



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:13 AM UTC

PDB ID : 4RY7 / pdb_00004ry7
Title : C-terminal mutant (D559E) of HCV/J4 RNA polymerase
Authors : Jaeger, J.; Cherry, A.; Dennis, C.
Deposited on : 2014-12-13
Resolution : 3.00 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

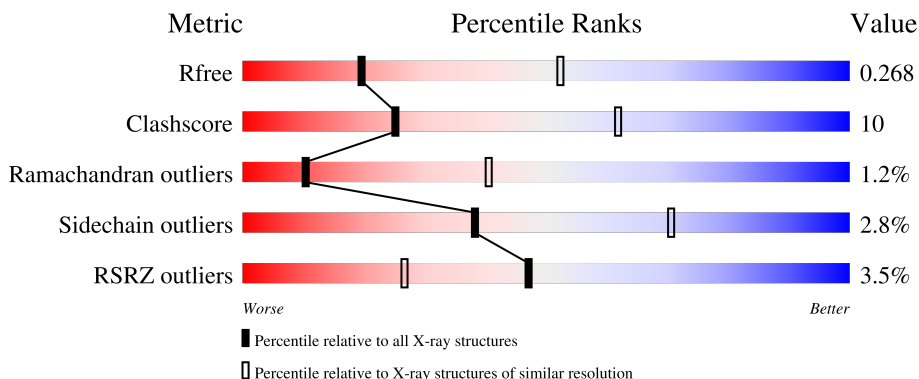
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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% 77% 20% ...
1	B	570	3% 78% 18% ...

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9315 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
			4417	2779	780	824	34			
1	B	565	Total	C	N	O	S	0	4	0
			4419	2779	781	826	33			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	GLU	ASP	engineered mutation	UNP O92972
B	559	GLU	ASP	engineered mutation	UNP O92972

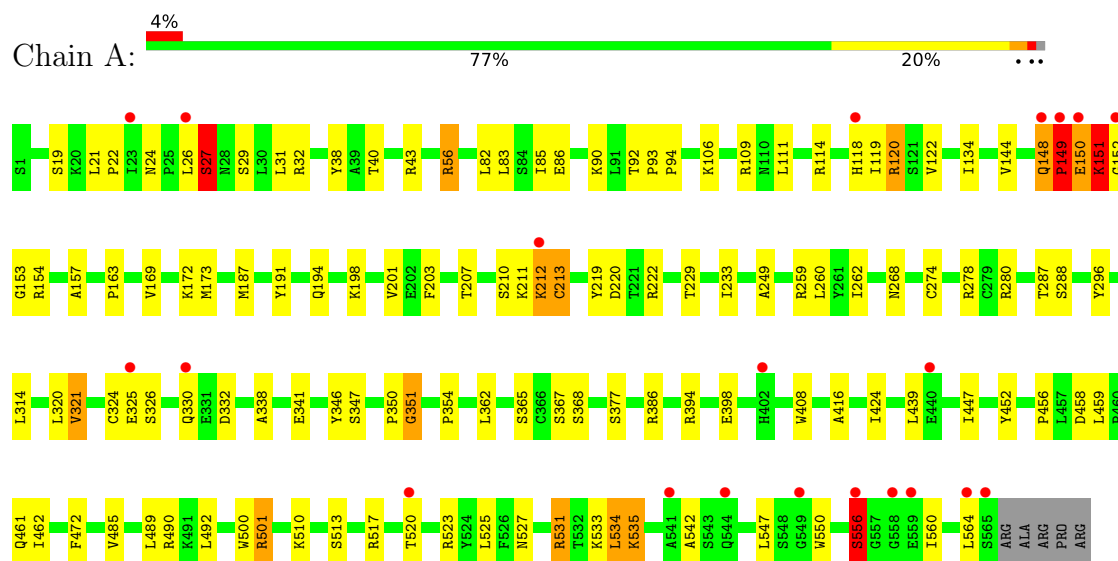
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	274	Total	O	0	0
			274	274		
2	B	205	Total	O	0	0
			205	205		

