo Initiation to Elongation
Authors : Wright, S.; Poranen, M.M.; Bamford, D.H.; Stuart, D.I.; Grimes, J.M.
Deposited on : 2011-11-21
Resolution : 2.67 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

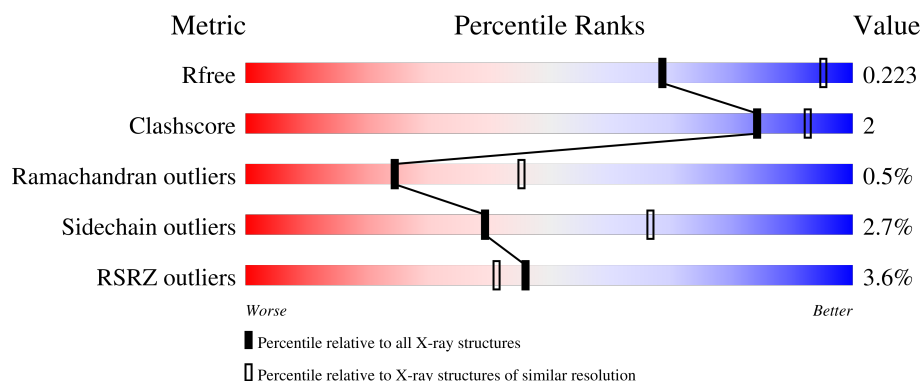
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	665	2% 89% 10%
1	B	665	4% 90% 9%
1	C	665	5% 91% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15798 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 RNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	0	0
			5265	3342	915	976	32			
1	B	664	Total	C	N	O	S	0	0	0
			5265	3342	915	976	32			
1	C	664	Total	C	N	O	S	0	0	0
			5265	3342	915	976	32			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	MET	ILE	conflict	UNP P11124
A	634	GLN	GLU	conflict	UNP P11124
B	456	MET	ILE	conflict	UNP P11124
B	634	GLN	GLU	conflict	UNP P11124
C	456	MET	ILE	conflict	UNP P11124
C	634	GLN	GLU	conflict	UNP P11124

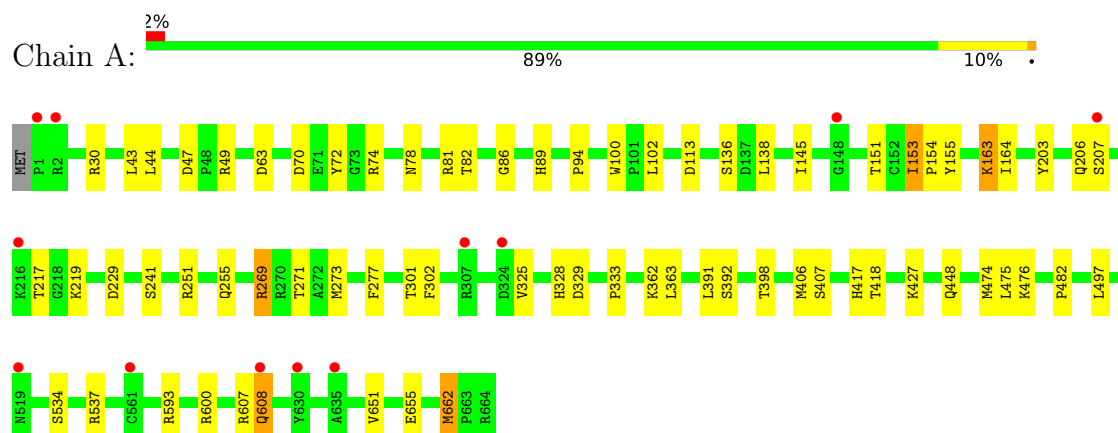
- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

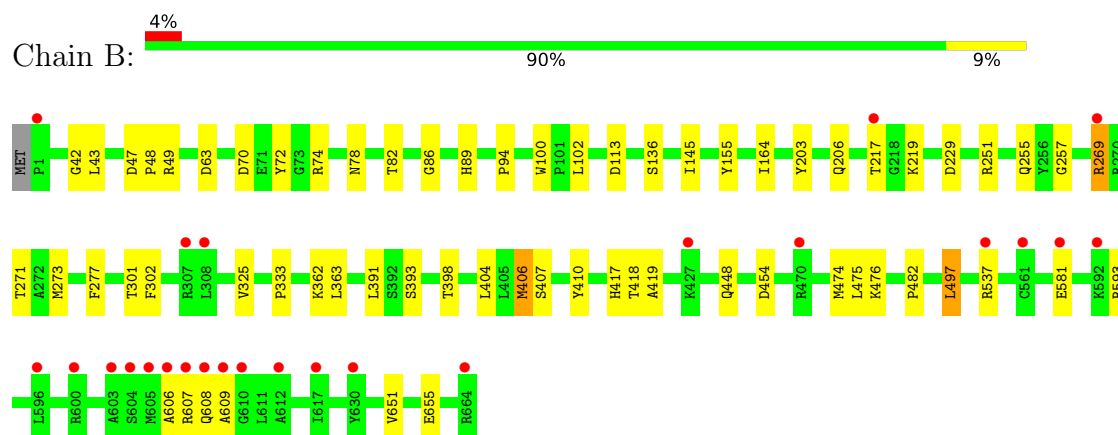
3 Residue-property plots [i](#)

