



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:03 PM UTC

PDB ID : 7Z36 / pdb_00007z36
Title : Crystal structure of the KAP1 tripartite motif in complex with the ZNF93 KRAB domain
Authors : Stoll, G.A.; Modis, Y.
Deposited on : 2022-03-01
Resolution : 2.80 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

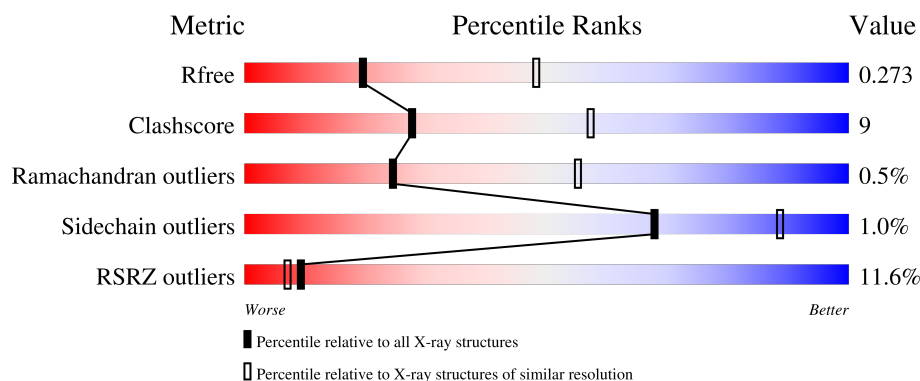
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	482	6% 79% 10% 10%
1	B	482	12% 79% 13% 7%
2	C	73	3% 52% 10% 37%
2	S	73	12% 58% 5% 36%
3	D	70	30% 50% 10% 40%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15589 atoms, of which 7692 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,Isoform 2 of Transcription intermediary factor 1-beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	433	Total	C	H	N	O	S	0	0	0
			6799	2145	3378	626	625	25			
1	B	446	Total	C	H	N	O	S	0	0	0
			6842	2173	3366	632	646	25			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P00720
A	2	GLY	-	expression tag	UNP P00720
A	3	SER	-	expression tag	UNP P00720
A	4	SER	-	expression tag	UNP P00720
A	5	HIS	-	expression tag	UNP P00720
A	6	HIS	-	expression tag	UNP P00720
A	7	HIS	-	expression tag	UNP P00720
A	8	HIS	-	expression tag	UNP P00720
A	9	HIS	-	expression tag	UNP P00720
A	10	HIS	-	expression tag	UNP P00720
A	11	SER	-	expression tag	UNP P00720
A	12	GLN	-	expression tag	UNP P00720
A	13	ASP	-	expression tag	UNP P00720
A	14	PRO	-	expression tag	UNP P00720
A	15	ASN	-	expression tag	UNP P00720
A	16	SER	-	expression tag	UNP P00720
A	17	SER	-	expression tag	UNP P00720
A	18	SER	-	expression tag	UNP P00720
A	19	GLU	-	expression tag	UNP P00720
A	20	ASN	-	expression tag	UNP P00720
A	21	LEU	-	expression tag	UNP P00720
A	22	TYR	-	expression tag	UNP P00720
A	23	PHE	-	expression tag	UNP P00720
A	24	GLN	-	expression tag	UNP P00720

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Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP P00720
A	186	ALA	-	linker	UNP P00720
B	1	MET	-	initiating methionine	UNP P00720
B	2	GLY	-	expression tag	UNP P00720
B	3	SER	-	expression tag	UNP P00720
B	4	SER	-	expression tag	UNP P00720
B	5	HIS	-	expression tag	UNP P00720
B	6	HIS	-	expression tag	UNP P00720
B	7	HIS	-	expression tag	UNP P00720
B	8	HIS	-	expression tag	UNP P00720
B	9	HIS	-	expression tag	UNP P00720
B	10	HIS	-	expression tag	UNP P00720
B	11	SER	-	expression tag	UNP P00720
B	12	GLN	-	expression tag	UNP P00720
B	13	ASP	-	expression tag	UNP P00720
B	14	PRO	-	expression tag	UNP P00720
B	15	ASN	-	expression tag	UNP P00720
B	16	SER	-	expression tag	UNP P00720
B	17	SER	-	expression tag	UNP P00720
B	18	SER	-	expression tag	UNP P00720
B	19	GLU	-	expression tag	UNP P00720
B	20	ASN	-	expression tag	UNP P00720
B	21	LEU	-	expression tag	UNP P00720
B	22	TYR	-	expression tag	UNP P00720
B	23	PHE	-	expression tag	UNP P00720
B	24	GLN	-	expression tag	UNP P00720
B	25	GLY	-	expression tag	UNP P00720
B	186	ALA	-	linker	UNP P00720

