



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:09 PM UTC

PDB ID : 6QAJ / pdb_00006qaj
Title : Structure of the tripartite motif of KAP1/TRIM28
Authors : Stoll, G.A.; Oda, S.; Yu, M.; Modis, Y.
Deposited on : 2018-12-19
Resolution : 2.90 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

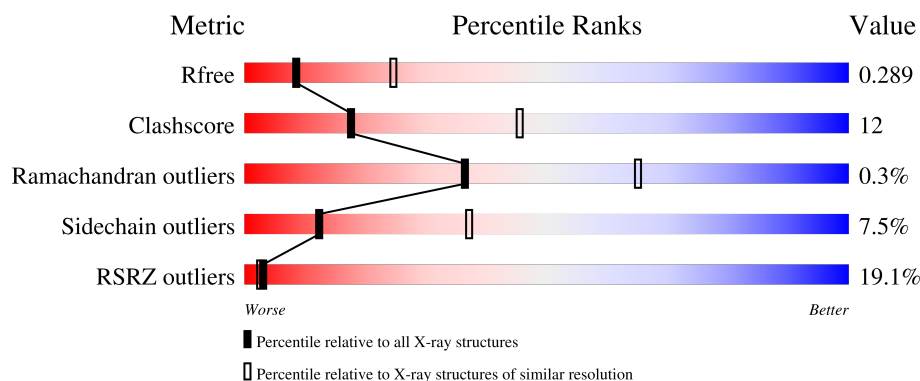
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	544	15% 59% 18% • 19%
1	B	544	16% 61% 18% • 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13867 atoms, of which 6904 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 Endolysin,Transcription intermediary factor 1-beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	439	Total	C	H	N	O	S	0	0	0
			6891	2166	3424	633	644	24			
1	B	441	Total	C	H	N	O	S	0	0	0
			6968	2179	3480	644	640	25			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-130	MET	-	initiating methionine	UNP P00720
A	-129	GLY	-	expression tag	UNP P00720
A	-128	SER	-	expression tag	UNP P00720
A	-127	SER	-	expression tag	UNP P00720
A	-126	HIS	-	expression tag	UNP P00720
A	-125	HIS	-	expression tag	UNP P00720
A	-124	HIS	-	expression tag	UNP P00720
A	-123	HIS	-	expression tag	UNP P00720
A	-122	HIS	-	expression tag	UNP P00720
A	-121	HIS	-	expression tag	UNP P00720
A	-120	SER	-	expression tag	UNP P00720
A	-119	GLN	-	expression tag	UNP P00720
A	-118	ASP	-	expression tag	UNP P00720
A	-117	PRO	-	expression tag	UNP P00720
A	-116	ASN	-	expression tag	UNP P00720
A	-115	SER	-	expression tag	UNP P00720
A	-114	SER	-	expression tag	UNP P00720
A	-113	SER	-	expression tag	UNP P00720
A	-112	GLU	-	expression tag	UNP P00720
A	-111	ASN	-	expression tag	UNP P00720
A	-110	LEU	-	expression tag	UNP P00720
A	-109	TYR	-	expression tag	UNP P00720
A	-108	PHE	-	expression tag	UNP P00720
A	-107	GLN	-	expression tag	UNP P00720
A	-106	GLY	-	expression tag	UNP P00720

