



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:28 PM EDT

PDB ID : 4B02 / pdb_00004b02
Title : The C-terminal Priming Domain is Strongly Associated with the Main Body of Bacteriophage phi6 RNA-Dependent RNA Polymerase
Authors : Sarin, L.P.; Wright, S.; Chen, Q.; Degerth, L.H.; Stuart, D.I.; Grimes, J.M.; Bamford, D.H.; Poranen, M.M.
Deposited on : 2012-06-27
Resolution : 3.30 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

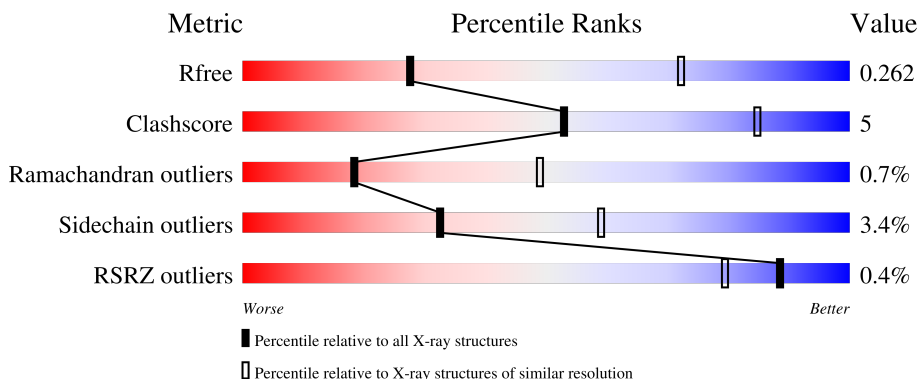
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	664	 88% 11% .
1	B	664	 83% 15% .
1	C	664	 84% 14% ..

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	914	977	32			
1	B	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			
1	C	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			

There are 3 discrepancies between the modelled and reference sequences:

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

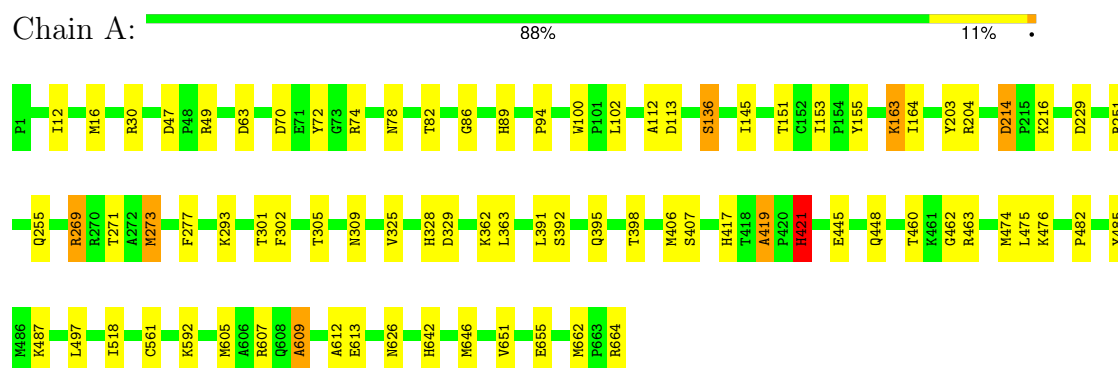
- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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		

