



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 02:57 am GMT

PDB ID : 4B02
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 : 4.02b-467
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

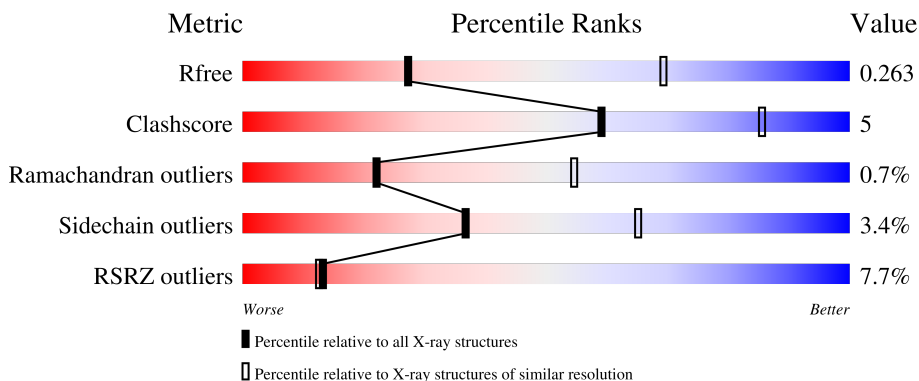
1 Overall quality at a glance

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	
1	B	664	
1	C	664	

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

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

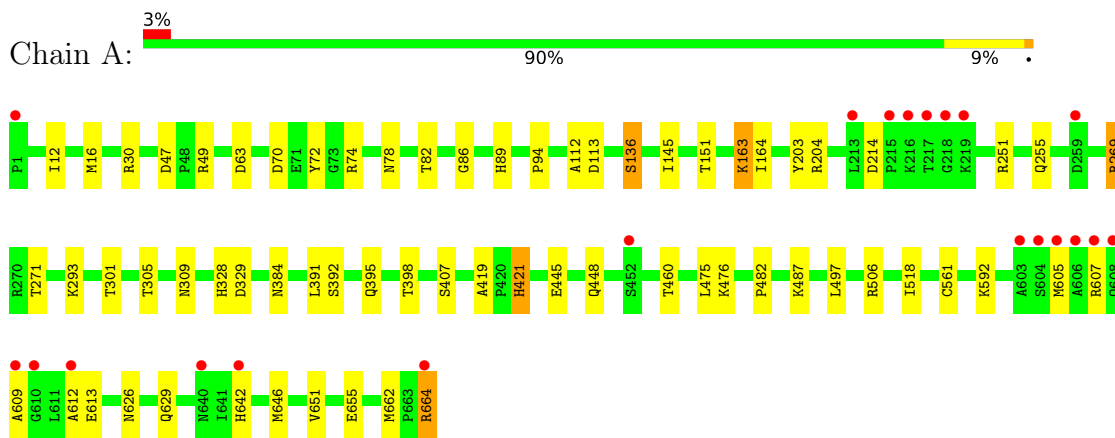
- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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		

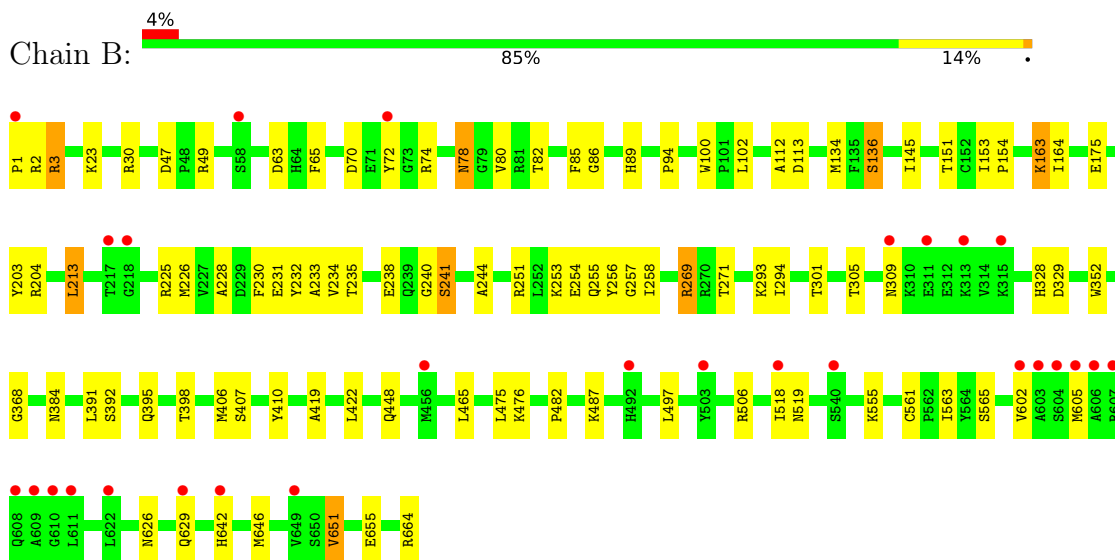
3 Residue-property plots [i](#)

