Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 04:07 am GMT

PDB ID	:	2CJQ
Title	:	Bovine viral diarrhea virus CP7-R12 RNA-dependent RNA polymerase
Authors	:	Choi, K.H.; Gallei, A.; Becher, P.; Rossmann, M.G.
Deposited on	:	2006-04-05
Resolution	:	2.60 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 2.60 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	Percentile Ranks	Value
Rfree		0.268
Clashscore		21
Ramachandran outliers		1.5%
Sidechain outliers		10.8%
RSRZ outliers		3.5%

Worse *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
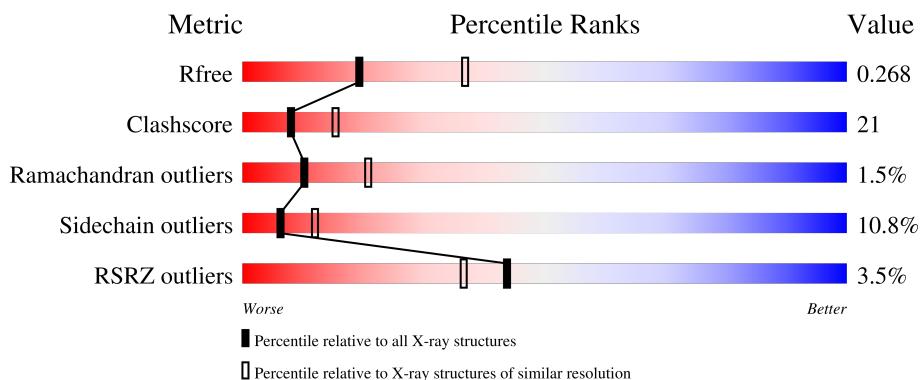
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	720	3% / 47% / 23% / 5% / 24%
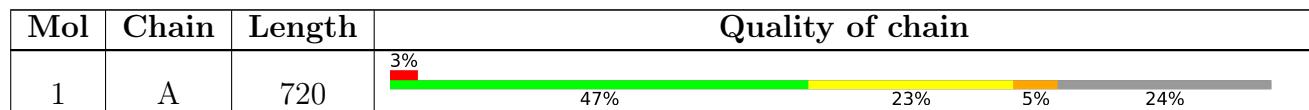
2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 4424 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	546	Total 4393	C 2794	N 771	O 811	S 17	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	THR	ILE	conflict	UNP Q96662
A	148	ILE	SER	conflict	UNP Q96662
A	348	ASN	ALA	conflict	UNP Q96662

