



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:32 AM UTC

PDB ID : 5D68 / pdb_00005d68
Title : Crystal structure of KRIT1 ARD-FERM
Authors : Zhang, R.; Li, X.; Boggon, T.J.
Deposited on : 2015-08-11
Resolution : 2.91 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

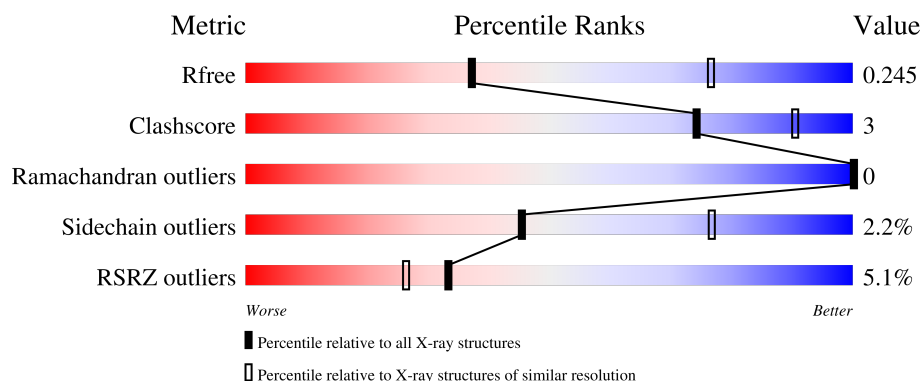
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	486	4% 81% 8% 11%
1	B	486	5% 78% 12% 10%
1	C	486	4% 78% 10% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10652 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 Krev interaction trapped protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3524	2254	613	638	19			
1	B	437	Total	C	N	O	S	0	0	0
			3555	2269	619	648	19			
1	C	431	Total	C	N	O	S	0	0	0
			3507	2243	610	636	18			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	GLY	-	expression tag	UNP O00522
A	252	SER	-	expression tag	UNP O00522
A	253	ASP	-	expression tag	UNP O00522
A	254	ILE	-	expression tag	UNP O00522
A	255	LEU	-	expression tag	UNP O00522
A	256	GLN	-	expression tag	UNP O00522
A	257	GLY	-	expression tag	UNP O00522
A	258	THR	-	expression tag	UNP O00522
B	251	GLY	-	expression tag	UNP O00522
B	252	SER	-	expression tag	UNP O00522
B	253	ASP	-	expression tag	UNP O00522
B	254	ILE	-	expression tag	UNP O00522
B	255	LEU	-	expression tag	UNP O00522
B	256	GLN	-	expression tag	UNP O00522
B	257	GLY	-	expression tag	UNP O00522
B	258	THR	-	expression tag	UNP O00522
C	251	GLY	-	expression tag	UNP O00522
C	252	SER	-	expression tag	UNP O00522
C	253	ASP	-	expression tag	UNP O00522
C	254	ILE	-	expression tag	UNP O00522
C	255	LEU	-	expression tag	UNP O00522
C	256	GLN	-	expression tag	UNP O00522
C	257	GLY	-	expression tag	UNP O00522

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Chain	Residue	Modelled	Actual	Comment	Reference
C	258	THR	-	expression tag	UNP O00522

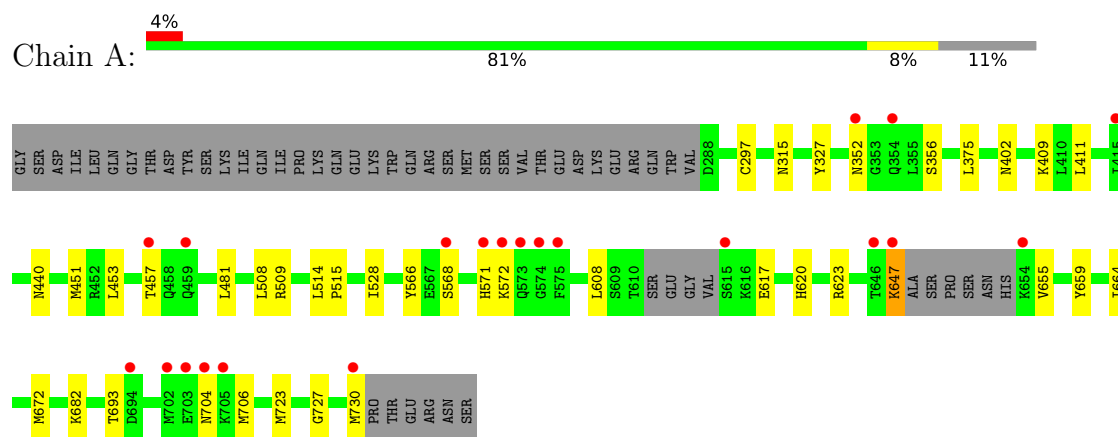
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	26	Total	O	0	0
			26	26		
2	C	21	Total	O	0	0
			21	21		

