



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:09 AM UTC

PDB ID : 4RY6 / pdb_00004ry6
Title : C-terminal mutant (W550A) of HCV/J4 RNA polymerase
Authors : Jaeger, J.; Cherry, A.; Dennis, C.
Deposited on : 2014-12-13
Resolution : 2.52 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

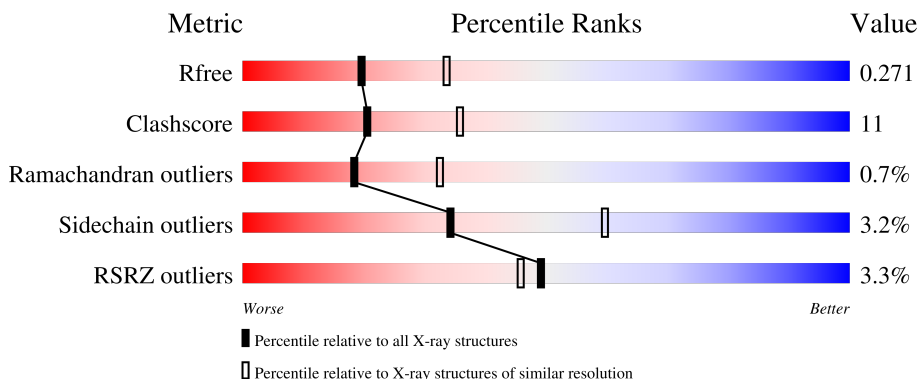
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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 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	570	 4% 73% 24% ...
1	B	570	 2% 79% 17% ...

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9260 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 HCV J4 RNA polymerase (NS5B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	0	3	0
			4407	2770	779	824	34			
1	B	564	Total	C	N	O	S	0	4	0
			4404	2767	779	825	33			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	550	ALA	TRP	engineered mutation	UNP O92972
B	550	ALA	TRP	engineered mutation	UNP O92972

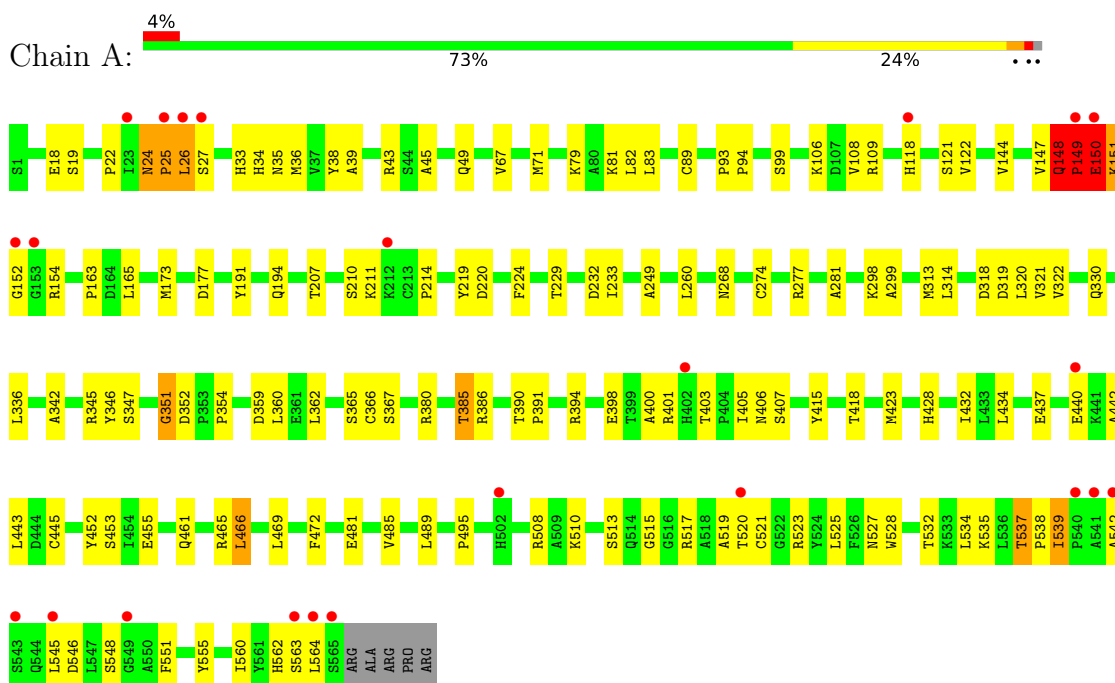
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	265	Total	O	0	0
			265	265		
2	B	184	Total	O	0	0
			184	184		