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total 31	O 31	0	0

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
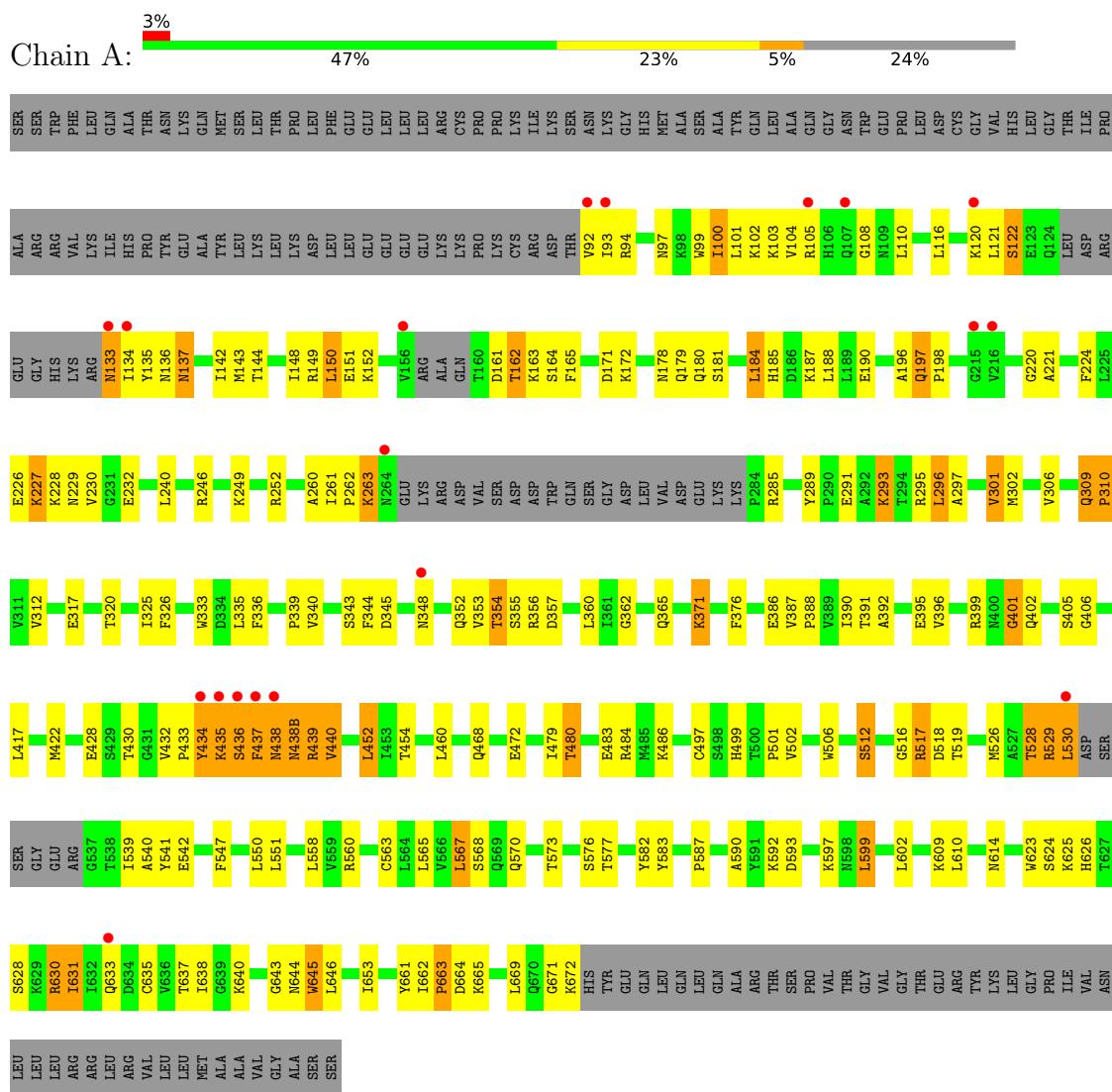
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	106.24Å 106.24Å 55.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.60 47.45 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.8 (50.00-2.60) 95.4 (47.45-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.259 0.260 , 0.268	Depositor DCC
R_{free} test set	1890 reflections (9.88%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l 0.046 for h,-h-k,-l 0.024 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	4424	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \|L\| >$, $< L^2 >$ 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	0.41	0/4484	0.67	2/6056 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	437	PHE	N-CA-C	-8.55	87.91	111.00
1	A	310	PRO	N-CA-C	-5.20	98.59	112.10

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	4393	0	4427	189	0
2	A	31	0	0	0	0
All	All	4424	0	4427	189	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 21.

