



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:44 AM UTC

PDB ID : 3WIV / pdb_00003wiv
Title : Crystal structure of Pro-S324A/D356A
Authors : Uehara, R.; Angkawidjaja, C.; Koga, Y.; Kanaya, S.
Deposited on : 2013-09-25
Resolution : 1.90 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

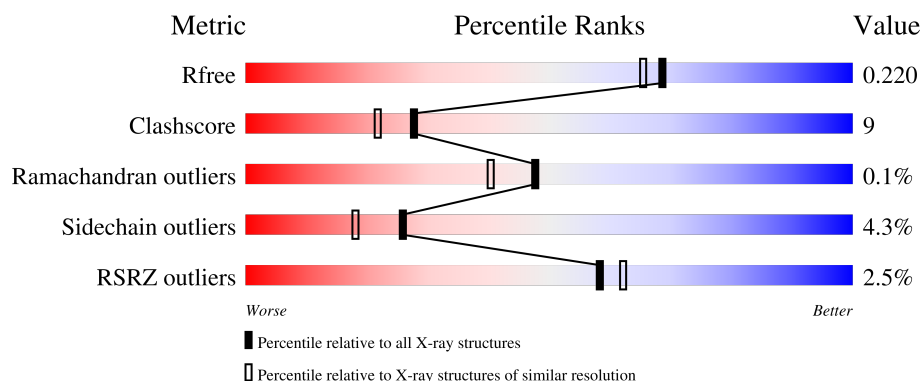
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	398	2% 79% 18% ...
1	B	398	2% 80% 16% ..
1	C	398	3% 82% 15% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9489 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 Tk-subtilisin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			2871	1818	480	566	7			
1	B	389	Total	C	N	O	S	0	0	0
			2858	1811	478	562	7			
1	C	397	Total	C	N	O	S	0	0	0
			2909	1840	487	575	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	ALA	SER	engineered mutation	UNP P58502
A	356	ALA	ASP	engineered mutation	UNP P58502
B	324	ALA	SER	engineered mutation	UNP P58502
B	356	ALA	ASP	engineered mutation	UNP P58502
C	324	ALA	SER	engineered mutation	UNP P58502
C	356	ALA	ASP	engineered mutation	UNP P58502

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Ca	0	0
			6	6		
2	B	6	Total	Ca	0	0
			6	6		
2	C	6	Total	Ca	0	0
			6	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	270	Total	O	0	0
			270	270		

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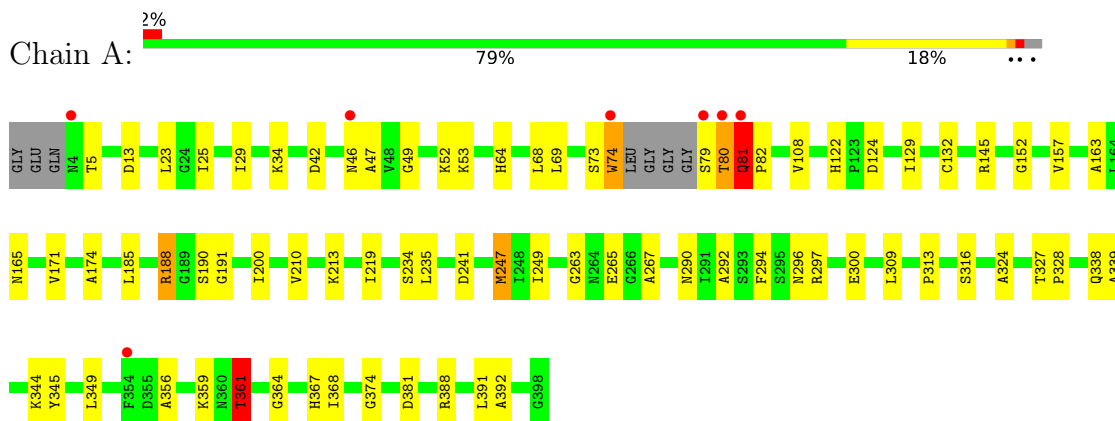
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	288	Total	O	0	0
			288	288		
3	C	275	Total	O	0	0
			275	275		

