



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:18 AM UTC

PDB ID : 3MWV / pdb_00003mwv
Title : Crystal structure of HCV NS5B polymerase
Authors : Coulombe, R.
Deposited on : 2010-05-06
Resolution : 2.20 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

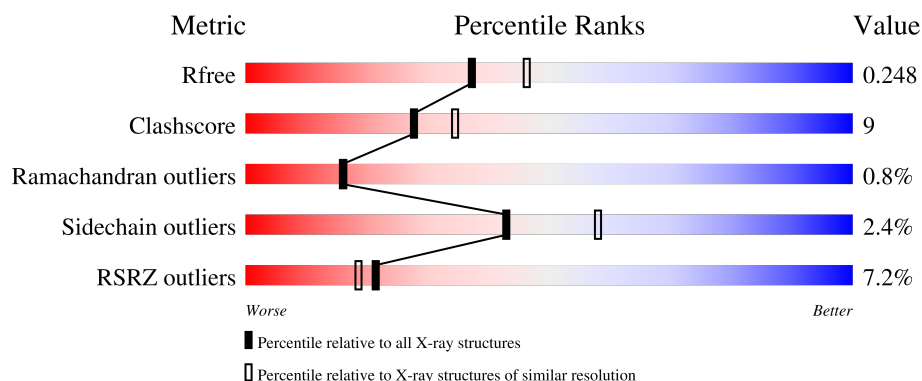
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	576	 4% 79% 15% . .
1	B	576	 10% 74% 19% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8959 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4358	2745	770	811	32			
1	B	558	Total	C	N	O	S	0	0	0
			4346	2737	768	809	32			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	571	HIS	-	expression tag	UNP O92972
A	572	HIS	-	expression tag	UNP O92972
A	573	HIS	-	expression tag	UNP O92972
A	574	HIS	-	expression tag	UNP O92972
A	575	HIS	-	expression tag	UNP O92972
A	576	HIS	-	expression tag	UNP O92972
B	571	HIS	-	expression tag	UNP O92972
B	572	HIS	-	expression tag	UNP O92972
B	573	HIS	-	expression tag	UNP O92972
B	574	HIS	-	expression tag	UNP O92972
B	575	HIS	-	expression tag	UNP O92972
B	576	HIS	-	expression tag	UNP O92972

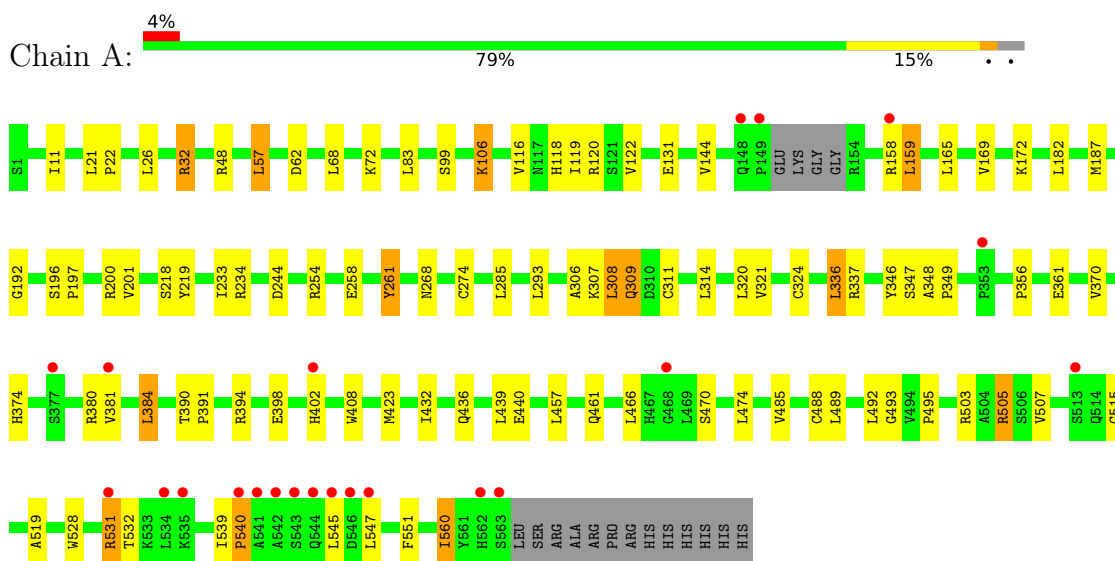
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	154	Total	O	0	0
			154	154		
2	B	101	Total	O	0	0
			101	101		

