



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2025 – 02:10 PM EDT

PDB ID : 9O0D / pdb_00009o0d
Title : crystal structure of rSAMD9 tRNase domain
Authors : Deng, J.P.
Deposited on : 2025-04-02
Resolution : 2.39 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 Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

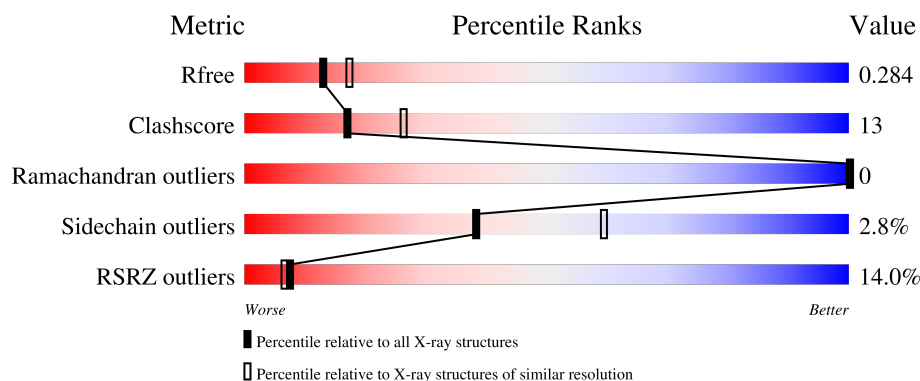
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (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	234	<div> <div>12%</div> <div>68%</div> <div>22%</div> <div>8%</div> </div>
1	B	234	<div> <div>15%</div> <div>68%</div> <div>22%</div> <div>8%</div> </div>
1	C	234	<div> <div>12%</div> <div>67%</div> <div>22%</div> <div>8%</div> </div>
1	D	234	<div> <div>13%</div> <div>72%</div> <div>18%</div> <div>8%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7064 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 rSAMD9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	82	0	0
			1753	1118	304	322	9			
1	B	216	Total	C	N	O	S	106	0	0
			1768	1125	307	327	9			
1	C	216	Total	C	N	O	S	92	0	0
			1765	1126	307	323	9			
1	D	215	Total	C	N	O	S	94	0	0
			1757	1122	305	321	9			

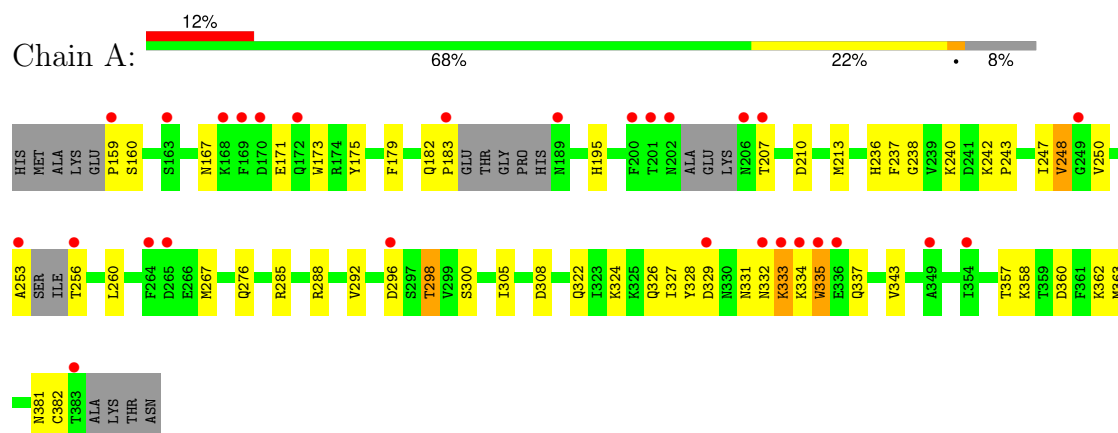
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	O	0	0
			4	4		
2	B	8	Total	O	0	0
			8	8		
2	C	3	Total	O	0	0
			3	3		
2	D	6	Total	O	0	0
			6	6		