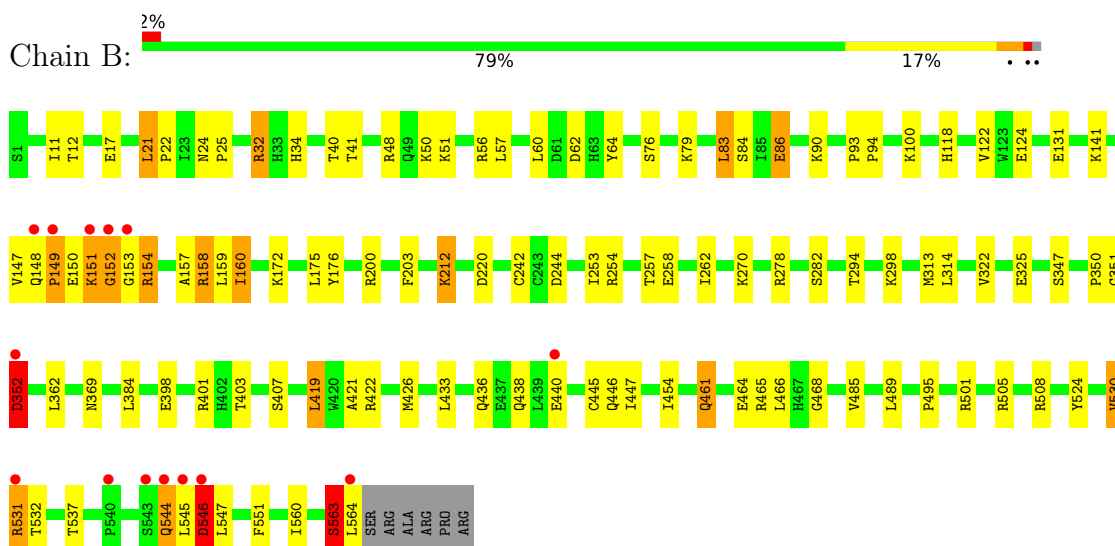
3 Residue-property plots

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: HCV J4 RNA polymerase (NS5B)



• Molecule 1: HCV J4 RNA polymerase (NS5B)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.15Å 107.80Å 133.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.52 19.90 – 2.52	Depositor EDS
% Data completeness (in resolution range)	93.0 (19.90-2.52) 92.9 (19.90-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8.4	Depositor
R, R_{free}	0.186 , 0.266 0.198 , 0.271	Depositor DCC
R_{free} test set	3398 reflections (6.93%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.046 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9260	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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	0.58	1/4501 (0.0%)	0.93	13/6107 (0.2%)
1	B	0.59	0/4498	0.95	13/6103 (0.2%)
All	All	0.59	1/8999 (0.0%)	0.94	26/12210 (0.2%)

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
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	GLU	CA-C	10.06	1.59	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	GLY	N-CA-C	-10.06	100.52	115.00
1	B	352	ASP	CA-C-N	-9.62	110.48	120.38
1	B	352	ASP	C-N-CA	-9.62	110.48	120.38
1	A	149	PRO	N-CA-C	7.41	127.74	112.47
1	A	148	GLN	N-CA-C	7.28	121.11	108.82
1	B	152	GLY	N-CA-C	-6.70	97.30	113.18
1	B	544	GLN	N-CA-C	-6.67	105.47	112.93
1	A	24	ASN	CA-C-N	6.40	127.84	119.84
1	A	24	ASN	C-N-CA	6.40	127.84	119.84
1	A	148	GLN	CA-C-N	6.32	127.74	119.84
1	A	148	GLN	C-N-CA	6.32	127.74	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	21	LEU	CA-C-N	6.26	126.62	119.92
1	B	21	LEU	C-N-CA	6.26	126.62	119.92
1	B	563	SER	CA-C-N	5.88	132.28	121.70
1	B	563	SER	C-N-CA	5.88	132.28	121.70
1	B	403	THR	CA-C-N	5.83	125.97	119.32
1	B	403	THR	C-N-CA	5.83	125.97	119.32
1	B	530	VAL	N-CA-C	5.78	116.91	108.53
1	A	537	THR	CA-C-N	-5.63	114.46	120.03
1	A	537	THR	C-N-CA	-5.63	114.46	120.03
1	B	546	ASP	CA-C-N	-5.57	113.83	123.25
1	B	546	ASP	C-N-CA	-5.57	113.83	123.25
1	A	495	PRO	CA-C-N	5.18	125.17	119.89
1	A	495	PRO	C-N-CA	5.18	125.17	119.89
1	A	352	ASP	CA-C-N	5.08	125.61	120.38
1	A	352	ASP	C-N-CA	5.08	125.61	120.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	GLN	Peptide
1	B	351	GLY	Peptide

