



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:01 AM UTC

PDB ID : 3KQH / pdb_00003kqh
Title : Three Conformational Snapshots of the Hepatitis C Virus NS3 Helicase Reveal a Ratchet Translocation Mechanism
Authors : Gu, M.; Rice, C.M.
Deposited on : 2009-11-17
Resolution : 2.40 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

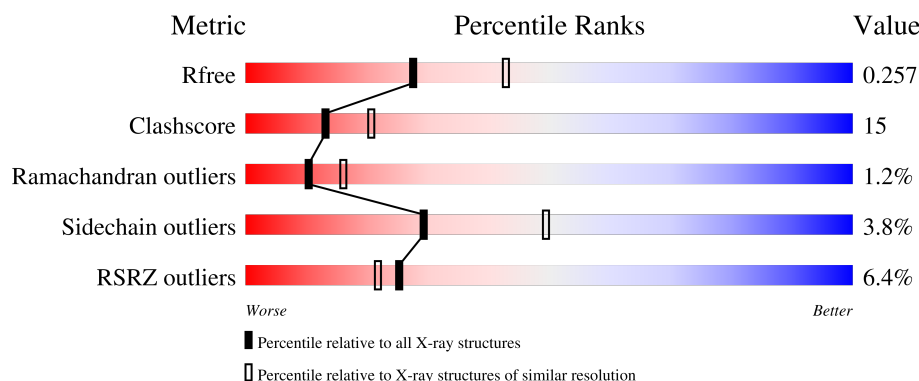
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	436	4% 68% 31% .
1	B	436	8% 67% 30% .
2	C	6	50% 50%
2	D	6	17% 17% 83%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6934 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 Serine protease/NTPase/helicase NS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3275	2074	555	625	21			
1	B	436	Total	C	N	O	S	0	0	0
			3275	2074	555	625	21			

- Molecule 2 is a DNA chain called 5'-D(*AP*AP*AP*AP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	P	0	0	0
			123	60	30	28	5			
2	D	6	Total	C	N	O	P	0	0	0
			123	60	30	28	5			

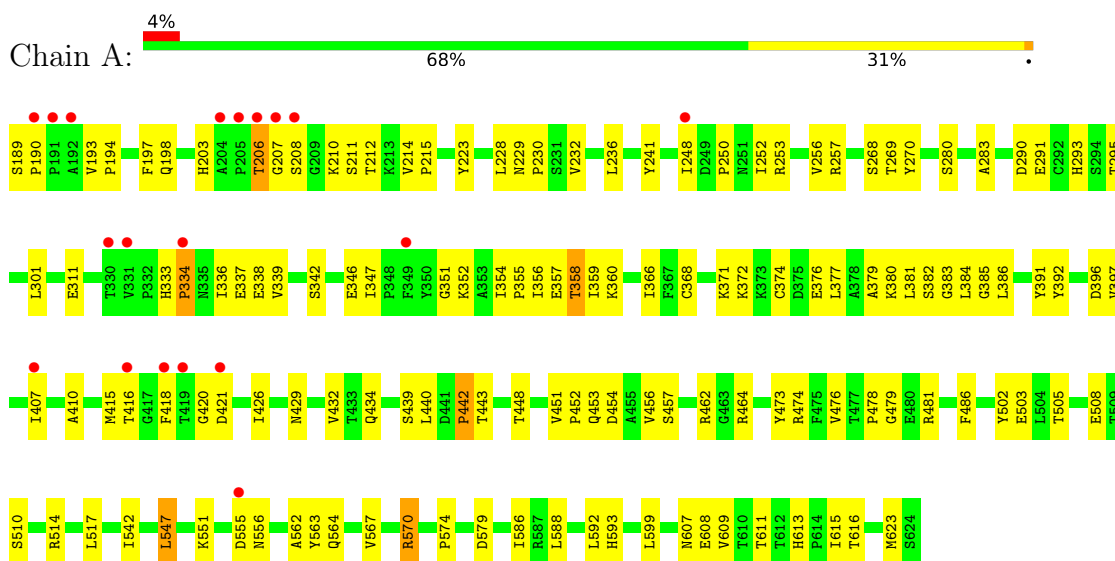
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total	O	0	0
			72	72		
3	B	60	Total	O	0	0
			60	60		
3	C	5	Total	O	0	0
			5	5		
3	D	1	Total	O	0	0
			1	1		