- Molecule 2 is a protein called SMARCAD1 CUE1 domain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	46	Total	C	H	N	O	S	0	0	0
			718	221	365	56	74	2			
2	S	47	Total	C	H	N	O	S	0	0	0
			651	208	318	54	70	1			

- Molecule 3 is a protein called Zinc finger protein 93.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	42	Total	C	H	N	O	S	0	0	0
			571	200	265	47	57	2			

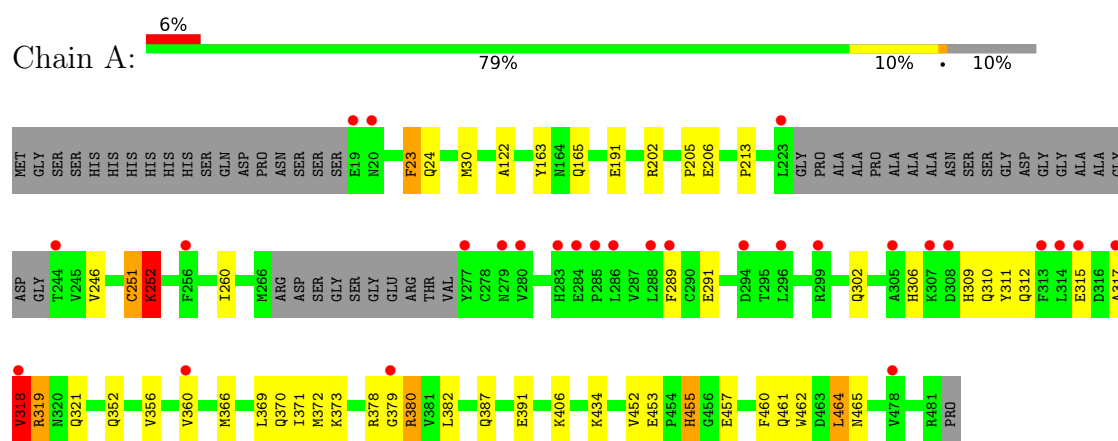
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