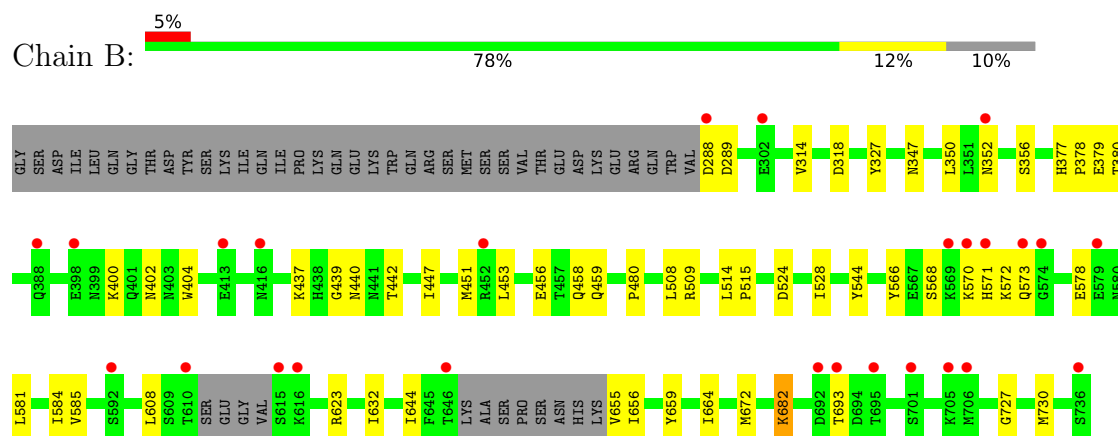
3 Residue-property plots

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.

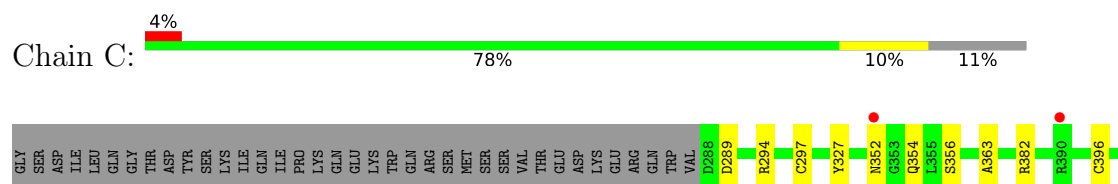
- Molecule 1: Krev interaction trapped protein 1