All (189) 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:435:LYS:HA	1:A:435:LYS:HE2	1.31	1.13
1:A:665:LYS:HD2	1:A:665:LYS:H	1.20	1.06
1:A:530:LEU:H	1:A:530:LEU:HD23	1.15	1.04
1:A:438:ASN:CG	1:A:438(B):ASN:H	1.59	1.03
1:A:92:VAL:HG12	1:A:93:ILE:H	1.34	0.90
1:A:309:GLN:HA	1:A:309:GLN:OE1	1.68	0.90
1:A:227:LYS:HD2	1:A:227:LYS:H	1.42	0.84
1:A:435:LYS:HA	1:A:435:LYS:CE	1.98	0.84
1:A:150:LEU:H	1:A:150:LEU:HD22	1.42	0.83
1:A:664:ASP:HB3	1:A:665:LYS:HD2	1.60	0.83
1:A:438:ASN:CG	1:A:438(B):ASN:N	2.31	0.82
1:A:530:LEU:H	1:A:530:LEU:CD2	1.92	0.80
1:A:480:THR:HG21	1:A:484:ARG:O	1.82	0.80
1:A:517:ARG:HG2	1:A:517:ARG:HH11	1.45	0.80
1:A:143:MET:HG2	1:A:148:ILE:HD12	1.63	0.78
1:A:371:LYS:N	1:A:371:LYS:HD2	1.97	0.78
1:A:371:LYS:H	1:A:371:LYS:CD	1.98	0.77
1:A:165:PHE:CD1	1:A:262:PRO:HG3	2.20	0.76
1:A:221:ALA:O	1:A:295:ARG:NH2	2.19	0.74
1:A:285:ARG:HH11	1:A:285:ARG:HG3	1.53	0.73
1:A:178:ASN:HD21	1:A:352:GLN:HA	1.54	0.72
1:A:501:PRO:O	1:A:609:LYS:HE2	1.89	0.72
1:A:134:ILE:HG22	1:A:135:TYR:N	2.04	0.72
1:A:120:LYS:HG2	1:A:121:LEU:N	2.05	0.71
1:A:644:ASN:C	1:A:645:TRP:HE3	1.94	0.70
1:A:437:PHE:HB2	1:A:440:VAL:HG11	1.72	0.70
1:A:172:LYS:HE2	1:A:348:ASN:HD21	1.56	0.69
1:A:665:LYS:H	1:A:665:LYS:CD	1.97	0.69
1:A:540:ALA:O	1:A:576:SER:N	2.25	0.68
1:A:371:LYS:HD2	1:A:371:LYS:H	1.52	0.68
1:A:150:LEU:H	1:A:150:LEU:CD2	2.07	0.68
1:A:354:THR:HG22	1:A:356:ARG:N	2.09	0.67
1:A:517:ARG:HH11	1:A:517:ARG:CG	2.06	0.67
1:A:92:VAL:HG12	1:A:93:ILE:N	2.08	0.67
1:A:261:ILE:HG22	1:A:392:ALA:HB2	1.75	0.66
1:A:437:PHE:CD2	1:A:437:PHE:O	2.48	0.66
1:A:343:SER:OG	1:A:486:LYS:HG3	1.95	0.66
1:A:530:LEU:HD23	1:A:530:LEU:N	2.00	0.65
1:A:110:LEU:HB2	1:A:395:GLU:HG2	1.78	0.65
1:A:583:TYR:CE1	1:A:587:PRO:HG3	2.32	0.65
1:A:577:THR:HG23	1:A:582:TYR:CE2	2.31	0.65
1:A:326:PHE:CD2	1:A:501:PRO:HG3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PRO:C	1:A:435:LYS:H	2.01	0.64
1:A:354:THR:HG22	1:A:356:ARG:H	1.61	0.64
1:A:438:ASN:ND2	1:A:438(B):ASN:H	1.97	0.63
1:A:563:CYS:O	1:A:567:LEU:HD12	1.98	0.63
1:A:93:ILE:HG22	1:A:94:ARG:N	2.14	0.62
1:A:635:CYS:HB3	1:A:653:ILE:HG12	1.81	0.62
1:A:590:ALA:O	1:A:593:ASP:HB3	2.00	0.62
1:A:228:LYS:HB3	1:A:232:GLU:CB	2.30	0.61
1:A:357:ASP:HB3	1:A:417:LEU:HD21	1.80	0.61
1:A:161:ASP:HB3	1:A:164:SER:HB3	1.83	0.61
1:A:438(B):ASN:O	1:A:439:ARG:HB2	2.02	0.60
1:A:497:CYS:O	1:A:499:HIS:HD2	1.85	0.59
1:A:100:ILE:HD13	1:A:100:ILE:O	2.02	0.59
1:A:628:SER:O	1:A:631:ILE:HG22	2.02	0.59
1:A:134:ILE:CG2	1:A:135:TYR:N	2.65	0.58
1:A:433:PRO:C	1:A:435:LYS:N	2.53	0.58
1:A:285:ARG:NH2	1:A:405:SER:HB3	2.18	0.58
1:A:228:LYS:HB3	1:A:232:GLU:HB2	1.86	0.58
1:A:669:LEU:HD12	1:A:669:LEU:N	2.19	0.58
1:A:184:LEU:O	1:A:188:LEU:HG	2.04	0.58
1:A:468:GLN:O	1:A:472:GLU:HG3	2.03	0.58
1:A:672:LYS:NZ	1:A:672:LYS:HB2	2.19	0.58
