



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:20 AM UTC

PDB ID : 1B47 / pdb_00001b47
Title : STRUCTURE OF THE N-TERMINAL DOMAIN OF CBL IN COMPLEX
WITH ITS BINDING SITE IN ZAP-70
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Deposited on : 1999-01-06
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

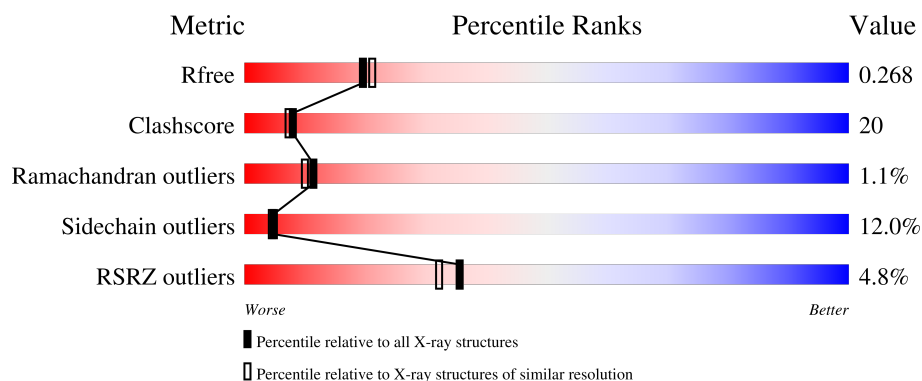
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	304	3% 57% 31% 9% .
1	B	304	3% 61% 31% 7% .
1	C	304	9% 51% 35% 11% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8092 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 CBL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2475	1604	423	435	13			
1	B	304	Total	C	N	O	S	0	0	0
			2472	1603	422	434	13			
1	C	304	Total	C	N	O	S	0	0	0
			2476	1605	422	436	13			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

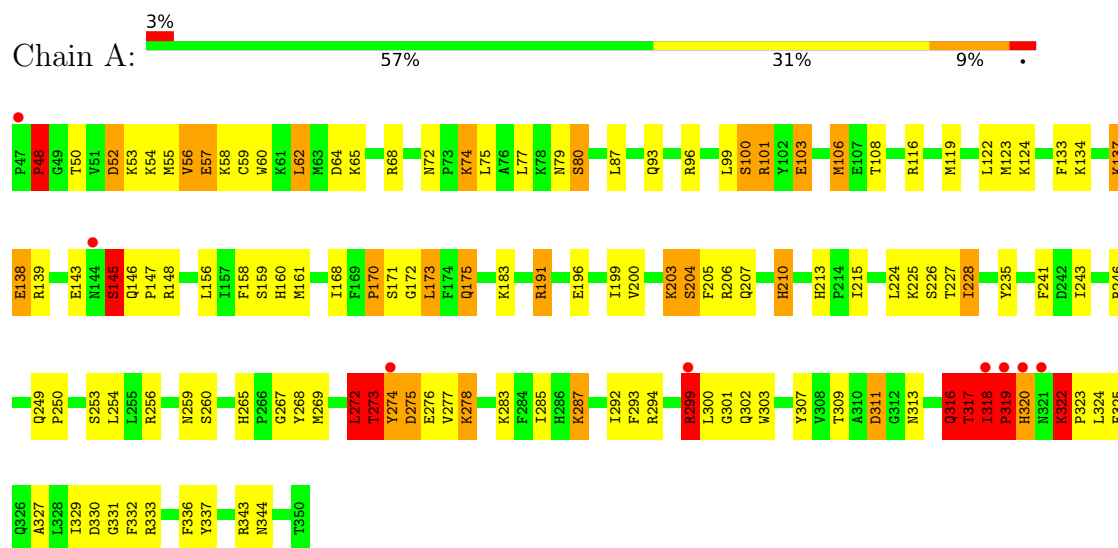
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	221	Total	O	0	0
			221	221		
3	B	261	Total	O	0	0
			261	261		
3	C	184	Total	O	0	0
			184	184		

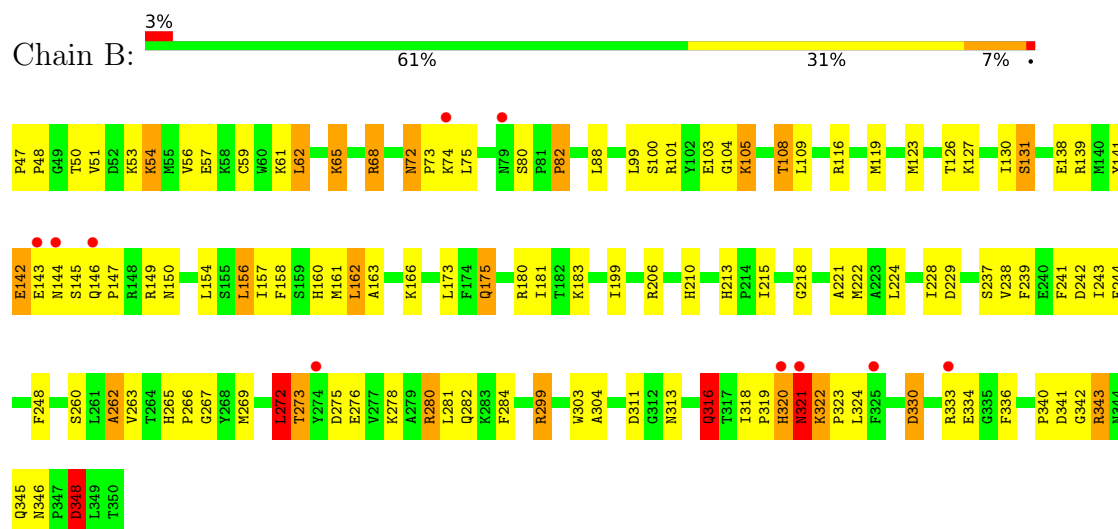
3 Residue-property plots [i](#)