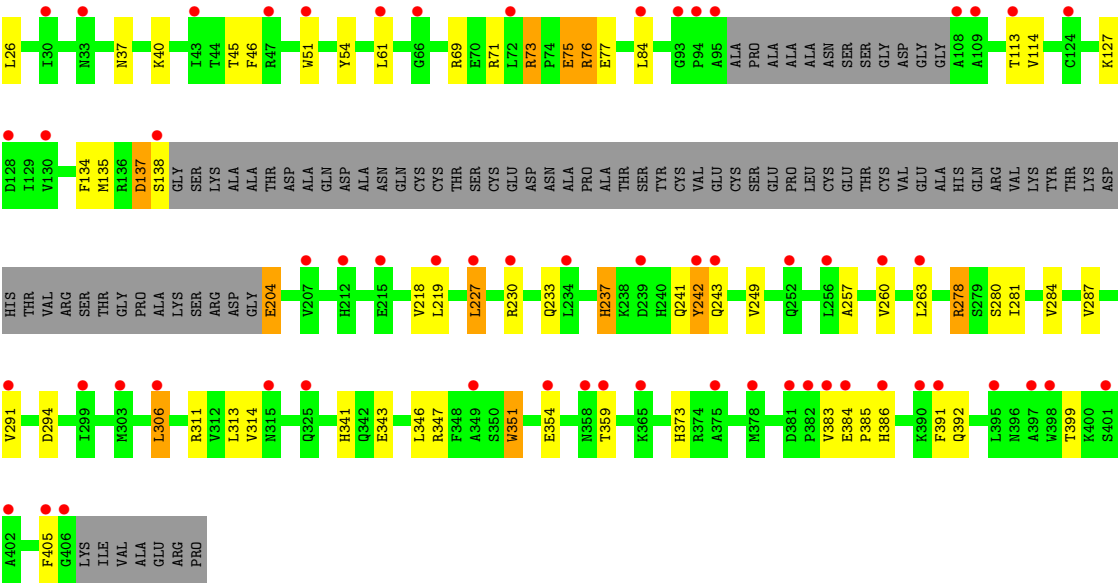
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Chain	Residue	Modelled	Actual	Comment	Reference
A	55	ALA	-	linker	UNP P00720
B	-130	MET	-	initiating methionine	UNP P00720
B	-129	GLY	-	expression tag	UNP P00720
B	-128	SER	-	expression tag	UNP P00720
B	-127	SER	-	expression tag	UNP P00720
B	-126	HIS	-	expression tag	UNP P00720
B	-125	HIS	-	expression tag	UNP P00720
B	-124	HIS	-	expression tag	UNP P00720
B	-123	HIS	-	expression tag	UNP P00720
B	-122	HIS	-	expression tag	UNP P00720
B	-121	HIS	-	expression tag	UNP P00720
B	-120	SER	-	expression tag	UNP P00720
B	-119	GLN	-	expression tag	UNP P00720
B	-118	ASP	-	expression tag	UNP P00720
B	-117	PRO	-	expression tag	UNP P00720
B	-116	ASN	-	expression tag	UNP P00720
B	-115	SER	-	expression tag	UNP P00720
B	-114	SER	-	expression tag	UNP P00720
B	-113	SER	-	expression tag	UNP P00720
B	-112	GLU	-	expression tag	UNP P00720
B	-111	ASN	-	expression tag	UNP P00720
B	-110	LEU	-	expression tag	UNP P00720
B	-109	TYR	-	expression tag	UNP P00720
B	-108	PHE	-	expression tag	UNP P00720
B	-107	GLN	-	expression tag	UNP P00720
B	-106	GLY	-	expression tag	UNP P00720
B	55	ALA	-	linker	UNP P00720

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Zn 4 4	0	0
2	B	4	Total Zn 4 4	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	59.77Å 169.33Å 374.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.80 – 2.90 62.80 – 2.90	Depositor EDS
% Data completeness (in resolution range)	41.4 (62.80-2.90) 39.1 (62.80-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.33 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.14-3260	Depositor
R, R_{free}	0.261 , 0.291 0.265 , 0.289	Depositor DCC
R_{free} test set	898 reflections (1.57%)	wwPDB-VP
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 73.5	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	0.88	EDS
Total number of atoms	13867	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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:
ZN

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	0.28	0/3523	0.52	1/4755 (0.0%)
1	B	0.28	0/3543	0.55	4/4775 (0.1%)
All	All	0.28	0/7066	0.54	5/9530 (0.1%)

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	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	73	ARG	NE-CZ-NH1	-6.78	114.72	121.50
1	B	73	ARG	NE-CZ-NH2	6.29	124.86	119.20
1	A	373	HIS	N-CA-C	5.28	116.98	108.32
1	B	-105	ASN	CA-C-N	-5.26	112.50	121.97
1	B	-105	ASN	C-N-CA	-5.26	112.50	121.97

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	373	HIS	Peptide
1	A	374	ARG	Peptide
1	A	75	GLU	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	3467	3424	3426	93	0
1	B	3488	3480	3483	110	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
All	All	6963	6904	6909	172	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 12.