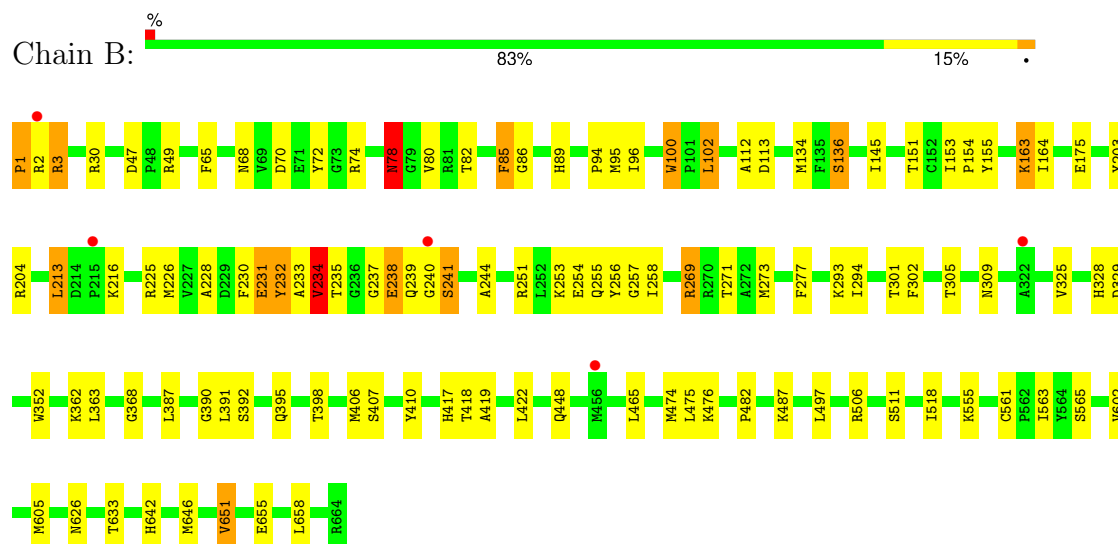
3 Residue-property plots

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.

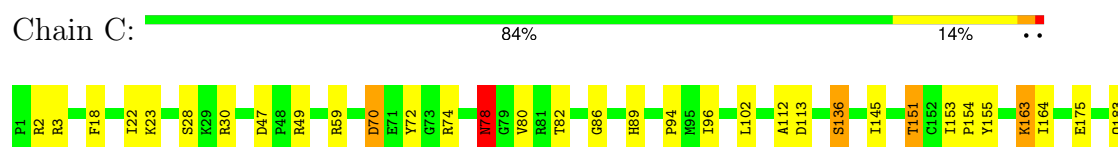
• Molecule 1: RNA-DIRECTED RNA POLYMERASE

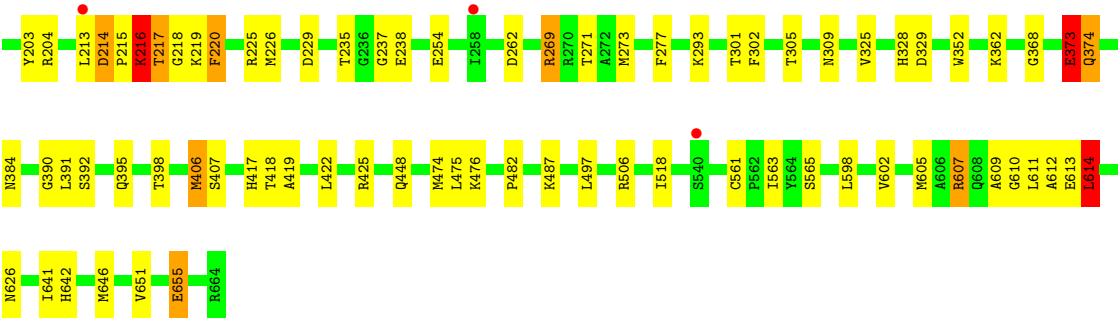


• Molecule 1: RNA-DIRECTED RNA POLYMERASE



• Molecule 1: RNA-DIRECTED RNA POLYMERASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	105.07Å 105.07Å 157.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.39 – 3.30 34.39 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (34.39-3.30) 96.5 (34.39-3.30)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.218 , 0.242 0.245 , 0.262	Depositor DCC
R_{free} test set	1426 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.811	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.063 for -h,-k,l 0.078 for h,-h-k,-l 0.075 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	15798	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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	0.77	1/5396 (0.0%)	1.26	14/7297 (0.2%)
1	B	0.83	1/5396 (0.0%)	1.38	31/7297 (0.4%)
1	C	0.81	2/5396 (0.0%)	1.39	30/7297 (0.4%)
All	All	0.80	4/16188 (0.0%)	1.34	75/21891 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	217	THR	CA-C	7.62	1.62	1.52
1	B	240	GLY	C-N	6.79	1.42	1.33
1	A	273	MET	SD-CE	-6.55	1.63	1.79
1	C	216	LYS	C-N	5.58	1.41	1.33

