



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 10:46 AM EST

PDB ID : 1QUV
Title : CRYSTAL STRUCTURE OF THE RNA DIRECTED RNA POLYMERASE
OF HEPATITIS C VIRUS
Authors : Ago, H.; Miyano, M.; Adachi, T.; Habuka, N.
Deposited on : 1999-07-04
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

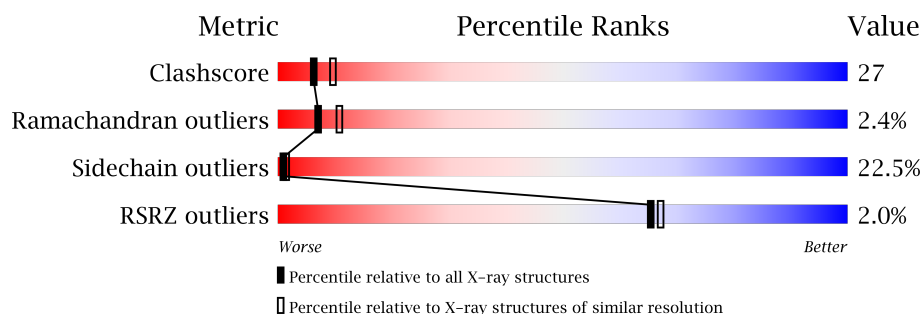
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

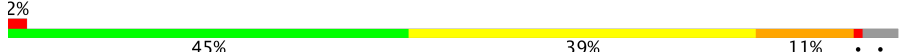
The reported resolution of this entry is 2.50 Å.

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))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	578	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4580 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 PROTEIN (RNA-DIRECTED RNA POLYMERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4296	2711	758	796	31			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	544	GLN	ARG	ENGINEERED MUTATION	UNP P26663

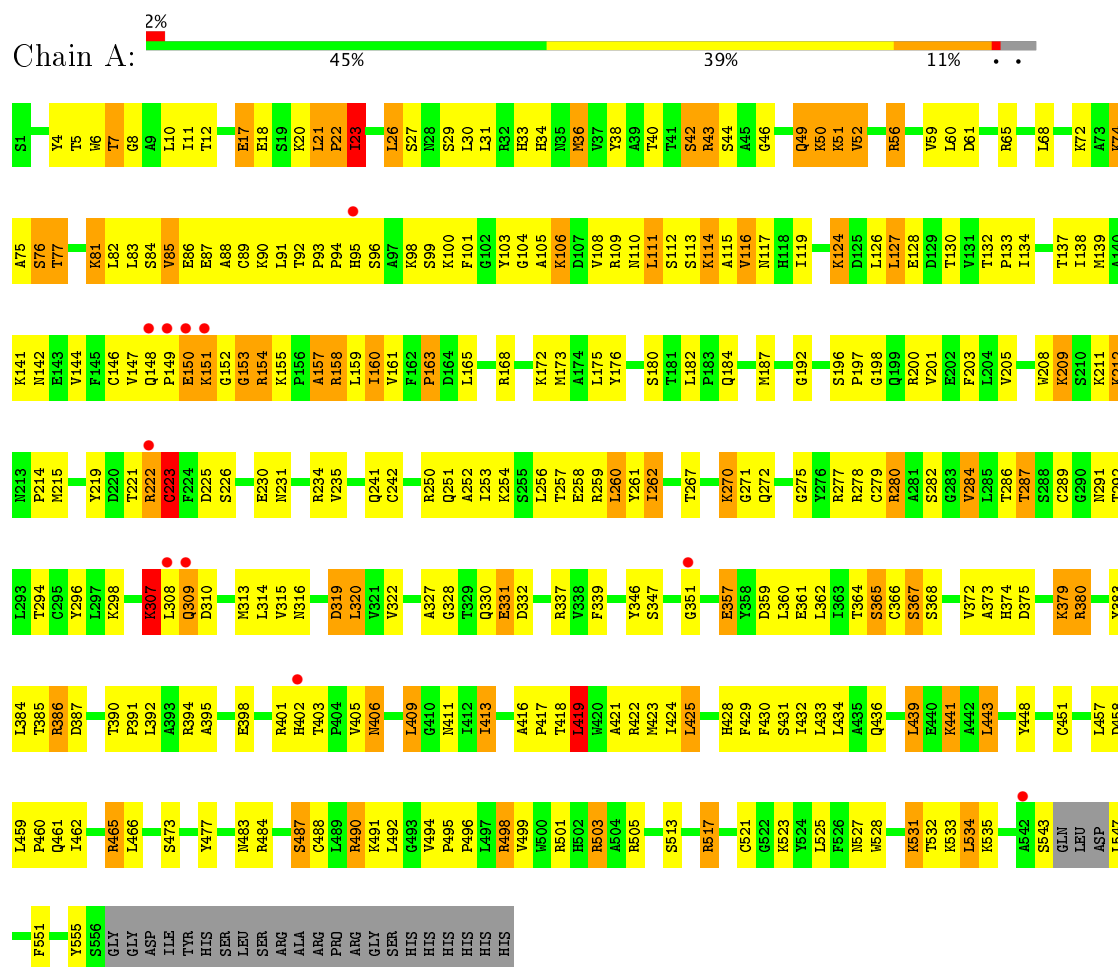
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	284	Total	O	0	0
			284	284		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: PROTEIN (RNA-DIRECTED RNA POLYMERASE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	63.65Å 63.65Å 262.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-2.50) 97.5 (19.70-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	15.56 (at 2.50Å)	Xtriage
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.223 , 0.316 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4580	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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	0.50	0/4389	0.72	1/5955 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	LEU	CA-CB-CG	5.73	128.48	115.30

