



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:36 PM EDT

PDB ID : 2YIB / pdb_00002yib
Title : Structure of the RNA polymerase VP1 from Infectious Pancreatic Necrosis Virus
Authors : Graham, S.C.; Sarin, L.P.; Bahar, M.W.; Myers, R.A.; Stuart, D.I.; Bamford, D.H.; Grimes, J.M.
Deposited on : 2011-05-11
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

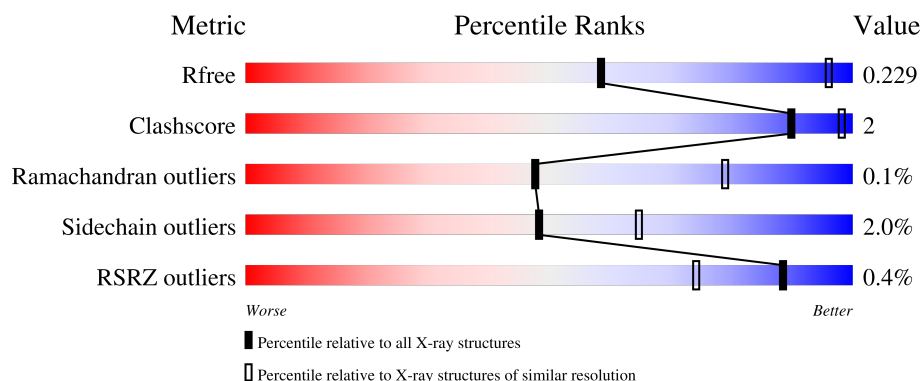
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	853	
1	B	853	
1	C	853	
2	D	770	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24183 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	789	Total	C	N	O	S	0	0	0
			6159	3908	1038	1187	26			
1	B	789	Total	C	N	O	S	0	0	0
			6155	3906	1038	1185	26			
1	C	789	Total	C	N	O	S	0	0	0
			6159	3908	1038	1187	26			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	846	VAL	-	expression tag	UNP P22173
A	847	GLU	-	expression tag	UNP P22173
A	848	HIS	-	expression tag	UNP P22173
A	849	HIS	-	expression tag	UNP P22173
A	850	HIS	-	expression tag	UNP P22173
A	851	HIS	-	expression tag	UNP P22173
A	852	HIS	-	expression tag	UNP P22173
A	853	HIS	-	expression tag	UNP P22173
B	846	VAL	-	expression tag	UNP P22173
B	847	GLU	-	expression tag	UNP P22173
B	848	HIS	-	expression tag	UNP P22173
B	849	HIS	-	expression tag	UNP P22173
B	850	HIS	-	expression tag	UNP P22173
B	851	HIS	-	expression tag	UNP P22173
B	852	HIS	-	expression tag	UNP P22173
B	853	HIS	-	expression tag	UNP P22173
C	846	VAL	-	expression tag	UNP P22173
C	847	GLU	-	expression tag	UNP P22173
C	848	HIS	-	expression tag	UNP P22173
C	849	HIS	-	expression tag	UNP P22173
C	850	HIS	-	expression tag	UNP P22173
C	851	HIS	-	expression tag	UNP P22173
C	852	HIS	-	expression tag	UNP P22173

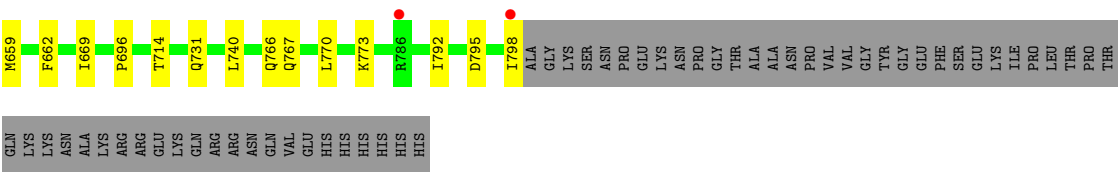
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Chain	Residue	Modelled	Actual	Comment	Reference
C	853	HIS	-	expression tag	UNP P22173

- Molecule 2 is a protein called RNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	761	Total	C	N	O	S	415	0	0
			5710	3622	966	1097	25			