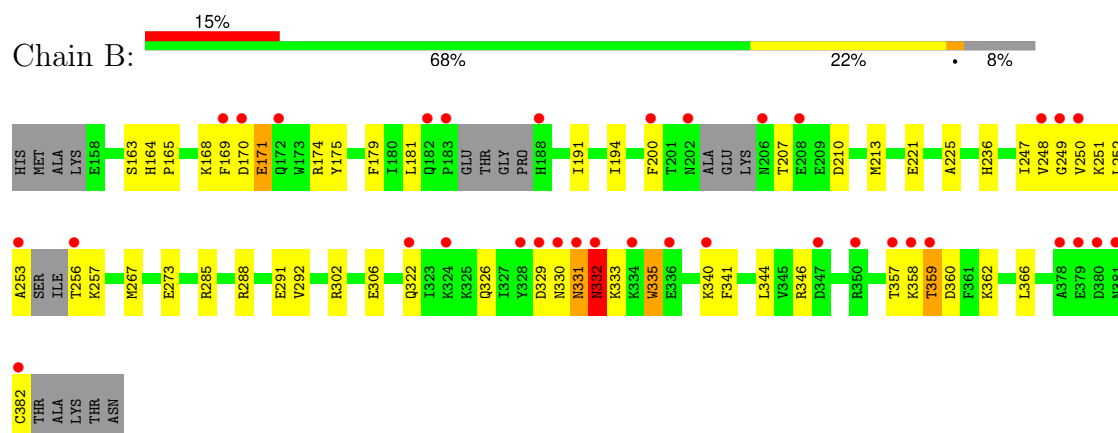
3 Residue-property plots [i](#)

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.

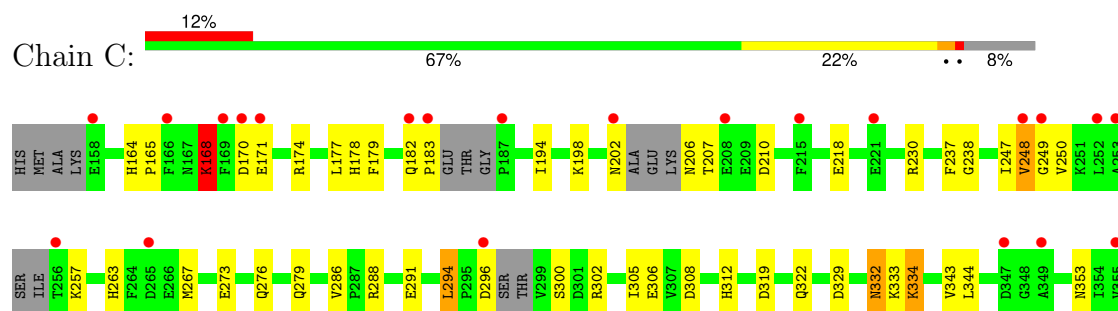
• Molecule 1: rSAMD9

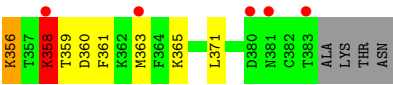


• Molecule 1: rSAMD9

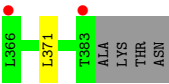
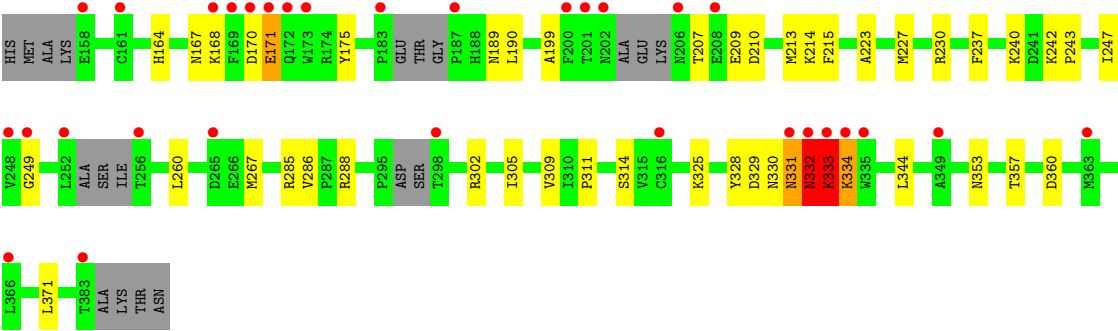