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	4296	0	4326	232	0
2	A	284	0	0	17	0
All	All	4580	0	4326	232	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 27.

All (232) 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:531:LYS:H	1:A:531:LYS:HD2	1.21	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LEU:HD13	1:A:432:ILE:HD12	1.41	1.01
1:A:52:VAL:HG22	1:A:226:SER:OG	1.63	0.98
1:A:127:LEU:HD23	1:A:251:GLN:HG2	1.46	0.97
1:A:222:ARG:HG3	1:A:351:GLY:HA2	1.48	0.95
1:A:498:ARG:HG2	1:A:499:VAL:N	1.88	0.89
1:A:141:LYS:HD2	1:A:158:ARG:HH12	1.37	0.88
1:A:12:THR:HG21	1:A:270:LYS:HZ2	1.36	0.88
1:A:134:ILE:HG13	1:A:259:ARG:HB3	1.56	0.87
1:A:158:ARG:HH11	1:A:158:ARG:CB	1.91	0.82
1:A:141:LYS:HD2	1:A:158:ARG:NH1	1.94	0.80
1:A:89:CYS:HB3	1:A:108:VAL:O	1.82	0.80
1:A:284:VAL:O	1:A:287:THR:HG22	1.80	0.80
1:A:531:LYS:H	1:A:531:LYS:CD	1.92	0.80
1:A:205:VAL:HG12	1:A:209:LYS:HE2	1.64	0.79
1:A:359:ASP:HB3	1:A:362:LEU:HD13	1.64	0.78
1:A:113:SER:O	1:A:117:ASN:HB2	1.84	0.77
1:A:547:LEU:N	2:A:695:HOH:O	2.17	0.77
1:A:307:LYS:H	1:A:307:LYS:HD3	1.50	0.77
1:A:132:THR:O	1:A:259:ARG:HD3	1.85	0.76
1:A:367:SER:O	1:A:386:ARG:HG3	1.86	0.75
1:A:380:ARG:NH1	2:A:606:HOH:O	2.19	0.74
1:A:272:GLN:NE2	2:A:692:HOH:O	2.22	0.73
1:A:222:ARG:HG3	1:A:351:GLY:CA	2.16	0.73
1:A:307:LYS:HG3	1:A:309:GLN:OE1	1.87	0.73
1:A:457:LEU:HB3	1:A:517:ARG:HD2	1.70	0.73
1:A:196:SER:HB2	1:A:466:LEU:HD22	1.70	0.73
1:A:386:ARG:HG2	1:A:387:ASP:N	2.03	0.72
1:A:234:ARG:HG3	1:A:262:ILE:HD11	1.72	0.72
1:A:74:LYS:O	1:A:77:THR:HB	1.91	0.71
1:A:531:LYS:HD2	1:A:531:LYS:N	2.03	0.70
1:A:30:LEU:HB2	1:A:428:HIS:CD2	2.27	0.70
1:A:379:LYS:HG3	2:A:620:HOH:O	1.91	0.69
1:A:357:GLU:OE1	1:A:357:GLU:HA	1.90	0.69
1:A:458:ASP:HA	1:A:461:GLN:NE2	2.07	0.69
1:A:180:SER:HB3	1:A:555:TYR:OH	1.92	0.69
1:A:81:LYS:HD3	2:A:686:HOH:O	1.93	0.68
1:A:398:GLU:HG2	1:A:403:THR:OG1	1.92	0.67
1:A:198:GLY:O	1:A:201:VAL:HG12	1.94	0.67
1:A:36:MET:HE3	1:A:147:VAL:HG22	1.75	0.67
1:A:46:GLY:HA2	1:A:49:GLN:HE21	1.58	0.67