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	4407	0	4420	103	0
1	B	4404	0	4410	94	0
2	A	265	0	0	9	0
2	B	184	0	0	8	0
All	All	9260	0	8830	197	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 11.

All (197) 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:517:ARG:O	1:A:520:THR:HG22	1.53	1.04
1:A:150:GLU:HB2	1:A:151:LYS:HA	1.55	0.89
1:A:149:PRO:HA	1:A:151:LYS:HE2	1.61	0.81
1:B:545:LEU:HB3	1:B:547:LEU:HD13	1.62	0.81
1:B:149:PRO:HA	1:B:151:LYS:HB2	1.62	0.80
1:B:148:GLN:N	1:B:151:LYS:HZ1	1.83	0.77
1:B:151:LYS:HG2	1:B:152:GLY:N	2.01	0.76
1:B:440:GLU:HB3	2:B:715:HOH:O	1.84	0.76
1:A:523:ARG:HG3	1:A:534:LEU:HD13	1.70	0.74
1:A:319:ASP:OD2	1:A:366:CYS:N	2.21	0.73
1:B:79:LYS:HG3	1:B:244:ASP:HB3	1.69	0.72
1:A:385:THR:HG21	1:A:481:GLU:OE2	1.91	0.71
1:B:151:LYS:HG2	1:B:152:GLY:H	1.55	0.70
1:A:380:ARG:NH2	2:A:706:HOH:O	2.24	0.70
1:A:144:VAL:HB	1:A:394:ARG:HG2	1.75	0.68
1:A:18:GLU:HG3	1:A:401:ARG:HH12	1.61	0.66
1:A:150:GLU:CB	1:A:151:LYS:HA	2.25	0.66
1:B:151:LYS:CG	1:B:152:GLY:H	2.09	0.66
1:B:369:ASN:ND2	2:B:744:HOH:O	2.27	0.66
1:B:505:ARG:NH2	1:B:531:ARG:HG2	2.11	0.65
1:A:79:LYS:NZ	2:A:716:HOH:O	2.29	0.65
1:A:83:LEU:HB2	1:A:173:MET:HA	1.80	0.63
1:A:367:SER:O	1:A:386:ARG:HB3	1.98	0.63
1:A:461:GLN:HB2	1:A:545:LEU:HD11	1.82	0.61
1:B:563:SER:OG	1:B:564:LEU:O	2.16	0.61
1:A:148:GLN:CA	1:A:151:LYS:HD3	2.31	0.61
1:A:523:ARG:NH2	1:A:535:LYS:O	2.35	0.60
1:B:151:LYS:CG	1:B:152:GLY:N	2.64	0.60
1:A:563:SER:OG	1:A:564:LEU:N	2.29	0.60
1:B:84:SER:HB2	1:B:86:GLU:HG2	1.83	0.60
1:B:149:PRO:HA	1:B:151:LYS:HD2	1.84	0.60
1:A:81:LYS:HG2	1:A:177:ASP:OD2	2.02	0.59
1:B:350:PRO:HB2	1:B:352:ASP:O	2.02	0.59
1:B:465:ARG:NH1	1:B:547:LEU:HB2	2.17	0.59
1:B:220:ASP:HB3	1:B:352:ASP:HB3	1.84	0.58
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.84	0.58
1:B:147:VAL:HB	1:B:151:LYS:NZ	2.19	0.58
1:A:527:ASN:HA	2:A:628:HOH:O	2.04	0.58
1:A:148:GLN:N	1:A:151:LYS:HD3	2.19	0.57
1:A:434:LEU:HD11	1:A:510:LYS:HB3	1.86	0.57
1:B:325:GLU:HG3	2:B:720:HOH:O	2.02	0.57
1:B:147:VAL:C	1:B:151:LYS:HZ1	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:SER:HG	1:B:564:LEU:C	2.11	0.57
1:A:26:LEU:HD21	1:A:432:ILE:HG12	1.86	0.56
1:A:465:ARG:NH2	2:A:817:HOH:O	2.37	0.56
1:A:211:LYS:HB2	1:A:214:PRO:HB3	1.88	0.56
1:A:347:SER:O	1:A:347:SER:OG	2.23	0.56
1:B:203:PHE:CD2	1:B:314:LEU:HD22	2.41	0.56