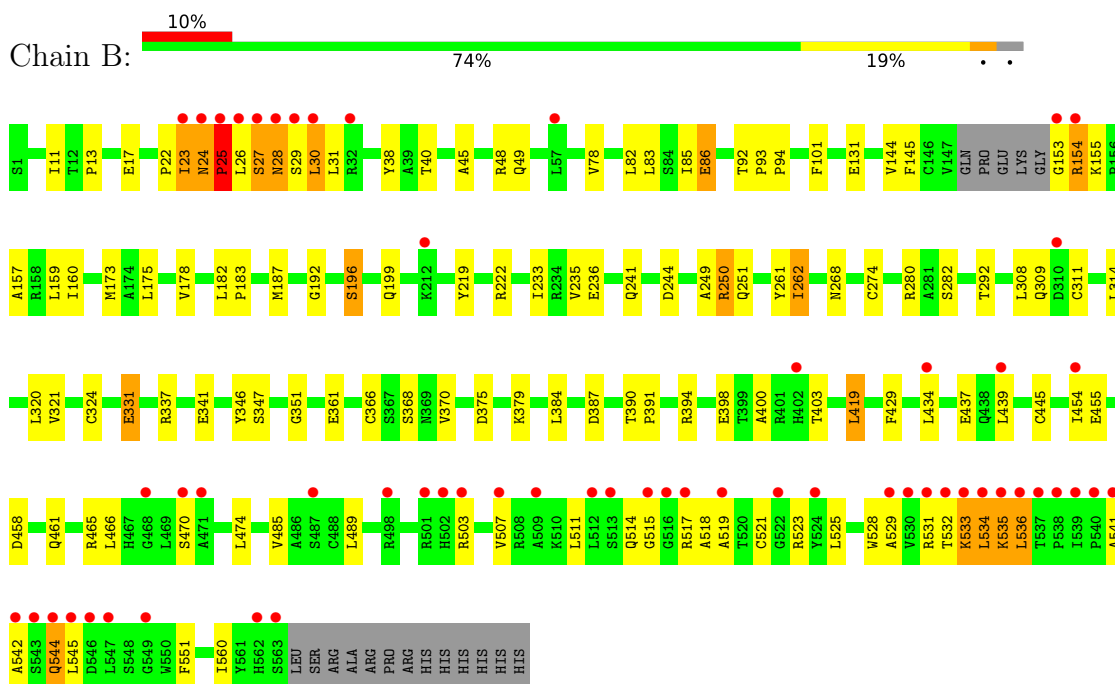
3 Residue-property plots [i](#)