1:A:103:TYR:HB3	1:A:114:LYS:HG3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LEU:HD13	1:A:168:ARG:HH11	1.59	0.66
1:A:490:ARG:HD3	2:A:787:HOH:O	1.95	0.66
1:A:18:GLU:HG3	1:A:401:ARG:NH1	2.12	0.65
1:A:12:THR:HG21	1:A:270:LYS:NZ	2.12	0.65
1:A:374:HIS:NE2	1:A:380:ARG:HG3	2.11	0.65
1:A:212:LYS:HB2	1:A:212:LYS:HZ3	1.61	0.65
1:A:187:MET:HE3	1:A:296:TYR:HB2	1.79	0.65
1:A:6:TRP:CE2	1:A:49:GLN:HG2	2.32	0.64
1:A:76:SER:HA	1:A:242:CYS:O	1.97	0.64
1:A:4:TYR:CE1	1:A:52:VAL:HG13	2.32	0.64
1:A:315:VAL:HG22	1:A:320:LEU:HD12	1.80	0.64
1:A:258:GLU:OE2	2:A:766:HOH:O	2.15	0.63
1:A:205:VAL:CG1	1:A:209:LYS:HE2	2.28	0.63
1:A:434:LEU:HD13	1:A:439:LEU:HD21	1.81	0.63
1:A:230:GLU:CD	2:A:760:HOH:O	2.38	0.63
1:A:158:ARG:HB2	1:A:158:ARG:HH11	1.64	0.62
1:A:465:ARG:HG3	1:A:465:ARG:NH1	2.14	0.62
1:A:465:ARG:HG3	1:A:465:ARG:HH11	1.64	0.62
1:A:51:LYS:HB3	1:A:222:ARG:HH22	1.63	0.62
1:A:330:GLN:HA	2:A:828:HOH:O	2.00	0.61
1:A:392:LEU:O	1:A:395:ALA:HB3	2.01	0.61
1:A:429:PHE:O	1:A:433:LEU:HB2	2.00	0.61
1:A:82:LEU:HD13	2:A:612:HOH:O	2.00	0.61
1:A:430:PHE:O	1:A:434:LEU:HB2	2.02	0.60
1:A:6:TRP:CZ2	1:A:49:GLN:HG2	2.36	0.60
1:A:158:ARG:CG	1:A:158:ARG:HH11	2.14	0.60
1:A:260:LEU:O	1:A:277:ARG:NH2	2.33	0.60
1:A:327:ALA:O	1:A:331:GLU:HG3	2.01	0.60
1:A:521:CYS:O	1:A:525:LEU:HG	2.02	0.60
1:A:94:PRO:HG3	1:A:109:ARG:NH1	2.17	0.59
1:A:460:PRO:HG3	1:A:525:LEU:HD21	1.84	0.59
1:A:91:LEU:HD13	1:A:176:TYR:CE1	2.38	0.59
1:A:83:LEU:O	1:A:173:MET:HG2	2.04	0.58
1:A:132:THR:O	1:A:259:ARG:CD	2.49	0.58
1:A:498:ARG:O	1:A:501:ARG:HB2	2.04	0.58
1:A:419:LEU:HD12	1:A:423:MET:SD	2.44	0.57
1:A:160:ILE:HA	1:A:282:SER:OG	2.05	0.57
1:A:357:GLU:OE1	1:A:357:GLU:CA	2.52	0.57
1:A:434:LEU:HD13	1:A:439:LEU:CD2	2.35	0.57
1:A:527:ASN:OD1	1:A:534:LEU:HG	2.05	0.56
1:A:192:GLY:HA3	1:A:316:ASN:ND2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:NH2	1:A:278:ARG:O	2.38	0.56
1:A:365:SER:O	1:A:366:CYS:HB2	2.03	0.56
1:A:380:ARG:HD2	2:A:606:HOH:O	2.05	0.56
1:A:40:THR:O	1:A:142:ASN:HA	2.05	0.56
1:A:159:LEU:HD23	1:A:159:LEU:N	2.21	0.55
1:A:146:CYS:SG	1:A:492:LEU:HD21	2.46	0.55