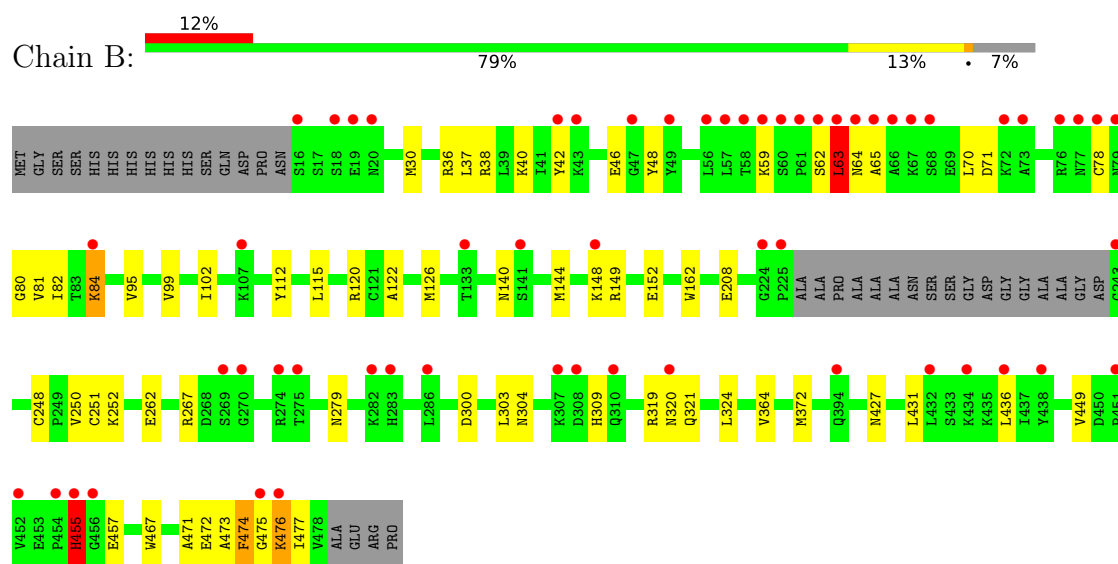
3 Residue-property plots

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: Endolysin,Transcription intermediary factor 1-beta,Isoform 2 of Transcription intermediary factor 1-beta

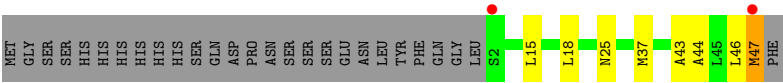


- Molecule 1: Endolysin,Transcription intermediary factor 1-beta,Isoform 2 of Transcription intermediary factor 1-beta

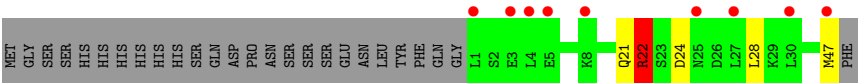


- Molecule 2: SMARCAD1 CUE1 domain

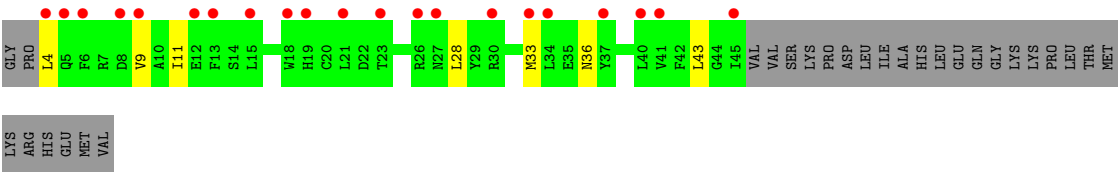




● Molecule 2: SMARCAD1 CUE1 domain



● Molecule 3: Zinc finger protein 93



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	190.28Å 68.58Å 149.11Å 90.00° 114.05° 90.00°	Depositor
Resolution (Å)	63.79 – 2.80 63.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (63.79-2.80) 97.3 (63.79-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.227 , 0.274 0.226 , 0.273	Depositor DCC
R_{free} test set	2761 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15589	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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	0.50	0/3477	0.90	11/4696 (0.2%)
1	B	0.54	4/3535 (0.1%)	0.94	13/4784 (0.3%)
2	C	0.57	0/354	0.85	1/475 (0.2%)
2	S	1.13	2/334 (0.6%)	1.02	4/453 (0.9%)
3	D	0.30	0/311	0.69	0/425
All	All	0.56	6/8011 (0.1%)	0.91	29/10833 (0.3%)