• Molecule 1: rSAMD9





● Molecule 1: rSAMd9



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.98Å 142.49Å 83.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.48 – 2.39 43.48 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.8 (43.48-2.39) 98.8 (43.48-2.39)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.228 , 0.277 0.244 , 0.284	Depositor DCC
R_{free} test set	49440 reflections (3.92%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7064	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.36 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.1281e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.49	0/1792	0.81	7/2411 (0.3%)
1	B	0.69	3/1807 (0.2%)	1.04	18/2430 (0.7%)
1	C	0.64	1/1804 (0.1%)	1.08	11/2425 (0.5%)
1	D	0.57	1/1796 (0.1%)	0.83	9/2414 (0.4%)
All	All	0.60	5/7199 (0.1%)	0.95	45/9680 (0.5%)

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	B	0	1
1	C	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	ARG	CD-NE	-10.11	1.32	1.46
1	B	332	ASN	C-N	-9.37	1.22	1.33
1	C	358	LYS	C-N	-8.75	1.22	1.33
1	B	285	ARG	CZ-NH1	6.54	1.42	1.32
1	D	332	ASN	C-N	-5.49	1.27	1.33

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	358	LYS	CA-C-N	24.42	159.19	122.56
1	C	358	LYS	C-N-CA	24.42	159.19	122.56
1	D	170	ASP	N-CA-C	15.42	131.40	112.58
1	B	168	LYS	N-CA-C	-15.09	86.75	110.14
1	B	171	GLU	N-CA-CB	-13.46	85.28	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	ARG	NE-CZ-NH1	-11.37	110.13	121.50
1	B	360	ASP	N-CA-C	-10.66	100.00	113.43
1	A	298	THR	N-CA-C	-10.66	100.33	113.97
1	A	248	VAL	N-CA-C	-10.21	92.10	108.95
1	B	332	ASN	O-C-N	-10.10	112.66	123.26
1	D	171	GLU	N-CA-CB	-9.69	94.50	111.08
1	C	358	LYS	CB-CA-C	-9.38	91.75	110.42
1	C	248	VAL	N-CA-C	-9.05	94.01	108.95
1	B	285	ARG	CD-NE-CZ	8.60	136.43	124.40
1	C	358	LYS	O-C-N	-8.42	111.39	122.59
1	D	331	ASN	CB-CA-C	8.22	126.78	110.42
1	B	332	ASN	CB-CA-C	7.87	126.59	111.17
1	B	359	THR	CB-CA-C	-7.81	96.30	111.06
1	B	333	LYS	N-CA-C	-7.20	94.77	107.73
1	D	332	ASN	CA-C-N	7.04	132.39	121.19
1	D	332	ASN	C-N-CA	7.04	132.39	121.19
1	A	250	VAL	N-CA-C	-6.96	98.37	108.11
1	D	171	GLU	N-CA-C	6.79	120.59	109.72
1	B	171	GLU	CB-CA-C	-6.73	102.54	113.37
1	B	169	PHE	CB-CA-C	-6.72	96.48	110.40
1	B	170	ASP	N-CA-C	6.72	120.11	110.10
1	C	168	LYS	N-CA-C	-6.66	99.82	110.14
1	B	171	GLU	N-CA-C	6.55	120.93	109.80
1	A	335	TRP	N-CA-C	-6.54	100.96	110.64
1	C	359	THR	N-CA-C	6.36	120.84	112.13
1	A	335	TRP	CB-CA-C	6.34	117.60	109.80
1	B	191	ILE	N-CA-C	-6.26	106.83	111.90
1	C	250	VAL	N-CA-C	-5.77	99.81	108.12
1	B	168	LYS	N-CA-CB	5.75	119.70	110.85
1	B	335	TRP	N-CA-C	-5.75	99.83	108.96
1	B	357	THR	N-CA-C	-5.64	98.80	110.80
1	D	332	ASN	CB-CA-C	-5.55	101.65	114.41
1	B	285	ARG	CG-CD-NE	-5.52	99.86	112.00
1	C	247	ILE	N-CA-C	5.37	116.45	108.23
1	A	296	ASP	N-CA-CB	-5.35	102.89	110.81
1	D	167	ASN	CB-CA-C	-5.35	102.97	111.48
1	A	296	ASP	N-CA-C	5.07	120.33	114.04
1	C	286	VAL	CA-C-N	-5.07	114.56	119.78
1	C	286	VAL	C-N-CA	-5.07	114.56	119.78
1	D	333	LYS	N-CA-C	-5.00	103.17	111.37