1:A:110:ASN:O	1:A:111:LEU:HB2	2.06	0.55
1:A:92:THR:O	1:A:109:ARG:NH2	2.40	0.55
1:A:105:ALA:O	1:A:108:VAL:HB	2.06	0.55
1:A:21:LEU:HD13	1:A:22:PRO:HD2	1.87	0.55
1:A:163:PRO:HB3	1:A:260:LEU:HD13	1.88	0.55
1:A:72:LYS:HD3	2:A:653:HOH:O	2.07	0.55
1:A:11:ILE:CD1	1:A:138:ILE:HD13	2.37	0.54
1:A:163:PRO:HB3	1:A:260:LEU:CD1	2.37	0.54
1:A:406:ASN:C	1:A:406:ASN:HD22	2.10	0.54
1:A:439:LEU:HB3	1:A:457:LEU:HD11	1.90	0.54
1:A:187:MET:CE	1:A:292:THR:HG22	2.37	0.54
1:A:346:TYR:O	1:A:347:SER:HB3	2.07	0.54
1:A:280:ARG:NH1	1:A:291:ASN:OD1	2.38	0.54
1:A:383:TYR:CE2	1:A:418:THR:HG22	2.43	0.54
1:A:187:MET:CE	1:A:296:TYR:HB2	2.38	0.54
1:A:90:LYS:HG2	2:A:607:HOH:O	2.08	0.54
1:A:175:LEU:HD13	1:A:286:THR:CG2	2.37	0.54
1:A:465:ARG:CG	1:A:465:ARG:HH11	2.21	0.53
1:A:112:SER:O	1:A:116:VAL:HG13	2.08	0.53
1:A:160:ILE:HD12	1:A:282:SER:OG	2.08	0.53
1:A:18:GLU:CG	1:A:401:ARG:NH1	2.71	0.53
1:A:5:THR:O	1:A:275:GLY:HA3	2.08	0.53
1:A:198:GLY:O	1:A:201:VAL:CG1	2.57	0.53
1:A:60:LEU:O	1:A:65:ARG:NH2	2.42	0.53
1:A:284:VAL:O	1:A:287:THR:CG2	2.55	0.53
1:A:46:GLY:HA2	1:A:49:GLN:NE2	2.24	0.53
1:A:294:THR:CG2	1:A:298:LYS:HE3	2.39	0.52
1:A:383:TYR:HE2	1:A:418:THR:HG22	1.74	0.52
1:A:231:ASN:O	1:A:235:VAL:HG23	2.09	0.52
1:A:160:ILE:HG13	1:A:161:VAL:N	2.24	0.52
1:A:448:TYR:CE1	1:A:551:PHE:HD2	2.27	0.52
1:A:390:THR:HB	1:A:391:PRO:HD3	1.92	0.51
1:A:401:ARG:O	1:A:403:THR:HG23	2.10	0.51
1:A:119:ILE:HD13	1:A:119:ILE:N	2.24	0.51
1:A:23:ILE:HD11	1:A:34:HIS:CE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ILE:CG1	1:A:259:ARG:HD2	2.40	0.51
1:A:86:GLU:HG2	1:A:90:LYS:HE2	1.92	0.51
1:A:87:GLU:O	1:A:90:LYS:HB2	2.11	0.50
1:A:160:ILE:HG13	1:A:161:VAL:H	1.76	0.50
1:A:84:SER:OG	1:A:87:GLU:HG3	2.12	0.50
1:A:124:LYS:O	1:A:128:GLU:HG3	2.12	0.50
1:A:409:LEU:HD12	1:A:409:LEU:O	2.11	0.50
1:A:11:ILE:HD12	1:A:138:ILE:HD13	1.93	0.50
1:A:94:PRO:HD3	1:A:109:ARG:HH22	1.76	0.50
1:A:86:GLU:O	1:A:90:LYS:HG3	2.12	0.49
1:A:458:ASP:HA	1:A:461:GLN:HE22	1.74	0.49
1:A:421:ALA:HA	1:A:425:LEU:HB2	1.94	0.49
1:A:42:SER:O	1:A:44:SER:N	2.46	0.49