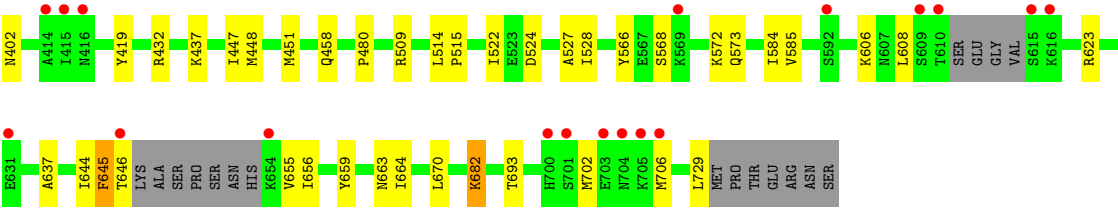


- Molecule 1: Krev interaction trapped protein 1



- Molecule 1: Krev interaction trapped protein 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.73Å 80.24Å 213.15Å 90.00° 91.69° 90.00°	Depositor
Resolution (Å)	49.37 – 2.91 49.37 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.37-2.91) 90.3 (49.37-2.91)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.91Å)	Xtriage
Refinement program	PHENIX dev_1760	Depositor
R, R_{free}	0.207 , 0.246 0.209 , 0.245	Depositor DCC
R_{free} test set	2378 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 28.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10652	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 4.33% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.36	0/3604	0.72	1/4872 (0.0%)
1	B	0.36	0/3636	0.71	3/4917 (0.1%)
1	C	0.36	0/3587	0.73	4/4851 (0.1%)
All	All	0.36	0/10827	0.72	8/14640 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	645	PHE	N-CA-C	6.61	122.26	112.94
1	B	402	ASN	CB-CA-C	-5.84	109.82	116.54
1	A	402	ASN	CB-CA-C	-5.68	110.01	116.54
1	C	402	ASN	CB-CA-C	-5.39	110.34	116.54
1	B	524	ASP	CA-C-N	5.30	124.75	119.24
1	B	524	ASP	C-N-CA	5.30	124.75	119.24
1	C	524	ASP	CA-C-N	5.28	125.34	119.32
1	C	524	ASP	C-N-CA	5.28	125.34	119.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3524	0	3540	15	0
1	B	3555	0	3558	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3507	0	3518	25	0
2	A	19	0	0	0	0
2	B	26	0	0	0	0
2	C	21	0	0	1	0
All	All	10652	0	10616	66	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 3.

All (66) 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:451:MET:HB3	1:B:453:LEU:HD13	1.77	0.67
1:A:451:MET:HE2	1:A:508:LEU:HD22	1.85	0.59
1:C:645:PHE:N	1:C:646:THR:HA	2.17	0.59
1:C:297:CYS:HB3	1:C:327:TYR:HB3	1.85	0.58
1:B:727:GLY:HA2	1:B:730:MET:HG3	1.86	0.58
1:C:432:ARG:HD2	1:C:451:MET:HE3	1.88	0.56
1:C:448:MET:HE3	1:C:458:GLN:HG3	1.90	0.53
1:A:297:CYS:HB3	1:A:327:TYR:HB3	1.90	0.53
1:C:352:ASN:ND2	1:C:354:GLN:OE1	2.43	0.51
1:B:566:TYR:CE2	1:B:571:HIS:HB2	2.45	0.51
1:C:352:ASN:HB3	1:C:356:SER:H	1.76	0.51
1:B:439:GLY:O	1:B:442:THR:OG1	2.28	0.51
1:C:572:LYS:HG2	1:C:573:GLN:HG3	1.93	0.51
1:A:352:ASN:HB3	1:A:356:SER:H	1.75	0.50
1:A:659:TYR:CE2	1:A:672:MET:HG3	2.46	0.50
1:C:528:ILE:HD12	1:C:623:ARG:HG3	1.94	0.50
1:B:447:ILE:HD12	1:B:480:PRO:HG2	1.93	0.49
1:C:568:SER:O	1:C:572:LYS:HB2	2.14	0.48
1:B:572:LYS:HG2	1:B:573:GLN:HG3	1.96	0.47
1:B:437:LYS:HE3	1:C:702:MET:O	2.14	0.47
1:C:419:TYR:CD1	1:C:437:LYS:HA	2.50	0.47
1:A:568:SER:O	1:A:572:LYS:HB2	2.16	0.46
1:C:584:ILE:HG13	1:C:585:VAL:HG13	1.97	0.46
1:C:447:ILE:HD12	1:C:480:PRO:HG2	1.97	0.46
1:A:566:TYR:CE2	1:A:571:HIS:HB2	2.50	0.46
1:B:288:ASP:OD1	1:B:289:ASP:N	2.49	0.46
1:A:727:GLY:O	1:A:730:MET:HG3	2.16	0.46
1:B:451:MET:HE2	1:B:508:LEU:HD22	1.98	0.45
1:B:352:ASN:HB3	1:B:356:SER:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:644:ILE:HG12	1:C:656:ILE:HB	1.98	0.45
