



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:19 AM UTC

PDB ID : 4WSE / pdb_00004wse
Title : Crystal structure of the Mimivirus polyadenylate synthase
Authors : Priet, S.; Lartigue, A.; Claverie, J.M.; Abergel, C.
Deposited on : 2014-10-27
Resolution : 2.84 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

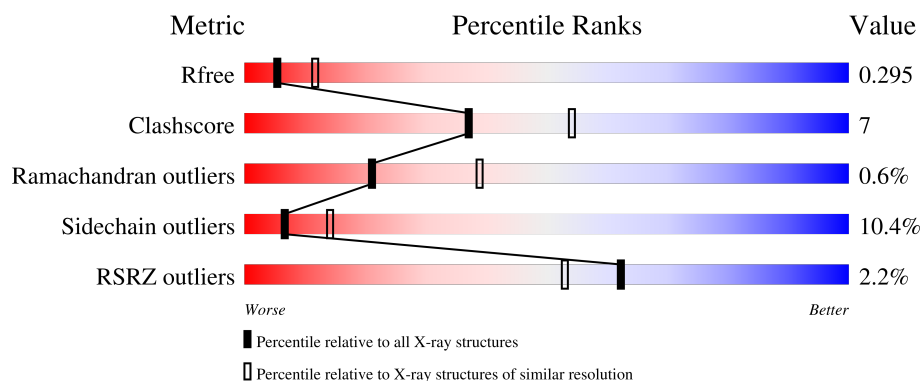
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	584	 63% 18% 15% 4%
1	B	584	 61% 20% 15% 4%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8506 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 Putative poly(A) polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	1	0
			4132	2662	677	780	13			
1	B	495	Total	C	N	O	S	0	0	0
			4134	2666	675	780	13			

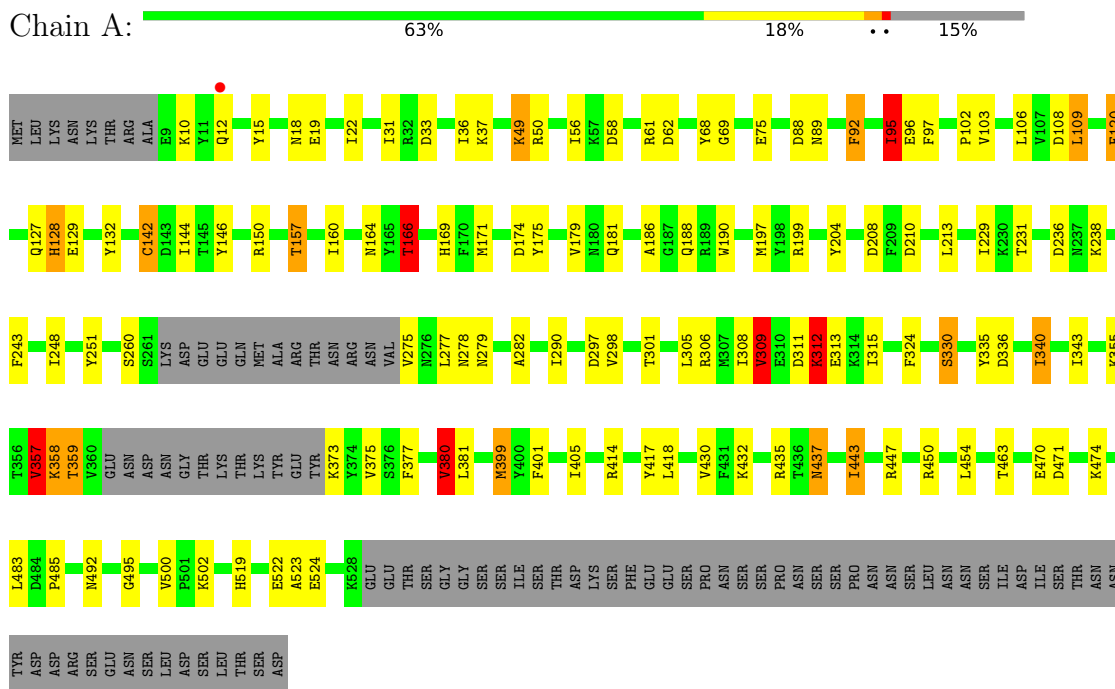
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	122	Total	O	0	0
			122	122		
2	B	118	Total	O	0	0
			118	118		