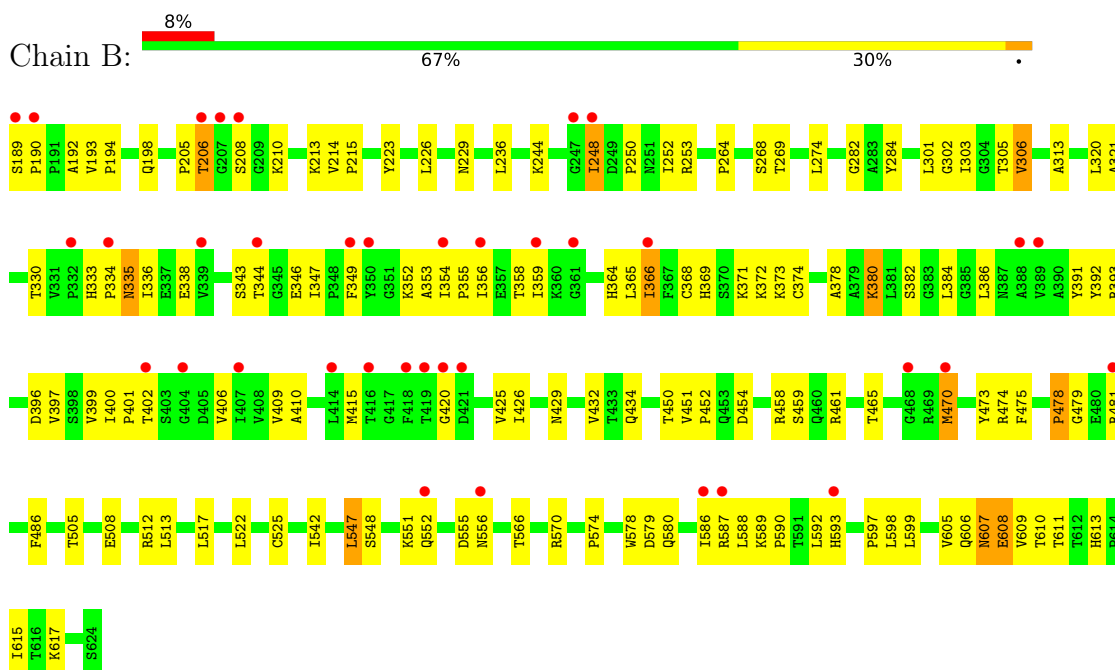
3 Residue-property plots [i](#)

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: Serine protease/NTPase/helicase NS3



- Molecule 1: Serine protease/NTPase/helicase NS3



- Molecule 2: 5'-D(*AP*AP*AP*AP*AP*A)-3'

Chain C:  50% 50%



- Molecule 2: 5'-D(*AP*AP*AP*AP*AP*A)-3'

Chain D:  17% 17% 83%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	45.20Å 115.38Å 197.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.5 (50.00-2.40) 93.4 (50.00-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.258 0.225 , 0.257	Depositor DCC
R_{free} test set	1930 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6934	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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	0.52	0/3356	0.85	3/4585 (0.1%)
1	B	0.49	0/3356	0.86	1/4585 (0.0%)
2	C	0.32	0/140	0.89	1/214 (0.5%)
2	D	0.31	0/140	0.77	1/214 (0.5%)
All	All	0.50	0/6992	0.86	6/9598 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	556	ASN	N-CA-C	6.31	118.04	111.03
2	C	6	DA	C2'-C3'-O3'	5.68	120.03	111.50
1	A	609	VAL	N-CA-C	5.44	116.31	108.48
1	A	564	GLN	N-CA-C	-5.26	105.62	111.36
2	D	4	DA	C2'-C3'-O3'	-5.13	103.80	111.50
1	A	579	ASP	N-CA-C	-5.06	103.84	110.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	563	TYR	Sidechain

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	3275	0	3236	95	0
1	B	3275	0	3236	106	0
2	C	123	0	68	2	0
2	D	123	0	68	5	0
3	A	72	0	0	7	0
3	B	60	0	0	7	0
3	C	5	0	0	1	0
3	D	1	0	0	0	0
All	All	6934	0	6608	199	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 15.