1:B:524:TYR:OH	1:B:537:THR:O	2.16	0.56
1:A:313:MET:HG2	1:A:322:VAL:HG22	1.88	0.56
1:B:22:PRO:HG2	1:B:401:ARG:HE	1.71	0.55
1:A:415:TYR:O	1:A:418:THR:HG23	2.07	0.55
1:A:149:PRO:CA	1:A:151:LYS:HE2	2.34	0.55
1:A:465:ARG:NH1	2:A:770:HOH:O	2.38	0.55
1:B:419:LEU:HD22	1:B:485:VAL:HG21	1.89	0.55
1:A:537:THR:HB	1:A:538:PRO:HD2	1.89	0.55
1:A:150:GLU:H	1:A:151:LYS:HG3	1.71	0.55
1:A:465:ARG:NH1	1:A:545:LEU:O	2.40	0.54
1:A:99:SER:HB2	1:A:165:LEU:HB3	1.88	0.54
1:A:24:ASN:HB3	1:A:27:SER:OG	2.07	0.54
1:B:421:ALA:O	1:B:426:MET:HG3	2.07	0.54
1:B:501:ARG:O	1:B:505:ARG:HG3	2.08	0.54
1:A:485:VAL:O	1:A:489:LEU:HG	2.08	0.54
1:B:118:HIS:O	1:B:122:VAL:HG23	2.08	0.54
1:B:254:ARG:NH2	1:B:258:GLU:HG2	2.23	0.54
1:A:442:ALA:HB2	1:A:455:GLU:HG3	1.90	0.54
1:A:453:SER:H	1:A:563:SER:HB2	1.72	0.54
1:B:203:PHE:HD2	1:B:314:LEU:HD22	1.74	0.53
1:A:268:ASN:HB3	1:A:274[B]:CYS:SG	2.49	0.52
1:A:220:ASP:OD2	1:A:351:GLY:HA3	2.09	0.52
1:A:67:VAL:O	1:A:71:MET:HG3	2.10	0.52
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.92	0.52
1:A:148:GLN:HA	1:A:151:LYS:HD3	1.92	0.51
1:B:56:ARG:NH2	1:B:278:ARG:O	2.40	0.51
1:A:191:TYR:O	1:A:194:GLN:HG2	2.11	0.50
1:A:465:ARG:NH1	1:A:545:LEU:HB2	2.27	0.50
1:B:150:GLU:N	1:B:151:LYS:HB2	2.26	0.50
1:B:150:GLU:HB3	1:B:151:LYS:HA	1.93	0.50
1:B:445:CYS:SG	1:B:454:ILE:HD12	2.51	0.50
1:B:124:GLU:HB2	2:B:724:HOH:O	2.11	0.50
1:B:148:GLN:HG3	1:B:149:PRO:HD2	1.93	0.50
1:B:505:ARG:HH22	1:B:531:ARG:HG2	1.76	0.50
1:A:45:ALA:O	1:A:49:GLN:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:LEU:HD21	1:A:551:PHE:CZ	2.47	0.49
1:B:563:SER:HA	1:B:564:LEU:CB	2.42	0.49
1:B:436:GLN:O	1:B:438:GLN:HG3	2.13	0.48
1:A:428:HIS:O	1:A:432:ILE:HG13	2.13	0.48
1:A:461:GLN:HG2	1:A:539:ILE:HG21	1.94	0.48
1:A:89:CYS:SG	1:A:108:VAL:HG13	2.53	0.48
1:A:38:TYR:CE2	1:A:154:ARG:HB3	2.48	0.47
1:B:83:LEU:HD22	1:B:176:TYR:HB3	1.96	0.47
1:B:294:THR:HG22	1:B:298:LYS:HE3	1.96	0.47
1:B:147:VAL:HG12	1:B:153:GLY:HA2	1.96	0.47
1:B:153:GLY:HA3	1:B:154:ARG:HG3	1.97	0.47
1:B:485:VAL:O	1:B:489:LEU:HG	2.14	0.47
1:A:224:PHE:CD2	1:A:318:ASP:HB2	2.50	0.47
1:A:469:LEU:HD11	1:A:538:PRO:HA	1.96	0.47
1:B:147:VAL:HB	1:B:151:LYS:HE3	1.96	0.47
1:B:436:GLN:OE1	1:B:438:GLN:NE2	2.48	0.47
1:A:207:THR:O	1:A:210:SER:OG	2.33	0.47
1:B:175:LEU:HD21	1:B:253:ILE:HG12	1.96	0.47