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	1
1	B	0	1
2	S	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	22	ARG	CG-CD	14.00	1.94	1.52
1	B	63	LEU	CG-CD2	10.68	1.87	1.52
2	S	22	ARG	CD-NE	-9.20	1.33	1.46
1	B	455	HIS	CA-CB	-6.88	1.40	1.53
1	B	208	GLU	C-O	6.58	1.27	1.23
1	B	63	LEU	CG-CD1	-6.32	1.31	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	476	LYS	CA-C-N	13.90	146.72	121.70
1	B	476	LYS	C-N-CA	13.90	146.72	121.70
1	A	252	LYS	CG-CD-CE	-10.94	86.13	111.30
1	B	455	HIS	N-CA-CB	-10.84	91.72	111.13
1	B	63	LEU	CD1-CG-CD2	-10.74	87.16	110.80
1	A	464	LEU	CD1-CG-CD2	-10.42	87.88	110.80
1	A	318	VAL	CG1-CB-CG2	-10.28	88.20	110.80
1	A	252	LYS	N-CA-CB	-9.24	98.09	113.15
1	B	84	LYS	CG-CD-CE	-8.95	90.71	111.30
1	B	63	LEU	CB-CG-CD2	-8.94	83.87	110.70
1	B	455	HIS	CB-CG-CD2	-8.85	119.70	131.20
2	S	22	ARG	CB-CG-CD	8.12	129.97	111.30
1	A	23	PHE	N-CA-C	7.09	125.91	110.80
1	B	63	LEU	CB-CG-CD1	6.46	130.09	110.70
2	C	47	MET	CB-CG-SD	-6.02	94.63	112.70
2	S	22	ARG	CA-CB-CG	-5.85	102.40	114.10
1	B	309	HIS	CA-CB-CG	5.60	119.40	113.80
1	B	455	HIS	CB-CA-C	5.58	120.71	109.38
2	S	22	ARG	N-CA-CB	5.56	119.74	110.85
1	A	251	CYS	CA-CB-SG	5.45	126.93	114.40
1	A	251	CYS	CB-CA-C	-5.40	98.59	109.55
1	B	252	LYS	N-CA-C	5.33	119.61	113.38
1	A	252	LYS	CB-CG-CD	5.30	123.50	111.30
2	S	22	ARG	NH1-CZ-NH2	-5.24	112.49	119.30
1	B	63	LEU	CA-CB-CG	-5.23	97.98	116.30
1	A	318	VAL	CA-CB-CG2	-5.18	101.59	110.40
1	A	380	ARG	CD-NE-CZ	-5.09	117.27	124.40
1	A	252	LYS	CB-CA-C	5.08	120.66	111.06
1	B	474	PHE	N-CA-CB	-5.06	102.53	109.91

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	319	ARG	Sidechain
1	B	455	HIS	Sidechain
2	S	22	ARG	Sidechain

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	3421	3378	3374	67	1
1	B	3476	3366	3364	62	1
2	C	353	365	365	13	0
2	S	333	318	320	5	0
3	D	306	265	265	13	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
All	All	7897	7692	7688	140	1