All (199) 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:611:THR:HB	3:A:49:HOH:O	1.55	1.04
1:B:366:ILE:HG23	1:B:426:ILE:HB	1.59	0.83
1:B:607:ASN:ND2	1:B:608:GLU:H	1.77	0.82
1:A:397:VAL:HG11	1:A:418:PHE:HB2	1.63	0.81
1:B:555:ASP:HB2	3:B:45:HOH:O	1.84	0.78
1:B:366:ILE:HD12	1:B:426:ILE:HD12	1.67	0.76
1:B:415:MET:HB2	3:B:43:HOH:O	1.87	0.74
1:A:208:SER:HB2	1:B:470:MET:SD	2.28	0.73
1:A:359:ILE:HD12	1:A:407:ILE:HD13	1.72	0.71
1:A:194:PRO:HG3	1:A:198:GLN:HB2	1.71	0.71
1:B:320:LEU:HD13	1:B:522:LEU:HD21	1.73	0.71
1:A:379:ALA:HA	3:A:76:HOH:O	1.92	0.70
1:A:611:THR:HG23	1:A:616:THR:HG21	1.72	0.70
1:B:505:THR:OG1	1:B:508:GLU:HG3	1.92	0.69
1:A:256:VAL:HG23	1:A:257:ARG:H	1.58	0.67
1:A:611:THR:HG22	1:A:611:THR:O	1.95	0.67
1:A:357:GLU:HA	1:A:360:LYS:HB2	1.76	0.66
1:A:415:MET:HE3	1:A:464:ARG:HH12	1.60	0.66
1:A:547:LEU:O	1:A:551:LYS:HG3	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:GLU:HG2	1:B:473:TYR:HD2	1.61	0.65
1:A:207:GLY:HA2	1:A:210:LYS:HE3	1.78	0.64
1:B:210:LYS:HD2	1:B:321:ALA:HB1	1.80	0.63
1:A:351:GLY:C	1:A:352:LYS:HD2	2.25	0.61
1:A:236:LEU:HD23	1:A:252:ILE:HG21	1.83	0.60
1:A:253:ARG:HB2	1:A:268:SER:HB2	1.84	0.59
1:B:274:LEU:HD21	1:B:302:GLY:HA2	1.83	0.59
1:A:229:ASN:O	1:A:269:THR:HA	2.03	0.58
1:B:349:PHE:HB3	3:B:39:HOH:O	2.03	0.58
1:B:371:LYS:HG3	1:B:392:TYR:CD2	2.37	0.58
1:A:451:VAL:HG23	1:A:452:PRO:HD2	1.83	0.58
1:B:486:PHE:O	1:B:525:CYS:HB2	2.04	0.58
1:B:589:LYS:HB3	1:B:590:PRO:HD3	1.85	0.57
1:A:366:ILE:HG21	1:A:377:LEU:HD21	1.86	0.57
1:A:371:LYS:HG3	1:A:392:TYR:CD2	2.40	0.57
1:B:401:PRO:HG2	1:B:406:VAL:HG11	1.87	0.56
1:B:548:SER:O	1:B:552:GLN:HG3	2.05	0.56
1:A:391:TYR:HB3	1:A:410:ALA:HB2	1.88	0.56
1:B:356:ILE:HD11	1:B:386:LEU:HD11	1.86	0.56
1:B:248:ILE:HD11	1:B:264:PRO:HD2	1.87	0.55
1:B:282:GLY:HA2	1:B:313:ALA:O	2.06	0.55
1:B:305:THR:OG1	1:B:512:ARG:HD3	2.06	0.55
1:B:574:PRO:HG2	1:B:607:ASN:OD1	2.05	0.55
1:B:586:ILE:HG13	1:B:587:ARG:N	2.22	0.55
1:B:192:ALA:O	1:B:194:PRO:HD3	2.06	0.55
1:B:333:HIS:HB3	1:B:336:ILE:HB	1.89	0.55
1:B:391:TYR:HB3	1:B:410:ALA:HB2	1.87	0.55
1:B:425:VAL:HG23	1:B:465:THR:HB	1.88	0.55
1:B:393:ARG:HG2	1:B:393:ARG:HH11	1.71	0.54
1:A:429:ASN:HD22	1:A:429:ASN:N	2.06	0.54
1:B:607:ASN:ND2	1:B:608:GLU:N	2.51	0.54
1:B:599:LEU:HD22	1:B:615:ILE:HG22	1.90	0.54
1:A:339:VAL:O	1:A:474:ARG:HA	2.07	0.53
1:A:334:PRO:HA	3:B:73:HOH:O	2.08	0.53
1:A:189:SER:N	1:A:190:PRO:HD2	2.24	0.53
1:B:365:LEU:C	1:B:366:ILE:HD13	2.34	0.53
1:B:193:VAL:HG21	1:B:223:TYR:CE2	2.44	0.52
1:B:335:ASN:ND2	1:B:335:ASN:H	2.07	0.52
1:B:229:ASN:O	1:B:269:THR:HA	2.10	0.52
1:B:335:ASN:H	1:B:335:ASN:HD22	1.58	0.52
1:B:189:SER:HB3	1:B:190:PRO:HD3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:HIS:HE1	1:B:615:ILE:HD13	1.74	0.52
1:B:607:ASN:HD22	1:B:608:GLU:H	1.56	0.51
1:B:429:ASN:OD1	1:B:475:PHE:HB2	2.10	0.51
1:A:228:LEU:HA	1:A:268:SER:O	2.10	0.51
1:A:502:TYR:OH	2:D:6:DA:H1'	2.11	0.51
1:B:336:ILE:HD11	1:B:465:THR:O	2.11	0.51