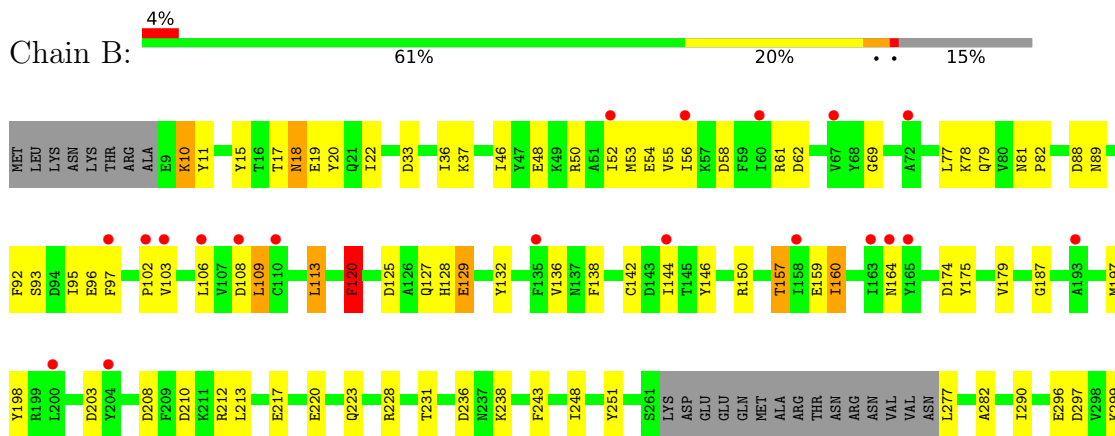
3 Residue-property plots [i](#)

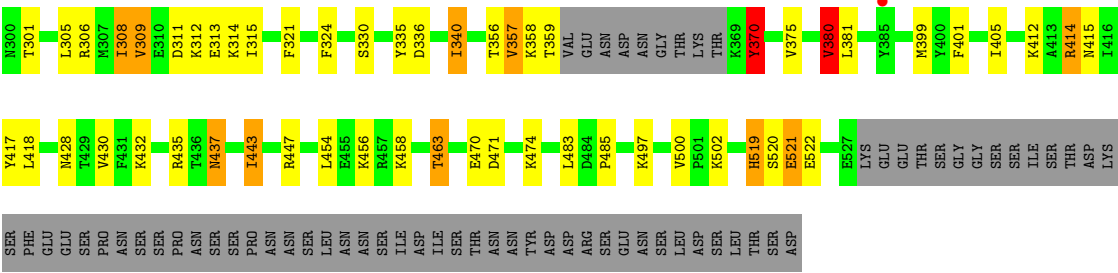
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Putative poly(A) polymerase catalytic subunit



- Molecule 1: Putative poly(A) polymerase catalytic subunit





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	200.03Å 69.65Å 97.49Å 90.00° 105.75° 90.00°	Depositor
Resolution (Å)	46.01 – 2.84 46.01 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.01-2.84) 99.3 (46.01-2.84)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.86Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.2	Depositor
R, R_{free}	0.227 , 0.268 0.248 , 0.295	Depositor DCC
R_{free} test set	1521 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	70.1	Xtriage
Anisotropy	0.888	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 99.1	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	0.94	EDS
Total number of atoms	8506	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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	0.87	1/4225 (0.0%)	1.46	42/5706 (0.7%)
1	B	0.88	0/4229	1.53	43/5711 (0.8%)
All	All	0.87	1/8454 (0.0%)	1.50	85/11417 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	GLN	CA-C	5.24	1.59	1.52