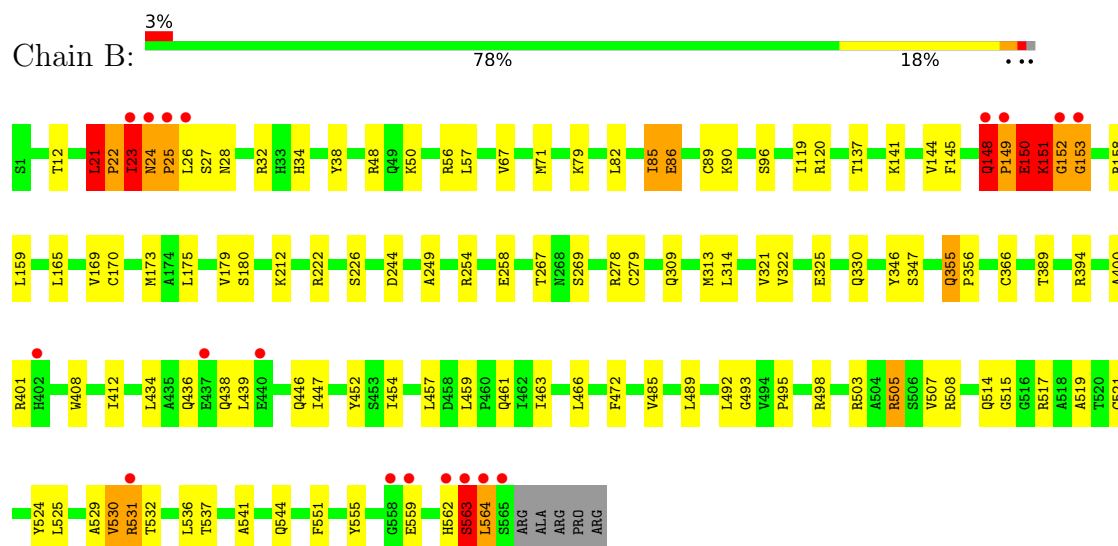
3 Residue-property plots [i](#)

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: 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	106.00Å 107.65Å 133.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 3.00 19.95 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.2 (19.95-3.00) 94.8 (19.95-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8.4	Depositor
R, R_{free}	0.173 , 0.258 0.192 , 0.268	Depositor DCC
R_{free} test set	2128 reflections (7.14%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9315	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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	0.62	2/4513 (0.0%)	0.94	14/6124 (0.2%)
1	B	0.69	3/4515 (0.1%)	1.02	20/6127 (0.3%)
All	All	0.65	5/9028 (0.1%)	0.98	34/12251 (0.3%)