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.

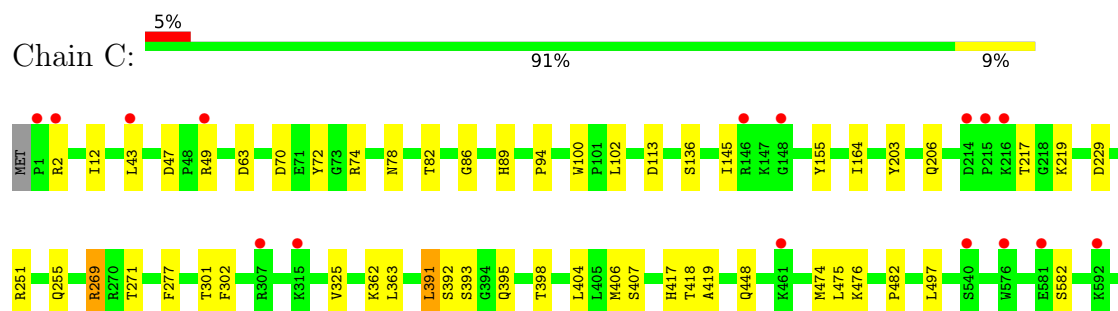
• Molecule 1: RNA-DIRECTED RNA POLYMERASE

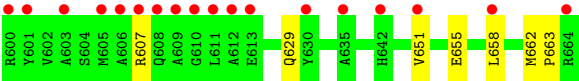


• Molecule 1: RNA-DIRECTED RNA POLYMERASE



• Molecule 1: RNA-DIRECTED RNA POLYMERASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.19Å 92.45Å 141.04Å 90.00° 101.47° 90.00°	Depositor
Resolution (Å)	39.09 – 2.67 39.09 – 2.67	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.09-2.67) 97.4 (39.09-2.67)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.215 , 0.225 0.215 , 0.223	Depositor DCC
R_{free} test set	3738 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.871	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.7	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	0.94	EDS
Total number of atoms	15798	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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

5.1 Standard geometry

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

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	0.69	1/5396 (0.0%)	1.20	11/7297 (0.2%)
1	B	0.69	0/5396	1.25	12/7297 (0.2%)
1	C	0.68	0/5396	1.26	13/7297 (0.2%)
All	All	0.69	1/16188 (0.0%)	1.24	36/21891 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	MET	SD-CE	-5.48	1.65	1.79

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	PHE	N-CA-C	6.64	122.05	113.88
1	A	302	PHE	N-CA-C	6.60	122.00	113.88
1	C	302	PHE	N-CA-C	6.55	121.94	113.88
1	C	663	PRO	CA-C-N	6.24	132.93	121.70
1	C	663	PRO	C-N-CA	6.24	132.93	121.70
1	A	100	TRP	N-CA-C	-6.14	102.04	109.72
1	B	100	TRP	N-CA-C	-6.14	102.05	109.72
1	C	363	LEU	N-CA-C	6.04	117.31	109.64
1	B	229	ASP	CA-CB-CG	6.02	118.62	112.60
1	B	277	PHE	N-CA-C	5.99	118.57	111.33
1	C	277	PHE	N-CA-C	5.98	118.56	111.33
1	A	229	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	277	PHE	N-CA-C	5.86	118.42	111.33
1	C	100	TRP	N-CA-C	-5.79	102.48	109.72
1	B	155	TYR	N-CA-C	5.74	119.46	112.23
1	C	406	MET	N-CA-C	5.71	117.31	111.14
1	A	363	LEU	N-CA-C	5.66	116.83	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	PRO	N-CA-C	5.64	119.74	110.55
1	A	333	PRO	N-CA-C	5.60	119.68	110.55
1	C	155	TYR	N-CA-C	5.57	119.25	112.23
1	B	363	LEU	N-CA-C	5.45	116.56	109.64
1	A	206	GLN	N-CA-C	-5.30	96.70	107.41
1	C	229	ASP	CA-CB-CG	5.23	117.83	112.60
1	B	454	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	241	SER	N-CA-C	5.22	117.74	109.50
1	C	419	ALA	N-CA-C	5.22	118.14	109.79
1	A	153	ILE	N-CA-C	5.18	114.61	108.96
1	A	155	TYR	N-CA-C	5.14	118.70	112.23
1	A	207	SER	N-CA-C	5.11	117.59	111.71
1	B	419	ALA	N-CA-C	5.11	117.97	109.79
1	B	206	GLN	CA-C-N	5.07	127.79	120.38
1	B	206	GLN	C-N-CA	5.07	127.79	120.38
1	B	406	MET	N-CA-C	5.07	116.49	111.07
1	C	206	GLN	N-CA-C	-5.02	97.83	107.57
1	C	206	GLN	CA-C-N	5.00	127.69	120.38
1	C	206	GLN	C-N-CA	5.00	127.69	120.38