1:A:192:GLY:HA3	1:A:316:ASN:HD21	1.77	0.49
1:A:134:ILE:CG1	1:A:259:ARG:HB3	2.36	0.48
1:A:208:TRP:CE2	1:A:214:PRO:HB2	2.49	0.48
1:A:36:MET:HE3	1:A:147:VAL:CG2	2.43	0.48
1:A:391:PRO:HB3	1:A:411:ASN:ND2	2.29	0.48
1:A:413:ILE:HD13	1:A:462:ILE:HG21	1.95	0.48
1:A:423:MET:HG2	1:A:528:TRP:CZ3	2.49	0.48
1:A:100:LYS:HG3	2:A:817:HOH:O	2.13	0.48
1:A:23:ILE:HG13	1:A:34:HIS:CD2	2.49	0.48
1:A:428:HIS:O	1:A:432:ILE:HG12	2.14	0.47
1:A:91:LEU:HD13	1:A:176:TYR:CD1	2.49	0.47
1:A:18:GLU:HB2	1:A:401:ARG:NH1	2.29	0.47
1:A:494:VAL:HG13	1:A:495:PRO:HD2	1.95	0.47
1:A:36:MET:O	1:A:147:VAL:HG13	2.14	0.47
1:A:203:PHE:CE1	1:A:314:LEU:HD13	2.49	0.47
1:A:152:GLY:O	1:A:153:GLY:C	2.53	0.47
1:A:94:PRO:HG3	1:A:109:ARG:HH12	1.80	0.47
1:A:215:MET:HG3	1:A:332:ASP:OD1	2.15	0.47
1:A:104:GLY:O	1:A:108:VAL:HG23	2.15	0.47
1:A:139:MET:HB3	1:A:139:MET:HE3	1.75	0.47
1:A:203:PHE:CD1	1:A:314:LEU:HD13	2.50	0.47
1:A:368:SER:HB2	1:A:385:THR:O	2.15	0.47
1:A:391:PRO:O	1:A:395:ALA:HB2	2.15	0.47
1:A:17:GLU:HB3	1:A:142:ASN:OD1	2.15	0.46
1:A:405:VAL:HG12	1:A:405:VAL:O	2.15	0.46
1:A:416:ALA:O	1:A:422:ARG:HG3	2.15	0.46
1:A:201:VAL:O	1:A:205:VAL:HG23	2.16	0.46
1:A:359:ASP:CB	1:A:362:LEU:HD13	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASP:O	1:A:279:CYS:HB2	2.15	0.46
1:A:144:VAL:HG22	1:A:394:ARG:HG2	1.98	0.46
1:A:280:ARG:HD2	1:A:291:ASN:OD1	2.15	0.45
1:A:148:GLN:O	1:A:149:PRO:C	2.54	0.45
1:A:319:ASP:OD1	1:A:366:CYS:HA	2.15	0.45
1:A:402:HIS:ND1	1:A:402:HIS:C	2.69	0.45
1:A:222:ARG:NH2	1:A:223:CYS:SG	2.86	0.45
1:A:361:GLU:CD	2:A:637:HOH:O	2.55	0.45
1:A:483:ASN:O	1:A:487:SER:HB2	2.15	0.45
1:A:75:ALA:C	1:A:77:THR:H	2.19	0.45
1:A:175:LEU:HD13	1:A:286:THR:HG23	1.98	0.45
1:A:158:ARG:C	1:A:159:LEU:HD23	2.37	0.45
1:A:252:ALA:O	1:A:256:LEU:HD12	2.17	0.45
1:A:99:SER:C	1:A:101:PHE:H	2.19	0.45
1:A:150:GLU:HG2	1:A:150:GLU:H	1.46	0.45
1:A:495:PRO:HA	1:A:496:PRO:HD3	1.91	0.44
1:A:21:LEU:HD12	1:A:21:LEU:C	2.38	0.44
1:A:313:MET:HE2	1:A:313:MET:HB3	1.74	0.44
1:A:212:LYS:HB2	1:A:212:LYS:NZ	2.32	0.44
1:A:523:LYS:HG3	1:A:534:LEU:HD11	1.99	0.44