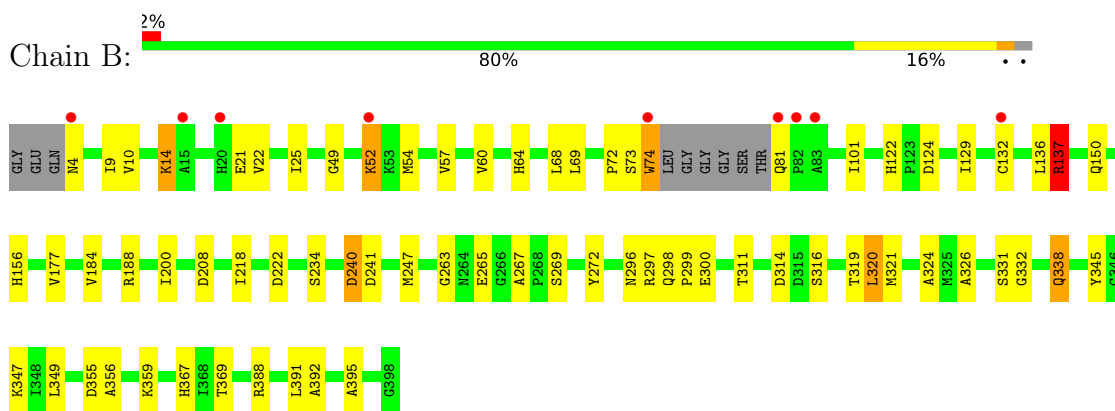
3 Residue-property plots [i](#)

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.