● Molecule 2: RNA-DIRECTED RNA POLYMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.74Å 195.45Å 197.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.43 – 3.80 44.43 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (44.43-3.80) 98.0 (44.43-3.80)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.77Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.184 , 0.213 0.203 , 0.229	Depositor DCC
R_{free} test set	2307 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	88.6	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 115.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.056 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	24183	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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

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	0.79	0/6296	1.25	13/8573 (0.2%)
1	B	0.77	0/6292	1.31	22/8568 (0.3%)
1	C	0.81	0/6296	1.31	18/8573 (0.2%)
2	D	0.79	0/5420	1.29	14/7383 (0.2%)
All	All	0.79	0/24304	1.29	67/33097 (0.2%)

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	773	LYS	N-CA-C	-7.43	104.19	113.55
1	C	773	LYS	N-CA-C	-7.26	104.28	113.43
1	B	118	GLY	CA-C-N	6.90	129.84	120.38
1	B	118	GLY	C-N-CA	6.90	129.84	120.38
1	A	773	LYS	N-CA-C	-6.41	105.38	113.72
1	B	6	ASN	CA-CB-CG	6.40	119.00	112.60
1	C	740	LEU	N-CA-C	6.21	118.85	111.33
1	C	543	ASP	CA-CB-CG	6.21	118.81	112.60
1	C	766	GLN	CA-C-N	6.07	128.66	120.65
1	C	766	GLN	C-N-CA	6.07	128.66	120.65
2	D	113	ASP	CA-CB-CG	6.04	118.64	112.60
1	C	258	ASP	CA-CB-CG	6.03	118.62	112.60
2	D	6	ASN	CA-CB-CG	6.01	118.61	112.60
1	B	113	ASP	CA-CB-CG	5.99	118.58	112.60
2	D	473	ASN	CA-CB-CG	5.95	118.55	112.60
1	C	113	ASP	CA-CB-CG	5.92	118.52	112.60
1	B	740	LEU	N-CA-C	5.90	118.47	111.33
1	C	6	ASN	CA-CB-CG	5.86	118.46	112.60
1	C	473	ASN	CA-CB-CG	5.86	118.45	112.60
1	A	258	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	258	ASP	CA-CB-CG	5.68	118.28	112.60
2	D	406	GLY	CA-C-N	5.60	128.05	120.38
2	D	406	GLY	C-N-CA	5.60	128.05	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	662	PHE	CA-C-N	5.59	126.31	119.99
1	B	662	PHE	C-N-CA	5.59	126.31	119.99
1	C	43	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	113	ASP	CA-CB-CG	5.49	118.09	112.60
1	B	43	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	6	ASN	CA-CB-CG	5.48	118.08	112.60
2	D	543	ASP	CA-CB-CG	5.47	118.07	112.60
2	D	662	PHE	CA-C-N	5.41	126.11	119.99
2	D	662	PHE	C-N-CA	5.41	126.11	119.99
1	C	731	GLN	CA-C-N	5.41	128.28	120.38
1	C	731	GLN	C-N-CA	5.41	128.28	120.38
1	B	3	ASP	CA-CB-CG	5.40	118.00	112.60
2	D	230	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	594	GLU	N-CA-C	-5.37	104.98	112.45
2	D	670	THR	N-CA-C	5.36	118.55	109.76
2	D	336	SER	N-CA-C	5.33	116.94	111.03
1	B	766	GLN	CA-C-N	5.32	127.86	120.63
1	B	766	GLN	C-N-CA	5.32	127.86	120.63
1	A	731	GLN	CA-C-N	5.31	127.93	120.28
1	A	731	GLN	C-N-CA	5.31	127.93	120.28
1	C	230	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	268	ASP	CA-CB-CG	5.26	117.86	112.60
1	C	662	PHE	CA-C-N	5.26	125.93	119.99
1	C	662	PHE	C-N-CA	5.26	125.93	119.99
1	B	731	GLN	CA-C-N	5.25	128.04	120.38
1	B	731	GLN	C-N-CA	5.25	128.04	120.38
1	A	268	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	473	ASN	CA-CB-CG	5.21	117.81	112.60
2	D	268	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	268	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	118	GLY	CA-C-N	5.16	127.45	120.38
1	A	118	GLY	C-N-CA	5.16	127.45	120.38
1	B	543	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	118	GLY	CA-C-N	5.11	127.83	120.38
1	C	118	GLY	C-N-CA	5.11	127.83	120.38
1	A	406	GLY	CA-C-N	5.10	127.36	120.38
1	A	406	GLY	C-N-CA	5.10	127.36	120.38
2	D	610	ILE	CA-C-N	5.07	127.14	120.60
2	D	610	ILE	C-N-CA	5.07	127.14	120.60
1	B	193	THR	N-CA-C	-5.05	104.02	110.53
1	A	3	ASP	CA-CB-CG	5.02	117.62	112.60
1	B	28	ASP	N-CA-C	5.02	116.49	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	ALA	CA-C-N	5.01	126.95	120.44
1	B	261	ALA	C-N-CA	5.01	126.95	120.44