1:A:358:THR:HG22	1:A:359:ILE:HG23	1.92	0.51
1:B:380:LYS:HB2	1:B:380:LYS:NZ	2.26	0.51
1:A:452:PRO:HG2	1:A:481:ARG:HH12	1.76	0.51
1:A:397:VAL:CG1	1:A:418:PHE:HB2	2.39	0.50
1:B:335:ASN:HD22	1:B:335:ASN:N	2.08	0.50
1:A:280:SER:HB2	1:A:283:ALA:HB2	1.93	0.50
1:A:366:ILE:HD12	1:A:426:ILE:HD12	1.93	0.50
1:A:333:HIS:HB3	1:A:336:ILE:HB	1.93	0.50
1:A:542:ILE:HD13	1:A:547:LEU:HG	1.94	0.50
1:A:611:THR:HG23	1:A:616:THR:CG2	2.41	0.50
1:A:434:GLN:NE2	1:A:556:ASN:HD22	2.10	0.49
1:B:248:ILE:O	1:B:250:PRO:HD3	2.11	0.49
1:A:453:GLN:HB2	1:A:457:SER:HB3	1.94	0.49
1:A:197:PHE:O	1:A:198:GLN:HG2	2.12	0.49
1:A:232:VAL:HG23	2:D:5:DA:H5''	1.95	0.49
1:B:578:TRP:CZ2	1:B:589:LYS:HG3	2.48	0.49
1:A:382:SER:HA	1:A:386:LEU:O	2.12	0.48
1:A:574:PRO:HG2	1:A:607:ASN:OD1	2.13	0.48
1:B:478:PRO:HG2	1:B:479:GLY:H	1.77	0.48
1:A:451:VAL:CG2	1:A:452:PRO:HD2	2.43	0.48
1:A:505:THR:OG1	1:A:508:GLU:HG3	2.12	0.48
1:A:567:VAL:HG21	1:A:599:LEU:HD11	1.93	0.48
1:B:451:VAL:HG23	1:B:452:PRO:HD2	1.93	0.48
1:B:542:ILE:HD13	1:B:547:LEU:HG	1.94	0.48
1:B:599:LEU:HD22	1:B:615:ILE:CG2	2.44	0.48
1:A:593:HIS:HB3	3:A:10:HOH:O	2.13	0.48
1:A:368:CYS:HB2	1:A:374:CYS:SG	2.54	0.48
1:A:380:LYS:HE2	1:A:384:LEU:HD11	1.94	0.48
1:A:442:PRO:HG2	1:A:443:THR:HG23	1.96	0.48
1:B:349:PHE:CG	1:B:354:ILE:HD11	2.49	0.48
1:B:358:THR:HG23	1:B:474:ARG:CZ	2.44	0.48
1:A:337:GLU:OE2	1:B:213:LYS:HG2	2.14	0.48
1:B:330:THR:HG21	1:B:458:ARG:HB3	1.96	0.48
1:B:372:LYS:HG3	1:B:373:LYS:N	2.27	0.48
1:A:462:ARG:HG3	1:A:473:TYR:CG	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:LEU:O	1:A:386:LEU:HB2	2.14	0.47
1:B:566:THR:O	1:B:570:ARG:HD3	2.15	0.47
1:A:358:THR:HG23	1:A:474:ARG:NE	2.30	0.47
1:A:397:VAL:HG21	1:A:416:THR:O	2.15	0.47
1:B:372:LYS:HE3	3:C:37:HOH:O	2.15	0.47
1:B:210:LYS:HA	1:B:214:VAL:CG2	2.45	0.47
1:B:359:ILE:HA	1:B:364:HIS:CD2	2.49	0.47
1:B:579:ASP:CG	1:B:580:GLN:H	2.23	0.47
1:B:248:ILE:O	1:B:248:ILE:HG23	2.15	0.46
1:B:303:ILE:O	1:B:306:VAL:HG13	2.14	0.46
1:B:391:TYR:OH	1:B:397:VAL:HG22	2.15	0.46
1:B:236:LEU:HD23	1:B:252:ILE:HG21	1.96	0.46
1:A:510:SER:O	1:A:514:ARG:HB2	2.15	0.46
1:B:391:TYR:O	1:B:410:ALA:CB	2.64	0.46
1:B:461:ARG:HG3	1:B:461:ARG:HH11	1.81	0.46
1:B:333:HIS:ND1	1:B:334:PRO:HD2	2.31	0.46
1:B:508:GLU:HB3	3:B:7:HOH:O	2.15	0.46
1:A:193:VAL:HG21	1:A:223:TYR:CE2	2.51	0.45
1:B:344:THR:O	1:B:355:PRO:HG3	2.16	0.45
1:B:391:TYR:CE2	1:B:415:MET:HG2	2.52	0.45
1:B:588:LEU:O	1:B:592:LEU:HG	2.16	0.45
1:A:478:PRO:HG2	1:A:479:GLY:H	1.81	0.45
1:B:356:ILE:CD1	1:B:386:LEU:HD11	2.46	0.45
1:B:371:LYS:HG3	1:B:392:TYR:CG	2.51	0.45
1:B:429:ASN:HD22	1:B:429:ASN:N	2.14	0.45
1:A:352:LYS:HD3	1:A:476:VAL:HG13	1.99	0.45
1:B:451:VAL:CG2	1:B:452:PRO:HD2	2.47	0.45
1:B:368:CYS:HB2	1:B:374:CYS:SG	2.57	0.45
1:B:380:LYS:O	1:B:384:LEU:HB2	2.17	0.44
1:B:597:PRO:HA	1:B:610:THR:HG23	2.00	0.44
1:A:440:LEU:HD23	1:A:623:MET:HE2	1.99	0.44
1:A:230:PRO:HD3	1:A:270:TYR:HE2	1.83	0.44
1:B:432:VAL:HG21	2:C:2:DA:H5"	2.00	0.44
1:A:376:GLU:O	1:A:379:ALA:HB3	2.17	0.44