1:A:22:PRO:HD3	1:A:401:ARG:HE	1.80	0.47
1:A:472:PHE:HE1	1:A:525:LEU:HD23	1.79	0.47
1:B:147:VAL:HB	1:B:151:LYS:CE	2.44	0.47
1:A:539:ILE:HG22	1:A:542:ALA:H	1.79	0.46
1:B:60:LEU:HD13	1:B:64:TYR:CE1	2.50	0.46
1:B:220:ASP:HB3	1:B:352:ASP:CB	2.45	0.46
1:A:109:ARG:HH11	1:A:109:ARG:HG2	1.79	0.46
1:A:534:LEU:HD12	2:A:628:HOH:O	2.15	0.46
1:B:32:ARG:NH2	1:B:495:PRO:HG3	2.30	0.46
1:B:62:ASP:HB2	2:B:671:HOH:O	2.15	0.46
1:B:294:THR:O	1:B:298:LYS:HG3	2.15	0.46
1:B:12:THR:HG21	1:B:270:LYS:HD2	1.97	0.46
1:B:21:LEU:HD23	1:B:34:HIS:HA	1.98	0.46
1:A:360:LEU:O	2:A:632:HOH:O	2.21	0.46
1:A:521:CYS:HB3	1:A:525:LEU:HD12	1.98	0.46
1:B:158:ARG:HA	1:B:158:ARG:HD2	1.67	0.46
1:A:34:HIS:ND1	1:A:35:ASN:OD1	2.49	0.46
1:A:19:SER:HB2	1:A:43:ARG:HH21	1.82	0.45
1:B:313:MET:HG2	1:B:322:VAL:HG22	1.97	0.45
1:A:106:LYS:HA	1:A:106:LYS:HD2	1.63	0.45
1:A:423:MET:HA	1:A:528:TRP:CH2	2.52	0.45
1:A:118:HIS:O	1:A:122:VAL:HG23	2.16	0.45
1:A:298:LYS:NZ	1:A:346:TYR:O	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:PRO:CA	1:B:151:LYS:HB2	2.39	0.45
1:B:531:ARG:HB2	1:B:532:THR:H	1.36	0.45
1:A:277:ARG:CZ	1:A:281:ALA:HB2	2.47	0.45
1:A:452:TYR:CE2	1:A:562:HIS:HB2	2.52	0.45
1:A:415:TYR:HB3	1:A:418:THR:HG21	1.99	0.44
1:A:26:LEU:CD2	1:A:432:ILE:HG12	2.48	0.44
1:A:465:ARG:HH11	1:A:545:LEU:HB2	1.82	0.44
1:A:299:ALA:C	1:A:313:MET:HE1	2.42	0.44
1:B:508:ARG:NH1	1:B:530:VAL:HG11	2.33	0.44
1:A:423:MET:HA	1:A:528:TRP:CZ2	2.53	0.44
1:B:446:GLN:O	1:B:447:ILE:HD13	2.18	0.44
1:A:406:ASN:HD21	1:A:443:LEU:HD22	1.83	0.43
1:A:440:GLU:HB3	2:A:667:HOH:O	2.18	0.43
1:B:200:ARG:HD3	1:B:384:LEU:CD2	2.48	0.43
1:A:163:PRO:HG3	1:A:260:LEU:HD21	2.00	0.43
1:B:149:PRO:HA	1:B:151:LYS:CB	2.41	0.43
1:B:172:LYS:HE3	1:B:560:ILE:HD13	2.00	0.43
1:B:546:ASP:C	1:B:547:LEU:HD12	2.43	0.43
1:B:433:LEU:HD23	1:B:433:LEU:HA	1.84	0.43
1:A:314:LEU:HD12	1:A:314:LEU:HA	1.78	0.43
1:A:336:LEU:HD21	1:A:354:PRO:HB2	2.01	0.43
1:A:18:GLU:CG	1:A:401:ARG:HH12	2.28	0.43
1:A:466:LEU:HD21	1:A:551:PHE:HZ	1.83	0.43
1:B:76[A]:SER:HA	1:B:242:CYS:O	2.18	0.43
1:B:508:ARG:CZ	1:B:530:VAL:HG11	2.49	0.43
1:A:36:MET:HE2	1:A:147:VAL:HG23	2.00	0.43
1:A:398:GLU:OE2	1:A:407:SER:N	2.45	0.42
1:A:510:LYS:O	1:A:513:SER:HB3	2.19	0.42
1:B:21:LEU:HD12	1:B:22:PRO:HD2	2.01	0.42
1:B:282:SER:HB3	2:B:731:HOH:O	2.18	0.42
1:B:398:GLU:OE2	1:B:407:SER:OG	2.32	0.42