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	2
1	B	0	4
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	23	ILE	CA-CB	8.86	1.66	1.54
1	B	24	ASN	CA-C	6.74	1.61	1.52
1	A	149	PRO	CA-C	5.99	1.60	1.52
1	B	24	ASN	C-O	5.62	1.31	1.24
1	A	150	GLU	N-CA	5.54	1.52	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	ASN	CA-C-N	11.66	134.42	119.84
1	B	24	ASN	C-N-CA	11.66	134.42	119.84
1	B	148	GLN	N-CA-C	9.47	130.74	109.81
1	A	151	LYS	N-CA-C	8.28	128.45	110.80
1	B	22	PRO	N-CA-C	8.13	123.82	111.14
1	B	150	GLU	N-CA-C	8.09	128.03	110.80
1	B	21	LEU	CA-C-N	7.91	127.90	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	21	LEU	C-N-CA	7.91	127.90	119.76
1	B	529	ALA	CB-CA-C	7.01	122.77	110.85
1	B	530	VAL	N-CA-C	6.67	119.66	109.12
1	B	153	GLY	N-CA-C	6.49	128.56	113.18
1	B	150	GLU	CA-C-N	6.40	134.82	122.53
1	B	150	GLU	C-N-CA	6.40	134.82	122.53
1	A	213	CYS	CA-C-N	6.28	126.23	119.76
1	A	213	CYS	C-N-CA	6.28	126.23	119.76
1	B	563	SER	CA-C-N	6.02	132.53	121.70
1	B	563	SER	C-N-CA	6.02	132.53	121.70
1	A	212	LYS	CG-CD-CE	-5.93	97.65	111.30
1	A	459	LEU	CA-C-N	-5.52	112.94	119.84
1	A	459	LEU	C-N-CA	-5.52	112.94	119.84
1	A	534	LEU	CA-C-N	-5.52	113.98	122.87
1	A	534	LEU	C-N-CA	-5.52	113.98	122.87
1	A	27	SER	N-CA-C	5.41	117.61	111.11
1	B	151	LYS	CB-CA-C	-5.41	100.63	109.56
1	A	368	SER	N-CA-C	5.31	116.91	108.79
1	B	24	ASN	N-CA-C	5.27	121.45	109.81
1	A	416	ALA	CA-C-N	-5.19	114.44	120.04
1	A	416	ALA	C-N-CA	-5.19	114.44	120.04
1	A	534	LEU	N-CA-C	-5.17	103.57	110.55
1	A	151	LYS	CB-CG-CD	5.05	122.92	111.30
1	B	149	PRO	CA-C-N	5.03	131.14	121.54
1	B	149	PRO	C-N-CA	5.03	131.14	121.54
1	B	454	ILE	N-CA-C	5.01	115.49	108.17
1	B	152	GLY	N-CA-C	-5.01	101.30	113.18

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	LYS	Peptide
1	A	535	LYS	Peptide
1	B	148	GLN	Peptide
1	B	151	LYS	Peptide
1	B	152	GLY	Peptide
1	B	562	HIS	Peptide

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	4417	0	4427	79	1
1	B	4419	0	4419	94	1
2	A	274	0	0	3	0
2	B	205	0	0	7	0
All	All	9315	0	8846	172	1

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 10.