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 (140) 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:63:LEU:CD2	1:B:63:LEU:CG	1.87	1.51
2:S:22:ARG:CD	2:S:22:ARG:CG	1.94	1.44
2:C:43:ALA:O	2:C:47:MET:HE1	1.18	1.28
1:B:63:LEU:CD2	1:B:63:LEU:CD1	2.23	1.15
2:C:43:ALA:O	2:C:47:MET:CE	1.98	1.11
1:B:63:LEU:CD2	1:B:63:LEU:CB	2.28	1.11
1:A:366:MET:HE3	3:D:43:LEU:HD13	1.32	1.05
1:B:63:LEU:CD2	1:B:63:LEU:HD13	1.87	0.99
1:A:206:GLU:OE1	1:A:206:GLU:N	2.00	0.93
2:C:47:MET:N	2:C:47:MET:HE3	1.87	0.89
1:A:457:GLU:N	1:A:457:GLU:OE1	2.06	0.89
1:B:140:ASN:O	1:B:144:MET:HG3	1.77	0.84
1:A:251:CYS:O	1:A:252:LYS:HB2	1.78	0.83
1:A:252:LYS:HD3	2:S:21:GLN:OE1	1.77	0.82
1:A:462:TRP:CH2	1:A:464:LEU:HD12	2.16	0.81
1:A:366:MET:HA	1:A:366:MET:HE2	1.63	0.80
1:B:63:LEU:CD2	1:B:63:LEU:HB3	2.10	0.79
1:A:372:MET:HE2	1:B:372:MET:HG2	1.68	0.76
1:B:300:ASP:O	1:B:304:ASN:OD1	2.05	0.74
1:A:302:GLN:HE21	1:A:302:GLN:HA	1.55	0.70
1:B:63:LEU:HD23	1:B:64:ASN:HD21	1.57	0.69
1:A:455:HIS:ND1	1:A:455:HIS:O	2.25	0.69
1:A:289:PHE:CD2	1:A:291:GLU:HG2	2.29	0.68
2:C:43:ALA:O	2:C:47:MET:SD	2.53	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:LEU:CD2	1:B:84:LYS:HE3	2.26	0.66
1:A:457:GLU:H	1:A:457:GLU:CD	2.04	0.64
3:D:28:LEU:C	3:D:28:LEU:HD23	2.23	0.64
1:A:312:GLN:HA	1:A:312:GLN:OE1	1.96	0.64
1:A:382:LEU:HD22	1:A:460:PHE:HE1	1.62	0.63
2:C:43:ALA:C	2:C:47:MET:HE1	2.14	0.63
1:B:250:VAL:O	1:B:251:CYS:SG	2.57	0.63
1:A:366:MET:CE	1:A:369:LEU:HD12	2.28	0.63
1:A:352:GLN:NE2	1:B:457:GLU:OE1	2.33	0.62
1:B:37:LEU:HD21	1:B:84:LYS:HE3	1.80	0.62
1:B:449:VAL:HG23	1:B:449:VAL:O	1.99	0.62
2:C:47:MET:CE	2:C:47:MET:N	2.60	0.62
1:A:251:CYS:O	1:A:252:LYS:CB	2.48	0.61
1:B:37:LEU:HD21	1:B:84:LYS:HG3	1.82	0.61
1:B:71:ASP:OD2	1:B:78:CYS:N	2.32	0.61
1:B:63:LEU:HD23	1:B:64:ASN:ND2	2.16	0.60
1:A:302:GLN:HA	1:A:302:GLN:NE2	2.16	0.60
1:B:372:MET:HE2	3:D:36:ASN:HD21	1.66	0.60
1:A:315:GLU:O	1:A:318:VAL:HG12	2.00	0.60
1:A:406:LYS:HD3	2:C:18:LEU:HD23	1.83	0.60
1:A:291:GLU:CD	1:A:312:GLN:HG2	2.26	0.59
1:A:462:TRP:HH2	1:A:464:LEU:HD12	1.66	0.59