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	5265	0	5167	33	0
1	B	5265	0	5167	29	0
1	C	5265	0	5167	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
All	All	15798	0	15501	72	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 2.

All (72) 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:251:ARG:HH11	1:A:255:GLN:HE22	1.41	0.69
1:B:251:ARG:HH11	1:B:255:GLN:HE22	1.40	0.67
1:C:251:ARG:HH11	1:C:255:GLN:HE22	1.42	0.67
1:B:606:ALA:HB3	1:B:609:ALA:HB2	1.80	0.63
1:A:608:GLN:HE22	1:B:593:ARG:CZ	2.12	0.63
1:A:600:ARG:HH12	1:B:581:GLU:HG3	1.66	0.61
1:A:600:ARG:NH1	1:B:581:GLU:HG3	2.15	0.60
1:A:593:ARG:HG2	1:B:42:GLY:HA2	1.83	0.60
1:C:391:LEU:HD22	1:C:398:THR:HG22	1.86	0.58
1:A:392:SER:O	1:A:398:THR:HG21	2.05	0.57
1:A:151:THR:HG22	1:A:163:LYS:HG3	1.89	0.53
1:C:651:VAL:O	1:C:655:GLU:HB2	2.10	0.52
1:A:651:VAL:O	1:A:655:GLU:HB2	2.10	0.52
1:A:203:TYR:HE1	1:A:271:THR:HG22	1.75	0.51
1:B:537:ARG:HG3	1:B:537:ARG:HH11	1.75	0.51
1:C:203:TYR:HE1	1:C:271:THR:HG22	1.75	0.51
1:B:203:TYR:HE1	1:B:271:THR:HG22	1.76	0.50
1:A:392:SER:O	1:A:398:THR:CG2	2.60	0.50
1:B:145:ILE:HD12	1:B:164:ILE:HD13	1.94	0.50
1:A:407:SER:HA	1:A:448:GLN:HE22	1.77	0.50
1:B:407:SER:HA	1:B:448:GLN:HE22	1.77	0.50
1:B:651:VAL:O	1:B:655:GLU:HB2	2.11	0.50
1:A:47:ASP:OD1	1:A:49:ARG:HD3	2.12	0.49
1:B:325:VAL:HG21	1:B:406:MET:HE2	1.94	0.49
1:A:534:SER:O	1:B:48:PRO:HG2	2.13	0.49
1:A:94:PRO:HB3	1:A:269:ARG:HG3	1.95	0.48
1:C:407:SER:HA	1:C:448:GLN:HE22	1.77	0.48
1:A:145:ILE:HD12	1:A:164:ILE:HD13	1.95	0.48
1:A:203:TYR:CE1	1:A:271:THR:HG22	2.48	0.48
1:A:70:ASP:OD2	1:A:74:ARG:HD2	2.13	0.48
1:C:70:ASP:OD2	1:C:74:ARG:HD2	2.14	0.48
1:B:70:ASP:OD2	1:B:74:ARG:HD2	2.14	0.47
1:C:203:TYR:CE1	1:C:271:THR:HG22	2.48	0.47
1:B:301:THR:HG23	1:B:448:GLN:HG3	1.96	0.47
1:B:391:LEU:HD22	1:B:398:THR:HG22	1.96	0.47
1:A:72:TYR:CE2	1:A:476:LYS:HD3	2.50	0.47
1:A:537:ARG:HD2	1:B:49:ARG:HG3	1.95	0.47
1:C:145:ILE:HD12	1:C:164:ILE:HD13	1.95	0.47
1:B:203:TYR:CE1	1:B:271:THR:HG22	2.49	0.47
1:B:417:HIS:CE1	1:B:474:MET:HE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:THR:HG23	1:C:448:GLN:HG3	1.96	0.47
1:C:86:GLY:O	1:C:89:HIS:HD2	1.98	0.47
1:C:94:PRO:HB3	1:C:269:ARG:HG3	1.97	0.46
1:A:325:VAL:HG21	1:A:406:MET:HE2	1.96	0.46
1:A:417:HIS:CE1	1:A:474:MET:HE1	2.51	0.46
1:B:47:ASP:OD1	1:B:49:ARG:HD3	2.15	0.46