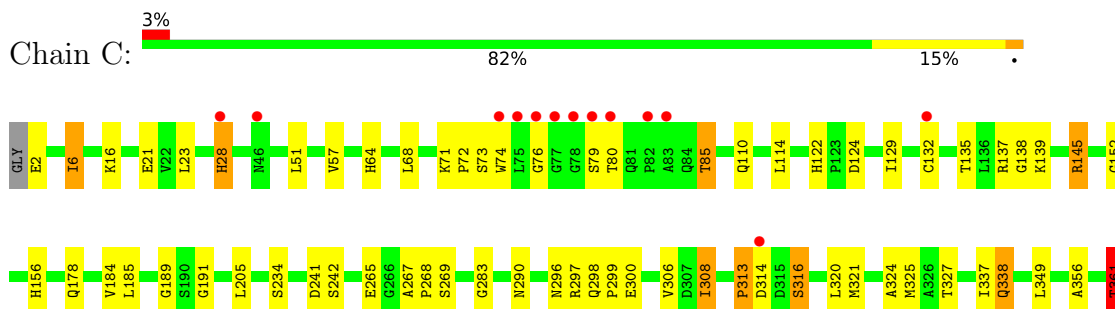
- Molecule 1: Tk-subtilisin



- Molecule 1: Tk-subtilisin



- Molecule 1: Tk-subtilisin





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.85Å 119.10Å 119.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.29 – 1.90 43.29 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.29-1.90) 99.9 (43.29-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.60 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.175 , 0.220 0.177 , 0.220	Depositor DCC
R_{free} test set	5241 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9489	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	1.48	13/2931 (0.4%)	1.22	5/4009 (0.1%)
1	B	1.47	8/2918 (0.3%)	1.24	3/3991 (0.1%)
1	C	1.42	13/2970 (0.4%)	1.25	17/4062 (0.4%)
All	All	1.46	34/8819 (0.4%)	1.24	25/12062 (0.2%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	ALA	CA-CB	8.10	1.62	1.53
1	C	184	VAL	N-CA	7.76	1.53	1.46
1	C	308	ILE	CA-CB	7.49	1.63	1.53
1	A	247	MET	SD-CE	-6.83	1.62	1.79
1	B	392	ALA	CA-CB	6.71	1.63	1.53
1	C	327	THR	CA-C	6.60	1.59	1.52
1	A	392	ALA	CA-CB	6.39	1.63	1.53
1	A	163	ALA	CA-CB	6.21	1.63	1.53
1	A	374	GLY	N-CA	6.13	1.53	1.44
1	A	157	VAL	CA-CB	6.13	1.61	1.54
1	B	136	LEU	C-O	6.10	1.31	1.23
1	B	184	VAL	CA-CB	6.01	1.62	1.54
1	C	314	ASP	CA-C	-5.98	1.45	1.53
1	C	135	THR	C-O	5.96	1.32	1.24
1	C	283	GLY	N-CA	5.93	1.50	1.44
1	B	331	SER	N-CA	5.84	1.53	1.46
1	C	57	VAL	CA-CB	-5.66	1.47	1.54
1	C	114	LEU	N-CA	-5.61	1.39	1.46
1	B	388	ARG	C-O	-5.58	1.17	1.24
1	A	249	ILE	N-CA	5.58	1.53	1.46
1	A	171	VAL	CA-CB	5.46	1.61	1.55
1	C	361	THR	CB-CG2	-5.45	1.34	1.52
1	C	6	ILE	N-CA	-5.42	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	306	VAL	C-O	-5.39	1.18	1.24
1	A	219	ILE	CA-C	5.36	1.59	1.52
1	B	269	SER	N-CA	5.30	1.51	1.45
1	A	339	ALA	CA-CB	5.30	1.61	1.53
1	B	177	VAL	N-CA	5.29	1.52	1.46
1	A	165	ASN	C-O	5.29	1.30	1.24
1	C	337	ILE	CA-CB	5.26	1.60	1.54
1	A	388	ARG	C-O	5.24	1.30	1.24
1	B	332	GLY	N-CA	5.22	1.52	1.45
1	A	263	GLY	N-CA	5.11	1.49	1.45
1	C	205	LEU	C-O	-5.06	1.18	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	ILE	N-CA-C	-7.20	104.75	111.45
1	C	298	GLN	CA-C-N	-7.01	113.48	120.98
1	C	298	GLN	C-N-CA	-7.01	113.48	120.98
1	C	85	THR	CB-CA-C	-6.43	98.15	110.24
1	A	73	SER	N-CA-C	-6.20	103.11	112.04
1	C	361	THR	N-CA-CB	-6.05	101.16	111.69
1	C	21	GLU	N-CA-C	-6.04	104.82	111.82
1	C	313	PRO	CA-C-N	6.02	131.53	122.68
1	C	313	PRO	C-N-CA	6.02	131.53	122.68
1	A	361	THR	OG1-CB-CG2	5.99	121.29	109.30
1	A	361	THR	CA-CB-CG2	5.97	120.65	110.50
1	C	374	GLY	CA-C-N	5.68	125.68	119.89
1	C	374	GLY	C-N-CA	5.68	125.68	119.89
1	C	156	HIS	N-CA-C	-5.59	105.11	111.14
1	C	361	THR	CA-CB-CG2	5.50	119.84	110.50
1	C	313	PRO	O-C-N	5.44	129.50	122.91
1	A	391	LEU	N-CA-C	5.28	117.03	111.28
1	B	137	ARG	CG-CD-NE	5.27	123.59	112.00
1	C	138	GLY	CA-C-N	-5.26	115.57	122.99
1	C	138	GLY	C-N-CA	-5.26	115.57	122.99
1	C	6	ILE	CB-CG1-CD1	-5.25	102.78	113.80
1	B	326	ALA	N-CA-C	-5.16	105.74	111.36
1	C	361	THR	OG1-CB-CG2	5.13	119.56	109.30
1	C	16	LYS	N-CA-C	5.11	119.57	113.23
1	A	361	THR	N-CA-CB	-5.02	102.20	111.53