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	241	SER	N-CA-C	10.71	125.81	108.99
1	B	240	GLY	N-CA-C	10.40	126.73	111.24
1	B	239	GLN	CA-C-N	9.71	130.44	121.31
1	B	239	GLN	C-N-CA	9.71	130.44	121.31
1	A	463	ARG	N-CA-C	-9.38	101.97	113.41
1	A	462	GLY	N-CA-C	9.28	124.65	111.10
1	C	217	THR	N-CA-C	9.18	130.36	110.80
1	B	238	GLU	N-CA-C	8.66	121.50	111.11
1	B	239	GLN	CA-C-O	-8.49	111.72	121.58
1	B	239	GLN	N-CA-C	-7.55	97.93	109.41
1	C	229	ASP	CA-CB-CG	7.54	120.14	112.60
1	B	234	VAL	N-CA-C	7.46	118.25	110.72
1	C	216	LYS	CA-C-O	-7.37	111.23	119.78
1	A	153	ILE	N-CA-C	7.25	116.86	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	218	GLY	CA-C-N	7.14	132.26	122.77
1	C	218	GLY	C-N-CA	7.14	132.26	122.77
1	C	611	LEU	CA-C-N	6.93	134.77	121.54
1	C	611	LEU	C-N-CA	6.93	134.77	121.54
1	C	373	GLU	CB-CG-CD	6.71	124.01	112.60
1	B	363	LEU	N-CA-C	6.60	119.20	109.50
1	C	302	PHE	N-CA-C	6.59	121.99	113.88
1	B	302	PHE	N-CA-C	6.57	121.95	113.88
1	B	216	LYS	N-CA-C	6.52	119.22	111.33
1	B	155	TYR	N-CA-C	6.51	119.69	111.69
1	A	302	PHE	N-CA-C	6.50	121.87	113.88
1	C	611	LEU	N-CA-C	-6.41	106.17	112.97
1	C	214	ASP	CA-CB-CG	6.41	119.01	112.60
1	B	231	GLU	CB-CG-CD	6.34	123.39	112.60
1	A	229	ASP	CA-CB-CG	6.33	118.93	112.60
1	C	155	TYR	N-CA-C	6.33	119.47	111.69
1	B	85	PHE	CA-CB-CG	6.25	120.06	113.80
1	B	232	TYR	N-CA-C	-6.18	104.54	111.28
1	B	100	TRP	N-CA-C	-6.01	100.53	109.42
1	C	598	LEU	CA-C-N	6.01	129.15	120.38
1	C	598	LEU	C-N-CA	6.01	129.15	120.38
1	A	100	TRP	N-CA-C	-6.00	102.22	109.72
1	A	363	LEU	N-CA-C	5.95	117.19	109.64
1	C	614	LEU	N-CA-C	5.89	118.28	108.20
1	A	609	ALA	N-CA-C	5.88	117.68	111.28
1	B	1	PRO	CA-C-N	5.87	132.76	121.54
1	B	1	PRO	C-N-CA	5.87	132.76	121.54
1	C	277	PHE	N-CA-C	5.84	118.39	111.33
1	C	237	GLY	CA-C-N	5.57	128.06	120.54
1	C	237	GLY	C-N-CA	5.57	128.06	120.54
1	C	655	GLU	CA-C-N	5.57	127.68	120.44
1	C	655	GLU	C-N-CA	5.57	127.68	120.44
1	A	214	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	421	HIS	CA-CB-CG	-5.48	108.32	113.80
1	B	658	LEU	CA-C-N	5.46	127.59	120.28
1	B	658	LEU	C-N-CA	5.46	127.59	120.28
1	B	511	SER	CA-C-N	5.43	129.46	120.94
1	B	511	SER	C-N-CA	5.43	129.46	120.94
1	C	151	THR	N-CA-C	-5.42	106.67	113.28
1	A	277	PHE	N-CA-C	5.41	117.88	111.33
1	A	155	TYR	N-CA-C	5.40	119.04	112.23
1	A	419	ALA	N-CA-C	5.38	118.40	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	PHE	N-CA-C	5.37	117.83	111.33
1	B	78	ASN	CA-CB-CG	5.33	117.92	112.60
1	B	96	ILE	CB-CA-C	5.28	115.25	110.13
1	C	70	ASP	CA-CB-CG	5.26	117.86	112.60
1	C	565	SER	CA-C-N	5.24	127.25	120.44
1	C	565	SER	C-N-CA	5.24	127.25	120.44
1	B	390	GLY	N-CA-C	-5.23	105.02	111.45
1	C	22	ILE	CA-C-N	5.15	127.18	120.28
1	C	22	ILE	C-N-CA	5.15	127.18	120.28
1	C	226	MET	N-CA-C	5.14	117.11	109.25
1	B	633	THR	CA-C-N	5.10	127.43	120.54
1	B	633	THR	C-N-CA	5.10	127.43	120.54
1	B	237	GLY	CA-C-N	5.04	127.35	120.54
1	B	237	GLY	C-N-CA	5.04	127.35	120.54
1	C	406	MET	N-CA-C	5.04	116.86	111.36
1	C	78	ASN	CA-CB-CG	5.03	117.63	112.60
1	B	68	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	485	TYR	N-CA-C	5.03	119.44	112.45
1	C	390	GLY	N-CA-C	-5.00	105.30	111.45