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: Genome polypeptide



- Molecule 1: Genome polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.27Å 108.33Å 133.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (50.00-2.20) 96.8 (50.00-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.248 0.219 , 0.248	Depositor DCC
R_{free} test set	7690 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8959	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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	0.39	0/4453	0.88	9/6044 (0.1%)
1	B	0.37	0/4440	0.92	19/6025 (0.3%)
All	All	0.38	0/8893	0.90	28/12069 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	ASN	N-CA-C	-13.57	96.72	113.28
1	A	196	SER	N-CA-C	-8.76	100.06	110.13
1	B	244	ASP	N-CA-C	-7.27	98.20	109.76
1	A	261	TYR	N-CA-C	6.88	118.86	111.36
1	B	27	SER	N-CA-C	-6.86	104.03	113.56
1	B	25	PRO	N-CA-C	-6.83	98.41	112.47
1	A	11	ILE	N-CA-C	-6.23	98.58	107.98
1	A	244	ASP	N-CA-C	-6.18	99.94	109.76
1	B	196	SER	N-CA-C	-5.85	101.52	110.07
1	B	24	ASN	N-CA-C	5.74	122.50	109.81
1	B	11	ILE	N-CA-C	-5.73	98.79	107.73
1	B	531	ARG	N-CA-C	-5.72	102.72	110.68
1	A	192	GLY	N-CA-C	5.53	120.49	113.24
1	A	131	GLU	N-CA-C	5.46	120.44	113.18
1	A	218	SER	N-CA-C	-5.39	101.49	110.17
1	B	387	ASP	N-CA-C	-5.35	101.78	109.48
1	B	351	GLY	N-CA-C	-5.34	100.52	113.18
1	B	192	GLY	N-CA-C	5.24	120.10	113.24
1	B	101	PHE	N-CA-C	5.19	118.44	112.57
1	A	560	ILE	N-CA-C	5.17	115.36	108.11
1	B	175	LEU	N-CA-C	5.15	121.34	113.61
1	A	285	LEU	N-CA-C	5.13	117.54	111.33
1	B	131	GLU	N-CA-C	5.12	121.69	110.80
1	B	78	VAL	N-CA-C	5.07	116.11	109.21
1	B	429	PHE	N-CA-C	5.06	116.88	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	VAL	N-CA-C	-5.02	105.65	110.72
1	B	544	GLN	N-CA-C	-5.00	107.17	113.28
1	B	560	ILE	N-CA-C	5.00	115.17	108.17

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	4358	0	4371	69	0
1	B	4346	0	4359	89	0
2	A	154	0	0	1	0
2	B	101	0	0	1	0
All	All	8959	0	8730	157	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 9.