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	6159	0	6090	24	0
1	B	6155	0	6086	26	0
1	C	6159	0	6090	28	0
2	D	5710	0	5296	24	0
All	All	24183	0	23562	87	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 (87) 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:B:644:VAL:HG22	2:D:92:THR:CG2	1.90	1.01
1:A:731:GLN:HG2	1:A:772:MET:HE1	1.50	0.93
1:B:644:VAL:HG22	2:D:92:THR:HG21	1.54	0.88
1:B:644:VAL:HG22	2:D:92:THR:HG23	1.61	0.81
1:C:187:PRO:HB3	1:C:197:LEU:HD11	1.73	0.70
1:A:187:PRO:HB3	1:A:197:LEU:HD11	1.74	0.69
1:C:12:ALA:HB3	2:D:243:ILE:HD11	1.76	0.67
1:C:493:LYS:HE2	1:C:714:THR:HG22	1.77	0.66
1:A:673:GLU:HG3	1:C:798:ILE:HG12	1.80	0.63
1:B:644:VAL:CG2	2:D:92:THR:HG21	2.28	0.63
1:B:187:PRO:HB3	1:B:197:LEU:HD11	1.81	0.63
2:D:187:PRO:HB3	2:D:197:LEU:HD11	1.80	0.62
1:C:74:ASP:HB2	1:C:81:ARG:HG2	1.86	0.57
1:A:74:ASP:HB2	1:A:81:ARG:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:TRP:HB3	1:B:521:LEU:HB3	1.87	0.57
1:B:74:ASP:HB2	1:B:81:ARG:HG2	1.87	0.56
2:D:398:TRP:HB3	2:D:521:LEU:HB3	1.87	0.56
1:A:593:LEU:CD1	1:A:659:MET:HB2	2.36	0.56
1:B:593:LEU:CD1	1:B:659:MET:HB2	2.35	0.56
2:D:74:ASP:HB2	2:D:81:ARG:HG2	1.88	0.55
1:C:19:MET:HB3	2:D:88:LYS:O	2.08	0.54
1:C:593:LEU:CD1	1:C:659:MET:HB2	2.38	0.53
2:D:593:LEU:CD1	2:D:659:MET:HB2	2.39	0.52
1:A:31:ILE:HD13	1:B:602:PRO:HG2	1.90	0.52
1:C:398:TRP:HB3	1:C:521:LEU:HB3	1.90	0.52
1:A:398:TRP:HB3	1:A:521:LEU:HB3	1.91	0.51
2:D:45:PRO:HB3	2:D:461:ASN:OD1	2.10	0.51
1:A:570:GLN:HG3	1:C:46:GLN:NE2	2.26	0.51
1:C:45:PRO:HB3	1:C:461:ASN:OD1	2.12	0.50
1:C:360:PRO:HB2	1:C:576:PRO:HB3	1.94	0.49
1:C:349:ASN:O	1:C:696:PRO:HD2	2.13	0.48
1:C:418:MET:HE2	1:C:482:LEU:HD12	1.95	0.48
1:A:551:ARG:NH2	2:D:85:GLU:HA	2.29	0.48
2:D:368:ILE:HG21	2:D:560:LEU:HD22	1.95	0.47
2:D:360:PRO:HB2	2:D:576:PRO:HB3	1.96	0.47
1:C:177:VAL:HG21	1:C:405:LYS:HB2	1.96	0.47
1:C:368:ILE:HG21	1:C:560:LEU:HD22	1.96	0.47
1:B:368:ILE:HG21	1:B:560:LEU:HD22	1.97	0.46
1:A:31:ILE:CD1	1:B:602:PRO:HG2	2.46	0.46
1:B:45:PRO:HB3	1:B:461:ASN:OD1	2.15	0.46
1:A:349:ASN:O	1:A:696:PRO:HD2	2.16	0.46
1:A:608:TYR:HB2	1:A:659:MET:HE2	1.98	0.46
1:B:767:GLN:HA	1:B:770:LEU:HD12	1.98	0.46
1:A:387:ALA:HB2	1:A:477:PHE:CD2	2.51	0.46
1:B:177:VAL:HG21	1:B:405:LYS:HB2	1.98	0.45