All (172) 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:B:148:GLN:HG3	1:B:150:GLU:HB2	1.23	1.14
1:A:148:GLN:HB3	1:A:149:PRO:HD2	1.15	1.14
1:B:148:GLN:HG2	1:B:153:GLY:HA3	1.37	1.03
1:B:148:GLN:HG3	1:B:150:GLU:CB	1.98	0.94
1:A:533:LYS:HB2	1:A:535:LYS:NZ	1.84	0.92
1:A:501:ARG:HH12	1:A:531:ARG:CZ	1.88	0.86
1:A:148:GLN:HB3	1:A:149:PRO:CD	2.02	0.84
1:A:533:LYS:HB2	1:A:535:LYS:HZ3	1.42	0.84
1:A:148:GLN:CB	1:A:149:PRO:HD2	2.00	0.83
1:A:501:ARG:HH22	1:A:531:ARG:NH1	1.81	0.78
1:B:313:MET:HG2	1:B:322:VAL:HG22	1.70	0.71
1:B:148:GLN:HG2	1:B:153:GLY:CA	2.16	0.71
1:A:324:CYS:SG	1:A:325:GLU:N	2.63	0.71
1:B:24:ASN:OD1	1:B:25:PRO:HD2	1.92	0.70
1:A:501:ARG:HH12	1:A:531:ARG:NH2	1.89	0.69
1:A:330:GLN:H	1:A:330:GLN:CD	2.01	0.68
1:B:56:ARG:HH12	1:B:279:CYS:HB3	1.57	0.68
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.76	0.68
1:B:389:THR:HG23	1:B:492:LEU:HD21	1.75	0.67
1:B:86:GLU:N	1:B:86:GLU:OE1	2.26	0.67
1:A:220:ASP:OD2	1:A:351:GLY:HA3	1.94	0.66
1:B:505:ARG:HH22	1:B:531:ARG:HG2	1.59	0.66
1:A:490:ARG:O	1:B:212:LYS:NZ	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:ARG:HH12	1:B:530:VAL:HA	1.59	0.65
1:B:508:ARG:NH1	1:B:530:VAL:HG11	2.11	0.65
1:A:233:ILE:HD12	1:A:262:ILE:HA	1.79	0.64
1:B:32:ARG:HG2	1:B:493:GLY:O	1.97	0.64
1:B:559:GLU:HA	2:B:782:HOH:O	1.98	0.64
1:B:505:ARG:NH2	1:B:531:ARG:HG2	2.13	0.64
1:B:148:GLN:HG3	1:B:150:GLU:CG	2.26	0.64
1:A:268:ASN:HB3	1:A:274[B]:CYS:SG	2.39	0.63
1:B:347:SER:O	1:B:347:SER:OG	2.13	0.62
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.80	0.62
1:B:57:LEU:O	1:B:347:SER:HB2	2.00	0.61
1:A:31:LEU:HD11	1:A:492:LEU:HD22	1.82	0.61
1:A:144:VAL:HB	1:A:394:ARG:HG2	1.82	0.60
1:B:563:SER:HA	1:B:564:LEU:CB	2.31	0.60
1:B:148:GLN:CG	1:B:150:GLU:HB2	2.16	0.60
1:A:485:VAL:O	1:A:489:LEU:HG	2.03	0.59
1:B:21:LEU:HD23	1:B:22:PRO:HD2	1.84	0.59
1:B:24:ASN:CG	1:B:25:PRO:HD2	2.28	0.58
1:A:56:ARG:NH2	1:A:278:ARG:O	2.34	0.58
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.85	0.58
1:A:86:GLU:OE1	1:A:90:LYS:NZ	2.37	0.57
1:B:56:ARG:NH1	1:B:279:CYS:HB3	2.18	0.57
1:B:180:SER:OG	1:B:555:TYR:OH	2.20	0.56
1:B:524:TYR:OH	1:B:537:THR:O	2.20	0.56
1:B:434:LEU:HD13	1:B:439:LEU:HD11	1.88	0.56
1:B:148:GLN:OE1	1:B:150:GLU:HG2	2.06	0.56
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.87	0.55
1:A:56:ARG:NH1	1:A:229:THR:HA	2.22	0.55
1:A:501:ARG:NH2	1:A:531:ARG:NH1	2.52	0.55
1:B:466:LEU:HD22	1:B:551:PHE:HE2	1.71	0.54
1:A:222:ARG:NE	1:A:350:PRO:O	2.41	0.54
1:B:436:GLN:O	1:B:438:GLN:HG3	2.08	0.54
1:A:533:LYS:HB2	1:A:535:LYS:HZ2	1.68	0.54