All (172) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-101:MET:HE2	1:B:-6:ASN:HB2	1.40	1.01
1:B:-14:ALA:O	1:B:-10:CYS:SG	2.29	0.91
1:B:9:ASN:O	1:B:12:ARG:HG2	1.76	0.85
1:A:-12:ARG:NH1	1:A:46:PHE:O	2.10	0.84
1:A:299:ILE:HG23	1:B:306:LEU:HD23	1.63	0.80
1:B:-90:ILE:HG22	1:B:-80:ILE:HD12	1.68	0.76
1:B:-13:VAL:O	1:B:-10:CYS:HB2	1.87	0.75
1:B:-4:VAL:HG22	1:B:4:VAL:HG11	1.69	0.73
1:B:-104:ILE:HG12	1:B:-104:ILE:O	1.88	0.71
1:A:75:GLU:O	1:A:76:ARG:HB2	1.90	0.70
1:B:-101:MET:HE1	1:B:-9:ALA:HA	1.73	0.70
1:B:-90:ILE:HD12	1:B:-68:LEU:HD11	1.72	0.69
1:A:-20:VAL:O	1:A:-16:LEU:HD13	1.93	0.69
1:B:-104:ILE:O	1:B:-104:ILE:CG1	2.40	0.68
1:A:204:GLU:N	1:A:204:GLU:OE1	2.27	0.68
1:B:-105:ASN:OD1	1:B:-104:ILE:N	2.25	0.68
1:A:287:VAL:O	1:A:291:VAL:HG23	1.93	0.68
1:A:295:VAL:HG22	1:B:386:HIS:ND1	2.09	0.67
1:B:-101:MET:SD	1:B:51:TRP:HZ3	2.18	0.66
1:B:9:ASN:HA	1:B:12:ARG:HG2	1.78	0.65
1:A:291:VAL:HG22	1:B:384:GLU:HA	1.78	0.65
1:A:302:ILE:HD11	1:B:306:LEU:HD22	1.79	0.65
1:B:45:THR:HG21	1:B:54:TYR:CE2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-20:VAL:O	1:B:-16:LEU:HD13	1.97	0.64
1:B:9:ASN:C	1:B:12:ARG:HG2	2.22	0.64
1:B:-20:VAL:HG22	1:B:15:GLN:HG3	1.80	0.64
1:B:-104:ILE:HD12	1:B:-10:CYS:HA	1.79	0.63
1:B:-101:MET:CE	1:B:-6:ASN:HB2	2.25	0.61
1:B:278:ARG:HE	1:B:281:ILE:HD11	1.67	0.59
1:A:37:ASN:O	1:A:40:LYS:HG2	2.03	0.58
1:A:72:LEU:HB2	1:A:135:MET:SD	2.43	0.58
1:B:45:THR:HG21	1:B:54:TYR:HE2	1.69	0.57
1:B:-107:GLN:HG2	1:B:51:TRP:HB3	1.85	0.57
1:A:44:THR:O	1:A:48:THR:OG1	2.21	0.57
1:A:302:ILE:HD11	1:B:306:LEU:CD2	2.35	0.57
1:B:9:ASN:CA	1:B:12:ARG:HG2	2.34	0.57
1:B:-90:ILE:CG2	1:B:-80:ILE:HD12	2.35	0.57
1:B:-5:MET:SD	1:B:46:PHE:HE2	2.27	0.57
1:A:-19:TYR:HD1	1:A:-8:LEU:HD23	1.69	0.57
1:A:402:ALA:HB3	1:B:386:HIS:O	2.05	0.56
1:B:-101:MET:HE2	1:B:-6:ASN:CB	2.26	0.56
1:A:348:PHE:HB3	1:B:84:LEU:HD23	1.87	0.56
1:A:401:SER:HB3	1:B:313:LEU:HD22	1.88	0.55