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.

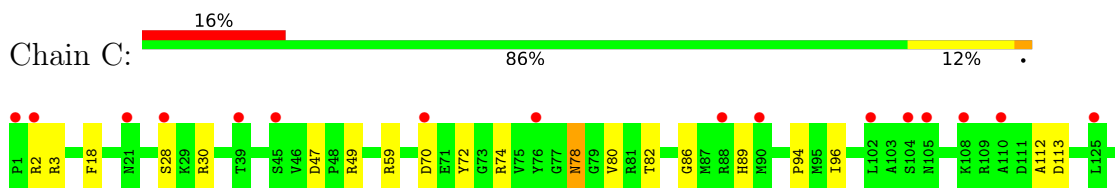
• Molecule 1: RNA-DIRECTED RNA POLYMERASE

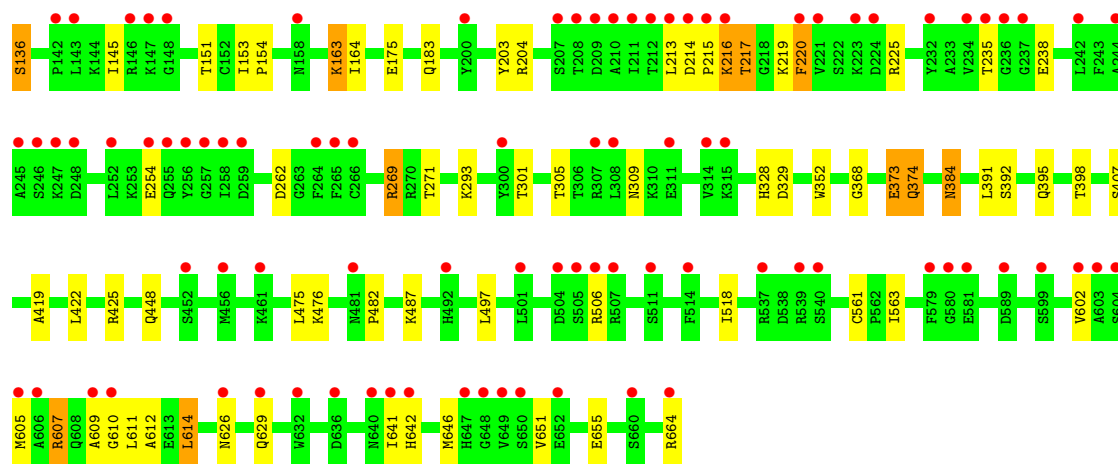


• Molecule 1: RNA-DIRECTED RNA POLYMERASE



• Molecule 1: RNA-DIRECTED RNA POLYMERASE





4 Data and refinement statistics i

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 0.246 , 0.263	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)	0.32 , 36.4	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 i

5.1 Standard geometry i

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	0.46	0/5396	0.66	0/7297
1	B	0.50	0/5396	0.71	2/7297 (0.0%)
1	C	0.48	0/5396	0.71	2/7297 (0.0%)
All	All	0.48	0/16188	0.69	4/21891 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	217	THR	N-CA-C	7.17	130.36	111.00
1	B	241	SER	N-CA-C	5.49	125.81	111.00
1	B	240	GLY	N-CA-C	5.45	126.73	113.10
1	C	611	LEU	C-N-CA	5.23	134.77	121.70