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	ASP	N-CA-C	21.86	147.22	111.37
1	B	11	TYR	N-CA-C	13.71	128.63	110.53
1	B	10	LYS	N-CA-C	13.49	139.54	110.80
1	A	357	VAL	N-CA-C	13.31	137.03	109.34
1	B	89	ASN	N-CA-CB	13.12	132.67	110.49
1	B	89	ASN	N-CA-C	-11.18	87.00	110.80
1	A	357	VAL	CB-CA-C	-10.64	93.84	111.29
1	B	120	PHE	CA-CB-CG	10.56	124.36	113.80
1	A	358	LYS	N-CA-C	10.45	123.81	110.33
1	B	128	HIS	N-CA-C	9.75	131.57	110.80
1	A	358	LYS	N-CA-CB	-9.73	97.06	110.29
1	B	10	LYS	CB-CA-C	-9.47	91.57	110.42
1	B	88	ASP	CB-CA-C	-9.37	95.28	110.84
1	B	92	PHE	CA-CB-CG	9.03	122.83	113.80
1	B	463	THR	N-CA-C	8.70	120.45	110.97
1	B	11	TYR	N-CA-CB	-8.46	98.26	110.36
1	B	129	GLU	N-CA-C	-8.33	98.12	109.54
1	A	358	LYS	CA-C-N	8.23	136.51	121.70
1	A	358	LYS	C-N-CA	8.23	136.51	121.70
1	B	370	TYR	N-CA-C	8.18	128.23	110.80
1	B	311	ASP	CA-C-N	7.28	132.88	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	311	ASP	C-N-CA	7.28	132.88	120.72
1	B	520	SER	CA-C-N	6.59	130.11	120.82
1	B	520	SER	C-N-CA	6.59	130.11	120.82
1	A	50	ARG	CA-C-N	6.56	129.30	120.65
1	A	50	ARG	C-N-CA	6.56	129.30	120.65
1	A	166	THR	CB-CA-C	6.16	118.63	110.06
1	B	324	PHE	CA-CB-CG	6.08	119.89	113.80
1	B	340	ILE	N-CA-C	-6.04	105.94	111.67
1	B	69	GLY	CA-C-N	5.98	126.45	119.94
1	B	69	GLY	C-N-CA	5.98	126.45	119.94
1	B	203	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	311	ASP	N-CA-C	5.87	123.30	110.80
1	A	58	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	278	ASN	CA-CB-CG	5.78	118.38	112.60
1	B	220	GLU	CA-C-N	5.76	128.28	120.44
1	B	220	GLU	C-N-CA	5.76	128.28	120.44
1	B	380	VAL	N-CA-CB	5.73	117.91	110.57
1	A	324	PHE	CA-CB-CG	5.70	119.50	113.80
1	A	95	ILE	N-CA-CB	5.68	118.42	111.60
1	A	340	ILE	N-CA-C	-5.67	106.28	111.67
1	A	380	VAL	N-CA-CB	5.63	117.78	110.57
1	B	62	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	77	LEU	CA-C-N	5.57	127.68	120.44
1	B	77	LEU	C-N-CA	5.57	127.68	120.44
1	A	92	PHE	CA-C-N	5.56	132.16	121.54
1	A	92	PHE	C-N-CA	5.56	132.16	121.54
1	A	89	ASN	CA-CB-CG	5.54	118.14	112.60
1	A	474	LYS	N-CA-C	-5.50	106.58	113.28
1	B	58	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	108	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	309	VAL	CA-C-N	5.45	130.10	121.99
1	A	309	VAL	C-N-CA	5.45	130.10	121.99
1	A	75	GLU	CA-C-N	5.41	127.80	120.44
1	A	75	GLU	C-N-CA	5.41	127.80	120.44
1	B	108	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	49	LYS	CA-C-N	5.30	127.39	120.28
1	A	49	LYS	C-N-CA	5.30	127.39	120.28
1	B	474	LYS	N-CA-C	-5.29	106.82	113.28
1	A	129	GLU	CA-C-N	5.26	131.59	121.54
1	A	129	GLU	C-N-CA	5.26	131.59	121.54
1	A	62	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	61	ARG	CA-C-N	5.19	127.50	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ARG	C-N-CA	5.19	127.50	120.65
1	A	524	GLU	N-CA-C	5.19	116.95	108.76
1	A	61	ARG	CA-C-N	5.17	127.47	120.65
1	A	61	ARG	C-N-CA	5.17	127.47	120.65
1	B	519	HIS	CB-CA-C	-5.14	105.09	113.37
1	A	495	GLY	CA-C-N	5.14	129.92	121.39
1	A	495	GLY	C-N-CA	5.14	129.92	121.39
1	B	48	GLU	N-CA-C	-5.12	106.36	113.18
1	A	88	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	277	LEU	CA-C-N	5.09	131.51	121.58
1	A	277	LEU	C-N-CA	5.09	131.51	121.58
1	B	125	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	521	GLU	CA-C-N	5.07	130.38	122.26
1	B	521	GLU	C-N-CA	5.07	130.38	122.26
1	B	198	TYR	CA-C-N	5.06	128.00	120.31
1	B	198	TYR	C-N-CA	5.06	128.00	120.31
1	A	69	GLY	CA-C-N	5.05	125.69	120.03
1	A	69	GLY	C-N-CA	5.05	125.69	120.03
1	A	128	HIS	CA-C-N	5.04	131.17	121.54
1	A	128	HIS	C-N-CA	5.04	131.17	121.54
1	B	89	ASN	CA-C-N	5.03	129.97	122.82
1	B	89	ASN	C-N-CA	5.03	129.97	122.82