1:B:384:GLU:N	1:B:385:PRO:CD	2.70	0.55
1:B:242:TYR:O	1:B:243:GLN:HG2	2.07	0.54
1:A:298:ALA:O	1:A:302:ILE:HG23	2.08	0.54
1:A:-95:ARG:HH11	1:A:-95:ARG:HG3	1.72	0.54
1:B:61:LEU:HD11	1:B:69:ARG:HH11	1.72	0.54
1:B:-101:MET:SD	1:B:51:TRP:CZ3	3.00	0.53
1:B:-32:VAL:HG22	1:B:-7:ILE:HD13	1.88	0.53
1:B:137:ASP:O	1:B:138:SER:HB2	2.08	0.53
1:A:386:HIS:NE2	1:B:294:ASP:OD2	2.42	0.53
1:B:37:ASN:O	1:B:40:LYS:HG2	2.08	0.53
1:A:65:CYS:HB3	1:A:72:LEU:HD21	1.89	0.53
1:B:113:THR:HG22	1:B:113:THR:O	2.09	0.53
1:B:383:VAL:HG23	1:B:383:VAL:O	2.08	0.53
1:B:237:HIS:N	1:B:237:HIS:CD2	2.77	0.52
1:B:71:ARG:HE	1:B:73:ARG:NH1	2.08	0.52
1:A:218:VAL:HG12	1:A:218:VAL:O	2.09	0.52
1:A:224:CYS:SG	1:A:237:HIS:HE1	2.32	0.52
1:B:76:ARG:O	1:B:76:ARG:HG2	2.10	0.51
1:A:-110:LEU:HD12	1:A:59:LEU:HD12	1.92	0.51
1:B:-19:TYR:HD1	1:B:-8:LEU:HD23	1.74	0.51
1:A:-109:TYR:HD1	1:A:-109:TYR:O	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:LEU:HD22	1:B:134:PHE:HE2	1.76	0.51
1:A:135:MET:HE2	1:B:351:TRP:HH2	1.76	0.51
1:A:-109:TYR:O	1:A:-109:TYR:CD1	2.64	0.51
1:B:-5:MET:O	1:B:-1:MET:HG2	2.11	0.51
1:B:281:ILE:O	1:B:284:VAL:HG22	2.11	0.51
1:B:73:ARG:O	1:B:75:GLU:N	2.44	0.50
1:A:-46:ASP:OD1	1:A:-46:ASP:N	2.42	0.50
1:B:73:ARG:HH11	1:B:73:ARG:HG2	1.75	0.50
1:A:263:LEU:HD22	1:B:346:LEU:HD21	1.94	0.50
1:A:346:LEU:HD21	1:B:263:LEU:HB3	1.94	0.50
1:A:-104:ILE:H	1:A:-104:ILE:HD13	1.77	0.49
1:A:340:LYS:HE3	1:B:-106:GLY:HA3	1.94	0.49
1:A:-68:LEU:HD12	1:A:-65:ALA:HB3	1.95	0.49
1:A:30:ILE:HG13	1:A:31:TRP:N	2.26	0.49
1:B:37:ASN:OD1	1:B:37:ASN:N	2.45	0.49
1:A:37:ASN:OD1	1:A:37:ASN:N	2.45	0.49
1:A:295:VAL:HG22	1:B:386:HIS:CG	2.48	0.49
1:A:7:PHE:O	1:A:11:LEU:HG	2.12	0.49
1:B:-46:ASP:OD1	1:B:-46:ASP:N	2.46	0.49
1:B:-22:LYS:N	1:B:-21:PRO:HD2	2.28	0.49
1:A:361:LEU:HD22	1:B:134:PHE:CE2	2.48	0.48
1:A:-49:ILE:HD12	1:A:-44:ALA:HB2	1.96	0.48
1:A:-22:LYS:N	1:A:-21:PRO:HD2	2.28	0.48
1:A:-4:VAL:HG22	1:A:4:VAL:HG11	1.95	0.48