1:A:289:PHE:CE2	1:A:291:GLU:HG2	2.38	0.59
1:A:318:VAL:CG1	1:A:319:ARG:N	2.66	0.58
1:B:455:HIS:C	1:B:455:HIS:HD1	2.11	0.58
1:B:372:MET:HE1	3:D:9:VAL:O	2.03	0.58
1:A:318:VAL:CG1	1:A:319:ARG:H	2.17	0.58
2:S:22:ARG:NH2	2:S:47:MET:HA	2.19	0.57
2:S:24:ASP:O	2:S:28:LEU:HD12	2.04	0.57
1:A:318:VAL:HG13	1:A:319:ARG:N	2.20	0.56
1:B:471:ALA:O	1:B:472:GLU:HB2	2.05	0.56
1:B:248:CYS:SG	1:B:250:VAL:O	2.64	0.56
2:C:47:MET:CE	2:C:47:MET:H	2.18	0.56
1:B:46:GLU:HB3	1:B:48:TYR:HE2	1.69	0.56
1:B:63:LEU:HB3	1:B:63:LEU:HD23	1.87	0.55
1:B:262:GLU:OE1	1:B:267:ARG:HD2	2.06	0.55
1:B:38:ARG:HG3	1:B:42:TYR:CE1	2.42	0.55
1:B:455:HIS:C	1:B:455:HIS:ND1	2.65	0.55
2:C:15:LEU:HG	2:C:37:MET:HE1	1.89	0.54
1:A:370:GLN:HE22	1:A:373:LYS:HD3	1.73	0.54
1:A:163:TYR:C	1:A:163:TYR:CD1	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4:LEU:C	3:D:4:LEU:HD23	2.34	0.52
2:C:46:LEU:HB3	2:C:47:MET:CE	2.40	0.52
1:A:370:GLN:NE2	1:A:373:LYS:HD3	2.25	0.52
2:C:44:ALA:HA	2:C:47:MET:SD	2.50	0.52
1:B:112:TYR:CE1	1:B:120:ARG:HD3	2.45	0.52
2:C:46:LEU:HB3	2:C:47:MET:HE3	1.93	0.51
3:D:28:LEU:HD23	3:D:28:LEU:O	2.09	0.51
1:A:213:PRO:HA	1:B:436:LEU:HD22	1.92	0.51
1:A:302:GLN:HE21	1:A:302:GLN:CA	2.23	0.51
1:A:378:ARG:HG2	1:B:474:PHE:HB3	1.91	0.51
1:A:372:MET:HE2	1:B:372:MET:CG	2.39	0.51
1:A:302:GLN:OE1	1:A:311:TYR:HD1	1.94	0.50
1:A:455:HIS:O	1:A:455:HIS:CG	2.63	0.50
3:D:11:ILE:O	3:D:33:MET:HE2	2.11	0.50
1:A:206:GLU:H	1:A:206:GLU:CD	2.00	0.50
1:B:37:LEU:CD2	1:B:84:LYS:CE	2.89	0.50
1:A:321:GLN:HA	1:A:321:GLN:OE1	2.11	0.50
1:B:70:LEU:HD11	1:B:82:ILE:CG2	2.43	0.49
1:A:378:ARG:NH2	1:B:475:GLY:O	2.44	0.49
1:B:126:MET:HE3	1:B:162:TRP:CZ3	2.48	0.49
2:S:22:ARG:HH22	2:S:47:MET:HA	1.76	0.49
1:A:246:VAL:HG11	1:A:260:ILE:HD11	1.94	0.48
1:A:302:GLN:OE1	1:A:311:TYR:CD1	2.66	0.48
1:A:461:GLN:N	1:B:476:LYS:O	2.40	0.48
1:B:471:ALA:O	1:B:473:ALA:N	2.41	0.48
1:A:191:GLU:OE2	1:A:202:ARG:NH2	2.45	0.48
1:B:372:MET:HE2	3:D:36:ASN:ND2	2.29	0.48
1:B:449:VAL:O	1:B:449:VAL:CG2	2.61	0.47
2:C:47:MET:N	2:C:47:MET:SD	2.87	0.47