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	4132	0	4077	63	0
1	B	4134	0	4072	63	0
2	A	122	0	0	3	0
2	B	118	0	0	6	0
All	All	8506	0	8149	116	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 7.

All (116) 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:12:GLN:NE2	1:B:412:LYS:HG3	1.46	1.29
1:B:357:VAL:HA	1:B:370:TYR:O	1.46	1.14
1:A:208:ASP:HB3	1:B:10:LYS:O	1.44	1.14
1:A:12:GLN:HE22	1:B:412:LYS:HG3	0.94	1.08
1:A:358:LYS:HB3	1:A:359:THR:HB	1.48	0.93
1:A:12:GLN:NE2	1:B:412:LYS:CG	2.34	0.89
1:A:208:ASP:CB	1:B:10:LYS:O	2.22	0.87
1:A:357:VAL:HG12	1:A:357:VAL:O	1.79	0.82
1:B:321:PHE:HE1	1:B:522:GLU:HG2	1.45	0.79
1:A:298:VAL:HG22	1:A:343:ILE:HG21	1.67	0.77
1:B:305:LEU:O	1:B:309:VAL:HB	1.87	0.74
1:A:95:ILE:O	1:A:142:CYS:HB2	1.90	0.71
1:A:56:ILE:HG23	1:A:109:LEU:HD11	1.74	0.70
1:A:443:ILE:HG23	1:A:447:ARG:HB3	1.76	0.68
1:A:12:GLN:HE22	1:B:412:LYS:CG	1.89	0.68
1:B:443:ILE:HG23	1:B:447:ARG:HB3	1.75	0.68
1:A:375:VAL:HG23	1:A:380:VAL:HG12	1.74	0.68
1:B:375:VAL:HG23	1:B:380:VAL:HG12	1.74	0.68
1:B:56:ILE:HG23	1:B:109:LEU:HD11	1.77	0.67
1:A:157:THR:HG21	1:A:164:ASN:HB3	1.77	0.67
1:A:492:ASN:H	1:A:523:ALA:HB1	1.62	0.64
1:A:401:PHE:O	1:A:405:ILE:HG12	1.98	0.64
1:A:492:ASN:N	1:A:523:ALA:HB1	2.12	0.63
1:B:401:PHE:O	1:B:405:ILE:HG12	1.99	0.62
1:B:502:LYS:O	1:B:519:HIS:HB2	1.98	0.62
1:A:502:LYS:O	1:A:519:HIS:HB2	1.99	0.62
1:A:166:THR:CG2	1:A:171:MET:CG	2.79	0.61
1:B:321:PHE:CE1	1:B:522:GLU:HG2	2.32	0.61
1:A:166:THR:HG22	1:A:171:MET:CG	2.31	0.61
1:A:298:VAL:HG22	1:A:343:ILE:HD13	1.82	0.61
1:A:166:THR:CG2	1:A:171:MET:HG3	2.31	0.60
1:B:497:LYS:HG3	2:B:700:HOH:O	2.01	0.59
1:A:309:VAL:HG21	1:A:315:ILE:HD11	1.85	0.58
1:A:312:LYS:HD2	1:A:312:LYS:H	1.68	0.58
1:B:213:LEU:HD13	1:B:282:ALA:HB2	1.87	0.57
1:B:50:ARG:HA	1:B:53:MET:HE2	1.88	0.56