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	332	ASN	Mainchain
1	C	358	LYS	Mainchain,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	1753	0	1708	43	0
1	B	1768	0	1728	47	0
1	C	1765	0	1723	34	0
1	D	1757	0	1715	40	0
2	A	4	0	0	1	0
2	B	8	0	0	1	0
2	C	3	0	0	1	0
2	D	6	0	0	1	0
All	All	7064	0	6874	162	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 13.

All (162) 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:329:ASP:HB3	1:A:334:LYS:CB	1.60	1.29
1:A:329:ASP:CB	1:A:334:LYS:HB3	1.68	1.23
1:B:252:LEU:HB2	1:B:256:THR:CG2	1.70	1.21
1:D:332:ASN:C	1:D:334:LYS:HB2	1.71	1.15
1:D:329:ASP:HB3	1:D:334:LYS:CB	1.86	1.04
1:A:331:ASN:HD21	1:C:206:ASN:HD22	1.08	1.01
1:B:252:LEU:CB	1:B:256:THR:HG21	1.91	1.01
1:D:329:ASP:CB	1:D:334:LYS:HB3	1.90	1.00
1:A:333:LYS:H	1:A:334:LYS:HB2	1.22	1.00
1:B:252:LEU:HB2	1:B:256:THR:HG21	0.99	0.98
1:B:250:VAL:HG12	1:B:251:LYS:H	1.28	0.97
1:D:329:ASP:HB3	1:D:334:LYS:HB3	1.00	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:GLY:HA3	1:D:302:ARG:HB3	1.49	0.94
1:D:332:ASN:O	1:D:334:LYS:HB2	1.71	0.90
1:B:329:ASP:O	1:B:332:ASN:O	1.89	0.90
1:B:359:THR:HG22	1:B:359:THR:O	1.69	0.89
1:A:238:GLY:O	1:A:248:VAL:O	1.90	0.88
1:A:333:LYS:H	1:A:334:LYS:CB	1.88	0.86
1:B:250:VAL:HG12	1:B:251:LYS:N	1.93	0.84
1:A:328:TYR:CE1	1:A:333:LYS:O	2.32	0.83
1:A:328:TYR:CZ	1:A:333:LYS:O	2.33	0.82
1:D:329:ASP:O	1:D:332:ASN:O	1.98	0.82
1:C:238:GLY:O	1:C:248:VAL:O	1.97	0.82
1:B:359:THR:O	1:B:359:THR:CG2	2.31	0.79
1:B:248:VAL:HG23	1:B:248:VAL:O	1.85	0.74
1:D:213:MET:HE1	1:D:267:MET:HE2	1.69	0.74
1:D:333:LYS:N	1:D:334:LYS:HB2	2.01	0.74
1:A:213:MET:HE1	1:A:267:MET:HE2	1.69	0.73
1:B:273:GLU:OE2	1:B:322:GLN:NE2	2.22	0.73
1:B:249:GLY:O	1:B:302:ARG:CZ	2.37	0.72
1:B:322:GLN:NE2	1:B:341:PHE:CZ	2.57	0.72
1:B:207:THR:HG23	1:B:210:ASP:H	1.57	0.69
1:C:288:ARG:NH1	1:C:306:GLU:OE2	2.23	0.69
1:B:250:VAL:CG1	1:B:251:LYS:H	2.06	0.68
1:D:330:ASN:O	1:D:331:ASN:C	2.37	0.68
1:A:288:ARG:NH2	1:A:308:ASP:OD2	2.27	0.66
1:B:250:VAL:O	1:B:302:ARG:HA	1.95	0.66
1:C:288:ARG:NH2	1:C:308:ASP:OD2	2.27	0.66
1:B:249:GLY:O	1:B:302:ARG:NE	2.28	0.66
1:C:230:ARG:NH2	1:C:319:ASP:O	2.24	0.66
1:A:329:ASP:HB3	1:A:334:LYS:HB3	0.75	0.64
1:B:236:HIS:HD2	1:B:306:GLU:OE2	1.81	0.64
1:D:175:TYR:HB3	1:D:247:ILE:HD13	1.80	0.64
1:A:331:ASN:HD21	1:C:206:ASN:ND2	1.88	0.63
1:C:164:HIS:HD2	1:C:165:PRO:O	1.81	0.62
1:C:230:ARG:HG3	1:C:371:LEU:HG	1.81	0.61
1:B:322:GLN:NE2	1:B:341:PHE:CE2	2.70	0.60
1:C:273:GLU:OE2	1:C:322:GLN:NE2	2.33	0.60
1:A:334:LYS:O	1:A:335:TRP:C	2.45	0.60
1:D:207:THR:HG22	1:D:210:ASP:H	1.67	0.59
1:C:329:ASP:O	1:C:332:ASN:O	2.19	0.59
1:B:249:GLY:O	1:B:302:ARG:NH2	2.35	0.59