All (157) 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:201:VAL:HG22	1:A:384:LEU:HD13	1.44	0.99
1:B:532:THR:O	1:B:533:LYS:HB2	1.70	0.89
1:B:461:GLN:HB3	1:B:545:LEU:HD11	1.56	0.84
1:A:505:ARG:HH22	1:A:531:ARG:NH1	1.76	0.83
1:A:531:ARG:HE	1:A:532:THR:H	1.28	0.81
1:A:32:ARG:NH2	1:A:495:PRO:HG3	1.99	0.78
1:B:85:ILE:HD13	1:B:173:MET:SD	2.26	0.75
1:A:234:ARG:NH1	1:A:258:GLU:OE2	2.18	0.75
1:B:27:SER:CB	1:B:400:ALA:HB2	2.20	0.71
1:A:32:ARG:HH11	1:A:32:ARG:HG3	1.55	0.69
1:B:29:SER:O	1:B:30:LEU:HB3	1.94	0.68
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.76	0.67
1:B:515:GLY:HA2	1:B:519:ALA:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:GLN:CB	1:B:545:LEU:HD11	2.23	0.66
1:A:308:LEU:HB3	1:A:311:CYS:SG	2.36	0.65
1:B:470:SER:O	1:B:474:LEU:HG	1.96	0.65
1:B:523:ARG:HH21	1:B:534:LEU:HG	1.62	0.65
1:A:106:LYS:HA	1:A:106:LYS:HE2	1.77	0.64
1:A:57:LEU:C	1:A:57:LEU:HD23	2.23	0.64
1:A:197:PRO:O	1:A:201:VAL:HG23	2.00	0.62
1:B:533:LYS:O	1:B:534:LEU:HB2	1.98	0.62
1:B:535:LYS:O	1:B:536:LEU:C	2.43	0.62
1:B:523:ARG:NH2	1:B:534:LEU:HG	2.15	0.61
1:B:541:ALA:HA	1:B:544:GLN:NE2	2.17	0.60
1:A:440:GLU:HG2	1:A:457:LEU:CD1	2.32	0.60
1:B:38:TYR:CE2	1:B:154:ARG:HG3	2.37	0.60
1:A:440:GLU:HG2	1:A:457:LEU:HD12	1.84	0.59
1:A:461:GLN:HB2	1:A:545:LEU:HD11	1.84	0.58
1:A:32:ARG:HG3	1:A:32:ARG:NH1	2.19	0.58
1:B:48:ARG:HG2	1:B:159:LEU:HG	1.86	0.58
1:B:27:SER:OG	1:B:400:ALA:HB2	2.04	0.57
1:A:390:THR:HB	1:A:391:PRO:HD3	1.85	0.57
1:B:187:MET:HE1	1:B:292:THR:HG22	1.86	0.57
1:B:236:GLU:OE2	1:B:280:ARG:NH2	2.35	0.56
1:A:201:VAL:CG2	1:A:384:LEU:HD13	2.28	0.56
1:B:390:THR:HB	1:B:391:PRO:HD3	1.87	0.56
1:A:32:ARG:HH21	1:A:495:PRO:HG3	1.70	0.56
1:B:29:SER:O	1:B:30:LEU:CB	2.53	0.56
1:B:233:ILE:HB	1:B:262:ILE:HD12	1.88	0.55
1:B:517:ARG:HG3	1:B:517:ARG:HH11	1.71	0.55
1:A:144:VAL:HB	1:A:394:ARG:HG2	1.87	0.55
1:B:22:PRO:HD2	1:B:400:ALA:HB1	1.89	0.55
1:B:368:SER:HB3	1:B:384:LEU:HG	1.88	0.54
1:A:381:VAL:HG11	1:A:474:LEU:CD2	2.38	0.54
1:B:503:ARG:O	1:B:507:VAL:HG23	2.08	0.54
1:B:485:VAL:O	1:B:489:LEU:HG	2.08	0.53
1:A:432:ILE:O	1:A:436:GLN:HG3	2.07	0.53
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.39	0.52
1:A:48:ARG:NH2	1:A:158:ARG:NH1	2.58	0.52
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.91	0.52
1:A:48:ARG:HG2	1:A:159:LEU:HD13	1.93	0.51
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.93	0.51
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.93	0.51