1:A:21:LEU:C	1:A:23:ILE:H	2.21	0.44
1:A:93:PRO:HA	1:A:94:PRO:HD3	1.75	0.44
1:A:416:ALA:N	1:A:417:PRO:CD	2.81	0.43
1:A:328:GLY:O	1:A:332:ASP:HB2	2.17	0.43
1:A:419:LEU:HB2	1:A:477:TYR:CE1	2.54	0.43
1:A:50:LYS:NZ	2:A:643:HOH:O	2.36	0.43
1:A:7:THR:OG1	1:A:8:GLY:N	2.51	0.43
1:A:106:LYS:O	1:A:109:ARG:N	2.52	0.43
1:A:309:GLN:H	1:A:309:GLN:HG2	1.65	0.43
1:A:115:ALA:O	1:A:119:ILE:HG12	2.19	0.43
1:A:433:LEU:HB3	1:A:439:LEU:HD13	2.00	0.43
1:A:223:CYS:HB3	2:A:672:HOH:O	2.17	0.43
1:A:175:LEU:HD21	1:A:253:ILE:HG12	2.01	0.42
1:A:137:THR:HA	1:A:267:THR:O	2.17	0.42
1:A:77:THR:HG23	1:A:77:THR:O	2.17	0.42
1:A:38:TYR:CZ	1:A:154:ARG:HG2	2.54	0.42
1:A:23:ILE:CG2	1:A:23:ILE:O	2.67	0.42
1:A:257:THR:O	1:A:262:ILE:HB	2.19	0.42
1:A:222:ARG:O	1:A:223:CYS:C	2.57	0.42
1:A:406:ASN:C	1:A:406:ASN:ND2	2.73	0.42
1:A:50:LYS:H	1:A:50:LYS:HG2	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:HG21	1:A:165:LEU:HD21	2.02	0.41
1:A:496:PRO:HB2	1:A:498:ARG:HD2	2.00	0.41
1:A:134:ILE:HG13	1:A:259:ARG:HD2	2.01	0.41
1:A:270:LYS:HG3	1:A:270:LYS:HZ2	1.42	0.41
1:A:132:THR:O	1:A:133:PRO:C	2.59	0.41
1:A:372:VAL:HG12	1:A:373:ALA:N	2.35	0.41
1:A:257:THR:HA	1:A:261:TYR:HB2	2.01	0.41
1:A:219:TYR:CD1	1:A:339:PHE:HE2	2.38	0.41
1:A:386:ARG:HG2	1:A:387:ASP:H	1.80	0.41
1:A:180:SER:CB	1:A:555:TYR:OH	2.64	0.41
1:A:113:SER:O	1:A:117:ASN:CB	2.61	0.41
1:A:148:GLN:HB2	1:A:153:GLY:O	2.21	0.41
1:A:250:ARG:HH11	1:A:250:ARG:HG2	1.85	0.41
1:A:93:PRO:C	1:A:95:HIS:H	2.24	0.41
1:A:241:GLN:OE1	1:A:250:ARG:HG2	2.20	0.41
1:A:152:GLY:O	1:A:153:GLY:O	2.39	0.41
1:A:85:VAL:O	1:A:88:ALA:HB3	2.21	0.41
1:A:40:THR:HB	1:A:157:ALA:HA	2.02	0.40
1:A:5:THR:O	1:A:275:GLY:CA	2.69	0.40
1:A:441:LYS:HD3	1:A:443:LEU:CD2	2.51	0.40
1:A:154:ARG:HH11	1:A:154:ARG:HG3	1.87	0.40
1:A:499:VAL:HG12	1:A:503:ARG:CD	2.51	0.40
1:A:142:ASN:N	1:A:142:ASN:HD22	2.19	0.40
1:A:197:PRO:HB3	1:A:384:LEU:HD12	2.03	0.40
1:A:33:HIS:HB2	1:A:492:LEU:O	2.21	0.40
1:A:402:HIS:ND1	1:A:403:THR:N	2.70	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	549/578 (95%)	496 (90%)	40 (7%)	13 (2%)	7	11