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: CBL

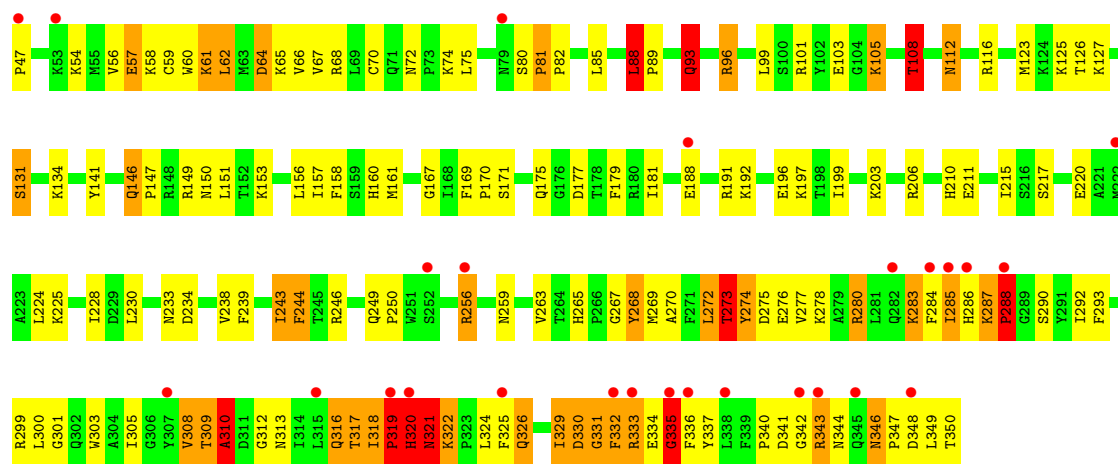


• Molecule 1: CBL



• Molecule 1: CBL





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	159.96Å 105.48Å 84.92Å 90.00° 92.06° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.20) 99.1 (50.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.19Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.218 , 0.266 0.220 , 0.268	Depositor DCC
R_{free} test set	3595 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8092	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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	1.20	4/2541 (0.2%)	1.81	48/3433 (1.4%)
1	B	1.26	6/2538 (0.2%)	1.77	35/3429 (1.0%)
1	C	1.05	1/2542 (0.0%)	1.66	40/3434 (1.2%)
All	All	1.17	11/7621 (0.1%)	1.75	123/10296 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	16
1	B	0	14
1	C	0	12
All	All	0	42

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	343	ARG	NE-CZ	-6.97	1.25	1.33
1	B	343	ARG	CD-NE	-6.51	1.37	1.46
1	A	205	PHE	CA-CB	6.23	1.63	1.53
1	B	242	ASP	N-CA	5.64	1.53	1.46
1	C	167	GLY	N-CA	5.45	1.52	1.45
1	B	241	PHE	CA-CB	5.37	1.61	1.53
1	B	82	PRO	N-CD	5.33	1.55	1.47
1	B	162	LEU	C-O	-5.30	1.17	1.24
1	A	319	PRO	N-CA	-5.24	1.40	1.47
1	A	243	ILE	N-CA	5.16	1.52	1.46
1	A	273	THR	N-CA	5.00	1.51	1.45