1:A:82:LEU:HD12	1:A:173:MET:O	2.19	0.42
1:A:151:LYS:HB2	1:A:151:LYS:HE3	1.59	0.42
1:B:254:ARG:HH22	1:B:258:GLU:HG2	1.84	0.42
1:A:398:GLU:HG2	1:A:403:THR:OG1	2.19	0.42
1:B:160:ILE:HA	1:B:282:SER:OG	2.19	0.42
1:B:466:LEU:HD21	1:B:551:PHE:HZ	1.84	0.42
1:B:148:GLN:O	1:B:150:GLU:N	2.52	0.42
1:A:515:GLY:HA2	1:A:519:ALA:HB2	2.02	0.42
1:A:118:HIS:HD2	1:A:121:SER:OG	2.02	0.42
1:B:93:PRO:HA	1:B:94:PRO:HD3	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:THR:O	1:A:232:ASP:HB2	2.20	0.42
1:A:359:ASP:HB3	1:A:362:LEU:HG	2.02	0.42
1:B:461:GLN:HB2	1:B:545:LEU:HD11	2.02	0.42
1:B:546:ASP:OD2	1:B:564:LEU:C	2.63	0.42
1:A:345:ARG:C	1:A:347:SER:H	2.28	0.41
1:A:555:TYR:CD1	1:A:560:ILE:HG13	2.55	0.41
1:B:122:VAL:HG13	2:B:716:HOH:O	2.20	0.41
1:B:545:LEU:HD23	1:B:545:LEU:HA	1.81	0.41
1:A:33:HIS:HB3	1:A:36:MET:HG3	2.02	0.41
1:A:24:ASN:HA	1:A:25:PRO:HD2	1.83	0.41
1:B:21:LEU:HA	1:B:22:PRO:HD3	1.86	0.41
1:B:40:THR:HB	1:B:157:ALA:HB2	2.01	0.41
1:B:149:PRO:HA	1:B:151:LYS:CD	2.49	0.41
1:B:257:THR:O	1:B:262:ILE:HG23	2.19	0.41
1:A:405:ILE:HG23	1:A:445:CYS:HA	2.03	0.41
1:B:212:LYS:H	1:B:212:LYS:HG3	1.59	0.41
1:A:342:ALA:HA	1:A:345:ARG:CZ	2.50	0.41
1:A:27:SER:OG	1:A:400:ALA:HB2	2.20	0.41
1:B:422:ARG:NH2	2:B:767:HOH:O	2.28	0.41
1:B:436:GLN:HB3	1:B:438:GLN:HE21	1.85	0.41
1:B:362:LEU:HD23	1:B:362:LEU:HA	1.88	0.40
1:A:365:SER:HB2	2:A:695:HOH:O	2.21	0.40
1:A:93:PRO:HA	1:A:94:PRO:HD3	1.89	0.40
1:B:48:ARG:HG2	1:B:159:LEU:HG	2.03	0.40
1:B:86:GLU:O	1:B:90:LYS:HG2	2.21	0.40
1:A:39:ALA:HB2	1:A:144:VAL:HG22	2.02	0.40
1:A:390:THR:HB	1:A:391:PRO:HD3	2.04	0.40
1:A:508:ARG:HH21	1:A:534:LEU:HD11	1.86	0.40
1:B:17:GLU:HB3	1:B:41:THR:CG2	2.52	0.40
1:B:24:ASN:HA	1:B:25:PRO:HD3	1.99	0.40
1:B:464:GLU:O	1:B:468:GLY:N	2.49	0.40
1:B:57:LEU:O	1:B:347:SER:HB2	2.22	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	566/570 (99%)	532 (94%)	30 (5%)	4 (1%)	18	32
1	B	566/570 (99%)	535 (94%)	27 (5%)	4 (1%)	18	32
All	All	1132/1140 (99%)	1067 (94%)	57 (5%)	8 (1%)	18	32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	PRO
1	B	531	ARG
1	B	546	ASP
1	A	351	GLY
1	A	546	ASP
1	B	352	ASP
1	A	25	PRO
1	B	149	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	483/484 (100%)	470 (97%)	13 (3%)	39	65
1	B	482/484 (100%)	464 (96%)	18 (4%)	30	54
All	All	965/968 (100%)	934 (97%)	31 (3%)	34	60