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	2871	0	2832	70	0
1	B	2858	0	2820	62	0
1	C	2909	0	2867	36	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
3	A	270	0	0	7	0
3	B	288	0	0	7	0
3	C	275	0	0	4	0
All	All	9489	0	8519	154	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 (154) 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:49:GLY:CA	1:B:74:TRP:HB2	1.63	1.29
1:A:81:GLN:HG3	1:A:82:PRO:CD	1.73	1.19
1:A:188:ARG:HH11	1:A:188:ARG:HG3	1.07	1.11
1:A:81:GLN:HG3	1:A:82:PRO:HD2	1.31	1.07
1:A:49:GLY:HA2	1:B:74:TRP:HB2	1.34	1.07
1:A:49:GLY:HA2	1:B:74:TRP:CB	1.84	1.07
1:A:74:TRP:HB3	1:B:49:GLY:HA3	1.35	1.05
1:A:49:GLY:HA3	1:B:74:TRP:HB2	1.41	1.02
1:A:81:GLN:CG	1:A:82:PRO:HD2	1.94	0.96
1:A:49:GLY:CA	1:B:74:TRP:CB	2.42	0.92
1:A:81:GLN:HG3	1:A:82:PRO:HD3	1.53	0.91
1:A:122:HIS:HD2	1:A:124:ASP:H	1.16	0.91
1:A:188:ARG:HH11	1:A:188:ARG:CG	1.87	0.87
1:B:122:HIS:HD2	1:B:124:ASP:H	1.24	0.86
1:C:361:THR:HG22	1:C:364:GLY:H	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLN:CG	1:A:82:PRO:CD	2.51	0.84
1:C:338:GLN:HE22	1:C:349:LEU:H	1.25	0.84
1:A:25:ILE:HD12	1:A:47:ALA:HB1	1.62	0.82
1:A:338:GLN:HE22	1:A:349:LEU:H	1.29	0.80
1:A:64:HIS:HD2	1:A:241:ASP:OD2	1.64	0.80
1:A:188:ARG:HG3	1:A:188:ARG:NH1	1.87	0.80
1:A:79:SER:O	1:A:80:THR:HG23	1.82	0.79
1:A:49:GLY:HA2	1:B:74:TRP:HB3	1.63	0.79
1:B:338:GLN:HE22	1:B:349:LEU:H	1.29	0.79
1:C:300:GLU:OE2	1:C:367:HIS:HE1	1.66	0.79
1:C:145:ARG:O	1:C:145:ARG:HD3	1.83	0.78
1:C:361:THR:CG2	1:C:364:GLY:H	1.96	0.78
1:C:122:HIS:HD2	1:C:124:ASP:H	1.30	0.77
1:A:356:ALA:O	1:A:367:HIS:HD2	1.70	0.74
1:A:361:THR:CG2	1:A:364:GLY:H	1.99	0.73
1:A:34:LYS:CE	3:A:1300:HOH:O	2.37	0.73
1:B:267:ALA:H	1:B:296:ASN:ND2	1.88	0.71
1:A:74:TRP:HD1	3:A:1109:HOH:O	1.74	0.71
1:B:137:ARG:HD2	3:B:1217:HOH:O	1.90	0.71
1:C:290:ASN:ND2	3:C:1349:HOH:O	2.24	0.69
1:B:64:HIS:HD2	1:B:241:ASP:OD2	1.76	0.69
1:A:338:GLN:HA	1:A:338:GLN:HE21	1.59	0.67
1:B:300:GLU:OE2	1:B:367:HIS:HE1	1.78	0.67
1:A:34:LYS:HE3	3:A:1300:HOH:O	1.95	0.67
1:C:300:GLU:OE2	1:C:367:HIS:CE1	2.48	0.65
1:A:300:GLU:OE2	1:A:367:HIS:HE1	1.79	0.64
1:A:361:THR:HG22	1:A:364:GLY:H	1.61	0.63
1:B:356:ALA:O	1:B:367:HIS:HD2	1.79	0.63
1:A:122:HIS:CD2	1:A:124:ASP:H	2.08	0.63
1:A:265:GLU:H	1:A:296:ASN:HD21	1.47	0.63
1:B:338:GLN:HE21	1:B:338:GLN:HA	1.65	0.61
1:A:34:LYS:HE2	3:A:1300:HOH:O	1.97	0.61
1:C:71:LYS:HE3	1:C:321:MET:HE3	1.82	0.61