1:B:86:GLY:O	1:B:89:HIS:HD2	1.99	0.46
1:A:301:THR:HG23	1:A:448:GLN:HG3	1.98	0.45
1:A:86:GLY:O	1:A:89:HIS:HD2	1.99	0.45
1:A:44:LEU:HD21	1:B:257:GLY:HA3	1.98	0.45
1:B:72:TYR:CE2	1:B:476:LYS:HD3	2.52	0.45
1:A:217:THR:HG23	1:A:219:LYS:H	1.81	0.45
1:B:94:PRO:HB3	1:B:269:ARG:HG3	1.99	0.45
1:C:47:ASP:OD1	1:C:49:ARG:HD3	2.18	0.44
1:A:427:LYS:HE3	1:C:12:ILE:HG21	2.00	0.44
1:C:417:HIS:CE1	1:C:474:MET:HE1	2.53	0.44
1:C:72:TYR:CE2	1:C:476:LYS:HD3	2.51	0.44
1:A:328:HIS:HD2	1:A:329:ASP:OD1	2.00	0.44
1:A:163:LYS:HE3	1:A:163:LYS:HB2	1.68	0.43
1:A:608:GLN:NE2	1:B:593:ARG:CZ	2.80	0.43
1:B:217:THR:HG23	1:B:219:LYS:H	1.84	0.43
1:C:217:THR:HG23	1:C:219:LYS:H	1.83	0.43
1:A:153:ILE:HA	1:A:154:PRO:HA	1.87	0.43
1:B:406:MET:HB3	1:B:410:TYR:CE2	2.54	0.43
1:C:658:LEU:HG	1:C:662:MET:HG3	2.01	0.42
1:B:475:LEU:HD21	1:B:482:PRO:HG3	1.99	0.42
1:A:138:LEU:HB2	1:A:662:MET:HE1	2.01	0.42
1:A:94:PRO:CB	1:A:269:ARG:HG3	2.50	0.41
1:A:475:LEU:HD21	1:A:482:PRO:HG3	2.02	0.41
1:C:395:GLN:HB3	1:C:398:THR:HG23	2.03	0.41
1:B:497:LEU:HD12	1:B:497:LEU:HA	1.99	0.40
1:C:475:LEU:HD21	1:C:482:PRO:HG3	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	662/665 (100%)	641 (97%)	19 (3%)	2 (0%)	36	57
1	B	662/665 (100%)	640 (97%)	19 (3%)	3 (0%)	24	45
1	C	662/665 (100%)	640 (97%)	18 (3%)	4 (1%)	21	41
All	All	1986/1995 (100%)	1921 (97%)	56 (3%)	9 (0%)	24	45

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	607	ARG
1	B	607	ARG
1	C	393	SER
1	A	136	SER
1	B	136	SER
1	B	393	SER
1	C	136	SER
1	C	607	ARG
1	C	2	ARG

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	557/558 (100%)	541 (97%)	16 (3%)	37	64
1	B	557/558 (100%)	544 (98%)	13 (2%)	44	71
1	C	557/558 (100%)	541 (97%)	16 (3%)	37	64
All	All	1671/1674 (100%)	1626 (97%)	45 (3%)	39	67

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	43	LEU
1	A	63	ASP
1	A	78	ASN
1	A	81	ARG
1	A	82	THR
1	A	102	LEU
1	A	113	ASP
1	A	163	LYS
1	A	269	ARG
1	A	362	LYS
1	A	391	LEU
1	A	418	THR
1	A	497	LEU
1	A	608	GLN
1	A	662	MET
1	B	43	LEU
1	B	63	ASP
1	B	78	ASN
1	B	82	THR
1	B	102	LEU
1	B	113	ASP
1	B	269	ARG
1	B	273	MET
1	B	362	LYS
1	B	404	LEU
1	B	418	THR
1	B	497	LEU
1	B	608	GLN
1	C	43	LEU
1	C	63	ASP
1	C	78	ASN
1	C	82	THR
1	C	102	LEU
1	C	113	ASP
1	C	269	ARG
1	C	325	VAL
1	C	362	LYS
1	C	391	LEU
1	C	392	SER
1	C	404	LEU
1	C	418	THR
1	C	497	LEU