1:A:236:ASP:OD1	1:A:238:LYS:HG2	2.06	0.56
1:A:213:LEU:HD13	1:A:282:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:TYR:HB3	1:A:340:ILE:HD11	1.88	0.55
1:B:197:MET:HA	2:B:654:HOH:O	2.07	0.54
1:A:248:ILE:HA	1:A:251:TYR:HB3	1.88	0.54
1:B:236:ASP:OD1	1:B:238:LYS:HG2	2.08	0.54
1:B:248:ILE:HA	1:B:251:TYR:HB3	1.88	0.54
1:A:305:LEU:O	1:A:309:VAL:HB	2.07	0.54
1:A:10:LYS:HB3	1:B:208:ASP:HB3	1.89	0.54
1:A:106:LEU:HD13	1:A:132:TYR:HB3	1.90	0.53
1:B:290:ILE:HD12	1:B:375:VAL:HG11	1.91	0.53
1:A:432:LYS:HB3	1:A:435:ARG:HH11	1.73	0.52
1:A:290:ILE:HD12	1:A:375:VAL:HG11	1.92	0.52
1:A:243:PHE:CZ	1:A:297:ASP:HB3	2.45	0.52
1:A:492:ASN:H	1:A:523:ALA:CB	2.22	0.52
1:B:357:VAL:HG23	1:B:370:TYR:HB3	1.91	0.52
1:B:55:VAL:HG11	1:B:113:LEU:HD22	1.92	0.52
1:B:19:GLU:HA	1:B:22:ILE:HD12	1.92	0.52
1:B:243:PHE:CZ	1:B:297:ASP:HB3	2.45	0.51
1:A:188:GLN:HG2	2:A:629:HOH:O	2.11	0.50
1:B:228:ARG:CZ	1:B:308:ILE:HG13	2.42	0.50
1:A:357:VAL:O	1:A:357:VAL:CG1	2.45	0.49
1:A:166:THR:HG22	1:A:171:MET:HG3	1.92	0.49
1:A:315:ILE:HD13	1:A:335:TYR:HB2	1.94	0.49
1:B:106:LEU:HD13	1:B:132:TYR:HB3	1.93	0.49
1:A:120:PHE:N	1:A:120:PHE:CD1	2.81	0.49
1:A:56:ILE:HB	1:A:95:ILE:HD11	1.95	0.48
1:A:450:ARG:HD2	1:B:138:PHE:HB3	1.97	0.47
1:A:103:VAL:HG12	2:A:617:HOH:O	2.15	0.47
1:A:19:GLU:HA	1:A:22:ILE:HD12	1.96	0.47
1:B:522:GLU:H	1:B:522:GLU:CD	2.22	0.47
1:A:399:MET:HG2	2:A:645:HOH:O	2.14	0.47
1:B:217:GLU:HG2	1:B:223:GLN:NE2	2.30	0.47
1:B:197:MET:CA	2:B:654:HOH:O	2.63	0.47
1:A:31:ILE:HG23	1:B:187:GLY:HA2	1.97	0.46
1:A:437:ASN:ND2	1:A:437:ASN:H	2.13	0.46
1:A:103:VAL:HG22	1:A:485:PRO:HB3	1.97	0.46
1:B:314:LYS:HB2	1:B:335:TYR:CE1	2.51	0.46
1:A:298:VAL:HG22	1:A:343:ILE:CG2	2.42	0.46
1:B:97:PHE:CZ	1:B:144:ILE:HG12	2.50	0.46
1:B:414:ARG:HG3	1:B:415:ASN:N	2.30	0.46
1:B:159:GLU:HB2	2:B:716:HOH:O	2.14	0.46