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	5265	0	5165	41	1
1	B	5265	0	5165	64	0
1	C	5265	0	5165	55	1
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
All	All	15798	0	15495	146	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 (146) 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: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:214:ASP:C	1:C:216:LYS:H	2.07	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:614:LEU:HD22	1:C:641:ILE:HD11	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:392:SER:O	1:A:398:THR:HG21	2.07	0.55
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: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: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: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: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:C:395:GLN:HB3	1:C:398:THR:HG23	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:C:610:GLY:C	1:C:612:ALA:H	2.18	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:565:SER:HB2	1:C:183:GLN:C	2.41	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%)	41	71
1	B	662/664 (100%)	634 (96%)	24 (4%)	4 (1%)	25	57
1	C	662/664 (100%)	628 (95%)	26 (4%)	8 (1%)	13	42
All	All	1986/1992 (100%)	1903 (96%)	69 (4%)	14 (1%)	22	54

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%)	540 (97%)	17 (3%)	40	67
1	B	557/557 (100%)	537 (96%)	20 (4%)	35	63
1	C	557/557 (100%)	538 (97%)	19 (3%)	37	65
All	All	1671/1671 (100%)	1615 (97%)	56 (3%)	37	65

All (56) 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	113	ASP
1	A	163	LYS
1	A	214	ASP
1	A	269	ARG
1	A	384	ASN
1	A	391	LEU
1	A	421	HIS
1	A	445	GLU
1	A	497	LEU
1	A	506	ARG
1	A	629	GLN
1	A	662	MET
1	A	664	ARG
1	B	3	ARG
1	B	23	LYS
1	B	30	ARG
1	B	63	ASP
1	B	78	ASN
1	B	82	THR
1	B	113	ASP
1	B	163	LYS
1	B	213	LEU
1	B	241	SER
1	B	254	GLU
1	B	269	ARG
1	B	384	ASN
1	B	391	LEU
1	B	497	LEU
1	B	506	ARG
1	B	519	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	629	GLN
1	B	651	VAL
1	B	664	ARG
1	C	3	ARG
1	C	30	ARG
1	C	78	ASN
1	C	82	THR
1	C	113	ASP
1	C	163	LYS
1	C	216	LYS
1	C	269	ARG
1	C	374	GLN
1	C	384	ASN
1	C	391	LEU
1	C	425	ARG
1	C	497	LEU
1	C	506	ARG
1	C	602	VAL
1	C	605	MET
1	C	614	LEU
1	C	629	GLN
1	C	664	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
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	525	GLN
1	A	626	ASN
1	B	15	GLN
1	B	26	GLN
1	B	78	ASN
1	B	89	HIS
1	B	255	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	309	ASN
1	B	328	HIS
1	B	448	GLN
1	B	469	HIS
1	B	525	GLN
1	B	626	ASN
1	C	15	GLN
1	C	26	GLN
1	C	78	ASN
1	C	89	HIS
1	C	255	GLN
1	C	309	ASN
1	C	328	HIS
1	C	384	ASN
1	C	448	GLN
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 monosaccharides 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	664/664 (100%)	0.20	21 (3%) 47 46	35, 61, 93, 161	0
1	B	664/664 (100%)	0.23	28 (4%) 36 34	39, 68, 100, 170	0
1	C	664/664 (100%)	0.85	105 (15%) 2 2	61, 89, 129, 177	0