1:B:514:GLN:HB2	1:B:518:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:LEU:HD23	1:B:439:LEU:HD11	1.93	0.51
1:B:534:LEU:C	1:B:536:LEU:H	2.19	0.50
1:B:346:TYR:O	1:B:347:SER:HB3	2.12	0.50
1:A:336:LEU:HD12	1:A:356:PRO:HD3	1.93	0.50
1:A:233:ILE:HD13	1:A:261:TYR:O	2.12	0.50
1:A:515:GLY:HA2	1:A:519:ALA:HB2	1.94	0.50
1:B:455:GLU:HB2	1:B:458:ASP:OD2	2.11	0.50
1:A:547:LEU:HD12	1:A:547:LEU:N	2.28	0.49
1:B:461:GLN:OE1	1:B:545:LEU:HD21	2.12	0.49
1:A:48:ARG:NH2	1:A:158:ARG:HH12	2.11	0.49
1:B:31:LEU:HD12	1:B:31:LEU:O	2.13	0.49
1:A:182:LEU:HD23	1:A:182:LEU:C	2.38	0.48
1:B:31:LEU:HD12	1:B:31:LEU:C	2.38	0.48
1:B:86:GLU:H	1:B:86:GLU:CD	2.21	0.48
1:B:38:TYR:CZ	1:B:154:ARG:HG3	2.48	0.48
1:B:40:THR:HB	1:B:157:ALA:HB2	1.96	0.48
1:B:308:LEU:HB2	1:B:311:CYS:SG	2.53	0.48
1:B:187:MET:HE1	1:B:292:THR:CG2	2.42	0.47
1:B:337:ARG:O	1:B:341:GLU:HG3	2.13	0.47
1:B:419:LEU:HD23	1:B:419:LEU:C	2.39	0.47
1:A:470:SER:O	1:A:474:LEU:HG	2.14	0.47
1:B:445:CYS:SG	1:B:454:ILE:HD12	2.54	0.47
1:B:26:LEU:C	1:B:28:ASN:H	2.22	0.47
1:B:523:ARG:HE	1:B:534:LEU:CD2	2.28	0.47
1:B:534:LEU:O	1:B:536:LEU:N	2.47	0.47
1:A:488:CYS:O	1:A:492:LEU:HD13	2.15	0.47
1:B:23:ILE:O	1:B:23:ILE:HG22	2.14	0.46
1:A:200:ARG:HD3	1:A:384:LEU:HD21	1.97	0.46
1:B:222:ARG:HH11	1:B:222:ARG:HG2	1.80	0.46
1:B:48:ARG:CG	1:B:159:LEU:HG	2.45	0.46
1:A:466:LEU:HD22	1:A:551:PHE:HE2	1.80	0.46
1:B:434:LEU:HD21	1:B:511:LEU:HD23	1.97	0.46
1:A:106:LYS:HA	1:A:106:LYS:CE	2.46	0.45
1:B:45:ALA:O	1:B:49:GLN:HG3	2.16	0.45
1:B:515:GLY:CA	1:B:519:ALA:HB2	2.46	0.45
1:B:309:GLN:O	1:B:324:CYS:HB2	2.16	0.45
1:B:465:ARG:NH1	1:B:545:LEU:HB2	2.31	0.45
1:A:439:LEU:O	1:A:457:LEU:HG	2.17	0.45
1:A:515:GLY:CA	1:A:519:ALA:HB2	2.47	0.45
1:A:254:ARG:HG2	1:B:251:GLN:NE2	2.31	0.45
1:B:23:ILE:O	1:B:23:ILE:CG2	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ALA:O	1:A:307:LYS:HB2	2.17	0.45
1:B:153:GLY:O	1:B:154:ARG:O	2.35	0.45
1:A:314:LEU:HB3	1:A:321:VAL:CG1	2.47	0.44
1:B:458:ASP:HA	1:B:461:GLN:NE2	2.32	0.44
1:B:541:ALA:HA	1:B:544:GLN:CD	2.42	0.44
1:A:361:GLU:HG2	1:A:370:VAL:O	2.17	0.44
1:A:381:VAL:HG11	1:A:474:LEU:HD21	1.98	0.44
1:B:466:LEU:HD22	1:B:551:PHE:HE2	1.83	0.44
1:A:309:GLN:O	1:A:324:CYS:HB2	2.17	0.44
1:B:25:PRO:HD2	1:B:26:LEU:O	2.17	0.44
1:B:182:LEU:HB3	1:B:183:PRO:HD3	2.00	0.44
1:B:517:ARG:HG3	1:B:517:ARG:NH1	2.33	0.44
1:B:222:ARG:HG2	1:B:222:ARG:NH1	2.33	0.43
1:B:331:GLU:H	1:B:331:GLU:CD	2.25	0.43