1:A:321:GLN:OE1	1:A:321:GLN:CA	2.62	0.47
1:A:371:ILE:HD11	1:B:467:TRP:CG	2.50	0.46
1:A:23:PHE:O	1:A:23:PHE:CG	2.69	0.46
1:B:63:LEU:CD1	1:B:63:LEU:HD21	2.35	0.46
1:A:380:ARG:HH11	1:A:380:ARG:HD3	1.52	0.46
1:B:70:LEU:HD11	1:B:82:ILE:HG21	1.99	0.45
1:B:63:LEU:HD13	1:B:63:LEU:HD21	1.89	0.45
1:A:387:GLN:OE1	1:A:391:GLU:HG3	2.17	0.45
1:A:379:GLY:HA2	1:A:382:LEU:HD12	1.98	0.45
1:A:460:PHE:CD1	1:B:364:VAL:HG22	2.52	0.45
1:B:30:MET:HE1	1:B:122:ALA:HA	1.98	0.44
1:A:317:ALA:O	1:A:321:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4:LEU:C	3:D:4:LEU:CD2	2.91	0.44
1:A:23:PHE:O	1:A:24:GLN:HB2	2.18	0.43
1:A:205:PRO:N	1:A:206:GLU:OE1	2.51	0.43
1:A:371:ILE:HD11	1:B:467:TRP:CB	2.48	0.43
1:B:48:TYR:HD1	1:B:59:LYS:HA	1.83	0.43
1:B:455:HIS:ND1	1:B:455:HIS:O	2.43	0.43
3:D:11:ILE:O	3:D:33:MET:CE	2.66	0.43
1:B:320:ASN:O	1:B:324:LEU:HG	2.18	0.43
1:B:36:ARG:HD2	1:B:38:ARG:HD3	2.01	0.43
1:A:366:MET:HE2	1:A:369:LEU:HD12	1.97	0.43
1:A:465:ASN:HD22	1:A:465:ASN:HA	1.67	0.42
1:A:434:LYS:HE3	1:B:321:GLN:OE1	2.18	0.42
3:D:28:LEU:C	3:D:28:LEU:CD2	2.92	0.42
1:A:30:MET:HE1	1:A:122:ALA:HA	2.01	0.42
1:B:95:VAL:O	1:B:99:VAL:HG23	2.19	0.42
1:B:40:LYS:HG2	1:B:81:VAL:HG22	2.02	0.42
1:A:246:VAL:CG1	1:A:260:ILE:HD11	2.50	0.42
1:A:302:GLN:NE2	1:A:306:HIS:HB2	2.35	0.41
1:A:369:LEU:HB3	3:D:4:LEU:HD11	2.01	0.41
1:B:144:MET:HE1	1:B:152:GLU:HB3	2.02	0.41
1:B:427:ASN:O	1:B:431:LEU:HD13	2.20	0.41
1:A:372:MET:HG2	1:B:372:MET:HG2	2.02	0.41
1:B:115:LEU:O	1:B:120:ARG:NH2	2.54	0.41
1:B:62:SER:HB3	1:B:65:ALA:HB3	2.01	0.41
1:A:291:GLU:HB3	1:A:310:GLN:OE1	2.21	0.41
1:A:318:VAL:HG12	1:A:319:ARG:H	1.85	0.41
1:A:356:VAL:O	1:A:360:VAL:HG23	2.21	0.41
1:B:102:ILE:HG21	1:B:112:TYR:CD2	2.55	0.41
1:B:46:GLU:CB	1:B:48:TYR:HE2	2.33	0.41
1:B:148:LYS:O	1:B:149:ARG:C	2.63	0.41
1:B:144:MET:CE	1:B:152:GLU:HB3	2.51	0.40
1:A:452:VAL:O	1:A:452:VAL:HG13	2.22	0.40
1:A:453:GLU:OE1	1:A:453:GLU:N	2.50	0.40
1:A:366:MET:HE3	3:D:43:LEU:CD1	2.24	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:TYR:HH	1:B:303:LEU:O[1_454]	1.58	0.02