1:A:80:THR:HG21	1:A:309:LEU:CD2	2.32	0.60
1:C:72:PRO:HA	1:C:320:LEU:HD22	1.84	0.59
1:A:122:HIS:HE1	1:A:316:SER:O	1.85	0.59
1:B:188:ARG:NH1	3:B:1185:HOH:O	2.34	0.59
1:A:267:ALA:H	1:A:296:ASN:ND2	2.00	0.59
1:A:49:GLY:N	1:B:74:TRP:C	2.60	0.58
1:A:235:LEU:HD12	1:A:235:LEU:C	2.28	0.58
1:C:361:THR:HG22	1:C:364:GLY:N	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:HIS:HE1	1:B:316:SER:O	1.86	0.58
1:A:265:GLU:H	1:A:296:ASN:ND2	2.01	0.58
1:A:23:LEU:HD21	1:A:29:ILE:HG12	1.86	0.57
1:C:64:HIS:HD2	1:C:241:ASP:OD2	1.86	0.57
1:A:5:THR:HG22	3:A:1245:HOH:O	2.05	0.57
1:B:69:LEU:C	1:B:324:ALA:HB2	2.29	0.57
1:C:110:GLN:HE21	1:C:178:GLN:HE22	1.53	0.57
1:C:79:SER:HB3	3:C:1330:HOH:O	2.05	0.57
1:A:80:THR:HG21	1:A:309:LEU:HD21	1.87	0.57
1:A:49:GLY:H	1:B:74:TRP:C	2.13	0.56
1:C:122:HIS:HE1	1:C:316:SER:O	1.86	0.56
1:C:356:ALA:O	1:C:367:HIS:HD2	1.88	0.56
1:A:74:TRP:CB	1:B:49:GLY:HA3	2.22	0.55
1:C:267:ALA:H	1:C:296:ASN:ND2	2.04	0.55
1:B:21:GLU:HG2	1:B:54:MET:HE2	1.89	0.55
1:C:269:SER:HA	1:C:297:ARG:O	2.07	0.54
1:B:14:LYS:HB3	1:C:268:PRO:HB3	1.90	0.54
1:C:338:GLN:HE21	1:C:338:GLN:HA	1.71	0.54
1:C:110:GLN:HE21	1:C:178:GLN:NE2	2.06	0.53
1:A:356:ALA:O	1:A:367:HIS:CD2	2.58	0.53
1:C:129:ILE:CG2	1:C:132:CYS:SG	2.97	0.52
1:B:234:SER:HB3	1:B:324:ALA:HB1	1.91	0.52
1:A:81:GLN:HG2	1:A:82:PRO:HD2	1.90	0.51
1:B:150:GLN:HG3	3:B:1346:HOH:O	2.10	0.51
1:C:145:ARG:HD3	1:C:145:ARG:C	2.21	0.51
1:A:74:TRP:HA	1:B:49:GLY:CA	2.42	0.50
1:B:345:TYR:HB3	1:B:347:LYS:HE3	1.93	0.50
1:B:240:ASP:C	1:B:240:ASP:OD2	2.54	0.50
1:A:361:THR:HG23	1:A:364:GLY:H	1.74	0.49
1:B:72:PRO:HA	1:B:320:LEU:HD22	1.93	0.49
1:B:369:THR:HB	1:B:391:LEU:HB3	1.94	0.49
1:B:137:ARG:HH11	1:B:137:ARG:HG3	1.77	0.49
1:C:68:LEU:HD13	1:C:189:GLY:HA3	1.94	0.49
1:A:185:LEU:HD23	1:A:191:GLY:HA3	1.95	0.48
1:C:74:TRP:O	1:C:76:GLY:HA3	2.14	0.48
1:B:208:ASP:HB2	1:C:64:HIS:CE1	2.47	0.48
1:B:122:HIS:CD2	1:B:124:ASP:H	2.15	0.48
1:C:129:ILE:HG21	1:C:132:CYS:SG	2.53	0.48
1:C:137:ARG:HD3	3:C:1201:HOH:O	2.13	0.48
1:B:129:ILE:HG21	1:B:132:CYS:SG	2.54	0.48
1:B:10:VAL:HG23	1:B:57:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ASP:HB2	1:B:272:TYR:CE1	2.49	0.47
1:B:359:LYS:HG2	1:B:395:ALA:HB1	1.96	0.47
1:A:292:ALA:HB1	1:A:294:PHE:CE2	2.50	0.46
1:C:185:LEU:HD23	1:C:191:GLY:HA3	1.96	0.46
1:B:200:ILE:CG2	1:B:247:MET:HG3	2.45	0.46
1:A:290:ASN:ND2	3:A:1230:HOH:O	2.48	0.46
1:B:218:ILE:HG22	1:B:222:ASP:HB2	1.98	0.46