All	All	1992/1992 (100%)	0.42	154 (7%) 13 12	35, 72, 115, 177	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	PRO	8.5
1	B	608	GLN	7.7
1	C	610	GLY	7.7
1	B	609	ALA	7.3
1	C	220	PHE	6.9
1	A	609	ALA	6.9
1	C	213	LEU	6.8
1	B	610	GLY	6.8
1	B	604	SER	6.7
1	B	603	ALA	6.7
1	A	606	ALA	6.5
1	C	209	ASP	6.3
1	A	607	ARG	6.0
1	C	540	SER	5.9
1	C	664	ARG	5.9
1	C	207	SER	5.8
1	C	210	ALA	5.8
1	B	605	MET	5.7
1	A	608	GLN	5.7
1	A	604	SER	5.6
1	C	215	PRO	5.5
1	C	2	ARG	5.1
1	A	216	LYS	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	505	SER	4.7
1	C	604	SER	4.7
1	C	259	ASP	4.6
1	C	211	ILE	4.5
1	C	603	ALA	4.5
1	B	606	ALA	4.5
1	B	602	VAL	4.5
1	C	605	MET	4.4
1	C	308	LEU	4.4
1	C	245	ALA	4.4
1	C	148	GLY	4.2
1	C	208	THR	4.1
1	C	264	PHE	4.0
1	C	212	THR	3.9
1	C	602	VAL	3.9
1	C	609	ALA	3.8
1	C	104	SER	3.8
1	C	223	LYS	3.7
1	C	539	ARG	3.7
1	B	1	PRO	3.7
1	C	258	ILE	3.6
1	C	492	HIS	3.6
1	C	256	TYR	3.5
1	C	504	ASP	3.4
1	C	626	ASN	3.3
1	C	649	VAL	3.3
1	C	39	THR	3.3
1	C	314	VAL	3.3
1	B	611	LEU	3.3
1	B	629	GLN	3.3
1	A	1	PRO	3.2
1	C	650	SER	3.2
1	C	507	ARG	3.2
1	C	105	ASN	3.2
1	C	110	ALA	3.1
1	C	236	GLY	3.1
1	B	649	VAL	3.1
1	A	219	LYS	3.1
1	B	492	HIS	3.1
1	C	307	ARG	3.1
1	C	90	MET	3.0
1	C	506	ARG	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	213	LEU	3.0
1	C	257	GLY	2.9
1	C	660	SER	2.9
1	A	664	ARG	2.9
1	C	514	PHE	2.9
1	A	217	THR	2.8
1	A	215	PRO	2.8
1	A	218	GLY	2.8
1	C	579	PHE	2.8
1	C	266	CYS	2.8
1	C	237	GLY	2.8
1	C	252	LEU	2.8
1	C	146	ARG	2.8
1	C	246	SER	2.8
1	B	218	GLY	2.8
1	C	311	GLU	2.7
1	C	244	ALA	2.7
1	C	102	LEU	2.7
1	A	605	MET	2.7
1	C	599	SER	2.6
1	A	612	ALA	2.6
1	C	636	ASP	2.6
1	C	214	ASP	2.6
1	C	142	PRO	2.5
1	C	216	LYS	2.5
1	B	456	MET	2.5
1	C	70	ASP	2.5
1	C	158	ASN	2.5
1	C	255	GLN	2.5
1	C	235	THR	2.5
1	C	481	ASN	2.5
1	C	589	ASP	2.5
1	C	248	ASP	2.5
1	C	21	ASN	2.5
1	A	603	ALA	2.5
1	C	221	VAL	2.5
1	C	580	GLY	2.5
1	C	642	HIS	2.5
1	C	125	LEU	2.5
1	C	315	LYS	2.5
1	C	300	TYR	2.4
1	A	610	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	581	GLU	2.4
1	C	28	SER	2.4
1	C	76	TYR	2.4
1	C	641	ILE	2.4
1	C	45	SER	2.4
1	C	247	LYS	2.4
1	C	629	GLN	2.3
1	B	518	ILE	2.3
1	C	200	TYR	2.3
1	C	647	HIS	2.3
1	C	234	VAL	2.3
1	C	143	LEU	2.3
1	B	217	THR	2.3
1	B	311	GLU	2.3
1	B	540	SER	2.3
1	C	88	ARG	2.2
1	C	511	SER	2.2
1	B	72	TYR	2.2
1	C	537	ARG	2.2
1	C	242	LEU	2.2
1	C	632	TRP	2.2
1	B	58	SER	2.2
1	B	607	ARG	2.2
1	C	254	GLU	2.2
1	C	652	GLU	2.2
1	A	642	HIS	2.2
1	A	259	ASP	2.1
1	C	452	SER	2.1
1	A	640	ASN	2.1
1	C	224	ASP	2.1
1	C	640	ASN	2.1
1	C	501	LEU	2.1
1	B	503	TYR	2.1
1	B	622	LEU	2.1
1	C	648	GLY	2.1
1	A	452	SER	2.1
1	C	147	LYS	2.1
1	C	456	MET	2.1
1	B	309	ASN	2.0
1	C	265	PHE	2.0
1	C	232	TYR	2.0
1	C	461	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	606	ALA	2.0
1	B	642	HIS	2.0
1	B	313	LYS	2.0
1	B	315	LYS	2.0
1	C	108	LYS	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
2	MN	C	665	1/1	0.70	0.19	177,177,177,177	0
2	MN	B	665	1/1	0.76	0.22	158,158,158,158	0
2	MN	A	665	1/1	0.88	0.13	124,124,124,124	0

6.5 Other polymers [i](#)

There are no such residues in this entry.