1:A:-52:ASN:O	1:A:-52:ASN:ND2	2.32	0.48
1:B:219:LEU:HD13	1:B:233:GLN:OE1	2.13	0.48
1:A:-68:LEU:O	1:A:-65:ALA:N	2.47	0.48
1:B:22:ALA:O	1:B:26:LEU:HG	2.14	0.47
1:B:-24:LYS:HD2	1:B:5:ALA:HB1	1.96	0.47
1:A:-93:ARG:HD2	1:A:-89:TYR:CE1	2.50	0.47
1:A:113:THR:O	1:A:113:THR:HG22	2.15	0.47
1:A:295:VAL:HG22	1:B:386:HIS:CE1	2.49	0.47
1:B:287:VAL:O	1:B:291:VAL:HG23	2.14	0.47
1:A:405:PHE:HA	1:B:383:VAL:HG12	1.97	0.47
1:B:71:ARG:HE	1:B:73:ARG:HH12	1.62	0.47
1:B:9:ASN:O	1:B:12:ARG:CG	2.56	0.47
1:A:405:PHE:CB	1:B:383:VAL:HG12	2.46	0.46
1:A:134:PHE:HE1	1:B:354:GLU:HB2	1.80	0.46
1:B:-102:GLU:O	1:B:-99:ARG:N	2.48	0.46
1:A:227:LEU:HD12	1:B:359:THR:HB	1.97	0.46
1:A:45:THR:HG21	1:A:54:TYR:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:LEU:HD23	1:A:365:LYS:HE2	1.97	0.46
1:A:399:THR:O	1:A:399:THR:HG23	2.16	0.45
1:B:9:ASN:HA	1:B:12:ARG:CG	2.44	0.45
1:A:-104:ILE:HG12	1:A:-103:PHE:N	2.31	0.45
1:B:45:THR:HG21	1:B:54:TYR:CD2	2.52	0.45
1:A:359:THR:C	1:A:361:LEU:H	2.24	0.45
1:B:7:PHE:CD1	1:B:7:PHE:N	2.84	0.45
1:A:-57:ILE:HG21	1:A:-53:CYS:SG	2.56	0.45
1:B:280:SER:O	1:B:284:VAL:HG13	2.17	0.45
1:B:-10:CYS:HB3	1:B:51:TRP:HH2	1.81	0.45
1:A:351:TRP:HH2	1:B:135:MET:HE1	1.81	0.45
1:B:-61:LEU:HD21	1:B:-53:CYS:HB2	1.99	0.45
1:A:401:SER:CB	1:B:313:LEU:HD22	2.47	0.45
1:B:278:ARG:O	1:B:281:ILE:HG12	2.16	0.45
1:A:135:MET:CE	1:B:351:TRP:HH2	2.30	0.45
1:B:73:ARG:HH11	1:B:73:ARG:CG	2.31	0.45
1:A:257:ALA:O	1:A:260:VAL:HG22	2.17	0.44
1:A:389:MET:O	1:A:389:MET:HG2	2.17	0.44
1:A:209:CYS:SG	1:A:210:ASN:N	2.91	0.44
1:B:311:ARG:O	1:B:314:VAL:HG12	2.17	0.44
1:B:-92:LEU:C	1:B:-92:LEU:HD12	2.42	0.44
1:A:-27:ARG:NH2	1:A:1:GLU:OE2	2.51	0.44
1:A:393:TRP:HA	1:A:393:TRP:CE3	2.52	0.44
1:B:233:GLN:HA	1:B:237:HIS:HB2	2.00	0.44
1:A:270:LEU:C	1:A:270:LEU:HD13	2.43	0.44
1:A:-110:LEU:HD11	1:B:347:ARG:HG2	2.00	0.44
1:A:333:TRP:CH2	1:A:337:LYS:HD2	2.53	0.44
1:A:58:ALA:HB1	1:B:347:ARG:NH1	2.33	0.43
1:A:373:HIS:ND1	1:A:373:HIS:N	2.66	0.43