1:D:333:LYS:N	1:D:334:LYS:CB	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ALA:O	1:B:256:THR:N	2.36	0.58
1:A:333:LYS:N	1:A:334:LYS:HB2	2.04	0.57
1:A:175:TYR:HB3	1:A:247:ILE:HD13	1.87	0.57
1:C:291:GLU:OE2	1:C:300:SER:HB3	2.05	0.57
1:A:160:SER:HB2	1:A:182:GLN:HG3	1.87	0.57
1:D:357:THR:OG1	1:D:360:ASP:HB2	2.03	0.57
1:A:167:ASN:HD21	1:A:285:ARG:HE	1.53	0.57
1:A:207:THR:OG1	1:A:210:ASP:HB2	2.05	0.56
1:B:358:LYS:O	1:B:359:THR:HB	2.05	0.56
1:C:361:PHE:CZ	1:C:365:LYS:HE2	2.41	0.56
1:A:253:ALA:O	1:A:256:THR:N	2.39	0.56
1:B:175:TYR:HB3	1:B:247:ILE:HD13	1.88	0.55
1:A:213:MET:HE3	1:A:213:MET:HA	1.89	0.55
1:A:213:MET:HE1	1:A:326:GLN:HG3	1.87	0.55
1:C:207:THR:HG23	1:C:210:ASP:H	1.72	0.55
1:A:322:GLN:HG2	1:A:343:VAL:HG22	1.89	0.54
1:D:223:ALA:O	1:D:227:MET:HG3	2.06	0.54
1:D:230:ARG:HD3	1:D:371:LEU:HG	1.89	0.54
1:A:324:LYS:HE3	1:A:337:GLN:CD	2.33	0.54
1:B:252:LEU:HD13	1:B:257:LYS:HG2	1.90	0.54
1:C:276:GLN:HA	1:C:279:GLN:HE21	1.73	0.53
1:A:276:GLN:HA	2:A:403:HOH:O	2.08	0.53
1:A:240:LYS:HD2	1:A:248:VAL:HG11	1.89	0.53
1:D:332:ASN:HB2	1:D:334:LYS:CB	2.38	0.53
1:A:159:PRO:HB2	1:A:179:PHE:CE2	2.43	0.53
1:A:328:TYR:OH	1:A:333:LYS:O	2.27	0.53
1:C:332:ASN:O	1:C:334:LYS:N	2.43	0.52
1:B:322:GLN:HG2	2:B:404:HOH:O	2.09	0.51
1:C:249:GLY:HA3	1:C:302:ARG:HB3	1.92	0.51
1:C:177:LEU:HG	1:C:178:HIS:CD2	2.46	0.51
1:A:171:GLU:HB3	1:A:173:TRP:H	1.75	0.51
1:D:199:ALA:HB2	1:D:240:LYS:HA	1.91	0.51
1:A:357:THR:OG1	1:A:360:ASP:HB2	2.11	0.51
1:D:285:ARG:HD3	1:D:286:VAL:O	2.10	0.51
1:C:294:LEU:O	1:C:296:ASP:N	2.41	0.51
1:B:252:LEU:HD13	1:B:256:THR:HG23	1.93	0.51
1:C:356:LYS:C	1:C:358:LYS:H	2.18	0.50
1:B:362:LYS:O	1:B:366:LEU:HD12	2.12	0.50
1:A:195:HIS:HD2	1:A:236:HIS:NE2	2.10	0.50
1:A:213:MET:CE	1:A:326:GLN:HG3	2.42	0.49
1:A:381:ASN:ND2	1:A:382:CYS:SG	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:ASP:O	1:D:334:LYS:CB	2.61	0.49
1:C:263:HIS:O	1:C:267:MET:HG2	2.11	0.49
1:B:326:GLN:HG2	1:B:335:TRP:HB3	1.94	0.48
1:B:252:LEU:HD13	1:B:256:THR:CG2	2.44	0.48
1:C:312:HIS:HE1	2:C:403:HOH:O	1.95	0.48
1:B:164:HIS:HD2	1:B:165:PRO:O	1.96	0.48
1:D:332:ASN:O	1:D:333:LYS:C	2.57	0.48
1:A:292:VAL:O	1:A:300:SER:OG	2.29	0.48
1:C:322:GLN:HG2	1:C:343:VAL:HG22	1.94	0.48
1:D:215:PHE:CD1	1:D:260:LEU:HD22	2.49	0.48
1:D:237:PHE:HB2	1:D:305:ILE:HB	1.95	0.48
1:B:221:GLU:HG2	1:B:344:LEU:CD1	2.43	0.47
1:A:358:LYS:O	1:A:362:LYS:HG3	2.14	0.47
1:D:242:LYS:HA	1:D:243:PRO:HA	1.72	0.47
1:A:329:ASP:CB	1:A:334:LYS:CB	2.55	0.47
1:C:356:LYS:C	1:C:358:LYS:N	2.73	0.47
1:D:329:ASP:O	1:D:334:LYS:HB3	2.16	0.46
1:D:344:LEU:HD23	1:D:353:ASN:HA	1.98	0.45
1:B:331:ASN:OD1	1:B:331:ASN:N	2.50	0.45