1:A:354:THR:CG2	1:A:356:ARG:H	2.17	0.57
1:A:105:ARG:HG3	1:A:122:SER:OG	2.03	0.57
1:A:662:ILE:N	1:A:662:ILE:HD12	2.17	0.57
1:A:134:ILE:CG2	1:A:135:TYR:H	2.17	0.57
1:A:430:THR:OG1	1:A:432:VAL:HG23	2.04	0.57
1:A:143:MET:HG2	1:A:148:ILE:CD1	2.33	0.56
1:A:185:HIS:HE1	1:A:357:ASP:OD2	1.88	0.56
1:A:540:ALA:HB2	1:A:573:THR:CG2	2.36	0.56
1:A:519:THR:OG1	1:A:614:ASN:ND2	2.39	0.56
1:A:134:ILE:HG22	1:A:135:TYR:H	1.69	0.56
1:A:92:VAL:CG1	1:A:93:ILE:H	2.14	0.55
1:A:333:TRP:CE2	1:A:339:PRO:HB2	2.42	0.54
1:A:133:ASN:N	1:A:530:LEU:HB3	2.21	0.54
1:A:136:ASN:HB3	1:A:542:GLU:OE2	2.08	0.54
1:A:152:LYS:HA	1:A:152:LYS:HE2	1.90	0.54
1:A:390:ILE:HG12	1:A:396:VAL:HG22	1.89	0.54
1:A:110:LEU:HB2	1:A:395:GLU:CG	2.37	0.54
1:A:479:ILE:HD12	1:A:479:ILE:H	1.72	0.54
1:A:181:SER:O	1:A:184:LEU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:TRP:HE3	1:A:645:TRP:N	2.06	0.53
1:A:94:ARG:HG3	1:A:386:GLU:OE2	2.08	0.53
1:A:252:ARG:HG3	1:A:252:ARG:HH11	1.73	0.53
1:A:336:PHE:HB2	1:A:339:PRO:HG3	1.89	0.53
1:A:517:ARG:CG	1:A:517:ARG:NH1	2.69	0.53
1:A:162:THR:O	1:A:162:THR:HG22	2.09	0.53
1:A:103:LYS:O	1:A:121:LEU:HD22	2.09	0.52
1:A:226:GLU:OE2	1:A:293:LYS:NZ	2.42	0.52
1:A:93:ILE:CG2	1:A:94:ARG:N	2.73	0.52
1:A:165:PHE:CG	1:A:262:PRO:HG3	2.44	0.52
1:A:432:VAL:HG11	1:A:437:PHE:HB3	1.92	0.52
1:A:438(B):ASN:O	1:A:439:ARG:CB	2.58	0.52
1:A:540:ALA:HB2	1:A:573:THR:HG22	1.92	0.52
1:A:583:TYR:CZ	1:A:587:PRO:HG3	2.45	0.52
1:A:539:ILE:HD12	1:A:570:GLN:NE2	2.25	0.51
1:A:150:LEU:HD22	1:A:150:LEU:N	2.18	0.51
1:A:289:TYR:HB3	1:A:406:GLY:HA3	1.91	0.51
1:A:228:LYS:HB3	1:A:232:GLU:HB3	1.92	0.51
1:A:480:THR:CG2	1:A:484:ARG:H	2.23	0.51
1:A:310:PRO:O	1:A:312:VAL:HG13	2.11	0.51
1:A:336:PHE:CE1	1:A:454:THR:HA	2.46	0.51
1:A:452:LEU:C	1:A:452:LEU:HD23	2.31	0.51
1:A:120:LYS:HG2	1:A:121:LEU:O	2.11	0.50
1:A:631:ILE:HD13	1:A:631:ILE:O	2.11	0.50
1:A:637:THR:HA	1:A:640:LYS:HD2	1.94	0.50
1:A:180:GLN:OE1	1:A:354:THR:HG21	2.11	0.50
1:A:289:TYR:CB	1:A:406:GLY:HA3	2.42	0.50
1:A:577:THR:HG22	1:A:577:THR:O	2.12	0.49
1:A:635:CYS:CB	1:A:653:ILE:HG12	2.42	0.49
1:A:285:ARG:HG3	1:A:285:ARG:NH1	2.24	0.49
1:A:630:ARG:O	1:A:633:GLN:HG2	2.12	0.49
1:A:502:VAL:CG2	1:A:516:GLY:HA3	2.43	0.49
1:A:502:VAL:HG23	1:A:516:GLY:HA3	1.95	0.49
1:A:297:ALA:O	1:A:301:VAL:HG12	2.13	0.49
1:A:152:LYS:HA	1:A:152:LYS:CE	2.43	0.48
1:A:178:ASN:ND2	1:A:352:GLN:HA	2.25	0.48
1:A:645:TRP:N	1:A:645:TRP:CE3	2.81	0.48
1:A:399:ARG:HD2	1:A:402:GLN:HB2	1.96	0.48
1:A:624:SER:C	1:A:626:HIS:H	2.16	0.48
1:A:391:THR:HG23	1:A:395:GLU:O	2.14	0.47
1:A:149:ARG:O	1:A:152:LYS:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLN:HE21	1:A:197:GLN:HB2	1.57	0.47
1:A:301:VAL:HG22	1:A:302:MET:HE2	1.97	0.47
1:A:100:ILE:HD12	1:A:396:VAL:HG11	1.96	0.47
1:A:93:ILE:HD12	1:A:101:LEU:HD11	1.97	0.46
1:A:260:ALA:HB3	1:A:391:THR:HA	1.96	0.46