1:C:595:ASN:CB	1:C:659:MET:HA	2.47	0.45
1:A:771:LEU:HD22	1:A:777:LEU:CD1	2.47	0.45
1:A:368:ILE:HG21	1:A:560:LEU:HD22	1.97	0.45
1:B:595:ASN:CB	1:B:659:MET:HA	2.47	0.45
1:A:360:PRO:HB2	1:A:576:PRO:HB3	1.99	0.45
1:A:643:GLU:OE2	1:C:70:GLU:HG3	2.17	0.45
1:B:731:GLN:HG2	1:B:772:MET:SD	2.57	0.45
1:A:103:TYR:CE2	1:A:797:ILE:HG21	2.52	0.44
1:B:360:PRO:HB2	1:B:576:PRO:HB3	1.97	0.44
1:B:301:LEU:HB2	1:B:323:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:387:ALA:HB2	2:D:477:PHE:CD2	2.53	0.44
2:D:499:PRO:HA	2:D:504:PHE:CG	2.53	0.44
1:C:767:GLN:HA	1:C:770:LEU:HD12	1.99	0.44
2:D:369:MET:HE1	2:D:528:ILE:HG12	1.99	0.43
1:A:187:PRO:CB	1:A:197:LEU:HD11	2.46	0.43
1:B:493:LYS:HE2	1:B:714:THR:HG22	2.00	0.43
1:C:499:PRO:HA	1:C:504:PHE:CG	2.52	0.43
1:A:45:PRO:HB3	1:A:461:ASN:OD1	2.18	0.43
1:A:499:PRO:HA	1:A:504:PHE:CG	2.54	0.43
1:C:387:ALA:HB2	1:C:477:PHE:CD2	2.53	0.43
2:D:420:TYR:HB2	2:D:445:MET:HE1	2.00	0.43
2:D:305:LYS:HG3	2:D:321:ILE:HD11	2.01	0.42
2:D:301:LEU:HB2	2:D:323:SER:HB2	2.01	0.42
1:C:12:ALA:CB	2:D:243:ILE:HD11	2.47	0.42
1:C:608:TYR:HB2	1:C:659:MET:HE2	2.01	0.42
1:C:607:ALA:HB2	1:C:649:VAL:HB	2.02	0.41
1:B:12:ALA:HB3	1:C:243:ILE:HD11	2.01	0.41
1:B:349:ASN:O	1:B:696:PRO:HD2	2.20	0.41
1:B:607:ALA:HB2	1:B:649:VAL:HB	2.01	0.41
1:B:608:TYR:HB2	1:B:659:MET:HE2	2.01	0.41
1:A:28:ASP:OD2	1:B:602:PRO:HD2	2.20	0.41
2:D:608:TYR:HB2	2:D:659:MET:HE2	2.03	0.41
1:B:499:PRO:HA	1:B:504:PHE:CG	2.56	0.41
1:C:187:PRO:CB	1:C:197:LEU:HD11	2.47	0.41
2:D:490:GLU:HG3	2:D:511:THR:HG22	2.03	0.41
1:B:420:TYR:HB2	1:B:445:MET:HE1	2.03	0.40
1:C:96:PRO:HD2	1:C:266:LEU:HD21	2.03	0.40
1:C:355:LEU:HB2	1:C:386:TYR:HB2	2.03	0.40
1:A:595:ASN:CB	1:A:659:MET:HA	2.51	0.40
1:A:596:LYS:CB	1:A:598:LEU:HG	2.51	0.40
1:C:490:GLU:HB3	1:C:507:LEU:HD22	2.04	0.40
2:D:595:ASN:CB	2:D:659:MET:HA	2.51	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	785/853 (92%)	761 (97%)	23 (3%)	1 (0%)	48	79
1	B	785/853 (92%)	761 (97%)	23 (3%)	1 (0%)	48	79
1	C	785/853 (92%)	758 (97%)	26 (3%)	1 (0%)	48	79
2	D	674/770 (88%)	651 (97%)	22 (3%)	1 (0%)	48	79
All	All	3029/3329 (91%)	2931 (97%)	94 (3%)	4 (0%)	48	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	406	GLY
1	B	406	GLY
1	C	406	GLY
1	A	406	GLY