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	ARG	CD-NE-CZ	37.48	176.88	124.40
1	A	139	ARG	CD-NE-CZ	15.46	146.05	124.40
1	A	101	ARG	CD-NE-CZ	14.47	144.66	124.40
1	C	93	GLN	CB-CG-CD	12.11	133.18	112.60
1	A	318	ILE	CA-C-N	11.28	133.93	119.84
1	A	318	ILE	C-N-CA	11.28	133.93	119.84
1	A	319	PRO	N-CA-C	10.38	133.86	112.47
1	C	93	GLN	CA-CB-CG	9.75	133.60	114.10
1	B	320	HIS	CA-C-N	9.59	139.85	121.54
1	B	320	HIS	C-N-CA	9.59	139.85	121.54
1	A	48	PRO	CA-C-N	9.26	128.90	120.10
1	A	48	PRO	C-N-CA	9.26	128.90	120.10
1	A	275	ASP	CA-CB-CG	9.07	121.67	112.60
1	A	273	THR	N-CA-CB	-8.85	96.96	110.42
1	A	250	PRO	CA-C-N	8.74	132.35	120.38
1	A	250	PRO	C-N-CA	8.74	132.35	120.38
1	C	191	ARG	CD-NE-CZ	8.71	136.60	124.40
1	C	320	HIS	CA-CB-CG	8.31	122.11	113.80
1	C	273	THR	N-CA-CB	-8.19	98.01	110.45
1	A	124	LYS	CA-CB-CG	8.07	130.24	114.10
1	C	47	PRO	N-CA-CB	8.02	111.83	103.00
1	A	206	ARG	CD-NE-CZ	8.02	135.63	124.40
1	A	227	THR	N-CA-C	7.86	119.48	111.07
1	C	57	GLU	CA-CB-CG	7.81	129.72	114.10
1	C	321	ASN	CA-CB-CG	-7.23	105.37	112.60
1	C	318	ILE	CA-C-N	7.15	128.77	119.84
1	C	318	ILE	C-N-CA	7.15	128.77	119.84
1	C	273	THR	CA-CB-CG2	7.14	122.64	110.50
1	B	206	ARG	CD-NE-CZ	7.03	134.25	124.40
1	A	235	TYR	CA-C-N	7.00	132.51	123.13
1	A	235	TYR	C-N-CA	7.00	132.51	123.13
1	B	330	ASP	CA-CB-CG	6.94	119.54	112.60
1	C	244	PHE	N-CA-C	-6.79	103.96	111.36
1	C	274	TYR	CA-CB-CG	6.75	126.05	113.90
1	C	199	ILE	O-C-N	-6.73	115.28	123.09
1	A	205	PHE	CA-CB-CG	-6.70	107.10	113.80
1	A	311	ASP	CA-CB-CG	-6.65	105.95	112.60
1	C	81	PRO	O-C-N	6.51	124.21	121.15
1	B	320	HIS	CA-C-O	6.51	129.81	120.51
1	C	169	PHE	CA-CB-CG	6.49	120.29	113.80
1	A	319	PRO	O-C-N	-6.47	113.91	122.64
1	B	109	LEU	CA-C-N	6.47	128.28	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	LEU	C-N-CA	6.47	128.28	120.13
1	C	93	GLN	CB-CA-C	6.47	121.03	110.88
1	C	181	ILE	CA-C-N	6.45	129.21	120.44
1	C	181	ILE	C-N-CA	6.45	129.21	120.44
1	A	274	TYR	N-CA-CB	6.36	120.01	110.22
1	B	248	PHE	CA-C-O	6.30	127.39	119.95
1	B	175	GLN	CB-CA-C	-6.29	101.36	111.18
1	B	47	PRO	N-CA-CB	6.28	109.90	103.00
1	A	273	THR	O-C-N	-6.19	115.44	122.68
1	A	93	GLN	CA-C-O	-6.18	114.33	120.70
1	A	273	THR	OG1-CB-CG2	6.08	121.47	109.30
1	B	262	ALA	CA-C-N	-6.08	116.76	122.66
1	B	262	ALA	C-N-CA	-6.08	116.76	122.66
1	A	241	PHE	O-C-N	-6.07	115.68	122.12
1	C	332	PHE	CA-CB-CG	-6.05	107.75	113.80
1	B	280	ARG	CD-NE-CZ	-5.99	116.02	124.40
1	C	108	THR	N-CA-CB	5.98	119.01	110.16
1	A	228	ILE	CB-CA-C	-5.95	104.27	112.24
1	A	139	ARG	NE-CZ-NH2	5.94	124.54	119.20
1	A	320	HIS	CA-CB-CG	-5.93	107.87	113.80
1	C	316	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	A	299	ARG	CD-NE-CZ	5.85	132.59	124.40
1	B	282	GLN	OE1-CD-NE2	5.82	128.42	122.60
1	B	213	HIS	CA-CB-CG	5.79	119.59	113.80
1	C	273	THR	CA-C-N	5.79	128.03	120.28
1	C	273	THR	C-N-CA	5.79	128.03	120.28
1	B	348	ASP	CA-C-O	-5.78	114.07	120.60
1	A	106	MET	N-CA-C	5.76	119.92	113.01
1	B	206	ARG	NH1-CZ-NH2	-5.75	111.82	119.30
1	A	103	GLU	N-CA-C	5.75	118.28	111.33
1	A	191	ARG	CA-C-O	-5.72	114.81	120.70
1	C	309	THR	N-CA-C	5.71	120.38	112.45
1	A	106	MET	N-CA-CB	5.66	120.30	110.39
1	C	343	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	A	293	PHE	CA-CB-CG	5.62	119.42	113.80
1	C	88	LEU	CA-C-O	5.60	124.16	118.79
1	C	112	ASN	CA-CB-CG	5.55	118.15	112.60
1	B	206	ARG	NE-CZ-NH1	5.51	127.01	121.50
1	A	225	LYS	CA-C-O	5.48	126.55	120.63
1	A	243	ILE	N-CA-CB	-5.47	103.57	110.57
1	C	319	PRO	N-CA-C	5.46	123.72	112.47
1	B	154	LEU	CA-C-N	5.46	127.53	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	LEU	C-N-CA	5.46	127.53	120.44
1	B	321	ASN	N-CA-CB	-5.45	101.28	110.49
1	A	307	TYR	N-CA-C	5.41	117.30	109.07
1	C	268	TYR	O-C-N	-5.40	116.15	122.96
1	B	68	ARG	CA-CB-CG	5.37	124.84	114.10
1	C	336	PHE	N-CA-C	-5.36	106.88	113.41
1	C	220	GLU	CB-CG-CD	5.35	121.70	112.60
1	B	341	ASP	CA-CB-CG	5.33	117.93	112.60
1	C	321	ASN	N-CA-C	5.32	122.13	110.80
1	A	278	LYS	CB-CA-C	-5.30	102.32	110.81
1	A	210	HIS	CA-CB-CG	-5.29	108.50	113.80
1	B	348	ASP	CB-CA-C	-5.29	101.94	110.77
1	B	316	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	B	180	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	A	287	LYS	CA-C-N	5.26	126.42	119.84
1	A	287	LYS	C-N-CA	5.26	126.42	119.84
1	C	146	GLN	CA-C-N	5.26	124.71	119.24
1	C	146	GLN	C-N-CA	5.26	124.71	119.24
1	C	274	TYR	N-CA-CB	5.25	117.84	110.12
1	A	343	ARG	CG-CD-NE	-5.24	100.48	112.00
1	B	175	GLN	CA-C-O	-5.20	114.39	120.53
1	C	273	THR	CA-C-O	-5.20	115.68	121.81
1	B	180	ARG	CD-NE-CZ	5.20	131.67	124.40
1	B	101	ARG	CG-CD-NE	-5.19	100.58	112.00
1	C	275	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	204	SER	N-CA-C	5.18	117.00	111.36
1	C	96	ARG	CA-C-O	5.17	125.91	119.97
1	A	52	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	272	LEU	CA-CB-CG	5.15	134.32	116.30
1	B	242	ASP	N-CA-CB	-5.15	102.55	110.12
1	A	203	LYS	O-C-N	-5.14	116.29	122.15
1	A	317	THR	N-CA-CB	5.14	119.95	111.62
1	C	57	GLU	CB-CG-CD	5.08	121.24	112.60
1	B	345	GLN	CB-CG-CD	5.07	121.21	112.60
1	A	124	LYS	N-CA-C	-5.06	105.66	111.07
1	B	199	ILE	N-CA-C	5.04	115.00	108.35
1	B	242	ASP	O-C-N	-5.03	116.79	122.12
1	A	273	THR	CA-CB-OG1	5.03	117.14	109.60
1	A	316	GLN	OE1-CD-NE2	-5.01	117.59	122.60

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	SER	Mainchain
1	A	170	PRO	Mainchain
1	A	213	HIS	Mainchain
1	A	260	SER	Mainchain
1	A	268	TYR	Mainchain
1	A	272	LEU	Mainchain
1	A	277	VAL	Mainchain
1	A	283	LYS	Mainchain
1	A	292	ILE	Mainchain
1	A	301	GLY	Mainchain
1	A	318	ILE	Peptide
1	A	319	PRO	Mainchain
1	A	322	LYS	Mainchain
1	A	336	PHE	Mainchain
1	A	48	PRO	Mainchain
1	A	80	SER	Mainchain
1	B	104	GLY	Peptide
1	B	127	LYS	Mainchain
1	B	130	ILE	Mainchain
1	B	131	SER	Mainchain
1	B	163	ALA	Mainchain
1	B	229	ASP	Mainchain
1	B	237	SER	Mainchain
1	B	260	SER	Mainchain
1	B	262	ALA	Mainchain
1	B	266	PRO	Mainchain
1	B	281	LEU	Mainchain
1	B	336	PHE	Mainchain
1	B	348	ASP	Mainchain
1	B	72	ASN	Mainchain
1	C	131	SER	Mainchain
1	C	151	LEU	Mainchain
1	C	179	PHE	Mainchain
1	C	238	VAL	Mainchain
1	C	286	HIS	Mainchain
1	C	301	GLY	Mainchain
1	C	310	ALA	Mainchain
1	C	319	PRO	Mainchain,Peptide
1	C	320	HIS	Peptide
1	C	321	ASN	Peptide
1	C	335	GLY	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	2475	0	2474	85	0
1	B	2472	0	2470	78	0
1	C	2476	0	2474	132	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	221	0	0	16	0
3	B	261	0	0	8	0
3	C	184	0	0	18	0
All	All	8092	0	7418	291	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 20.