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	5165	44	1
1	B	5265	0	5165	68	0
1	C	5265	0	5165	59	1
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	15495	157	1

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 5.

All (157) 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:612:ALA:HB1	1:C:96:ILE:HG21	1.44	0.96
1:B:1:PRO:H2	1:B:238:GLU:HG3	1.35	0.91
1:A:605:MET:HA	1:C:373:GLU:HG3	1.67	0.77
1:C:213:LEU:HD13	1:C:220:PHE:CZ	2.22	0.74
1:A:613:GLU:OE2	1:C:374:GLN:HB2	1.89	0.72
1:C:219:LYS:HG2	1:C:262:ASP:OD1	1.90	0.71
1:B:251:ARG:HH11	1:B:255:GLN:HE22	1.39	0.71
1:A:612:ALA:HB1	1:C:96:ILE:CG2	2.20	0.69
1:B:228:ALA:HB1	1:B:232:TYR:HB3	1.75	0.69
1:A:609:ALA:HB1	1:C:373:GLU:HG2	1.75	0.68
1:C:651:VAL:O	1:C:655:GLU:HB2	1.94	0.66
1:A:419:ALA:HA	1:A:421:HIS:NE2	2.13	0.64
1:A:151:THR:HG22	1:A:163:LYS:HG3	1.79	0.63
1:C:214:ASP:C	1:C:216:LYS:H	2.07	0.62
1:A:251:ARG:HH11	1:A:255:GLN:HE22	1.47	0.62
1:B:235:THR:HB	1:B:238:GLU:HB2	1.81	0.61
1:C:419:ALA:HB1	1:C:422:LEU:HG	1.82	0.61
1:C:151:THR:HG22	1:C:163:LYS:HG3	1.81	0.61
1:B:256:TYR:HB2	1:B:258:ILE:HD12	1.83	0.60
1:A:203:TYR:HE1	1:A:271:THR:HG22	1.67	0.59
1:B:203:TYR:HE1	1:B:271:THR:HG22	1.67	0.59
1:A:47:ASP:OD1	1:A:49:ARG:HD3	2.03	0.58
1:A:94:PRO:HB3	1:A:269:ARG:HG3	1.87	0.57
1:B:392:SER:O	1:B:398:THR:HG21	2.04	0.57
1:B:407:SER:HA	1:B:448:GLN:HE22	1.69	0.57
1:C:203:TYR:HE1	1:C:271:THR:HG22	1.69	0.57
1:A:407:SER:HA	1:A:448:GLN:HE22	1.67	0.57
1:C:213:LEU:HD13	1:C:220:PHE:CE2	2.40	0.57
1:A:664:ARG:HD3	1:B:651:VAL:HG12	1.87	0.56
1:B:392:SER:O	1:B:398:THR:CG2	2.53	0.56
1:B:47:ASP:OD1	1:B:49:ARG:HD3	2.05	0.56
1:C:614:LEU:HD22	1:C:641:ILE:HD11	1.87	0.56
1:C:325:VAL:HG21	1:C:406:MET:HE2	1.87	0.56
1:C:407:SER:HA	1:C:448:GLN:HE22	1.70	0.56
1:B:102:LEU:HA	1:B:233:ALA:HA	1.88	0.56