1:D:164:HIS:HE1	1:D:168:LYS:O	1.99	0.45
1:A:167:ASN:ND2	1:A:285:ARG:HG3	2.32	0.45
1:C:202:ASN:HB3	1:C:206:ASN:OD1	2.16	0.45
1:B:248:VAL:O	1:B:248:VAL:CG2	2.58	0.44
1:C:344:LEU:HD23	1:C:353:ASN:HA	2.00	0.44
1:C:174:ARG:HH11	1:C:174:ARG:HG3	1.83	0.44
1:D:164:HIS:CD2	1:D:288:ARG:HD2	2.53	0.44
1:A:237:PHE:HB2	1:A:305:ILE:HB	1.99	0.44
1:A:327:ILE:O	1:A:335:TRP:HA	2.17	0.44
1:D:189:ASN:O	1:D:190:LEU:HB2	2.18	0.44
1:B:194:ILE:HD11	1:B:346:ARG:HD3	2.00	0.43
1:B:340:LYS:H	1:B:340:LYS:HG2	1.69	0.43
1:A:331:ASN:C	1:A:332:ASN:OD1	2.62	0.43
1:D:213:MET:HE1	1:D:267:MET:CE	2.46	0.43
1:B:322:GLN:NE2	1:B:341:PHE:CE1	2.87	0.43
1:B:213:MET:HE1	1:B:267:MET:HE2	2.00	0.43
1:B:225:ALA:HA	1:B:344:LEU:O	2.19	0.43
1:B:252:LEU:CD1	1:B:257:LYS:HG2	2.49	0.43
1:B:174:ARG:HD3	1:B:291:GLU:HB3	2.01	0.42
1:B:330:ASN:C	1:B:332:ASN:N	2.77	0.42
1:D:325:LYS:HG3	2:D:403:HOH:O	2.20	0.42
1:B:221:GLU:HG2	1:B:344:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:LYS:HA	1:C:168:LYS:HD2	1.54	0.42
1:C:237:PHE:HB2	1:C:305:ILE:HB	2.00	0.42
1:C:363:MET:HE3	1:C:363:MET:HB3	1.80	0.42
1:B:249:GLY:HA3	1:B:292:VAL:HG21	2.00	0.42
1:B:330:ASN:C	1:B:332:ASN:H	2.28	0.42
1:D:207:THR:HB	1:D:210:ASP:HB2	2.00	0.42
1:C:179:PHE:HD2	1:C:179:PHE:N	2.18	0.42
1:D:210:ASP:O	1:D:214:LYS:HG3	2.20	0.42
1:D:332:ASN:HB2	1:D:334:LYS:HB2	2.01	0.42
1:D:328:TYR:CE1	1:D:333:LYS:O	2.73	0.41
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.94	0.41
1:D:333:LYS:N	1:D:334:LYS:CA	2.83	0.41
1:C:257:LYS:HE3	1:C:257:LYS:HB2	1.81	0.41
1:D:207:THR:HG22	1:D:209:GLU:N	2.36	0.41
1:B:164:HIS:CE1	1:B:288:ARG:HD2	2.55	0.41
1:B:163:SER:HA	1:B:181:LEU:HD11	2.03	0.41
1:B:179:PHE:N	1:B:179:PHE:HD1	2.18	0.41
1:B:179:PHE:N	1:B:179:PHE:CD1	2.88	0.41
1:C:198:LYS:HE3	1:C:218:GLU:OE1	2.20	0.41
1:A:242:LYS:HA	1:A:243:PRO:HA	1.97	0.41
1:C:182:GLN:HB3	1:C:183:PRO:HD2	2.02	0.41
1:D:330:ASN:C	1:D:332:ASN:N	2.76	0.41
1:D:227:MET:HA	1:D:311:PRO:HB3	2.01	0.40
1:A:183:PRO:HB2	1:A:195:HIS:CE1	2.56	0.40
1:A:363:MET:HE3	1:A:363:MET:HB3	1.94	0.40
1:D:223:ALA:HA	1:D:309:VAL:HG21	2.03	0.40
1:C:179:PHE:N	1:C:179:PHE:CD2	2.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	207/234 (88%)	196 (95%)	11 (5%)	0	100	100
1	B	208/234 (89%)	193 (93%)	15 (7%)	0	100	100
1	C	206/234 (88%)	191 (93%)	15 (7%)	0	100	100
1	D	205/234 (88%)	193 (94%)	12 (6%)	0	100	100
All	All	826/936 (88%)	773 (94%)	53 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	194/214 (91%)	192 (99%)	2 (1%)	73	86
1	B	198/214 (92%)	194 (98%)	4 (2%)	50	70
1	C	196/214 (92%)	185 (94%)	11 (6%)	17	30
1	D	195/214 (91%)	190 (97%)	5 (3%)	41	62
All	All	783/856 (92%)	761 (97%)	22 (3%)	38	59