1:B:408:TRP:O	1:B:412:ILE:HG13	2.07	0.53
1:A:19:SER:HB3	1:A:43:ARG:HH21	1.72	0.53
1:A:24:ASN:HB3	1:A:27:SER:HB3	1.90	0.53
1:A:321:VAL:HG23	1:A:365:SER:HB3	1.89	0.52
1:B:485:VAL:O	1:B:489:LEU:HG	2.09	0.52
1:B:170:CYS:HA	1:B:173:MET:CE	2.39	0.52
1:B:32:ARG:HH21	1:B:495:PRO:HG3	1.74	0.52
1:B:151:LYS:HG3	1:B:153:GLY:HA3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:TYR:O	1:A:194:GLN:HG2	2.09	0.52
1:A:86:GLU:HG3	1:A:111:LEU:HD11	1.91	0.52
1:B:22:PRO:O	1:B:24:ASN:N	2.43	0.52
1:A:118:HIS:O	1:A:122:VAL:HG23	2.11	0.51
1:A:347:SER:O	1:A:347:SER:OG	2.25	0.51
1:B:434:LEU:HD11	1:B:514:GLN:NE2	2.24	0.51
1:B:56:ARG:NH2	1:B:278:ARG:O	2.38	0.51
1:B:148:GLN:HB2	1:B:153:GLY:H	1.75	0.51
1:B:457:LEU:HB3	1:B:517:ARG:HB3	1.93	0.51
1:B:505:ARG:HH11	1:B:505:ARG:CG	2.23	0.50
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.93	0.50
1:A:151:LYS:HE3	1:A:153:GLY:HA2	1.95	0.49
1:B:21:LEU:CD2	1:B:22:PRO:HD2	2.43	0.49
1:B:67:VAL:O	1:B:71:MET:HG3	2.13	0.49
1:B:254:ARG:HH12	1:B:258:GLU:HG3	1.76	0.49
1:B:148:GLN:OE1	1:B:148:GLN:HA	2.09	0.49
1:A:338:ALA:HA	1:A:341:GLU:HG2	1.94	0.49
1:A:398:GLU:OE1	1:A:408:TRP:HD1	1.96	0.48
1:B:48:ARG:HG2	1:B:159:LEU:HG	1.95	0.48
1:B:175:LEU:O	1:B:179:VAL:HG22	2.13	0.48
1:A:21:LEU:HD12	1:A:22:PRO:HD2	1.94	0.48
1:A:229:THR:O	1:A:233:ILE:HG13	2.14	0.48
1:A:517:ARG:O	1:A:520:THR:HG22	2.14	0.48
1:A:439:LEU:O	1:A:456:PRO:HD2	2.14	0.48
1:B:12:THR:OG1	1:B:269:SER:OG	2.24	0.48
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.43	0.48
1:B:85:ILE:HD12	1:B:120:ARG:HE	1.79	0.47
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.94	0.47
1:B:180:SER:HG	1:B:555:TYR:HH	1.56	0.47
1:A:150:GLU:O	1:A:152:GLY:N	2.48	0.47
1:B:170:CYS:HA	1:B:173:MET:HE3	1.98	0.46
1:B:23:ILE:O	1:B:23:ILE:HG22	2.15	0.46
1:B:472:PHE:O	2:B:693:HOH:O	2.21	0.46
1:A:38:TYR:CZ	1:A:154:ARG:HB3	2.51	0.46
1:A:501:ARG:NH1	1:A:531:ARG:NH2	2.62	0.46
1:B:346:TYR:O	1:B:347:SER:HB3	2.16	0.46
1:A:534:LEU:O	1:A:535:LYS:HD2	2.16	0.46
1:A:203:PHE:CE2	1:A:314:LEU:HD13	2.51	0.45
1:B:86:GLU:HA	1:B:89:CYS:HB2	1.97	0.45
1:B:461:GLN:HG2	1:B:541:ALA:HB3	1.97	0.45
1:A:85:ILE:HD11	1:A:120:ARG:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:LEU:HD11	1:B:514:GLN:HE22	1.81	0.45
1:B:563:SER:OG	1:B:564:LEU:O	2.28	0.45
1:B:325:GLU:HG3	2:B:735:HOH:O	2.16	0.45
1:B:26:LEU:O	1:B:27:SER:OG	2.26	0.45
1:B:26:LEU:O	1:B:28:ASN:N	2.50	0.45
1:B:226[B]:SER:HA	1:B:279:CYS:SG	2.57	0.45
1:A:93:PRO:HA	1:A:94:PRO:HD3	1.87	0.44
1:B:150:GLU:HB3	1:B:151:LYS:HG2	1.99	0.44
1:A:163:PRO:HG3	1:A:260:LEU:HD21	2.00	0.44