1:B:-97:ASP:OD2	1:B:-6:ASN:ND2	2.46	0.43
1:B:281:ILE:HA	1:B:284:VAL:HG22	2.00	0.43
1:A:357:ASN:N	1:A:357:ASN:OD1	2.50	0.43
1:A:-103:PHE:HE2	1:A:-36:VAL:HG13	1.83	0.43
1:B:257:ALA:HA	1:B:260:VAL:HG22	1.99	0.43
1:A:263:LEU:HD23	1:A:263:LEU:O	2.18	0.43
1:A:340:LYS:HE3	1:B:-106:GLY:CA	2.48	0.43
1:A:-29:ILE:HD11	1:A:-7:ILE:HA	1.99	0.43
1:B:137:ASP:OD1	1:B:204:GLU:N	2.52	0.43
1:A:384:GLU:O	1:B:291:VAL:HG22	2.19	0.43
1:A:-15:ASP:O	1:A:-11:ARG:HG3	2.18	0.42
1:B:-9:ALA:O	1:B:-5:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:VAL:O	1:A:380:VAL:CG1	2.67	0.42
1:B:-10:CYS:HB3	1:B:51:TRP:CH2	2.55	0.42
1:B:343:GLU:O	1:B:347:ARG:HG3	2.19	0.42
1:B:242:TYR:O	1:B:242:TYR:CD1	2.72	0.42
1:A:-5:MET:O	1:A:-1:MET:HG2	2.19	0.42
1:B:-5:MET:SD	1:B:46:PHE:CE2	3.09	0.42
1:B:-100:LEU:HD13	1:B:-100:LEU:HA	1.92	0.42
1:B:-104:ILE:O	1:B:-104:ILE:HG13	2.20	0.42
1:A:-11:ARG:O	1:A:-7:ILE:HG13	2.20	0.42
1:A:302:ILE:HG13	1:A:303:MET:N	2.33	0.41
1:A:351:TRP:HH2	1:B:135:MET:CE	2.33	0.41
1:A:359:THR:HG23	1:B:227:LEU:HD12	2.01	0.41
1:A:389:MET:SD	1:A:389:MET:N	2.93	0.41
1:A:257:ALA:HA	1:A:260:VAL:HG22	2.02	0.41
1:A:278:ARG:O	1:A:281:ILE:HG12	2.20	0.41
1:B:16:GLN:O	1:B:17:LYS:HB2	2.20	0.41
1:A:277:VAL:O	1:A:281:ILE:HG23	2.21	0.41
1:A:-29:ILE:HG12	1:A:-4:VAL:HG21	2.03	0.41
1:A:208:TYR:HA	1:A:216:PRO:HA	2.03	0.41
1:B:-43:GLU:O	1:B:-39:ASN:ND2	2.45	0.41
1:B:-11:ARG:O	1:B:-7:ILE:HG13	2.21	0.40
1:A:-101:MET:HE2	1:A:-6:ASN:HD22	1.86	0.40
1:A:129:ILE:O	1:A:129:ILE:HG13	2.20	0.40
1:B:76:ARG:HE	1:B:76:ARG:HB3	1.69	0.40
1:A:135:MET:HE3	1:A:135:MET:HB2	1.98	0.40
1:A:383:VAL:O	1:B:405:PHE:N	2.54	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	433/544 (80%)	403 (93%)	28 (6%)	2 (0%)	24	54
1	B	435/544 (80%)	406 (93%)	28 (6%)	1 (0%)	43	72
All	All	868/1088 (80%)	809 (93%)	56 (6%)	3 (0%)	36	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	218	VAL
1	A	360	ALA
1	A	385	PRO