1:B:94:PRO:HB3	1:B:269:ARG:HG3	1.86	0.56
1:C:220:PHE:H	1:C:220:PHE:HD1	1.53	0.55
1:C:94:PRO:HB3	1:C:269:ARG:HG3	1.87	0.55
1:A:325:VAL:HG21	1:A:406:MET:HE2	1.88	0.55
1:A:392:SER:O	1:A:398:THR:HG21	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ASP:OD1	1:C:49:ARG:HD3	2.07	0.54
1:B:203:TYR:CE1	1:B:271:THR:HG22	2.42	0.54
1:A:151:THR:CG2	1:A:163:LYS:HG3	2.37	0.54
1:C:203:TYR:CE1	1:C:271:THR:HG22	2.43	0.54
1:C:392:SER:O	1:C:398:THR:HG21	2.08	0.54
1:A:651:VAL:O	1:A:655:GLU:HB2	2.07	0.54
1:B:325:VAL:HG21	1:B:406:MET:HE2	1.87	0.54
1:A:203:TYR:CE1	1:A:271:THR:HG22	2.42	0.53
1:C:392:SER:O	1:C:398:THR:CG2	2.56	0.53
1:B:100:TRP:HB3	1:B:233:ALA:HB2	1.90	0.53
1:B:231:GLU:HA	1:B:234:VAL:HG13	1.92	0.52
1:A:392:SER:O	1:A:398:THR:CG2	2.57	0.52
1:C:610:GLY:C	1:C:612:ALA:H	2.18	0.52
1:C:216:LYS:O	1:C:217:THR:HB	2.09	0.52
1:B:602:VAL:HB	1:B:605:MET:HB2	1.91	0.52
1:B:475:LEU:HD21	1:B:482:PRO:HG3	1.93	0.51
1:C:59:ARG:NH2	1:C:220:PHE:HE1	2.10	0.50
1:B:417:HIS:CE1	1:B:474:MET:HE1	2.47	0.50
1:B:151:THR:HG22	1:B:163:LYS:HG3	1.94	0.50
1:B:642:HIS:CE1	1:B:646:MET:HG3	2.47	0.49
1:C:72:TYR:CE2	1:C:476:LYS:HD3	2.47	0.49
1:A:70:ASP:OD2	1:A:74:ARG:HD2	2.12	0.49
1:A:72:TYR:CE2	1:A:476:LYS:HD3	2.47	0.49
1:C:417:HIS:CE1	1:C:474:MET:HE1	2.48	0.49
1:B:230:PHE:CD2	1:B:231:GLU:HG3	2.47	0.49
1:C:213:LEU:HD13	1:C:220:PHE:CE1	2.47	0.49
1:C:475:LEU:HD21	1:C:482:PRO:HG3	1.93	0.49
1:B:3:ARG:HB2	1:B:235:THR:HG22	1.95	0.48
1:A:417:HIS:CE1	1:A:474:MET:HE1	2.48	0.48
1:C:395:GLN:HB3	1:C:398:THR:HG23	1.95	0.48
1:C:273:MET:HE3	1:C:392:SER:HA	1.95	0.48
1:C:642:HIS:CE1	1:C:646:MET:HG3	2.48	0.48
1:A:475:LEU:HD21	1:A:482:PRO:HG3	1.95	0.47
1:A:642:HIS:CE1	1:A:646:MET:HG3	2.49	0.47
1:B:72:TYR:CE2	1:B:476:LYS:HD3	2.50	0.47
1:B:145:ILE:HD12	1:B:164:ILE:HD13	1.96	0.47