1:A:314:LEU:HB3	1:A:321:VAL:HG12	1.99	0.43
1:A:62:ASP:HB2	2:A:1241:HOH:O	2.19	0.43
1:A:116:VAL:CG1	1:A:120:ARG:NH1	2.81	0.43
1:A:485:VAL:O	1:A:489:LEU:HG	2.19	0.43
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.58	0.43
1:B:196:SER:OG	1:B:199:GLN:HG3	2.19	0.43
1:A:57:LEU:C	1:A:57:LEU:CD2	2.91	0.43
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.99	0.43
1:A:374:HIS:CE1	1:A:380:ARG:HG2	2.54	0.43
1:A:346:TYR:O	1:A:347:SER:HB3	2.17	0.43
1:B:145:PHE:CE2	1:B:155:LYS:HD2	2.53	0.43
1:B:160:ILE:HA	1:B:282:SER:OG	2.18	0.43
1:B:233:ILE:HD13	1:B:261:TYR:O	2.18	0.43
1:A:503:ARG:O	1:A:507:VAL:HG23	2.19	0.43
1:A:423:MET:HA	1:A:528:TRP:CZ2	2.54	0.42
1:A:32:ARG:HG2	1:A:493:GLY:O	2.19	0.42
1:A:187:MET:HE2	1:A:293:LEU:HD23	2.02	0.42
1:B:528:TRP:CZ3	1:B:529:ALA:HB2	2.55	0.42
1:B:361:GLU:HG2	1:B:370:VAL:O	2.19	0.42
1:B:375:ASP:OD1	1:B:379:LYS:HB2	2.18	0.42
1:A:99:SER:HB2	1:A:165:LEU:HB3	2.02	0.42
1:A:539:ILE:HA	1:A:540:PRO:HD3	1.95	0.42
1:B:93:PRO:HA	1:B:94:PRO:HD3	1.94	0.42
1:B:398:GLU:HG2	1:B:403:THR:OG1	2.20	0.42
1:A:348:ALA:N	1:A:349:PRO:CD	2.82	0.42
1:B:534:LEU:HD12	1:B:534:LEU:HA	1.95	0.42
1:B:26:LEU:C	1:B:28:ASN:N	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:HIS:O	1:A:122:VAL:HG23	2.19	0.42
1:A:492:LEU:HD12	1:A:492:LEU:N	2.35	0.42
1:A:21:LEU:HD12	1:A:22:PRO:HD2	2.01	0.41
1:B:153:GLY:O	1:B:154:ARG:C	2.63	0.41
1:B:178:VAL:HG23	2:B:1125:HOH:O	2.18	0.41
1:A:106:LYS:HE2	1:A:106:LYS:CA	2.48	0.41
1:A:398:GLU:OE1	1:A:408:TRP:HD1	2.03	0.41
1:A:461:GLN:CB	1:A:545:LEU:HD11	2.48	0.41
1:A:466:LEU:CD2	1:A:551:PHE:HE2	2.33	0.41
1:B:92:THR:HA	1:B:93:PRO:HD3	1.98	0.41
1:B:321:VAL:O	1:B:321:VAL:HG13	2.19	0.41
1:A:116:VAL:HG12	1:A:120:ARG:NH1	2.36	0.41
1:B:26:LEU:HD23	1:B:26:LEU:HA	1.57	0.41
1:B:144:VAL:HB	1:B:394:ARG:HG2	2.02	0.41
1:B:268:ASN:HB3	1:B:274:CYS:SG	2.61	0.41
1:B:521:CYS:O	1:B:525:LEU:HB2	2.21	0.41
1:A:423:MET:HG2	1:A:528:TRP:CZ3	2.56	0.40
1:A:68:LEU:O	1:A:72:LYS:HG3	2.21	0.40
1:B:241:GLN:OE1	1:B:250:ARG:HG2	2.21	0.40
1:B:542:ALA:C	1:B:544:GLN:H	2.30	0.40
1:B:13:PRO:HB3	1:B:17:GLU:CD	2.47	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	555/576 (96%)	540 (97%)	14 (2%)	1 (0%)	43	51
1	B	554/576 (96%)	530 (96%)	16 (3%)	8 (1%)	9	7
All	All	1109/1152 (96%)	1070 (96%)	30 (3%)	9 (1%)	16	16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	PRO
1	B	30	LEU
1	B	154	ARG
1	B	533	LYS
1	B	534	LEU
1	B	535	LYS
1	B	536	LEU
1	A	540	PRO
1	B	24	ASN