1:A:206:THR:HA	3:A:50:HOH:O	2.18	0.44
1:A:542:ILE:HD11	1:A:562:ALA:HB3	2.00	0.44
1:B:391:TYR:O	1:B:410:ALA:HB1	2.18	0.44
1:B:356:ILE:C	1:B:358:THR:H	2.25	0.44
1:B:194:PRO:HG2	1:B:198:GLN:HB3	1.99	0.44
1:A:454:ASP:OD1	1:A:456:VAL:N	2.51	0.43
1:A:355:PRO:O	1:A:358:THR:HB	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:TYR:CE2	1:B:470:MET:HB3	2.54	0.43
1:B:611:THR:O	1:B:617:LYS:HE2	2.18	0.43
1:A:371:LYS:HG3	1:A:392:TYR:CG	2.54	0.43
1:A:613:HIS:CE1	1:A:615:ILE:HG12	2.54	0.43
1:A:338:GLU:HG2	1:A:473:TYR:HD2	1.84	0.43
1:B:400:ILE:CD1	1:B:415:MET:HE2	2.49	0.43
1:B:547:LEU:O	1:B:551:LYS:HG3	2.19	0.43
1:B:598:LEU:HB2	1:B:609:VAL:HG13	2.01	0.43
1:A:248:ILE:O	1:A:250:PRO:HD3	2.19	0.42
1:B:354:ILE:N	1:B:354:ILE:HD12	2.35	0.42
1:B:396:ASP:O	1:B:399:VAL:HG22	2.19	0.42
1:A:211:SER:HB3	1:A:290:ASP:OD1	2.19	0.42
1:A:214:VAL:N	1:A:215:PRO:HD2	2.34	0.42
1:A:347:ILE:HG21	1:A:381:LEU:HD21	2.01	0.42
1:A:383:GLY:C	1:A:385:GLY:H	2.27	0.42
1:A:434:GLN:HG3	2:D:2:DA:H62	1.84	0.42
1:A:588:LEU:O	1:A:592:LEU:HG	2.18	0.42
1:B:214:VAL:HB	1:B:215:PRO:CD	2.49	0.42
1:B:302:GLY:O	1:B:306:VAL:HG12	2.19	0.42
1:A:382:SER:HB3	3:A:76:HOH:O	2.19	0.42
1:B:226:LEU:HD22	1:B:284:TYR:CE2	2.53	0.42
1:A:212:THR:O	1:A:215:PRO:HG2	2.19	0.42
1:B:374:CYS:HA	1:B:409:VAL:CG1	2.49	0.42
1:B:454:ASP:HB2	1:B:481:ARG:O	2.19	0.42
1:B:369:HIS:HD2	1:B:450:THR:CG2	2.32	0.42
1:B:429:ASN:N	1:B:429:ASN:ND2	2.67	0.42
1:A:432:VAL:HG21	2:D:2:DA:H5'	2.01	0.42
1:A:354:ILE:HD13	1:A:426:ILE:HD13	2.02	0.42
1:A:429:ASN:N	1:A:429:ASN:ND2	2.64	0.42
1:A:342:SER:HB2	3:A:123:HOH:O	2.18	0.42
1:A:380:LYS:O	1:A:384:LEU:HD13	2.19	0.42
1:B:205:PRO:O	1:B:206:THR:C	2.63	0.41
1:A:291:GLU:C	1:A:293:HIS:H	2.27	0.41
1:B:593:HIS:HB2	3:B:27:HOH:O	2.19	0.41
1:A:256:VAL:HG23	1:A:257:ARG:N	2.29	0.41
1:A:354:ILE:HD11	1:A:426:ILE:HG21	2.02	0.41
1:A:502:TYR:O	1:A:503:GLU:C	2.62	0.41
1:B:450:THR:HG23	2:C:1:DA:C5	2.56	0.41
1:A:570:ARG:CG	1:A:570:ARG:HH11	2.33	0.41
1:B:330:THR:HG22	1:B:459:SER:OG	2.21	0.41
1:B:352:LYS:HB3	1:B:353:ALA:H	1.65	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ILE:HG23	1:A:357:GLU:N	2.36	0.41
1:B:253:ARG:HB2	1:B:268:SER:HB2	2.03	0.41
1:B:378:ALA:O	1:B:382:SER:HB2	2.21	0.41
1:B:513:LEU:O	1:B:517:LEU:HD13	2.21	0.41
1:A:203:HIS:HB2	3:A:63:HOH:O	2.20	0.41
1:B:338:GLU:HA	1:B:473:TYR:O	2.21	0.41
1:A:358:THR:HG23	1:A:474:ARG:CZ	2.51	0.40
1:B:402:THR:N	3:B:122:HOH:O	2.53	0.40
1:A:280:SER:HB2	1:A:283:ALA:CB	2.52	0.40
1:A:613:HIS:HE1	1:A:615:ILE:HG12	1.84	0.40
1:B:349:PHE:HB2	1:B:354:ILE:HD11	2.04	0.40
1:A:197:PHE:CD2	1:A:311:GLU:HB2	2.57	0.40
1:A:295:THR:HB	1:A:486:PHE:HB3	2.04	0.40
1:A:586:ILE:HD12	1:A:586:ILE:HA	1.91	0.40
1:B:347:ILE:O	1:B:353:ALA:HA	2.21	0.40
2:D:1:DA:HO5'	2:D:1:DA:H8	1.67	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	434/436 (100%)	398 (92%)	32 (7%)	4 (1%)	14	22
1	B	434/436 (100%)	396 (91%)	32 (7%)	6 (1%)	9	13
All	All	868/872 (100%)	794 (92%)	64 (7%)	10 (1%)	10	16