1:B:300:GLU:OE2	1:B:367:HIS:CE1	2.63	0.46
1:A:81:GLN:HE21	1:A:81:GLN:HB2	1.53	0.46
1:C:338:GLN:NE2	1:C:349:LEU:H	2.03	0.46
1:B:25:ILE:HD13	1:B:54:MET:HE3	1.97	0.46
1:A:13:ASP:OD1	1:A:13:ASP:C	2.59	0.45
1:A:300:GLU:OE2	1:A:367:HIS:CE1	2.66	0.45
1:A:74:TRP:HA	1:B:49:GLY:N	2.30	0.45
1:A:188:ARG:CG	1:A:188:ARG:NH1	2.55	0.45
1:B:265:GLU:H	1:B:296:ASN:HD21	1.64	0.45
1:A:361:THR:HG22	1:A:364:GLY:N	2.29	0.45
1:B:129:ILE:CG2	1:B:132:CYS:SG	3.03	0.45
1:C:308:ILE:HG13	1:C:325:MET:HB3	1.98	0.45
1:C:265:GLU:H	1:C:296:ASN:ND2	2.14	0.45
1:A:5:THR:OG1	1:A:42:ASP:HB3	2.17	0.45
1:C:234:SER:HB3	1:C:324:ALA:HB1	1.98	0.45
1:B:338:GLN:NE2	1:B:349:LEU:H	2.06	0.45
1:C:122:HIS:CD2	1:C:124:ASP:H	2.21	0.45
1:A:129:ILE:CG2	1:A:132:CYS:SG	3.06	0.44
1:B:69:LEU:HD13	1:B:263:GLY:HA2	1.99	0.44
1:B:267:ALA:H	1:B:296:ASN:HD22	1.63	0.44
1:B:4:ASN:HB3	3:B:1198:HOH:O	2.17	0.44
1:A:68:LEU:C	1:A:68:LEU:HD12	2.43	0.44
1:A:25:ILE:HD13	1:A:25:ILE:HG21	1.82	0.44
1:A:108:VAL:HG22	1:A:108:VAL:O	2.17	0.43
1:A:344:LYS:HD3	1:A:345:TYR:CZ	2.54	0.43
1:A:200:ILE:CG2	1:A:247:MET:HG3	2.50	0.42
1:A:364:GLY:O	1:A:368:ILE:HG23	2.19	0.42
1:B:52:LYS:HZ2	1:B:60:VAL:H	1.67	0.42
1:A:235:LEU:HD12	1:A:235:LEU:O	2.18	0.42
1:C:28:HIS:HB2	3:C:1298:HOH:O	2.19	0.42
1:B:298:GLN:N	1:B:299:PRO:CD	2.82	0.42
1:B:356:ALA:O	1:B:367:HIS:CD2	2.67	0.42
1:A:69:LEU:C	1:A:324:ALA:HB2	2.45	0.42
1:B:265:GLU:H	1:B:296:ASN:ND2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:GLY:HA2	1:C:313:PRO:CD	2.49	0.42
1:A:5:THR:HG23	3:A:1334:HOH:O	2.20	0.42
1:A:297:ARG:NE	1:A:381:ASP:OD1	2.52	0.42
1:B:81:GLN:HA	3:B:1169:HOH:O	2.20	0.42
1:B:9:ILE:HD12	1:B:9:ILE:N	2.35	0.41
1:B:314:ASP:OD2	3:B:1144:HOH:O	2.21	0.41
1:A:327:THR:N	1:A:328:PRO:HD2	2.35	0.41
1:B:156:HIS:HA	1:B:311:THR:O	2.20	0.41
1:B:338:GLN:HE22	1:B:349:LEU:N	2.07	0.41
1:A:152:GLY:HA2	1:A:313:PRO:CD	2.51	0.41
1:A:234:SER:HB3	1:A:324:ALA:HB1	2.03	0.41
1:B:73:SER:CB	1:B:319:THR:HG22	2.50	0.41
1:B:73:SER:HB2	1:B:319:THR:HG22	2.02	0.41
1:B:188:ARG:NH2	3:B:1351:HOH:O	2.54	0.40
1:B:265:GLU:N	1:B:265:GLU:CD	2.79	0.40
1:B:72:PRO:O	1:B:321:MET:HE2	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	387/398 (97%)	371 (96%)	15 (4%)	1 (0%)	36	29
1	B	385/398 (97%)	372 (97%)	13 (3%)	0	100	100
1	C	395/398 (99%)	379 (96%)	16 (4%)	0	100	100
All	All	1167/1194 (98%)	1122 (96%)	44 (4%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	GLN