1:A:592:LYS:HE2	1:C:254:GLU:HG2	1.96	0.47
1:C:18:PHE:CG	1:C:28:SER:HB3	2.49	0.47
1:C:70:ASP:OD2	1:C:74:ARG:HD2	2.15	0.47
1:A:664:ARG:CD	1:B:651:VAL:HG12	2.44	0.47
1:B:85:PHE:CE2	1:B:213:LEU:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:MET:HE3	1:B:392:SER:HA	1.96	0.47
1:A:612:ALA:CB	1:C:96:ILE:HG21	2.30	0.47
1:C:136:SER:OG	1:C:293:LYS:NZ	2.48	0.46
1:C:86:GLY:O	1:C:89:HIS:HD2	1.98	0.46
1:A:145:ILE:HD12	1:A:164:ILE:HD13	1.97	0.46
1:B:70:ASP:OD2	1:B:74:ARG:HD2	2.15	0.46
1:B:136:SER:OG	1:B:293:LYS:NZ	2.48	0.46
1:B:565:SER:HB2	1:C:183:GLN:C	2.41	0.46
1:B:395:GLN:HB3	1:B:398:THR:HG23	1.98	0.46
1:C:145:ILE:HD12	1:C:164:ILE:HD13	1.98	0.46
1:A:12:ILE:O	1:A:16:MET:HG2	2.16	0.46
1:B:86:GLY:O	1:B:89:HIS:HD2	1.99	0.45
1:C:204:ARG:HH12	1:C:626:ASN:HD21	1.64	0.45
1:C:112:ALA:HB1	1:C:487:LYS:HE2	1.99	0.45
1:B:555:LYS:NZ	1:C:384:ASN:ND2	2.65	0.45
1:C:94:PRO:CB	1:C:269:ARG:HG3	2.47	0.45
1:B:651:VAL:O	1:B:655:GLU:HB2	2.17	0.45
1:B:251:ARG:HB2	1:B:255:GLN:HE21	1.82	0.45
1:B:102:LEU:HD11	1:B:232:TYR:HD1	1.81	0.44
1:B:204:ARG:HH12	1:B:626:ASN:HD21	1.64	0.44
1:B:253:LYS:O	1:B:257:GLY:HA2	2.17	0.44
1:C:214:ASP:C	1:C:216:LYS:N	2.76	0.44
1:B:419:ALA:HB1	1:B:422:LEU:HD12	1.99	0.44
1:B:518:ILE:HB	1:B:561:CYS:SG	2.58	0.44
1:C:86:GLY:O	1:C:89:HIS:CD2	2.71	0.44
1:A:86:GLY:O	1:A:89:HIS:HD2	2.00	0.44
1:B:102:LEU:HD11	1:B:232:TYR:CD1	2.53	0.44
1:A:112:ALA:HB1	1:A:487:LYS:HE2	2.00	0.44
1:A:273:MET:HE3	1:A:392:SER:HA	2.00	0.43
1:B:86:GLY:O	1:B:89:HIS:CD2	2.72	0.43
1:B:94:PRO:CB	1:B:269:ARG:HG3	2.48	0.43
1:C:518:ILE:HB	1:C:561:CYS:SG	2.59	0.43
1:A:518:ILE:HB	1:A:561:CYS:SG	2.59	0.43
1:B:153:ILE:HA	1:B:154:PRO:HA	1.85	0.43
1:B:175:GLU:HA	1:B:352:TRP:CE3	2.54	0.43
1:B:231:GLU:HB3	1:B:234:VAL:HG22	2.00	0.43
1:B:95:MET:HE2	1:B:269:ARG:H	1.83	0.43