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	427/482 (89%)	415 (97%)	10 (2%)	2 (0%)	24	55
1	B	442/482 (92%)	426 (96%)	13 (3%)	3 (1%)	18	47
2	C	44/73 (60%)	44 (100%)	0	0	100	100
2	S	45/73 (62%)	45 (100%)	0	0	100	100
3	D	40/70 (57%)	40 (100%)	0	0	100	100
All	All	998/1180 (85%)	970 (97%)	23 (2%)	5 (0%)	24	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	455	HIS
1	B	63	LEU
1	B	80	GLY
1	B	477	ILE
1	A	309	HIS

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	362/415 (87%)	359 (99%)	3 (1%)	73	90
1	B	364/415 (88%)	360 (99%)	4 (1%)	65	87
2	C	40/65 (62%)	39 (98%)	1 (2%)	42	76
2	S	33/65 (51%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	28/64 (44%)	28 (100%)	0	100	100
All	All	827/1024 (81%)	819 (99%)	8 (1%)	68	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	252	LYS
1	A	318	VAL
1	B	63	LEU
1	B	279	ASN
1	B	319	ARG
1	B	455	HIS
2	C	25	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	GLN
1	A	306	HIS
1	A	309	HIS
1	A	370	GLN
1	A	442	HIS
1	A	455	HIS
1	A	465	ASN
1	B	64	ASN
1	B	304	ASN
1	B	370	GLN
1	B	387	GLN
1	B	461	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	433/482 (89%)	0.34	28 (6%) 25 18	28, 61, 130, 170	0
1	B	446/482 (92%)	0.66	58 (13%) 7 6	29, 74, 126, 160	0
2	C	46/73 (63%)	0.07	2 (4%) 40 31	37, 54, 97, 120	0
2	S	47/73 (64%)	1.23	9 (19%) 3 2	64, 88, 149, 158	0
3	D	42/70 (60%)	2.15	21 (50%) 0 0	84, 112, 131, 134	0
All	All	1014/1180 (85%)	0.58	118 (11%) 9 7	28, 70, 130, 170	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	TYR	7.1
1	B	308	ASP	6.6
1	B	58	THR	6.3
1	A	308	ASP	6.3
1	B	225	PRO	5.8
1	A	315	GLU	5.8
1	B	67	LYS	5.3
1	A	279	ASN	5.2
1	B	243	GLY	5.1
2	S	3	GLU	4.8
3	D	12	GLU	4.8
1	B	60	SER	4.8
2	S	1	LEU	4.7
1	A	294	ASP	4.6
1	A	20	ASN	4.6
2	S	4	LEU	4.6
1	B	270	GLY	4.5
2	C	47	MET	4.5
1	A	19	GLU	4.4
3	D	23	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	65	ALA	4.3
3	D	27	ASN	4.1
3	D	18	TRP	4.1
3	D	33	MET	4.1
3	D	45	ILE	4.1
1	A	288	LEU	4.0
1	B	283	HIS	4.0
1	B	57	LEU	3.9
1	B	66	ALA	3.8
2	S	47	MET	3.8
1	B	77	ASN	3.8
3	D	37	TYR	3.7
1	A	478	VAL	3.6
1	B	49	TYR	3.6
1	B	63	LEU	3.6
1	A	283	HIS	3.5
1	B	282	LYS	3.5
1	A	313	PHE	3.5
1	A	296	LEU	3.5
2	S	8	LYS	3.5
1	B	456	GLY	3.5
2	S	5	GLU	3.4
1	B	438	TYR	3.3
1	A	305	ALA	3.3
1	B	56	LEU	3.2
3	D	5	GLN	3.1
1	B	455	HIS	3.1
1	A	223	LEU	3.1
1	B	148	LYS	3.1
1	B	320	ASN	3.0
1	B	432	LEU	3.0
1	A	314	LEU	3.0
3	D	34	LEU	3.0
1	A	317	ALA	3.0
1	B	434	LYS	2.9
2	S	25	ASN	2.9
1	B	269	SER	2.8
1	B	43	LYS	2.8
1	B	76	ARG	2.8
1	B	307	LYS	2.8
3	D	19	HIS	2.7
1	B	18	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	475	GLY	2.7
1	B	310	GLN	2.7
1	B	436	LEU	2.7
3	D	15	LEU	2.7
3	D	30	ARG	2.7
1	B	16	SER	2.7
2	S	30	LEU	2.6
1	B	141	SER	2.6
2	C	2	SER	2.6
1	B	451	PRO	2.6
1	B	476	LYS	2.6
3	D	26	ARG	2.5
1	B	68	SER	2.5
1	B	78	CYS	2.5
1	A	307	LYS	2.5
2	S	27	LEU	2.4
1	B	64	ASN	2.4
1	A	286	LEU	2.4
1	A	256	PHE	2.4
1	B	62	SER	2.4
1	B	42	TYR	2.4
1	B	47	GLY	2.4
1	B	274	ARG	2.4
1	B	107	LYS	2.3
3	D	6	PHE	2.3
1	A	284	GLU	2.3
3	D	40	LEU	2.3
1	B	224	GLY	2.3
1	A	289	PHE	2.3
3	D	13	PHE	2.3
3	D	21	LEU	2.3
1	B	20	ASN	2.3
1	B	133	THR	2.3
1	A	285	PRO	2.3
1	B	286	LEU	2.2
3	D	4	LEU	2.2
3	D	41	VAL	2.2
1	A	280	VAL	2.2
1	B	275	THR	2.2
1	B	59	LYS	2.2
1	A	360	VAL	2.2
1	A	318	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	454	PRO	2.2
1	B	73	ALA	2.2
1	B	72	LYS	2.1
1	A	244	THR	2.1
1	B	79	ASN	2.1
3	D	9	VAL	2.1
3	D	8	ASP	2.1
1	B	19	GLU	2.0
1	B	394	GLN	2.0
1	B	452	VAL	2.0
1	B	61	PRO	2.0
1	A	299	ARG	2.0
1	A	379	GLY	2.0
1	B	84	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
4	ZN	A	503	1/1	0.92	0.09	138,138,138,138	0
4	ZN	A	504	1/1	0.95	0.07	132,132,132,132	0
4	ZN	A	502	1/1	0.98	0.05	77,77,77,77	0
4	ZN	B	502	1/1	0.98	0.03	39,39,39,39	0
4	ZN	B	503	1/1	0.98	0.04	91,91,91,91	0
4	ZN	B	504	1/1	0.98	0.06	74,74,74,74	0
4	ZN	B	501	1/1	0.99	0.07	39,39,39,39	0
4	ZN	A	501	1/1	0.99	0.04	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.