1:A:288:SER:HB2	1:A:556:SER:HB3	2.00	0.44
1:A:314:LEU:HD12	1:A:314:LEU:HA	1.85	0.44
1:A:472:PHE:HE1	1:A:525:LEU:HD23	1.82	0.44
1:A:86:GLU:O	1:A:90:LYS:HG3	2.18	0.43
1:A:510:LYS:NZ	2:A:822:HOH:O	2.48	0.43
1:B:144:VAL:HB	1:B:394:ARG:HG2	2.00	0.43
1:B:452:TYR:HA	1:B:563:SER:HB2	2.00	0.43
1:A:531:ARG:HH11	1:A:531:ARG:HG3	1.83	0.43
1:B:309:GLN:HG3	1:B:325:GLU:HB3	1.99	0.43
1:B:38:TYR:CZ	1:B:145:PHE:HB2	2.54	0.43
1:B:394:ARG:NH1	2:B:748:HOH:O	2.39	0.43
1:A:346:TYR:O	1:A:347:SER:HB3	2.18	0.43
1:A:83:LEU:HB2	1:A:173:MET:HA	2.01	0.43
1:A:280:ARG:HD2	1:A:287:THR:HA	1.99	0.43
1:A:326:SER:OG	1:A:332:ASP:OD2	2.30	0.43
1:B:137:THR:HA	1:B:267:THR:O	2.19	0.43
1:B:148:GLN:OE1	1:B:148:GLN:CA	2.63	0.43
1:B:515:GLY:HA2	1:B:519:ALA:HB2	1.99	0.43
1:A:354:PRO:HA	2:A:859:HOH:O	2.17	0.43
1:B:26:LEU:C	1:B:27:SER:HG	2.23	0.43
1:B:446:GLN:O	1:B:447:ILE:HD13	2.18	0.43
1:B:141:LYS:NZ	1:B:158:ARG:NH2	2.66	0.42
1:B:32:ARG:NH2	1:B:495:PRO:HG3	2.35	0.42
1:A:207:THR:O	1:A:210:SER:OG	2.31	0.42
1:B:79:LYS:HG3	1:B:244:ASP:HB3	2.02	0.42
1:B:503:ARG:O	1:B:507:VAL:HG23	2.19	0.42
1:A:19:SER:HB3	1:A:43:ARG:NH2	2.35	0.42
1:A:447:ILE:HB	1:A:452:TYR:HE1	1.84	0.42
1:B:23:ILE:O	1:B:23:ILE:CG2	2.67	0.42
1:B:22:PRO:HG2	1:B:400:ALA:HB1	2.01	0.42
1:B:96:SER:HA	2:B:641:HOH:O	2.20	0.42
1:A:547:LEU:O	1:A:550:TRP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:LEU:O	1:B:169:VAL:HG23	2.18	0.41
1:A:92:THR:O	1:A:109:ARG:HD2	2.21	0.41
1:A:458:ASP:O	1:A:462:ILE:HG13	2.20	0.41
1:B:32:ARG:O	1:B:34:HIS:N	2.53	0.41
1:B:524:TYR:CE2	1:B:536:LEU:HB3	2.55	0.41
1:A:29:SER:HA	2:A:819:HOH:O	2.19	0.41
1:A:40:THR:HB	1:A:157:ALA:HB2	2.03	0.41
1:B:48:ARG:NH1	2:B:774:HOH:O	2.51	0.41
1:B:90:LYS:HG2	2:B:723:HOH:O	2.19	0.41
1:B:226[A]:SER:HA	1:B:279:CYS:SG	2.60	0.41
1:A:26:LEU:O	1:A:29:SER:OG	2.38	0.41
1:A:134:ILE:HG13	1:A:259:ARG:HB3	2.03	0.41
1:B:401:ARG:HD3	1:B:401:ARG:HA	1.91	0.41
1:B:355:GLN:HA	1:B:356:PRO:HD3	1.88	0.41
1:B:521:CYS:O	1:B:525:LEU:HB2	2.21	0.41
1:B:531:ARG:HB2	1:B:532:THR:H	1.41	0.41
1:A:367:SER:CB	1:A:386:ARG:NH1	2.83	0.41
1:A:461:GLN:HB2	1:A:542:ALA:HA	2.02	0.41
1:B:459:LEU:O	1:B:463:ILE:HG13	2.20	0.41
1:A:187:MET:HG2	1:A:296:TYR:CD1	2.56	0.41
1:A:531:ARG:NH1	1:A:531:ARG:HG3	2.36	0.41
1:A:198:LYS:O	1:A:201:VAL:HG12	2.20	0.41
1:A:424:ILE:HG12	1:A:500:TRP:NE1	2.36	0.41
1:A:362:LEU:HD23	1:A:362:LEU:HA	1.86	0.40
1:A:523:ARG:O	1:A:527:ASN:HB2	2.21	0.40
1:A:490:ARG:HH11	1:A:490:ARG:HG3	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:NH1	1:B:24:ASN:OD1[1_565]	2.16	0.04