1:A:249:LYS:HA	1:A:376:PHE:HB2	1.97	0.46
1:A:644:ASN:N	1:A:645:TRP:CE3	2.83	0.46
1:A:671:GLY:O	1:A:672:LYS:C	2.54	0.46
1:A:93:ILE:HG22	1:A:97:ASN:HB2	1.98	0.46
1:A:560:ARG:HD2	1:A:599:LEU:HD21	1.98	0.46
1:A:104:VAL:HA	1:A:121:LEU:HD23	1.98	0.46
1:A:99:TRP:HA	1:A:102:LYS:CE	2.46	0.46
1:A:662:ILE:N	1:A:662:ILE:CD1	2.79	0.46
1:A:135:TYR:HE2	1:A:528:THR:HG23	1.81	0.46
1:A:301:VAL:HG22	1:A:302:MET:CE	2.46	0.45
1:A:220:GLY:O	1:A:229:ASN:HB2	2.16	0.45
1:A:144:THR:OG1	1:A:150:LEU:HD21	2.16	0.45
1:A:227:LYS:H	1:A:227:LYS:CD	2.12	0.45
1:A:93:ILE:CG2	1:A:97:ASN:HB2	2.47	0.44
1:A:101:LEU:C	1:A:103:LYS:H	2.20	0.44
1:A:592:LYS:HE3	1:A:597:LYS:HA	2.00	0.44
1:A:672:LYS:NZ	1:A:672:LYS:CB	2.79	0.44
1:A:480:THR:HG22	1:A:483:GLU:HA	2.00	0.44
1:A:226:GLU:OE2	1:A:291:GLU:HB3	2.17	0.44
1:A:638:ILE:O	1:A:645:TRP:CD1	2.71	0.44
1:A:387:VAL:HA	1:A:388:PRO:HD3	1.84	0.43
1:A:227:LYS:HE2	1:A:293:LYS:CE	2.47	0.43
1:A:344:PHE:N	1:A:344:PHE:CD2	2.86	0.43
1:A:547:PHE:CE2	1:A:551:LEU:HD11	2.53	0.43
1:A:661:TYR:O	1:A:663:PRO:HD3	2.18	0.43
1:A:335:LEU:HD13	1:A:439:ARG:HD3	2.00	0.43
1:A:438:ASN:OD1	1:A:438(B):ASN:N	2.48	0.43
1:A:643:GLY:HA3	1:A:645:TRP:CZ3	2.54	0.43
1:A:435:LYS:O	1:A:436:SER:HB2	2.18	0.43
1:A:638:ILE:HG22	1:A:645:TRP:HD1	1.84	0.43
1:A:526:MET:CE	1:A:563:CYS:SG	3.07	0.43
1:A:137:ASN:HD22	1:A:137:ASN:HA	1.62	0.42
1:A:438(B):ASN:HD22	1:A:438(B):ASN:HA	1.53	0.42
1:A:333:TRP:CZ2	1:A:339:PRO:HB2	2.54	0.42
1:A:526:MET:HE1	1:A:563:CYS:SG	2.59	0.42
1:A:353:VAL:O	1:A:401:GLY:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:THR:CG2	1:A:355:SER:N	2.83	0.42
1:A:152:LYS:HE2	1:A:152:LYS:CA	2.48	0.42
1:A:672:LYS:HB2	1:A:672:LYS:HZ2	1.83	0.42
1:A:110:LEU:HD12	1:A:110:LEU:HA	1.86	0.42
1:A:197:GLN:HE22	1:A:312:VAL:HB	1.85	0.42
1:A:296:LEU:HD12	1:A:296:LEU:HA	1.92	0.42
1:A:428:GLU:OE1	1:A:434:TYR:HE1	2.03	0.41
1:A:142:ILE:HD13	1:A:565:LEU:CB	2.50	0.41
1:A:506:TRP:HE1	1:A:512:SER:HB3	1.84	0.41
1:A:354:THR:O	1:A:357:ASP:HB2	2.20	0.41
1:A:135:TYR:CE2	1:A:528:THR:HG23	2.55	0.41
1:A:161:ASP:C	1:A:163:LYS:H	2.24	0.41
1:A:197:GLN:HE22	1:A:312:VAL:CB	2.33	0.41
1:A:541:TYR:HA	1:A:576:SER:HB3	2.03	0.41
1:A:220:GLY:HA3	1:A:230:VAL:CG2	2.51	0.41
1:A:136:ASN:OD1	1:A:529:ARG:HB2	2.20	0.41
1:A:320:THR:CG2	1:A:325:ILE:HG12	2.51	0.41
1:A:187:LYS:O	1:A:190:GLU:HB3	2.21	0.41
1:A:196:ALA:O	1:A:198:PRO:HD3	2.21	0.40
1:A:99:TRP:HA	1:A:102:LYS:HE3	2.03	0.40
1:A:301:VAL:HG11	1:A:376:PHE:CE1	2.55	0.40
1:A:344:PHE:CE1	1:A:422:MET:HG3	2.56	0.40
1:A:362:GLY:HA2	1:A:365:GLN:HE21	1.86	0.40
1:A:262:PRO:O	1:A:263:LYS:C	2.60	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	536/720 (74%)	500 (93%)	28 (5%)	8 (2%)	10	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	LYS
1	A	438	ASN
1	A	224	PHE
1	A	401	GLY
1	A	436	SER
1	A	625	LYS
1	A	108	GLY
1	A	162	THR