All (291) 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:C:157:ILE:HG22	1:C:161:MET:HE2	1.21	1.17
1:C:256:ARG:HG2	1:C:256:ARG:HH11	1.16	1.07
1:A:319:PRO:HA	3:A:474:HOH:O	1.61	0.99
1:B:265:HIS:HD2	1:B:267:GLY:H	1.12	0.96
1:C:82:PRO:HG3	1:C:156:LEU:HD22	1.49	0.95
1:B:157:ILE:HG22	1:B:161:MET:HE2	1.49	0.95
1:C:265:HIS:HD2	1:C:267:GLY:H	1.12	0.94
1:B:273:THR:HG22	1:B:276:GLU:H	1.28	0.94
1:A:273:THR:HG22	1:A:276:GLU:H	1.33	0.93
1:A:294:ARG:NH2	1:A:316:GLN:OE1	2.02	0.91
1:B:269:MET:HB3	1:B:272:LEU:HD22	1.55	0.89
1:B:210:HIS:HD2	1:B:215:ILE:H	1.12	0.88
1:C:273:THR:HG22	1:C:276:GLU:H	1.40	0.86
1:C:319:PRO:HA	1:C:320:HIS:CD2	2.10	0.86
1:A:210:HIS:HD2	1:A:215:ILE:H	1.23	0.85
1:B:218:GLY:HA3	1:C:64:ASP:OD1	1.76	0.84
1:C:210:HIS:HD2	1:C:215:ILE:H	1.25	0.83
1:A:265:HIS:HD2	1:A:267:GLY:H	1.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:CYS:SG	1:B:123:MET:HG2	2.21	0.80
1:C:340:PRO:HD3	1:C:346:ASN:HD22	1.47	0.80
1:C:256:ARG:HG2	1:C:256:ARG:NH1	1.89	0.80
1:C:123:MET:HE2	3:C:504:HOH:O	1.81	0.80
1:C:326:GLN:OE1	1:C:326:GLN:HA	1.82	0.80
1:B:53:LYS:O	1:B:57:GLU:HG2	1.82	0.79
1:B:82:PRO:HG3	1:B:156:LEU:HD13	1.65	0.78
1:B:210:HIS:CD2	1:B:215:ILE:H	1.99	0.78
1:A:320:HIS:HD2	3:A:474:HOH:O	1.66	0.78
1:C:265:HIS:CD2	1:C:267:GLY:H	2.00	0.78
1:A:285:ILE:HG22	3:A:547:HOH:O	1.85	0.76
1:A:259:ASN:HB3	3:A:432:HOH:O	1.87	0.75
1:A:60:TRP:CH2	1:A:96:ARG:HD3	2.21	0.75
1:A:311:ASP:OD2	1:A:313:ASN:OD1	2.05	0.75
1:A:299:ARG:NH1	1:A:302:GLN:OE1	2.20	0.74
1:C:59:CYS:SG	1:C:123:MET:CG	2.76	0.74
1:B:273:THR:CG2	1:B:276:GLU:H	1.99	0.73
1:B:263:VAL:O	3:B:455:HOH:O	2.06	0.73
1:C:259:ASN:HA	1:C:263:VAL:HB	1.70	0.73
3:B:455:HOH:O	1:C:93:GLN:CD	2.32	0.72
1:A:210:HIS:CD2	1:A:215:ILE:H	2.06	0.72
1:C:62:LEU:HB3	1:C:126:THR:HG21	1.70	0.72
1:B:299:ARG:NH1	1:B:318:ILE:HD13	2.06	0.71
1:A:53:LYS:O	1:A:56:VAL:HG22	1.91	0.71
1:C:158:PHE:HA	1:C:161:MET:HE3	1.72	0.71
1:A:145:SER:HB2	1:A:147:PRO:HD2	1.72	0.70
1:A:203:LYS:HZ3	1:A:207:GLN:NE2	1.90	0.70
1:B:72:ASN:HD21	1:B:74:LYS:NZ	1.88	0.70
1:A:273:THR:HG23	1:A:275:ASP:H	1.56	0.70
1:C:243:ILE:HD13	1:C:300:LEU:HB3	1.74	0.69
1:A:322:LYS:HD2	1:A:327:ALA:HA	1.76	0.68
1:C:274:TYR:CE1	1:C:278:LYS:HD2	2.28	0.68
1:C:329:ILE:O	1:C:330:ASP:C	2.36	0.67
1:B:59:CYS:SG	1:B:123:MET:CG	2.83	0.66
1:C:239:PHE:O	1:C:243:ILE:HG13	1.95	0.66
1:B:320:HIS:H	1:B:321:ASN:CG	2.04	0.65
1:A:119:MET:HA	1:A:119:MET:HE3	1.78	0.65
1:A:203:LYS:NZ	1:A:207:GLN:HE22	1.95	0.65
1:A:322:LYS:HE3	1:A:330:ASP:OD2	1.97	0.64
1:C:210:HIS:CD2	1:C:215:ILE:H	2.13	0.64
1:B:59:CYS:SG	1:B:123:MET:SD	2.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:THR:HG23	3:C:486:HOH:O	1.97	0.64
1:C:287:LYS:NZ	1:C:344:ASN:ND2	2.46	0.64
1:A:143:GLU:O	1:A:148:ARG:HG2	1.98	0.64
1:C:82:PRO:CG	1:C:156:LEU:HD22	2.26	0.64
1:C:58:LYS:HD3	1:C:123:MET:CE	2.28	0.64
1:C:59:CYS:SG	1:C:123:MET:SD	2.95	0.64
1:C:287:LYS:HZ1	1:C:344:ASN:ND2	1.96	0.64
1:C:170:PRO:HG2	1:C:175:GLN:HG3	1.79	0.63
1:C:62:LEU:HB3	1:C:126:THR:CG2	2.28	0.63
1:C:64:ASP:O	1:C:68:ARG:HG3	1.99	0.62
1:A:265:HIS:CD2	1:A:267:GLY:H	2.15	0.62
1:C:269:MET:O	1:C:270:ALA:HB3	1.99	0.62
1:B:265:HIS:HE1	3:B:601:HOH:O	1.82	0.61