1:B:50:ARG:HG2	1:B:53:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:THR:HA	2:B:710:HOH:O	2.15	0.46
1:B:102:PRO:HG3	1:B:146:TYR:HB2	1.98	0.46
1:B:335:TYR:HB2	1:B:340:ILE:HD11	1.98	0.46
1:A:166:THR:CG2	1:A:171:MET:HG2	2.45	0.45
1:B:17:THR:HA	1:B:18:ASN:HA	1.76	0.45
1:B:79:GLN:CD	1:B:160:ILE:HG12	2.42	0.45
1:A:175:TYR:HB3	1:A:197:MET:HE2	1.99	0.45
1:A:97:PHE:CZ	1:A:144:ILE:HG12	2.53	0.44
1:B:309:VAL:HG21	1:B:315:ILE:HD11	1.99	0.44
1:A:12:GLN:HE21	1:B:412:LYS:CG	2.25	0.44
1:B:296:GLU:HA	1:B:299:LYS:HZ2	1.82	0.44
1:B:437:ASN:ND2	1:B:437:ASN:H	2.15	0.44
1:B:95:ILE:HB	1:B:142:CYS:HB2	2.00	0.44
1:B:52:ILE:HG23	1:B:113:LEU:HD11	2.00	0.44
1:B:157:THR:HG21	1:B:164:ASN:HB3	1.99	0.44
1:B:103:VAL:HG22	1:B:485:PRO:HB3	2.01	0.43
1:A:229:ILE:HD11	1:A:305:LEU:HD21	2.00	0.43
1:A:102:PRO:HG3	1:A:146:TYR:HB2	2.00	0.43
1:B:78:LYS:HA	1:B:81:ASN:O	2.19	0.42
1:A:417:TYR:HD2	1:A:418:LEU:HD12	1.84	0.42
1:B:78:LYS:HG3	1:B:82:PRO:HA	2.01	0.42
1:B:212:ARG:HB3	1:B:212:ARG:NH1	2.34	0.42
1:A:377:PHE:CE2	1:A:414:ARG:HD3	2.53	0.42
1:A:169:HIS:HE1	1:A:204:TYR:O	2.03	0.42
1:B:432:LYS:HB3	1:B:435:ARG:NH1	2.35	0.42
1:B:335:TYR:CB	1:B:340:ILE:HD11	2.50	0.42
1:A:186:ALA:HA	1:A:190:TRP:CD1	2.55	0.42
1:A:335:TYR:CB	1:A:340:ILE:HD11	2.50	0.41
1:B:522:GLU:CD	1:B:522:GLU:N	2.78	0.41
1:B:175:TYR:HB3	1:B:197:MET:HE2	2.03	0.41
1:B:417:TYR:HD2	1:B:418:LEU:HD12	1.86	0.41
1:B:20:TYR:HB3	2:B:710:HOH:O	2.19	0.41
1:A:68:TYR:CZ	1:A:96:GLU:HB3	2.55	0.41
1:B:120:PHE:O	1:B:136:VAL:HA	2.20	0.40
1:B:212:ARG:HB3	1:B:212:ARG:HH11	1.86	0.40
1:A:49:LYS:HD2	1:A:92:PHE:HA	2.04	0.40
1:A:330:SER:HA	1:A:343:ILE:O	2.21	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	490/584 (84%)	443 (90%)	42 (9%)	5 (1%)	12	24
1	B	489/584 (84%)	446 (91%)	42 (9%)	1 (0%)	43	62
All	All	979/1168 (84%)	889 (91%)	84 (9%)	6 (1%)	21	39