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	607	ASN
1	A	420	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	206	THR
1	B	208	SER
1	B	248	ILE
1	B	420	GLY
1	A	421	ASP
1	A	206	THR
1	B	478	PRO
1	A	334	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	356/356 (100%)	343 (96%)	13 (4%)	30	51
1	B	356/356 (100%)	342 (96%)	14 (4%)	28	48
All	All	712/712 (100%)	685 (96%)	27 (4%)	29	49

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	301	LEU
1	A	346	GLU
1	A	358	THR
1	A	372	LYS
1	A	396	ASP
1	A	439	SER
1	A	442	PRO
1	A	448	THR
1	A	517	LEU
1	A	547	LEU
1	A	555	ASP
1	A	570	ARG
1	A	608	GLU
1	B	244	LYS
1	B	301	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	306	VAL
1	B	335	ASN
1	B	343	SER
1	B	346	GLU
1	B	366	ILE
1	B	380	LYS
1	B	434	GLN
1	B	470	MET
1	B	547	LEU
1	B	605	VAL
1	B	606	GLN
1	B	608	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	HIS
1	A	203	HIS
1	A	387	ASN
1	A	434	GLN
1	A	460	GLN
1	A	518	ASN
1	A	580	GLN
1	A	606	GLN
1	A	607	ASN
1	B	195	GLN
1	B	221	GLN
1	B	335	ASN
1	B	387	ASN
1	B	460	GLN
1	B	518	ASN
1	B	541	HIS
1	B	549	GLN
1	B	552	GLN
1	B	606	GLN
1	B	607	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](#)