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Mol	Chain	Res	Type
1	C	582	SER
1	C	629	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	78	ASN
1	A	89	HIS
1	A	91	ASN
1	A	255	GLN
1	A	309	ASN
1	A	328	HIS
1	A	448	GLN
1	A	492	HIS
1	A	519	ASN
1	A	525	GLN
1	A	608	GLN
1	A	626	ASN
1	A	634	GLN
1	B	25	GLN
1	B	26	GLN
1	B	78	ASN
1	B	89	HIS
1	B	91	ASN
1	B	191	GLN
1	B	255	GLN
1	B	309	ASN
1	B	328	HIS
1	B	448	GLN
1	B	492	HIS
1	B	519	ASN
1	B	525	GLN
1	B	626	ASN
1	C	26	GLN
1	C	78	ASN
1	C	89	HIS
1	C	91	ASN
1	C	255	GLN
1	C	309	ASN
1	C	328	HIS
1	C	448	GLN

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Mol	Chain	Res	Type
1	C	492	HIS
1	C	519	ASN
1	C	525	GLN
1	C	626	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	664/665 (99%)	0.19	12 (1%) 67 65	42, 55, 80, 108	0
1	B	664/665 (99%)	0.26	25 (3%) 44 39	43, 58, 85, 136	0
1	C	664/665 (99%)	0.31	34 (5%) 33 29	38, 59, 89, 157	0
All	All	1992/1995 (99%)	0.26	71 (3%) 46 41	38, 57, 84, 157	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	606	ALA	6.9
1	C	609	ALA	5.1
1	B	1	PRO	5.0
1	C	576	TRP	4.9
1	B	607	ARG	4.8
1	B	606	ALA	4.6
1	C	612	ALA	4.4
1	A	148	GLY	4.2
1	A	1	PRO	4.1
1	C	608	GLN	3.8
1	B	610	GLY	3.6
1	A	561	CYS	3.6
1	B	307	ARG	3.5
1	B	608	GLN	3.5
1	B	537	ARG	3.5
1	C	651	VAL	3.4
1	C	307	ARG	3.3
1	C	603	ALA	3.3
1	B	609	ALA	3.2
1	B	596	LEU	3.2
1	C	605	MET	3.1
1	B	581	GLU	3.1
1	C	610	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	630	TYR	3.1
1	B	470	ARG	3.1
1	B	612	ALA	3.0
1	B	600	ARG	3.0
1	B	604	SER	2.9
1	A	307	ARG	2.9
1	C	607	ARG	2.9
1	A	635	ALA	2.8
1	B	308	LEU	2.8
1	B	217	THR	2.8
1	C	1	PRO	2.8
1	B	427	LYS	2.7
1	A	608	GLN	2.6
1	C	461	LYS	2.6
1	C	215	PRO	2.6
1	C	611	LEU	2.5
1	C	642	HIS	2.5
1	C	216	LYS	2.4
1	C	315	LYS	2.4
1	B	664	ARG	2.4
1	C	613	GLU	2.4
1	C	214	ASP	2.4
1	C	2	ARG	2.4
1	A	216	LYS	2.3
1	A	2	ARG	2.3
1	C	664	ARG	2.3
1	B	561	CYS	2.3
1	B	269	ARG	2.3
1	C	635	ALA	2.3
1	C	148	GLY	2.3
1	C	601	TYR	2.2
1	B	630	TYR	2.2
1	C	49	ARG	2.2
1	A	324	ASP	2.2
1	B	603	ALA	2.1
1	A	519	ASN	2.1
1	C	630	TYR	2.1
1	C	581	GLU	2.1
1	C	600	ARG	2.1
1	C	658	LEU	2.1
1	B	605	MET	2.1
1	A	207	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	540	SER	2.1
1	C	592	LYS	2.0
1	B	592	LYS	2.0
1	C	43	LEU	2.0
1	B	617	ILE	2.0
1	C	146	ARG	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 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
2	MN	A	1665	1/1	0.61	0.31	191,191,191,191	0
2	MN	C	1665	1/1	0.65	0.22	165,165,165,165	0
2	MN	B	1665	1/1	0.91	0.12	114,114,114,114	0

6.5 Other polymers [i](#)

There are no such residues in this entry.