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	ASN
1	A	312	LYS
1	A	359	THR
1	A	15	TYR
1	B	15	TYR
1	A	357	VAL

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	459/542 (85%)	415 (90%)	44 (10%)	8	17
1	B	458/542 (84%)	407 (89%)	51 (11%)	6	12
All	All	917/1084 (85%)	822 (90%)	95 (10%)	7	14

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	33	ASP
1	A	36	ILE
1	A	37	LYS
1	A	95	ILE
1	A	109	LEU
1	A	120	PHE
1	A	127	GLN
1	A	128	HIS
1	A	142	CYS
1	A	150	ARG
1	A	157	THR
1	A	160	ILE
1	A	166	THR
1	A	174	ASP
1	A	179	VAL
1	A	199	ARG
1	A	210	ASP
1	A	231	THR
1	A	260	SER
1	A	275	VAL
1	A	301	THR
1	A	306	ARG
1	A	308	ILE
1	A	309	VAL
1	A	312	LYS
1	A	313	GLU
1	A	330	SER
1	A	336	ASP
1	A	355	LYS
1	A	373	LYS
1	A	380	VAL
1	A	381	LEU
1	A	399	MET
1	A	430	VAL
1	A	437	ASN
1	A	443	ILE
1	A	454	LEU
1	A	463	THR
1	A	470	GLU
1	A	471	ASP
1	A	483	LEU
1	A	500	VAL

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Mol	Chain	Res	Type
1	A	522	GLU
1	B	18	ASN
1	B	33	ASP
1	B	36	ILE
1	B	37	LYS
1	B	46	ILE
1	B	54	GLU
1	B	93	SER
1	B	96	GLU
1	B	109	LEU
1	B	113	LEU
1	B	120	PHE
1	B	127	GLN
1	B	129	GLU
1	B	150	ARG
1	B	157	THR
1	B	160	ILE
1	B	174	ASP
1	B	179	VAL
1	B	210	ASP
1	B	231	THR
1	B	277	LEU
1	B	301	THR
1	B	306	ARG
1	B	308	ILE
1	B	309	VAL
1	B	312	LYS
1	B	313	GLU
1	B	330	SER
1	B	336	ASP
1	B	356	THR
1	B	357	VAL
1	B	358	LYS
1	B	359	THR
1	B	370	TYR
1	B	380	VAL
1	B	381	LEU
1	B	399	MET
1	B	414	ARG
1	B	428	ASN
1	B	430	VAL
1	B	437	ASN

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Mol	Chain	Res	Type
1	B	443	ILE
1	B	454	LEU
1	B	456	LYS
1	B	458	LYS
1	B	463	THR
1	B	470	GLU
1	B	471	ASP
1	B	483	LEU
1	B	500	VAL
1	B	521	GLU

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	12	GLN
1	A	21	GLN
1	A	139	GLN
1	A	169	HIS
1	A	181	GLN
1	A	303	ASN
1	A	437	ASN
1	A	449	ASN
1	B	21	GLN
1	B	139	GLN
1	B	169	HIS
1	B	279	ASN
1	B	303	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	495/584 (84%)	0.10	1 (0%) 91 91	46, 93, 136, 164	1 (0%)
1	B	495/584 (84%)	0.45	21 (4%) 40 32	50, 103, 153, 183	5 (1%)
All	All	990/1168 (84%)	0.27	22 (2%) 62 53	46, 99, 142, 183	6 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	144	ILE	7.7
1	B	165	TYR	5.9
1	B	67	VAL	5.4
1	B	56	ILE	4.7
1	B	52	ILE	3.9
1	B	60	ILE	3.8
1	B	97	PHE	3.6
1	B	103	VAL	3.3
1	A	12	GLN	3.3
1	B	200	LEU	2.7
1	B	135	PHE	2.7
1	B	164	ASN	2.5
1	B	158	ILE	2.4
1	B	193	ALA	2.4
1	B	108	ASP	2.4
1	B	385	TYR	2.4
1	B	163	ILE	2.4
1	B	110	CYS	2.3
1	B	204	TYR	2.3
1	B	106	LEU	2.3
1	B	72	ALA	2.2
1	B	102	PRO	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.