1:C:303:TRP:CD2	1:C:324:LEU:HD22	2.35	0.61
1:B:265:HIS:CD2	1:B:267:GLY:H	2.05	0.61
1:C:350:THR:HG22	3:C:479:HOH:O	2.01	0.61
1:B:299:ARG:HH12	1:B:318:ILE:HD13	1.64	0.61
1:C:350:THR:HA	3:C:478:HOH:O	2.01	0.61
1:A:269:MET:HB3	1:A:272:LEU:HD22	1.82	0.60
1:C:134:LYS:HD3	3:C:516:HOH:O	2.00	0.60
1:B:273:THR:HG23	1:B:275:ASP:N	2.16	0.60
1:A:79:ASN:HB2	3:A:419:HOH:O	2.00	0.60
1:B:304:ALA:HB1	1:B:316:GLN:NE2	2.16	0.60
1:C:149:ARG:O	1:C:153:LYS:HG3	2.01	0.60
1:B:273:THR:HG23	1:B:275:ASP:H	1.67	0.60
1:A:274:TYR:CG	3:A:545:HOH:O	2.50	0.59
1:C:157:ILE:CG2	1:C:161:MET:HE2	2.14	0.59
1:C:170:PRO:CG	1:C:175:GLN:HG3	2.31	0.59
1:B:269:MET:CB	1:B:272:LEU:HD22	2.31	0.59
1:C:58:LYS:HD3	1:C:123:MET:HE3	1.84	0.59
1:A:53:LYS:O	1:A:57:GLU:HG2	2.02	0.59
1:C:72:ASN:O	1:C:75:LEU:HB2	2.03	0.59
1:C:103:GLU:HG2	3:C:495:HOH:O	2.03	0.59
1:B:322:LYS:HB2	1:B:323:PRO:HD2	1.84	0.59
1:A:318:ILE:HG13	3:A:464:HOH:O	2.03	0.58
1:C:125:LYS:HE3	3:C:508:HOH:O	2.03	0.58
1:A:274:TYR:O	1:A:274:TYR:CD1	2.57	0.58
1:A:58:LYS:O	1:A:62:LEU:HD22	2.04	0.57
1:A:146:GLN:HB3	1:A:147:PRO:HD3	1.86	0.56
1:A:275:ASP:OD1	1:A:278:LYS:NZ	2.38	0.56
1:B:228:ILE:HG12	1:B:244:PHE:CD1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ARG:HD3	3:C:393:HOH:O	2.05	0.56
1:C:146:GLN:OE1	1:C:149:ARG:NH1	2.33	0.56
1:C:105:LYS:HB2	1:C:108:THR:HG23	1.88	0.56
1:C:317:THR:O	1:C:318:ILE:HG13	2.06	0.56
1:A:203:LYS:NZ	1:A:207:GLN:NE2	2.54	0.56
1:C:59:CYS:SG	1:C:123:MET:HG2	2.46	0.56
1:A:160:HIS:HE1	3:A:372:HOH:O	1.88	0.55
1:C:269:MET:HB3	1:C:272:LEU:HD22	1.89	0.55
1:C:70:CYS:HA	1:C:75:LEU:CD1	2.37	0.55
1:C:341:ASP:HB3	1:C:343:ARG:NH1	2.21	0.55
1:A:317:THR:HG23	3:A:466:HOH:O	2.07	0.55
1:A:331:GLY:HA3	1:A:337:TYR:CD2	2.41	0.55
1:C:146:GLN:N	1:C:147:PRO:CD	2.70	0.54
1:A:52:ASP:O	1:A:55:MET:N	2.40	0.54
1:C:329:ILE:O	1:C:332:PHE:N	2.41	0.54
1:B:62:LEU:HB3	1:B:126:THR:CG2	2.37	0.54
1:B:278:LYS:NZ	1:B:278:LYS:HB3	2.23	0.54
1:C:332:PHE:C	1:C:332:PHE:CD1	2.85	0.54
1:A:320:HIS:CD2	3:A:474:HOH:O	2.50	0.53
1:C:287:LYS:O	1:C:288:PRO:C	2.51	0.53
1:A:119:MET:O	1:A:123:MET:HG2	2.09	0.53
1:C:233:ASN:O	1:C:234:ASP:HB2	2.09	0.53
1:B:144:ASN:O	1:B:149:ARG:NH2	2.42	0.53
1:A:196:GLU:HG3	3:A:561:HOH:O	2.09	0.52
1:A:253:SER:O	1:A:254:LEU:C	2.52	0.52
1:B:303:TRP:CD2	1:B:324:LEU:HD22	2.45	0.52
1:B:311:ASP:OD2	1:B:313:ASN:OD1	2.26	0.52
1:A:100:SER:O	1:A:103:GLU:HG2	2.09	0.52
1:C:269:MET:HG3	1:C:292:ILE:HB	1.92	0.52
1:B:146:GLN:HB3	1:B:147:PRO:HD3	1.90	0.52
1:C:225:LYS:NZ	3:C:379:HOH:O	2.38	0.52
1:C:303:TRP:HB2	1:C:319:PRO:HG2	1.91	0.52
1:C:305:ILE:O	1:C:316:GLN:HA	2.09	0.52
1:A:53:LYS:O	1:A:54:LYS:C	2.53	0.52
1:C:322:LYS:HG3	1:C:326:GLN:HB3	1.92	0.52
1:C:210:HIS:HD2	1:C:215:ILE:N	1.99	0.51
1:A:322:LYS:HD2	1:A:327:ALA:CA	2.40	0.51
1:C:330:ASP:O	1:C:333:ARG:N	2.43	0.51
1:B:157:ILE:O	1:B:161:MET:HG3	2.10	0.51
1:B:239:PHE:CZ	1:B:243:ILE:HD11	2.45	0.51
3:B:455:HOH:O	1:C:93:GLN:OE1	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:THR:HA	1:A:116:ARG:HD3	1.92	0.51
1:A:303:TRP:O	1:A:318:ILE:HG23	2.11	0.51
1:C:268:TYR:O	1:C:269:MET:HE2	2.10	0.51
1:C:273:THR:HG22	1:C:276:GLU:N	2.19	0.51
1:C:293:PHE:CD1	1:C:324:LEU:HD21	2.46	0.50
1:A:249:GLN:HG3	1:A:323:PRO:HB3	1.94	0.50