1:C:153:ILE:HA	1:C:154:PRO:HA	1.88	0.42
1:C:235:THR:HB	1:C:238:GLU:HB2	2.01	0.42
1:C:78:ASN:ND2	1:C:80:VAL:H	2.17	0.42
1:B:78:ASN:ND2	1:B:80:VAL:H	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLY:O	1:A:89:HIS:CD2	2.73	0.42
1:B:231:GLU:CB	1:B:234:VAL:HG22	2.48	0.42
1:C:219:LYS:CG	1:C:262:ASP:OD1	2.65	0.42
1:A:136:SER:OG	1:A:293:LYS:NZ	2.53	0.42
1:B:328:HIS:HD2	1:B:329:ASP:OD1	2.02	0.42
1:C:225:ARG:HA	1:C:225:ARG:HD3	1.90	0.42
1:A:163:LYS:HE3	1:A:163:LYS:HB2	1.74	0.42
1:A:328:HIS:HD2	1:A:329:ASP:OD1	2.03	0.42
1:B:301:THR:HG23	1:B:448:GLN:HG3	2.01	0.42
1:C:301:THR:HG23	1:C:448:GLN:HG3	2.01	0.42
1:A:664:ARG:HG3	1:B:651:VAL:HB	2.01	0.41
1:C:163:LYS:HE3	1:C:163:LYS:HB2	1.82	0.41
1:C:175:GLU:HA	1:C:352:TRP:CE3	2.55	0.41
1:B:112:ALA:HB1	1:B:487:LYS:HE2	2.02	0.41
1:B:163:LYS:HE3	1:B:163:LYS:HB2	1.82	0.41
1:A:204:ARG:HH12	1:A:626:ASN:HD21	1.66	0.41
1:C:305:THR:H	1:C:309:ASN:ND2	2.19	0.41
1:B:175:GLU:HA	1:B:352:TRP:CD2	2.56	0.41
1:B:226:MET:CE	1:B:244:ALA:HB2	2.51	0.41
1:B:305:THR:H	1:B:309:ASN:ND2	2.19	0.41
1:B:134:MET:HG2	1:B:294:ILE:HG21	2.03	0.41
1:A:301:THR:HG23	1:A:448:GLN:HG3	2.02	0.41
1:A:305:THR:H	1:A:309:ASN:ND2	2.19	0.41
1:A:664:ARG:HD3	1:B:651:VAL:CG1	2.50	0.41
1:A:395:GLN:HB3	1:A:398:THR:HG23	2.02	0.41
1:C:328:HIS:HD2	1:C:329:ASP:OD1	2.04	0.41
1:B:251:ARG:HH11	1:B:255:GLN:NE2	2.13	0.41
1:B:225:ARG:HA	1:B:225:ARG:HD3	1.89	0.41
1:B:3:ARG:HD3	1:B:234:VAL:HG23	2.03	0.40
1:B:230:PHE:O	1:B:234:VAL:HG13	2.21	0.40
1:B:555:LYS:NZ	1:C:384:ASN:HD21	2.19	0.40
1:A:94:PRO:CB	1:A:269:ARG:HG3	2.49	0.40
1:B:65:PHE:CG	1:B:563:ILE:HD13	2.56	0.40
1:B:406:MET:HB3	1:B:410:TYR:CE2	2.56	0.40
1:C:518:ILE:HG21	1:C:563:ILE:HD11	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:THR:O	1:C:607:ARG:NH2[3_455]	1.51	0.69