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	149	PRO
1	A	150	GLU
1	A	151	LYS

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Mol	Chain	Res	Type
1	A	233	ILE
1	A	321	VAL
1	A	330	GLN
1	A	385	THR
1	A	437	GLU
1	A	466	LEU
1	A	532	THR
1	A	539	ILE
1	A	548	SER
1	B	11	ILE
1	B	32	ARG
1	B	50	LYS
1	B	51	LYS
1	B	83	LEU
1	B	86	GLU
1	B	100	LYS
1	B	131	GLU
1	B	141	LYS
1	B	151	LYS
1	B	154	ARG
1	B	158	ARG
1	B	160	ILE
1	B	212	LYS
1	B	419	LEU
1	B	461	GLN
1	B	544	GLN
1	B	563	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	63	HIS
1	A	118	HIS
1	A	402	HIS
1	A	406	ASN
1	A	428	HIS
1	A	461	GLN
1	A	514	GLN
1	B	28	ASN
1	B	34	HIS
1	B	355	GLN

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Mol	Chain	Res	Type
1	B	406	ASN
1	B	438	GLN

5.3.3 RNA [i](#)

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	565/570 (99%)	0.02	23 (4%) 41 38	11, 41, 85, 108	3 (0%)
1	B	564/570 (98%)	-0.39	14 (2%) 58 55	7, 29, 59, 99	4 (0%)
All	All	1129/1140 (99%)	-0.18	37 (3%) 49 46	7, 33, 78, 108	7 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	565	SER	4.9
1	A	564	LEU	4.7
1	A	152	GLY	4.6
1	A	26	LEU	4.3
1	A	27	SER	4.3
1	A	563	SER	4.0
1	A	118	HIS	4.0
1	A	541	ALA	3.8
1	B	440	GLU	3.5
1	A	440	GLU	3.4
1	B	564	LEU	3.4
1	A	25	PRO	3.3
1	B	545	LEU	3.3
1	B	352	ASP	3.3
1	B	152	GLY	3.2
1	B	543	SER	2.8
1	B	149	PRO	2.8
1	B	153	GLY	2.7
1	A	149	PRO	2.7
1	A	542	ALA	2.7
1	A	502	HIS	2.6
1	A	153	GLY	2.6
1	B	531	ARG	2.5
1	A	540	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	148	GLN	2.5
1	B	546	ASP	2.4
1	B	540	PRO	2.3
1	B	544	GLN	2.3
1	A	545	LEU	2.3
1	A	23	ILE	2.2
1	A	150	GLU	2.2
1	A	212	LYS	2.2
1	B	151	LYS	2.2
1	A	402	HIS	2.1
1	A	549	GLY	2.1
1	A	520	THR	2.1
1	A	543	SER	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.