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	THR
1	A	333	LYS
1	B	171	GLU
1	B	200	PHE
1	B	331	ASN
1	B	382	CYS
1	C	168	LYS
1	C	170	ASP
1	C	171	GLU
1	C	194	ILE
1	C	294	LEU
1	C	332	ASN
1	C	333	LYS

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Mol	Chain	Res	Type
1	C	334	LYS
1	C	356	LYS
1	C	358	LYS
1	C	360	ASP
1	D	171	GLU
1	D	314	SER
1	D	332	ASN
1	D	333	LYS
1	D	334	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	195	HIS
1	A	381	ASN
1	B	164	HIS
1	B	178	HIS
1	B	236	HIS
1	B	244	GLN
1	B	276	GLN
1	B	312	HIS
1	B	322	GLN
1	B	381	ASN
1	C	164	HIS
1	C	178	HIS
1	C	206	ASN
1	C	278	GLN
1	C	279	GLN
1	C	312	HIS
1	C	331	ASN
1	D	189	ASN
1	D	278	GLN
1	D	279	GLN
1	D	322	GLN

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	215/234 (91%)	0.91	28 (13%) 9 7	25, 57, 93, 137	22 (10%)
1	B	216/234 (92%)	0.90	35 (16%) 5 5	24, 56, 98, 135	26 (12%)
1	C	216/234 (92%)	0.92	27 (12%) 9 8	24, 63, 100, 121	22 (10%)
1	D	215/234 (91%)	0.78	31 (14%) 7 6	27, 53, 90, 105	24 (11%)
All	All	862/936 (92%)	0.88	121 (14%) 7 6	24, 58, 96, 137	94 (10%)