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	662/664 (100%)	641 (97%)	19 (3%)	2 (0%)	36	65
1	B	662/664 (100%)	634 (96%)	24 (4%)	4 (1%)	21	52
1	C	662/664 (100%)	628 (95%)	26 (4%)	8 (1%)	10	37
All	All	1986/1992 (100%)	1903 (96%)	69 (4%)	14 (1%)	18	49

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	373	GLU
1	C	607	ARG
1	A	136	SER
1	A	607	ARG
1	B	136	SER
1	C	2	ARG
1	C	136	SER
1	C	220	PHE
1	B	465	LEU
1	C	609	ALA
1	B	2	ARG
1	B	368	GLY
1	C	215	PRO
1	C	368	GLY

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	557/557 (100%)	541 (97%)	16 (3%)	37	62
1	B	557/557 (100%)	538 (97%)	19 (3%)	32	59
1	C	557/557 (100%)	535 (96%)	22 (4%)	28	56
All	All	1671/1671 (100%)	1614 (97%)	57 (3%)	32	59

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	63	ASP
1	A	78	ASN
1	A	82	THR
1	A	102	LEU
1	A	113	ASP
1	A	163	LYS
1	A	214	ASP
1	A	216	LYS
1	A	269	ARG
1	A	362	LYS
1	A	391	LEU
1	A	421	HIS
1	A	445	GLU
1	A	497	LEU
1	A	662	MET
1	B	3	ARG
1	B	30	ARG
1	B	78	ASN
1	B	82	THR
1	B	102	LEU
1	B	113	ASP
1	B	163	LYS
1	B	213	LEU
1	B	234	VAL
1	B	241	SER
1	B	254	GLU
1	B	269	ARG
1	B	362	LYS
1	B	387	LEU
1	B	391	LEU
1	B	418	THR
1	B	497	LEU
1	B	506	ARG

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Mol	Chain	Res	Type
1	B	651	VAL
1	C	3	ARG
1	C	23	LYS
1	C	30	ARG
1	C	78	ASN
1	C	82	THR
1	C	102	LEU
1	C	113	ASP
1	C	163	LYS
1	C	216	LYS
1	C	269	ARG
1	C	362	LYS
1	C	373	GLU
1	C	374	GLN
1	C	391	LEU
1	C	418	THR
1	C	425	ARG
1	C	497	LEU
1	C	506	ARG
1	C	602	VAL
1	C	605	MET
1	C	613	GLU
1	C	614	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	25	GLN
1	A	26	GLN
1	A	78	ASN
1	A	89	HIS
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	626	ASN
1	B	26	GLN
1	B	78	ASN

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Mol	Chain	Res	Type
1	B	83	ASN
1	B	89	HIS
1	B	158	ASN
1	B	255	GLN
1	B	309	ASN
1	B	328	HIS
1	B	448	GLN
1	B	469	HIS
1	B	492	HIS
1	B	525	GLN
1	B	626	ASN
1	C	26	GLN
1	C	78	ASN
1	C	83	ASN
1	C	89	HIS
1	C	158	ASN
1	C	304	HIS
1	C	309	ASN
1	C	328	HIS
1	C	384	ASN
1	C	448	GLN
1	C	492	HIS
1	C	525	GLN
1	C	626	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 [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	664/664 (100%)	-0.26	0 100 100	35, 61, 93, 161	0
1	B	664/664 (100%)	-0.25	5 (0%) 82 68	39, 68, 100, 170	0
1	C	664/664 (100%)	-0.09	3 (0%) 87 76	61, 89, 129, 177	0
All	All	1992/1992 (100%)	-0.20	8 (0%) 88 79	35, 72, 115, 177	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	GLY	2.6
1	C	540	SER	2.6
1	B	456	MET	2.5
1	C	213	LEU	2.3
1	C	258	ILE	2.2
1	B	215	PRO	2.1
1	B	322	ALA	2.0
1	B	2	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(Å ²)	Q<0.9
2	MN	B	665	1/1	0.85	0.08	158,158,158,158	0
2	MN	A	665	1/1	0.86	0.06	124,124,124,124	0
2	MN	C	665	1/1	0.89	0.09	177,177,177,177	0

6.5 Other polymers [i](#)

There are no such residues in this entry.