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	482/634 (76%)	430 (89%)	52 (11%)	6	12

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

Mol	Chain	Res	Type
1	A	100	ILE
1	A	116	LEU
1	A	122	SER
1	A	133	ASN
1	A	137	ASN
1	A	150	LEU
1	A	151	GLU
1	A	171	ASP
1	A	179	GLN
1	A	184	LEU
1	A	197	GLN
1	A	227	LYS
1	A	240	LEU
1	A	246	ARG
1	A	293	LYS
1	A	296	LEU
1	A	301	VAL

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Mol	Chain	Res	Type
1	A	306	VAL
1	A	309	GLN
1	A	317	GLU
1	A	340	VAL
1	A	345	ASP
1	A	354	THR
1	A	360	LEU
1	A	371	LYS
1	A	434	TYR
1	A	435	LYS
1	A	438(B)	ASN
1	A	439	ARG
1	A	440	VAL
1	A	452	LEU
1	A	460	LEU
1	A	480	THR
1	A	512	SER
1	A	517	ARG
1	A	518	ASP
1	A	528	THR
1	A	529	ARG
1	A	530	LEU
1	A	550	LEU
1	A	558	LEU
1	A	567	LEU
1	A	568	SER
1	A	599	LEU
1	A	602	LEU
1	A	610	LEU
1	A	623	TRP
1	A	630	ARG
1	A	631	ILE
1	A	645	TRP
1	A	646	LEU
1	A	663	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	137	ASN
1	A	178	ASN

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Mol	Chain	Res	Type
1	A	197	GLN
1	A	202	HIS
1	A	211	GLN
1	A	304	ASN
1	A	337	ASN
1	A	348	ASN
1	A	365	GLN
1	A	438(B)	ASN
1	A	499	HIS
1	A	578	GLN
1	A	614	ASN
1	A	659	HIS

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 monosaccharides 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 (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(Å²)	Q<0.9
1	A	546/720 (75%)	0.32	19 (3%)	44	36	26, 48, 93, 128	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	ASN	5.4
1	A	530	LEU	4.6
1	A	438	ASN	3.6
1	A	348	ASN	3.3
1	A	134	ILE	3.0
1	A	156	VAL	2.8
1	A	434	TYR	2.8
1	A	92	VAL	2.6
1	A	435	LYS	2.3
1	A	633	GLN	2.3
1	A	93	ILE	2.3
1	A	120	LYS	2.2
1	A	436	SER	2.2
1	A	105	ARG	2.2
1	A	133	ASN	2.1
1	A	216	VAL	2.1
1	A	437	PHE	2.1
1	A	215	GLY	2.0
1	A	107	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.