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%)	524 (93%)	36 (6%)	6 (1%)	11	43
1	B	567/570 (100%)	535 (94%)	25 (4%)	7 (1%)	10	40
All	All	1133/1140 (99%)	1059 (94%)	61 (5%)	13 (1%)	10	43

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	LYS
1	B	23	ILE
1	B	25	PRO
1	B	148	GLN
1	B	150	GLU
1	B	531	ARG
1	A	149	PRO
1	A	151	LYS
1	A	213	CYS
1	A	351	GLY
1	A	556	SER
1	B	149	PRO
1	B	564	LEU

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	484/485 (100%)	471 (97%)	13 (3%)	39	71
1	B	483/485 (100%)	469 (97%)	14 (3%)	37	70
All	All	967/970 (100%)	940 (97%)	27 (3%)	38	70

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

Mol	Chain	Res	Type
1	A	27	SER
1	A	32	ARG
1	A	56	ARG
1	A	106	LYS
1	A	120	ARG
1	A	148	GLN
1	A	321	VAL
1	A	377	SER
1	A	501	ARG
1	A	513	SER
1	A	531	ARG
1	A	556	SER
1	A	564	LEU
1	B	21	LEU
1	B	50	LYS
1	B	85	ILE
1	B	86	GLU
1	B	148	GLN
1	B	151	LYS
1	B	222	ARG
1	B	330	GLN
1	B	355	GLN
1	B	366	CYS
1	B	498	ARG
1	B	505	ARG
1	B	544	GLN
1	B	563	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	HIS
1	B	206	ASN
1	B	514	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 [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 [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	565/570 (99%)	0.00	21 (3%)	45 25	11, 42, 101, 158	3 (0%)
1	B	565/570 (99%)	-0.27	18 (3%)	50 29	12, 31, 75, 151	4 (0%)
All	All	1130/1140 (99%)	-0.13	39 (3%)	47 27	11, 35, 96, 158	7 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	148	GLN	6.4
1	B	565	SER	5.8
1	B	23	ILE	4.8
1	A	118	HIS	4.5
1	A	325	GLU	4.4
1	B	24	ASN	4.3
1	B	25	PRO	3.9
1	B	402	HIS	3.6
1	B	152	GLY	3.6
1	A	152	GLY	3.5
1	A	440	GLU	3.3
1	A	565	SER	3.2
1	A	23	ILE	3.2
1	A	330	GLN	3.1
1	A	149	PRO	3.0
1	B	558	GLY	2.8
1	A	556	SER	2.8
1	B	26	LEU	2.8
1	B	564	LEU	2.7
1	A	212	LYS	2.7
1	A	559	GLU	2.7
1	B	563	SER	2.7
1	A	26	LEU	2.6
1	B	562	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	520	THR	2.5
1	A	150	GLU	2.5
1	B	153	GLY	2.4
1	A	541	ALA	2.3
1	B	440	GLU	2.3
1	A	549	GLY	2.2
1	A	564	LEU	2.2
1	B	148	GLN	2.2
1	B	559	GLU	2.2
1	B	437	GLU	2.1
1	B	149	PRO	2.1
1	A	558	GLY	2.1
1	A	402	HIS	2.1
1	A	544	GLN	2.0
1	B	531	ARG	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 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.