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	ILE
1	A	43	ARG
1	A	153	GLY
1	A	271	GLY
1	A	7	THR
1	A	307	LYS
1	A	151	LYS
1	A	157	ALA
1	A	360	LEU
1	A	513	SER
1	A	223	CYS
1	A	22	PRO
1	A	163	PRO

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	471/492 (96%)	365 (78%)	106 (22%)	1	1

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	17	GLU
1	A	20	LYS
1	A	21	LEU
1	A	23	ILE
1	A	26	LEU
1	A	27	SER
1	A	29	SER

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Mol	Chain	Res	Type
1	A	31	LEU
1	A	36	MET
1	A	42	SER
1	A	43	ARG
1	A	49	GLN
1	A	50	LYS
1	A	51	LYS
1	A	52	VAL
1	A	56	ARG
1	A	59	VAL
1	A	61	ASP
1	A	68	LEU
1	A	74	LYS
1	A	76	SER
1	A	77	THR
1	A	81	LYS
1	A	85	VAL
1	A	96	SER
1	A	98	LYS
1	A	106	LYS
1	A	111	LEU
1	A	114	LYS
1	A	116	VAL
1	A	124	LYS
1	A	126	LEU
1	A	127	LEU
1	A	130	THR
1	A	150	GLU
1	A	151	LYS
1	A	154	ARG
1	A	155	LYS
1	A	158	ARG
1	A	160	ILE
1	A	172	LYS
1	A	182	LEU
1	A	184	GLN
1	A	200	ARG
1	A	209	LYS
1	A	211	LYS
1	A	212	LYS
1	A	221	THR
1	A	222	ARG

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Mol	Chain	Res	Type
1	A	223	CYS
1	A	254	LYS
1	A	260	LEU
1	A	262	ILE
1	A	270	LYS
1	A	280	ARG
1	A	284	VAL
1	A	287	THR
1	A	289	CYS
1	A	307	LYS
1	A	308	LEU
1	A	309	GLN
1	A	310	ASP
1	A	319	ASP
1	A	320	LEU
1	A	322	VAL
1	A	331	GLU
1	A	337	ARG
1	A	357	GLU
1	A	364	THR
1	A	365	SER
1	A	367	SER
1	A	375	ASP
1	A	379	LYS
1	A	380	ARG
1	A	386	ARG
1	A	406	ASN
1	A	409	LEU
1	A	413	ILE
1	A	419	LEU
1	A	424	ILE
1	A	425	LEU
1	A	431	SER
1	A	436	GLN
1	A	439	LEU
1	A	441	LYS
1	A	443	LEU
1	A	451	CYS
1	A	459	LEU
1	A	465	ARG
1	A	473	SER
1	A	484	ARG

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Mol	Chain	Res	Type
1	A	487	SER
1	A	488	CYS
1	A	490	ARG
1	A	491	LYS
1	A	498	ARG
1	A	503	ARG
1	A	505	ARG
1	A	517	ARG
1	A	531	LYS
1	A	532	THR
1	A	533	LYS
1	A	534	LEU
1	A	535	LYS
1	A	543	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	35	ASN
1	A	49	GLN
1	A	206	ASN
1	A	272	GLN
1	A	316	ASN
1	A	355	GLN
1	A	406	ASN
1	A	483	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 carbohydrates 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(Å ²)	Q<0.9
1	A	553/578 (95%)	-0.09	11 (1%) 65 67	5, 26, 46, 65	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	351	GLY	4.0
1	A	151	LYS	3.8
1	A	149	PRO	3.3
1	A	308	LEU	3.2
1	A	148	GLN	3.0
1	A	309	GLN	2.9
1	A	150	GLU	2.5
1	A	95	HIS	2.5
1	A	222	ARG	2.2
1	A	542	ALA	2.1
1	A	402	HIS	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.