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	LYS	8.2
1	B	381	ASN	7.0
1	C	383	THR	6.2
1	B	250	VAL	6.2
1	A	168	LYS	6.1
1	B	382	CYS	6.0
1	A	253	ALA	6.0
1	B	170	ASP	5.8
1	A	333	LYS	5.5
1	B	380	ASP	5.5
1	A	170	ASP	5.4
1	A	206	ASN	5.3
1	B	331	ASN	5.2
1	B	249	GLY	5.1
1	A	383	THR	4.9
1	C	183	PRO	4.9
1	D	168	LYS	4.8
1	C	265	ASP	4.8
1	A	189	ASN	4.8
1	D	170	ASP	4.6
1	B	379	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	296	ASP	4.3
1	B	256	THR	4.1
1	C	187	PRO	4.1
1	B	253	ALA	4.0
1	C	253	ALA	4.0
1	A	169	PHE	4.0
1	D	171	GLU	4.0
1	A	202	ASN	3.9
1	D	256	THR	3.9
1	D	206	ASN	3.8
1	B	330	ASN	3.8
1	C	182	GLN	3.8
1	A	335	TRP	3.7
1	A	249	GLY	3.7
1	B	169	PHE	3.6
1	B	200	PHE	3.6
1	C	169	PHE	3.6
1	D	349	ALA	3.6
1	B	357	THR	3.6
1	D	248	VAL	3.6
1	D	383	THR	3.5
1	A	296	ASP	3.5
1	D	158	GLU	3.5
1	D	334	LYS	3.5
1	B	328	TYR	3.5
1	A	200	PHE	3.5
1	D	335	TRP	3.4
1	C	170	ASP	3.4
1	C	158	GLU	3.4
1	C	347	ASP	3.4
1	D	187	PRO	3.3
1	D	172	GLN	3.3
1	D	333	LYS	3.3
1	B	206	ASN	3.3
1	B	358	LYS	3.3
1	B	248	VAL	3.3
1	C	381	ASN	3.3
1	B	329	ASP	3.2
1	A	207	THR	3.2
1	D	202	ASN	3.1
1	A	329	ASP	3.1
1	B	378	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	171	GLU	3.1
1	D	183	PRO	3.1
1	A	256	THR	3.0
1	A	349	ALA	3.0
1	B	332	ASN	2.9
1	C	380	ASP	2.9
1	C	208	GLU	2.9
1	C	358	LYS	2.9
1	C	256	THR	2.8
1	C	252	LEU	2.7
1	C	202	ASN	2.7
1	D	169	PHE	2.7
1	D	208	GLU	2.7
1	D	331	ASN	2.6
1	B	322	GLN	2.6
1	D	200	PHE	2.6
1	D	249	GLY	2.6
1	D	173	TRP	2.6
1	A	183	PRO	2.5
1	C	215	PHE	2.5
1	C	248	VAL	2.5
1	D	298	THR	2.5
1	B	359	THR	2.5
1	A	265	ASP	2.4
1	A	172	GLN	2.4
1	D	252	LEU	2.4
1	D	366	LEU	2.4
1	B	336	GLU	2.4
1	C	221	GLU	2.4
1	D	161	CYS	2.4
1	A	354	ILE	2.4
1	C	349	ALA	2.3
1	C	363	MET	2.3
1	A	264	PHE	2.3
1	B	188	HIS	2.3
1	B	182	GLN	2.3
1	A	332	ASN	2.2
1	D	332	ASN	2.2
1	C	355	VAL	2.2
1	C	249	GLY	2.2
1	B	324	LYS	2.2
1	D	363	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	163	SER	2.2
1	D	265	ASP	2.2
1	D	316	CYS	2.2
1	A	201	THR	2.2
1	B	347	ASP	2.2
1	A	336	GLU	2.1
1	C	166	PHE	2.1
1	B	208	GLU	2.1
1	B	340	LYS	2.1
1	A	159	PRO	2.1
1	B	183	PRO	2.1
1	B	334	LYS	2.1
1	D	201	THR	2.1
1	B	350	ARG	2.1
1	B	172	GLN	2.1
1	B	202	ASN	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.