1:C:59:CYS:SG	1:C:123:MET:HG3	2.50	0.50
1:B:72:ASN:HD21	1:B:74:LYS:HZ2	1.56	0.50
1:A:299:ARG:NH1	1:A:302:GLN:CD	2.70	0.49
1:B:48:PRO:O	1:B:116:ARG:NH1	2.45	0.49
1:B:265:HIS:HD2	1:B:267:GLY:N	1.95	0.49
1:C:170:PRO:HD2	1:C:175:GLN:HG3	1.93	0.49
1:C:170:PRO:CD	1:C:175:GLN:HG3	2.43	0.49
1:A:317:THR:C	1:A:318:ILE:HG12	2.37	0.49
1:A:173:LEU:O	1:A:175:GLN:HG2	2.12	0.49
1:A:183:LYS:HE2	1:A:249:GLN:NE2	2.28	0.49
1:A:309:THR:OG1	1:A:311:ASP:OD1	2.23	0.48
1:A:119:MET:HE3	1:A:119:MET:CA	2.40	0.48
1:B:320:HIS:H	1:B:321:ASN:ND2	2.11	0.48
1:C:310:ALA:C	1:C:312:GLY:H	2.20	0.48
1:C:340:PRO:HG3	1:C:347:PRO:HD3	1.94	0.48
1:A:160:HIS:HD2	3:A:415:HOH:O	1.96	0.48
1:B:142:GLU:O	1:B:143:GLU:C	2.56	0.48
1:B:158:PHE:HA	1:B:161:MET:HE3	1.94	0.48
1:B:65:LYS:HG2	1:B:68:ARG:HH21	1.79	0.48
1:B:222:MET:SD	1:C:67:VAL:HG11	2.53	0.48
1:C:146:GLN:N	1:C:147:PRO:HD2	2.29	0.48
1:B:322:LYS:NZ	1:B:330:ASP:OD2	2.42	0.48
1:A:101:ARG:HH21	1:A:173:LEU:HB2	1.79	0.48
1:B:218:GLY:CA	1:C:64:ASP:OD1	2.55	0.48
1:C:273:THR:O	1:C:277:VAL:HG23	2.14	0.48
1:C:309:THR:O	1:C:310:ALA:CB	2.61	0.48
1:A:59:CYS:SG	1:A:122:LEU:HD23	2.53	0.47
1:B:105:LYS:O	1:B:108:THR:HG23	2.13	0.47
1:B:62:LEU:HB3	1:B:126:THR:HG21	1.95	0.47
1:B:72:ASN:OD1	1:B:74:LYS:HB2	2.14	0.47
1:A:170:PRO:HD2	1:A:175:GLN:HG3	1.96	0.47
1:C:285:ILE:HG13	1:C:285:ILE:O	2.14	0.47
1:C:322:LYS:NZ	1:C:330:ASP:OD2	2.39	0.47
1:C:334:GLU:O	1:C:335:GLY:C	2.58	0.47
1:A:158:PHE:HA	1:A:161:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:LYS:HD3	1:C:283:LYS:N	2.30	0.47
1:C:290:SER:O	1:C:308:VAL:HG23	2.14	0.47
1:C:310:ALA:O	1:C:312:GLY:N	2.48	0.47
1:C:70:CYS:HA	1:C:75:LEU:HD11	1.97	0.46
1:B:105:LYS:HB2	1:B:108:THR:HG23	1.98	0.46
1:C:329:ILE:O	1:C:330:ASP:O	2.34	0.46
1:A:77:LEU:HB3	3:A:420:HOH:O	2.15	0.46
1:C:64:ASP:HB3	1:C:68:ARG:NH1	2.30	0.46
1:B:284:PHE:CE1	1:B:342:GLY:HA3	2.51	0.46
1:B:348:ASP:HB2	3:B:526:HOH:O	2.15	0.46
1:C:332:PHE:O	1:C:335:GLY:N	2.45	0.46
1:B:72:ASN:OD1	1:B:74:LYS:HE3	2.16	0.46
1:B:343:ARG:NH2	1:C:171:SER:OG	2.49	0.46
1:A:170:PRO:HG2	1:A:175:GLN:HG3	1.98	0.45
1:C:310:ALA:C	1:C:312:GLY:N	2.73	0.45
1:A:287:LYS:HZ1	1:A:344:ASN:HD21	1.64	0.45
1:C:66:VAL:CG2	1:C:126:THR:HG23	2.47	0.45
1:C:285:ILE:HA	1:C:308:VAL:HG11	1.98	0.45
1:B:72:ASN:HA	1:B:73:PRO:HD3	1.76	0.45
1:C:249:GLN:HB2	1:C:250:PRO:HA	1.98	0.45
1:C:256:ARG:HH11	1:C:256:ARG:CG	2.06	0.45
1:C:101:ARG:NH1	3:C:456:HOH:O	2.50	0.45
1:B:146:GLN:N	1:B:147:PRO:CD	2.80	0.45
1:C:66:VAL:HG21	1:C:126:THR:HG23	1.97	0.45
1:C:150:ASN:HD22	1:C:153:LYS:HD2	1.82	0.45
1:B:54:LYS:HG2	3:B:610:HOH:O	2.16	0.45
1:C:74:LYS:NZ	1:C:141:TYR:CZ	2.85	0.45
1:A:79:ASN:OD1	1:A:79:ASN:C	2.59	0.45
1:A:299:ARG:HH22	1:A:318:ILE:CG2	2.30	0.45
1:B:144:ASN:ND2	1:B:149:ARG:HH21	2.15	0.45
1:C:283:LYS:N	1:C:283:LYS:CD	2.78	0.45
1:A:53:LYS:HA	1:A:56:VAL:HG22	1.99	0.45
1:A:64:ASP:OD2	1:A:68:ARG:NH1	2.50	0.44
1:C:74:LYS:O	1:C:75:LEU:C	2.61	0.44
1:B:330:ASP:O	1:B:334:GLU:HG3	2.18	0.44
1:A:265:HIS:HD2	1:A:267:GLY:N	2.05	0.44
1:C:284:PHE:HB3	1:C:290:SER:OG	2.16	0.44
1:C:85:LEU:O	1:C:89:PRO:HG2	2.18	0.44
1:A:287:LYS:NZ	1:A:344:ASN:HD21	2.15	0.44
1:B:269:MET:HB3	1:B:272:LEU:CD2	2.39	0.43