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	436/436 (100%)	0.31	19 (4%) 39 34	13, 46, 76, 84	0
1	B	436/436 (100%)	0.50	37 (8%) 16 13	21, 48, 76, 86	0
2	C	6/6 (100%)	0.06	0 100 100	36, 45, 50, 50	0
2	D	6/6 (100%)	0.17	1 (16%) 4 3	40, 46, 50, 51	0
All	All	884/884 (100%)	0.40	57 (6%) 25 22	13, 47, 76, 86	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	GLY	4.7
1	A	207	GLY	3.9
1	A	331	VAL	3.7
1	B	414	LEU	3.6
1	B	419	THR	3.5
1	B	359	ILE	3.5
1	B	420	GLY	3.4
1	B	418	PHE	3.4
1	B	349	PHE	3.1
1	A	204	ALA	3.1
1	A	418	PHE	3.0
1	B	354	ILE	3.0
1	A	206	THR	3.0
1	B	416	THR	3.0
1	A	421	ASP	2.9
1	A	248	ILE	2.9
1	A	416	THR	2.9
1	B	366	ILE	2.8
1	B	470	MET	2.8
1	B	421	ASP	2.8
1	B	208	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	190	PRO	2.7
1	B	407	ILE	2.6
1	B	350	TYR	2.6
1	B	206	THR	2.6
1	A	205	PRO	2.5
1	B	593	HIS	2.5
1	B	332	PRO	2.5
1	A	349	PHE	2.4
1	A	330	THR	2.4
1	A	334	PRO	2.4
2	D	1	DA	2.4
1	A	208	SER	2.3
1	B	404	GLY	2.3
1	B	247	GLY	2.3
1	B	361	GLY	2.3
1	B	587	ARG	2.3
1	B	248	ILE	2.3
1	B	356	ILE	2.3
1	B	334	PRO	2.3
1	B	388	ALA	2.3
1	B	552	GLN	2.2
1	B	402	THR	2.2
1	B	481	ARG	2.2
1	B	468	GLY	2.2
1	B	586	ILE	2.2
1	A	192	ALA	2.1
1	B	556	ASN	2.1
1	B	344	THR	2.1
1	A	555	ASP	2.1
1	A	191	PRO	2.1
1	A	419	THR	2.1
1	A	190	PRO	2.1
1	A	407	ILE	2.0
1	B	339	VAL	2.0
1	B	389	VAL	2.0
1	B	189	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.