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	303/306 (99%)	290 (96%)	13 (4%)	26	18
1	B	301/306 (98%)	290 (96%)	11 (4%)	30	22
1	C	306/306 (100%)	291 (95%)	15 (5%)	22	14
All	All	910/918 (99%)	871 (96%)	39 (4%)	26	18

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	52	LYS
1	A	53	LYS
1	A	74	TRP
1	A	80	THR
1	A	81	GLN
1	A	145	ARG
1	A	188	ARG
1	A	190	SER
1	A	210	VAL
1	A	213	LYS
1	A	359	LYS
1	A	361	THR
1	B	14	LYS
1	B	22	VAL
1	B	52	LYS
1	B	68	LEU
1	B	74	TRP
1	B	137	ARG
1	B	240	ASP
1	B	297	ARG
1	B	320	LEU
1	B	338	GLN
1	B	355	ASP
1	C	2	GLU
1	C	6	ILE

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Mol	Chain	Res	Type
1	C	23	LEU
1	C	28	HIS
1	C	51	LEU
1	C	73	SER
1	C	80	THR
1	C	85	THR
1	C	139	LYS
1	C	145	ARG
1	C	242	SER
1	C	299	PRO
1	C	316	SER
1	C	338	GLN
1	C	361	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	81	GLN
1	A	122	HIS
1	A	150	GLN
1	A	250	GLN
1	A	290	ASN
1	A	296	ASN
1	A	338	GLN
1	A	367	HIS
1	B	20	HIS
1	B	64	HIS
1	B	122	HIS
1	B	150	GLN
1	B	290	ASN
1	B	296	ASN
1	B	338	GLN
1	B	367	HIS
1	C	64	HIS
1	C	122	HIS
1	C	178	GLN
1	C	250	GLN
1	C	290	ASN
1	C	296	ASN
1	C	298	GLN
1	C	338	GLN

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Mol	Chain	Res	Type
1	C	367	HIS

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](#)

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	391/398 (98%)	-0.23	7 (1%) 67 71	14, 21, 39, 61	0
1	B	389/398 (97%)	-0.22	9 (2%) 61 65	14, 22, 38, 63	0
1	C	397/398 (99%)	-0.02	13 (3%) 49 52	14, 24, 44, 67	0
All	All	1177/1194 (98%)	-0.16	29 (2%) 58 62	14, 22, 41, 67	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	TRP	8.0
1	A	74	TRP	7.4
1	C	76	GLY	6.7
1	A	80	THR	6.4
1	A	79	SER	5.6
1	C	78	GLY	4.9
1	C	74	TRP	4.6
1	B	83	ALA	4.6
1	B	81	GLN	4.6
1	C	132	CYS	4.3
1	C	75	LEU	4.3
1	C	79	SER	3.2
1	C	80	THR	3.0
1	C	77	GLY	3.0
1	B	132	CYS	2.9
1	A	4	ASN	2.8
1	A	354	PHE	2.7
1	C	82	PRO	2.7
1	C	314	ASP	2.6
1	A	81	GLN	2.6
1	C	83	ALA	2.4
1	B	82	PRO	2.4
1	B	4	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	15	ALA	2.2
1	A	46	ASN	2.2
1	C	28	HIS	2.2
1	C	46	ASN	2.2
1	B	20	HIS	2.1
1	B	52	LYS	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	1004	1/1	0.94	0.12	34,34,34,34	0
2	CA	C	1006	1/1	0.95	0.09	36,36,36,36	0
2	CA	B	1004	1/1	0.96	0.18	40,40,40,40	0
2	CA	A	1006	1/1	0.97	0.05	30,30,30,30	0
2	CA	C	1001	1/1	0.98	0.03	27,27,27,27	0
2	CA	B	1001	1/1	0.98	0.03	25,25,25,25	0
2	CA	A	1003	1/1	0.99	0.04	25,25,25,25	0
2	CA	B	1002	1/1	0.99	0.04	21,21,21,21	0
2	CA	B	1003	1/1	0.99	0.04	22,22,22,22	0
2	CA	A	1001	1/1	0.99	0.02	17,17,17,17	0
2	CA	B	1006	1/1	0.99	0.03	22,22,22,22	0
2	CA	A	1005	1/1	0.99	0.02	20,20,20,20	0
2	CA	C	1002	1/1	0.99	0.02	19,19,19,19	0
2	CA	C	1003	1/1	0.99	0.02	18,18,18,18	0
2	CA	C	1004	1/1	0.99	0.03	17,17,17,17	0
2	CA	C	1005	1/1	0.99	0.02	19,19,19,19	0
2	CA	A	1002	1/1	0.99	0.05	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	B	1005	1/1	1.00	0.04	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.