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	372/468 (80%)	341 (92%)	31 (8%)	10	32
1	B	374/468 (80%)	349 (93%)	25 (7%)	15	43
All	All	746/936 (80%)	690 (92%)	56 (8%)	12	37

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-104	ILE
1	A	-103	PHE
1	A	-95	ARG
1	A	-67	ASN
1	A	-57	ILE
1	A	-52	ASN
1	A	-23	LEU
1	A	-13	VAL
1	A	48	THR
1	A	111	ASP
1	A	114	VAL
1	A	115	VAL
1	A	121	LYS

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Mol	Chain	Res	Type
1	A	134	PHE
1	A	302	ILE
1	A	303	MET
1	A	308	LYS
1	A	337	LYS
1	A	357	ASN
1	A	365	LYS
1	A	367	LEU
1	A	373	HIS
1	A	377	LYS
1	A	379	ILE
1	A	380	VAL
1	A	386	HIS
1	A	389	MET
1	A	393	TRP
1	A	394	ASP
1	A	395	LEU
1	A	400	LYS
1	B	-110	LEU
1	B	-87	ASP
1	B	-47	LYS
1	B	7	PHE
1	B	75	GLU
1	B	76	ARG
1	B	77	GLU
1	B	114	VAL
1	B	127	LYS
1	B	137	ASP
1	B	204	GLU
1	B	227	LEU
1	B	230	ARG
1	B	237	HIS
1	B	241	GLN
1	B	242	TYR
1	B	249	VAL
1	B	278	ARG
1	B	306	LEU
1	B	341	HIS
1	B	351	TRP
1	B	373	HIS
1	B	391	PHE
1	B	392	GLN