1:B:322:LYS:H	1:B:322:LYS:HG2	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ARG:HD3	3:A:487:HOH:O	2.18	0.43
1:A:332:PHE:O	1:A:333:ARG:C	2.62	0.43
1:C:256:ARG:HG3	3:C:476:HOH:O	2.18	0.43
1:A:303:TRP:CD2	1:A:324:LEU:HD22	2.52	0.43
1:B:74:LYS:HB3	1:B:141:TYR:CD1	2.54	0.43
1:B:160:HIS:HE1	3:B:464:HOH:O	2.00	0.43
1:C:123:MET:O	1:C:127:LYS:HG3	2.18	0.43
1:C:160:HIS:HE1	3:C:376:HOH:O	2.01	0.43
1:C:175:GLN:HB3	3:C:413:HOH:O	2.19	0.43
1:C:280:ARG:HG3	1:C:280:ARG:HH11	1.83	0.43
1:C:287:LYS:NZ	1:C:344:ASN:HD21	2.17	0.43
1:B:183:LYS:HA	1:B:183:LYS:HE3	2.01	0.43
1:B:100:SER:O	1:B:103:GLU:HG3	2.19	0.43
1:C:123:MET:HE1	3:C:503:HOH:O	2.18	0.43
1:B:142:GLU:O	1:B:144:ASN:N	2.52	0.43
1:B:181:ILE:HD11	1:B:238:VAL:HG23	2.01	0.43
1:A:72:ASN:OD1	1:A:74:LYS:HB2	2.19	0.42
1:C:246:ARG:O	1:C:249:GLN:HG2	2.19	0.42
1:B:62:LEU:HB3	1:B:126:THR:HG22	2.01	0.42
1:C:112:ASN:O	1:C:116:ARG:HG3	2.20	0.42
1:C:177:ASP:OD1	1:C:177:ASP:N	2.46	0.42
1:B:175:GLN:NE2	3:B:419:HOH:O	2.49	0.42
1:C:265:HIS:CE1	1:C:347:PRO:HG2	2.55	0.42
1:A:133:PHE:O	1:A:134:LYS:C	2.62	0.42
1:C:303:TRP:O	1:C:319:PRO:HD2	2.19	0.42
1:B:145:SER:HB2	1:B:147:PRO:HD2	2.01	0.42
1:C:256:ARG:NH1	1:C:256:ARG:CG	2.72	0.42
1:C:309:THR:HG23	1:C:313:ASN:O	2.19	0.42
1:A:134:LYS:O	1:A:137:LYS:HD3	2.19	0.42
1:A:325:PHE:O	1:A:329:ILE:HG13	2.19	0.42
1:B:119:MET:O	1:B:123:MET:HG3	2.18	0.42
1:A:138:GLU:H	1:A:138:GLU:HG3	1.36	0.42
1:B:72:ASN:OD1	1:B:74:LYS:N	2.41	0.42
1:B:162:LEU:HD11	1:B:166:LYS:HE3	2.01	0.42
1:A:75:LEU:HD21	1:A:133:PHE:HE1	1.85	0.42
1:A:265:HIS:HE1	3:A:519:HOH:O	2.02	0.42
1:A:299:ARG:O	1:A:300:LEU:C	2.61	0.42
1:C:192:LYS:HE3	3:C:400:HOH:O	2.19	0.42
1:C:196:GLU:HG3	3:C:465:HOH:O	2.19	0.42
1:C:228:ILE:HG12	1:C:244:PHE:CD1	2.55	0.42
1:C:325:PHE:CZ	1:C:349:LEU:HD22	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ARG:HH22	1:A:318:ILE:HG21	1.84	0.42
1:C:324:LEU:O	1:C:325:PHE:C	2.62	0.42
1:C:103:GLU:CG	3:C:495:HOH:O	2.66	0.41
1:B:318:ILE:O	1:B:319:PRO:C	2.62	0.41
1:C:88:LEU:HD12	1:C:88:LEU:HA	1.87	0.41
1:A:48:PRO:O	1:A:116:ARG:HD2	2.20	0.41
1:C:61:LYS:HB2	1:C:61:LYS:NZ	2.36	0.41
1:A:170:PRO:O	1:A:172:GLY:N	2.54	0.41
1:C:284:PHE:CZ	1:C:342:GLY:HA3	2.56	0.41
1:B:146:GLN:HE21	1:B:150:ASN:HD21	1.68	0.41
1:C:60:TRP:CH2	1:C:96:ARG:HD3	2.56	0.41
1:C:80:SER:HB2	1:C:81:PRO:HD2	2.01	0.41
1:C:284:PHE:CE1	1:C:342:GLY:HA3	2.56	0.41
1:C:349:LEU:N	3:C:479:HOH:O	2.54	0.41
1:B:215:ILE:HG21	1:B:221:ALA:HB2	2.02	0.41
1:C:321:ASN:HD22	1:C:321:ASN:HA	1.53	0.41
1:A:87:LEU:HD22	1:A:159:SER:HA	2.03	0.40
1:B:321:ASN:ND2	1:B:321:ASN:H	1.99	0.40
1:A:170:PRO:CG	1:A:175:GLN:HG3	2.51	0.40
1:A:246:ARG:NH1	3:A:460:HOH:O	2.50	0.40
1:B:280:ARG:HH11	1:B:280:ARG:HD2	1.58	0.40
1:C:330:ASP:O	1:C:331:GLY:C	2.64	0.40
1:C:331:GLY:HA3	1:C:337:TYR:CD2	2.57	0.40
1:A:170:PRO:CD	1:A:175:GLN:HG3	2.51	0.40
1:A:275:ASP:CG	1:A:278:LYS:HZ1	2.28	0.40
1:B:51:VAL:HG23	1:B:116:ARG:HG2	2.03	0.40
1:B:340:PRO:HG3	1:B:346:ASN:HD22	1.86	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	302/304 (99%)	284 (94%)	16 (5%)	2 (1%)	18	19
1	B	302/304 (99%)	292 (97%)	10 (3%)	0	100	100
1	C	302/304 (99%)	273 (90%)	21 (7%)	8 (3%)	4	2
All	All	906/912 (99%)	849 (94%)	47 (5%)	10 (1%)	11	10