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	669/739 (90%)	656 (98%)	13 (2%)	50	66
1	B	668/739 (90%)	654 (98%)	14 (2%)	47	64
1	C	669/739 (90%)	655 (98%)	14 (2%)	47	64
2	D	573/593 (97%)	562 (98%)	11 (2%)	50	66
All	All	2579/2810 (92%)	2527 (98%)	52 (2%)	48	65

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	14	ILE

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Mol	Chain	Res	Type
1	A	29	VAL
1	A	94	SER
1	A	231	LEU
1	A	393	LEU
1	A	566	ILE
1	A	669	ILE
1	A	772	MET
1	A	773	LYS
1	A	792	ILE
1	A	795	ASP
1	A	797	ILE
1	B	6	ASN
1	B	14	ILE
1	B	15	LEU
1	B	29	VAL
1	B	94	SER
1	B	231	LEU
1	B	393	LEU
1	B	450	SER
1	B	566	ILE
1	B	586	SER
1	B	669	ILE
1	B	773	LYS
1	B	792	ILE
1	B	795	ASP
1	C	6	ASN
1	C	14	ILE
1	C	15	LEU
1	C	19	MET
1	C	58	ARG
1	C	94	SER
1	C	231	LEU
1	C	393	LEU
1	C	450	SER
1	C	566	ILE
1	C	586	SER
1	C	669	ILE
1	C	792	ILE
1	C	795	ASP
2	D	6	ASN
2	D	14	ILE
2	D	29	VAL

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Mol	Chain	Res	Type
2	D	94	SER
2	D	231	LEU
2	D	393	LEU
2	D	450	SER
2	D	566	ILE
2	D	586	SER
2	D	669	ILE
2	D	687	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	429	ASN
1	A	623	ASN
1	A	731	GLN
1	A	793	GLN
1	B	226	ASN
1	B	329	HIS
1	B	429	ASN
1	B	623	ASN
1	B	768	GLN
1	C	46	GLN
1	C	50	GLN
1	C	203	GLN
1	C	226	ASN
1	C	378	ASN
1	C	429	ASN
1	C	623	ASN
1	C	768	GLN
1	C	793	GLN
2	D	226	ASN
2	D	329	HIS
2	D	378	ASN
2	D	429	ASN
2	D	623	ASN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	687:LEU	C	688:UNK	N	3.36
1	D	767:UNK	C	768:UNK	N	1.03
1	D	700:UNK	C	701:UNK	N	1.02

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	789/853 (92%)	-0.42	1 (0%) 92 87	50, 80, 118, 174	0
1	B	789/853 (92%)	-0.22	4 (0%) 87 71	62, 113, 183, 214	0
1	C	789/853 (92%)	-0.45	2 (0%) 90 78	49, 85, 131, 179	0
2	D	678/770 (88%)	-0.25	4 (0%) 85 68	58, 103, 162, 190	0
All	All	3045/3329 (91%)	-0.34	11 (0%) 88 74	49, 93, 158, 214	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	798	ILE	4.2
2	D	434	PRO	3.5
1	B	728	LEU	3.4
1	B	747	LEU	3.2
2	D	666	LEU	2.5
1	B	729	LEU	2.4
1	A	798	ILE	2.3
1	C	798	ILE	2.3
2	D	687	LEU	2.2
1	C	786	ARG	2.1
2	D	665	ASP	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.