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Mol	Chain	Res	Type
1	B	399	THR

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

Mol	Chain	Res	Type
1	A	9	ASN
1	A	344	HIS
1	A	371	GLN
1	B	267	HIS

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 ⓘ

Of 8 ligands modelled in this entry, 8 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 ⓘ

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	439/544 (80%)	1.16	79 (17%) 3 3	54, 115, 177, 267	1 (0%)
1	B	441/544 (81%)	1.19	89 (20%) 3 2	44, 123, 189, 380	0
All	All	880/1088 (80%)	1.17	168 (19%) 3 2	44, 118, 184, 380	1 (0%)

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	406	GLY	9.0
1	A	359	THR	5.8
1	A	-7	ILE	5.3
1	A	-103	PHE	4.8
1	A	357	ASN	4.5
1	B	108	ALA	4.2
1	A	405	PHE	4.2
1	B	-110	LEU	4.1
1	A	314	VAL	4.0
1	A	358	ASN	3.8
1	B	113	THR	3.8
1	B	-25	ALA	3.7
1	B	365	LYS	3.7
1	B	72	LEU	3.6
1	A	349	ALA	3.6
1	A	133	TYR	3.6
1	A	256	LEU	3.6
1	B	-90	ILE	3.6
1	B	234	LEU	3.6
1	A	-10	CYS	3.6
1	A	397	ALA	3.6
1	A	365	LYS	3.5
1	A	95	ALA	3.5
1	B	405	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	-70	PRO	3.4
1	A	257	ALA	3.4
1	A	213	LYS	3.4
1	B	51	TRP	3.3
1	A	140	SER	3.3
1	B	390	LYS	3.3
1	B	-7	ILE	3.3
1	B	386	HIS	3.3
1	A	134	PHE	3.3
1	A	-109	TYR	3.3
1	A	348	PHE	3.2
1	B	-40	PHE	3.2
1	A	246	GLU	3.2
1	A	350	SER	3.2
1	B	61	LEU	3.2
1	B	19	TRP	3.2
1	A	369	TYR	3.1
1	A	-29	ILE	3.1
1	A	244	PHE	3.1
1	B	130	VAL	3.1
1	B	383	VAL	3.1
1	B	95	ALA	3.1
1	B	30	ILE	3.1
1	B	-100	LEU	3.1
1	B	252	GLN	3.0
1	B	-94	LEU	3.0
1	B	219	LEU	3.0
1	B	384	GLU	3.0
1	B	11	LEU	2.9
1	B	239	ASP	2.9
1	B	47	ARG	2.9
1	A	382	PRO	2.9
1	B	358	ASN	2.9
1	B	124	CYS	2.9
1	B	242	TYR	2.9
1	B	212	HIS	2.9
1	B	230	ARG	2.9
1	B	402	ALA	2.8
1	A	372	LEU	2.8
1	B	-28	LEU	2.8
1	B	243	GLN	2.8
1	A	-75	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	398	TRP	2.7
1	A	-16	LEU	2.7
1	A	227	LEU	2.7
1	B	299	ILE	2.7
1	A	-67	ASN	2.7
1	B	359	THR	2.7
1	A	388	GLU	2.7
1	A	291	VAL	2.7
1	B	391	PHE	2.7
1	B	397	ALA	2.7
1	B	303	MET	2.7
1	B	66	GLY	2.7
1	A	375	ALA	2.7
1	B	-49	ILE	2.7
1	B	93	GLY	2.7
1	B	260	VAL	2.7
1	B	401	SER	2.7
1	A	403	GLU	2.6
1	B	-102	GLU	2.6
1	B	128	ASP	2.6
1	B	20	ASP	2.6
1	B	263	LEU	2.6
1	A	379	ILE	2.5
1	B	325	GLN	2.5
1	A	-52	ASN	2.5
1	A	-100	LEU	2.5
1	A	30	ILE	2.5
1	A	384	GLU	2.5
1	B	354	GLU	2.5
1	B	5	ALA	2.5
1	A	355	SER	2.5
1	B	378	MET	2.5
1	A	40	LYS	2.5
1	B	33	ASN	2.5
1	A	353	LEU	2.5
1	A	370	PHE	2.5
1	A	226	THR	2.5
1	B	-84	GLY	2.4
1	A	376	LEU	2.4
1	B	-20	VAL	2.4
1	A	306	LEU	2.4
1	A	207	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	242	TYR	2.4
1	A	113	THR	2.4
1	B	315	ASN	2.4
1	A	212	HIS	2.4
1	B	227	LEU	2.4
1	A	374	ARG	2.3
1	B	349	ALA	2.3
1	A	14	LEU	2.3
1	A	371	GLN	2.3
1	B	-74	LEU	2.3
1	A	35	THR	2.3
1	B	18	ARG	2.3
1	B	-23	LEU	2.2
1	B	138	SER	2.2
1	A	-56	GLY	2.2
1	B	109	ALA	2.2
1	B	256	LEU	2.2
1	B	395	LEU	2.2
1	A	-104	ILE	2.2
1	A	111	ASP	2.2
1	A	351	TRP	2.2
1	B	207	VAL	2.2
1	B	-83	TYR	2.2
1	A	66	GLY	2.2
1	A	-41	LEU	2.2
1	A	234	LEU	2.2
1	A	352	ALA	2.2
1	B	84	LEU	2.2
1	A	-105	ASN	2.2
1	B	-52	ASN	2.2
1	B	94	PRO	2.2
1	B	6	GLY	2.2
1	A	-71	SER	2.2
1	A	240	HIS	2.1
1	A	360	ALA	2.1
1	B	291	VAL	2.1
1	A	399	THR	2.1
1	B	-10	CYS	2.1
1	B	215	GLU	2.1
1	A	237	HIS	2.1
1	B	382	PRO	2.1
1	B	14	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	306	LEU	2.1
1	A	404	ALA	2.1
1	A	54	TYR	2.1
1	B	-78	ILE	2.1
1	A	119	VAL	2.1
1	B	-70	PRO	2.1
1	B	-3	PHE	2.1
1	A	137	ASP	2.1
1	B	375	ALA	2.1
1	A	135	MET	2.0
1	A	238	LYS	2.0
1	A	-111	ASN	2.0
1	A	72	LEU	2.0
1	B	43	ILE	2.0
1	B	381	ASP	2.0
1	A	216	PRO	2.0
1	B	8	THR	2.0
1	B	-85	GLU	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	ZN	A	503	1/1	0.82	0.18	342,342,342,342	0
2	ZN	B	504	1/1	0.86	0.25	247,247,247,247	0
2	ZN	A	502	1/1	0.89	0.10	132,132,132,132	0
2	ZN	B	502	1/1	0.92	0.15	262,262,262,262	0
2	ZN	B	501	1/1	0.95	0.12	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	500	1/1	0.98	0.04	79,79,79,79	0
2	ZN	B	503	1/1	0.99	0.05	70,70,70,70	0
2	ZN	A	501	1/1	0.99	0.08	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.