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	477/491 (97%)	463 (97%)	14 (3%)	37	51
1	B	475/491 (97%)	466 (98%)	9 (2%)	50	66
All	All	952/982 (97%)	929 (98%)	23 (2%)	43	58

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	32	ARG
1	A	57	LEU
1	A	83	LEU
1	A	106	LYS
1	A	159	LEU
1	A	308	LEU
1	A	309	GLN
1	A	336	LEU
1	A	337	ARG
1	A	384	LEU
1	A	402	HIS
1	A	505	ARG
1	A	531	ARG

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Mol	Chain	Res	Type
1	B	23	ILE
1	B	83	LEU
1	B	86	GLU
1	B	250	ARG
1	B	262	ILE
1	B	331	GLU
1	B	366	CYS
1	B	419	LEU
1	B	437	GLU

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	251	GLN
1	A	309	GLN
1	A	406	ASN
1	A	544	GLN
1	B	33	HIS
1	B	35	ASN
1	B	49	GLN
1	B	63	HIS
1	B	251	GLN
1	B	273	ASN
1	B	406	ASN
1	B	428	HIS
1	B	461	GLN
1	B	527	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 oligosaccharides 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

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	559/576 (97%)	0.00	22 (3%) 43 40	13, 24, 49, 82	0
1	B	558/576 (96%)	0.49	58 (10%) 11 9	13, 32, 65, 79	0
All	All	1117/1152 (96%)	0.25	80 (7%) 21 18	13, 27, 59, 82	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	SER	9.4
1	A	545	LEU	6.2
1	B	534	LEU	5.7
1	B	26	LEU	5.5
1	A	541	ALA	4.8
1	B	542	ALA	4.4
1	B	25	PRO	4.4
1	A	563	SER	4.3
1	A	542	ALA	4.2
1	A	149	PRO	4.2
1	B	543	SER	4.2
1	A	540	PRO	4.1
1	B	532	THR	4.0
1	A	534	LEU	3.8
1	B	545	LEU	3.8
1	B	530	VAL	3.6
1	B	563	SER	3.6
1	B	153	GLY	3.5
1	B	29	SER	3.5
1	B	529	ALA	3.4
1	B	24	ASN	3.4
1	B	531	ARG	3.3
1	A	402	HIS	3.3
1	B	544	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	536	LEU	3.2
1	B	541	ALA	3.2
1	A	513	SER	3.0
1	A	544	GLN	3.0
1	A	531	ARG	3.0
1	B	535	LYS	3.0
1	B	539	ILE	2.9
1	B	516	GLY	2.9
1	A	543	SER	2.8
1	B	507	VAL	2.8
1	A	562	HIS	2.7
1	B	402	HIS	2.7
1	B	517	ARG	2.7
1	B	547	LEU	2.7
1	B	537	THR	2.6
1	B	468	GLY	2.6
1	B	533	LYS	2.6
1	B	28	ASN	2.6
1	B	439	LEU	2.5
1	B	540	PRO	2.5
1	B	23	ILE	2.5
1	B	513	SER	2.5
1	B	512	LEU	2.5
1	B	546	ASP	2.5
1	A	546	ASP	2.5
1	B	503	ARG	2.4
1	B	515	GLY	2.4
1	B	30	LEU	2.4
1	B	498	ARG	2.4
1	B	549	GLY	2.3
1	B	57	LEU	2.3
1	B	509	ALA	2.3
1	B	562	HIS	2.3
1	A	381	VAL	2.3
1	B	434	LEU	2.2
1	B	310	ASP	2.2
1	A	353	PRO	2.2
1	A	468	GLY	2.2
1	B	522	GLY	2.2
1	B	502	HIS	2.2
1	A	535	LYS	2.2
1	A	148	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	538	PRO	2.2
1	B	487	SER	2.2
1	B	32	ARG	2.2
1	B	212	LYS	2.2
1	B	524	TYR	2.1
1	B	470	SER	2.1
1	B	519	ALA	2.1
1	B	471	ALA	2.1
1	A	547	LEU	2.1
1	B	154	ARG	2.1
1	A	158	ARG	2.0
1	B	501	ARG	2.0
1	A	377	SER	2.0
1	B	454	ILE	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 ⓘ

There are no oligosaccharides 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.