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	PRO
1	C	310	ALA
1	C	319	PRO
1	C	329	ILE
1	C	288	PRO
1	C	321	ASN
1	C	330	ASP
1	A	171	SER
1	C	335	GLY
1	C	331	GLY

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	267/272 (98%)	236 (88%)	31 (12%)	5	5
1	B	266/272 (98%)	239 (90%)	27 (10%)	7	7
1	C	267/272 (98%)	229 (86%)	38 (14%)	3	3
All	All	800/816 (98%)	704 (88%)	96 (12%)	5	4

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	VAL
1	A	57	GLU
1	A	62	LEU

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Mol	Chain	Res	Type
1	A	65	LYS
1	A	74	LYS
1	A	80	SER
1	A	99	LEU
1	A	100	SER
1	A	106	MET
1	A	108	THR
1	A	137	LYS
1	A	138	GLU
1	A	145	SER
1	A	156	LEU
1	A	168	ILE
1	A	173	LEU
1	A	175	GLN
1	A	199	ILE
1	A	200	VAL
1	A	204	SER
1	A	224	LEU
1	A	226	SER
1	A	228	ILE
1	A	256	ARG
1	A	272	LEU
1	A	273	THR
1	A	299	ARG
1	A	316	GLN
1	A	317	THR
1	A	318	ILE
1	A	322	LYS
1	B	50	THR
1	B	54	LYS
1	B	56	VAL
1	B	61	LYS
1	B	62	LEU
1	B	65	LYS
1	B	75	LEU
1	B	80	SER
1	B	88	LEU
1	B	99	LEU
1	B	105	LYS
1	B	108	THR
1	B	131	SER
1	B	138	GLU

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Mol	Chain	Res	Type
1	B	139	ARG
1	B	142	GLU
1	B	156	LEU
1	B	173	LEU
1	B	224	LEU
1	B	272	LEU
1	B	273	THR
1	B	299	ARG
1	B	316	GLN
1	B	321	ASN
1	B	322	LYS
1	B	333	ARG
1	B	348	ASP
1	C	54	LYS
1	C	56	VAL
1	C	57	GLU
1	C	61	LYS
1	C	62	LEU
1	C	64	ASP
1	C	65	LYS
1	C	88	LEU
1	C	93	GLN
1	C	99	LEU
1	C	105	LYS
1	C	108	THR
1	C	131	SER
1	C	188	GLU
1	C	197	LYS
1	C	203	LYS
1	C	211	GLU
1	C	217	SER
1	C	224	LEU
1	C	230	LEU
1	C	243	ILE
1	C	256	ARG
1	C	272	LEU
1	C	273	THR
1	C	280	ARG
1	C	283	LYS
1	C	285	ILE
1	C	287	LYS
1	C	288	PRO

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Mol	Chain	Res	Type
1	C	299	ARG
1	C	308	VAL
1	C	317	THR
1	C	320	HIS
1	C	322	LYS
1	C	326	GLN
1	C	333	ARG
1	C	346	ASN
1	C	348	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	160	HIS
1	A	207	GLN
1	A	210	HIS
1	A	249	GLN
1	A	265	HIS
1	A	320	HIS
1	A	344	ASN
1	A	346	ASN
1	B	144	ASN
1	B	150	ASN
1	B	160	HIS
1	B	210	HIS
1	B	249	GLN
1	B	265	HIS
1	B	302	GLN
1	B	313	ASN
1	B	320	HIS
1	B	344	ASN
1	B	346	ASN
1	C	150	ASN
1	C	207	GLN
1	C	210	HIS
1	C	265	HIS
1	C	320	HIS
1	C	321	ASN
1	C	344	ASN
1	C	346	ASN

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 3 ligands modelled in this entry, 3 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	304/304 (100%)	0.24	8 (2%) 57 54	27, 42, 68, 74	0
1	B	304/304 (100%)	0.05	10 (3%) 49 46	24, 36, 59, 68	0
1	C	304/304 (100%)	0.67	26 (8%) 16 14	30, 50, 75, 84	0
All	All	912/912 (100%)	0.32	44 (4%) 35 32	24, 43, 70, 84	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	342	GLY	6.1
1	C	320	HIS	5.2
1	C	336	PHE	4.5
1	C	319	PRO	4.1
1	C	285	ILE	3.3
1	A	318	ILE	3.3
1	A	47	PRO	3.3
1	C	315	LEU	3.1
1	C	307	TYR	3.1
1	B	320	HIS	2.9
1	B	79	ASN	2.9
1	C	345	GLN	2.9
1	C	47	PRO	2.8
1	C	284	PHE	2.8
1	C	348	ASP	2.8
1	A	274	TYR	2.8
1	C	338	LEU	2.8
1	C	256	ARG	2.7
1	C	79	ASN	2.7
1	C	335	GLY	2.7
1	A	319	PRO	2.6
1	C	286	HIS	2.5
1	C	343	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	144	ASN	2.5
1	A	299	ARG	2.4
1	A	320	HIS	2.4
1	C	333	ARG	2.4
1	C	288	PRO	2.3
1	C	252	SER	2.3
1	B	143	GLU	2.3
1	B	146	GLN	2.3
1	B	325	PHE	2.2
1	A	321	ASN	2.2
1	C	222	MET	2.2
1	C	325	PHE	2.2
1	B	74	LYS	2.2
1	C	188	GLU	2.1
1	C	53	LYS	2.1
1	B	274	TYR	2.1
1	C	282	GLN	2.0
1	B	144	ASN	2.0
1	B	321	ASN	2.0
1	C	332	PHE	2.0
1	B	333	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](#)

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($\text{\AA}^2$)	Q<0.9
2	CA	A	351	1/1	0.93	0.34	28,28,28,28	0
2	CA	C	351	1/1	0.96	0.25	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	B	351	1/1	0.97	0.39	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.