1:C:682:LYS:HE3	1:C:682:LYS:HB2	1.81	0.45
1:A:617:GLU:HB2	1:A:620:HIS:ND1	2.32	0.45
1:B:544:TYR:HB3	1:B:632:ILE:HD13	1.99	0.45
1:C:382:ARG:HG2	2:C:809:HOH:O	2.17	0.44
1:B:568:SER:O	1:B:572:LYS:HB2	2.16	0.44
1:A:528:ILE:HD12	1:A:623:ARG:HG3	2.00	0.44
1:B:528:ILE:HD12	1:B:623:ARG:HG3	1.98	0.44
1:C:659:TYR:HB2	1:C:670:LEU:HB2	1.99	0.43
1:B:347:ASN:HB3	1:B:350:LEU:HB2	1.99	0.43
1:B:377:HIS:HA	1:B:378:PRO:HD3	1.87	0.43
1:A:440:ASN:HA	1:A:481:LEU:HD12	2.00	0.43
1:C:566:TYR:CD1	1:C:606:LYS:HG2	2.53	0.43
1:C:363:ALA:HB1	1:C:396:CYS:HB2	2.00	0.43
1:C:637:ALA:HA	1:C:663:ASN:HB3	2.00	0.43
1:A:375:LEU:HD11	1:A:411:LEU:HD23	2.00	0.42
1:C:514:LEU:HA	1:C:515:PRO:HD3	1.90	0.42
1:B:400:LYS:HA	1:B:404:TRP:CG	2.54	0.42
1:A:514:LEU:HD12	1:A:515:PRO:HD2	2.02	0.42
1:C:289:ASP:OD1	1:C:294:ARG:NH1	2.52	0.42
1:A:704:ASN:HD22	1:A:706:MET:HE2	1.84	0.42
1:B:514:LEU:HA	1:B:515:PRO:HD3	1.94	0.42
1:C:706:MET:HE2	1:C:706:MET:HB3	1.93	0.42
1:C:514:LEU:HD12	1:C:515:PRO:HD2	2.02	0.42
1:B:456:GLU:O	1:B:459:GLN:HG2	2.20	0.42
1:B:659:TYR:CE2	1:B:672:MET:HG3	2.54	0.42
1:B:379:GLU:HB3	1:B:440:ASN:ND2	2.35	0.42
1:B:682:LYS:HB2	1:B:682:LYS:HE3	1.78	0.41
1:B:644:ILE:HG12	1:B:656:ILE:HB	2.02	0.41
1:A:453:LEU:HB3	1:A:457:THR:HG23	2.02	0.41
1:B:318:ASP:OD2	1:B:327:TYR:OH	2.34	0.41
1:B:377:HIS:HB3	1:B:380:THR:OG1	2.20	0.41
1:B:581:LEU:O	1:B:585:VAL:HG22	2.20	0.41
1:B:570:LYS:HE3	1:B:571:HIS:CE1	2.55	0.41
1:B:584:ILE:HG13	1:B:585:VAL:HG13	2.02	0.41
1:A:647:LYS:NZ	1:A:647:LYS:HB2	2.35	0.40
1:C:522:ILE:HD11	1:C:527:ALA:CB	2.51	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	427/486 (88%)	416 (97%)	11 (3%)	0	100	100
1	B	431/486 (89%)	418 (97%)	13 (3%)	0	100	100
1	C	425/486 (87%)	412 (97%)	13 (3%)	0	100	100
All	All	1283/1458 (88%)	1246 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	390/439 (89%)	380 (97%)	10 (3%)	40	73
1	B	394/439 (90%)	385 (98%)	9 (2%)	44	76
1	C	388/439 (88%)	381 (98%)	7 (2%)	51	80
All	All	1172/1317 (89%)	1146 (98%)	26 (2%)	45	77

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
1	A	409	LYS
1	A	509	ARG
1	A	608	LEU
1	A	647	LYS

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Mol	Chain	Res	Type
1	A	655	VAL
1	A	664	ILE
1	A	682	LYS
1	A	693	THR
1	A	723	MET
1	B	314	VAL
1	B	458	GLN
1	B	509	ARG
1	B	578	GLU
1	B	608	LEU
1	B	655	VAL
1	B	664	ILE
1	B	682	LYS
1	B	693	THR
1	C	509	ARG
1	C	608	LEU
1	C	655	VAL
1	C	664	ILE
1	C	682	LYS
1	C	693	THR
1	C	729	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	388	GLN
1	A	627	GLN
1	A	700	HIS
1	B	372	GLN
1	B	376	ASN
1	B	619	HIS
1	B	622	GLN
1	B	627	GLN
1	B	714	GLN
1	C	367	HIS
1	C	372	GLN
1	C	496	ASN
1	C	627	GLN
1	C	689	GLN
1	C	700	HIS
1	C	711	HIS
1	C	726	ASN

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Mol	Chain	Res	Type
1	C	728	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	433/486 (89%)	0.19	21 (4%) 35 28	21, 40, 83, 128	0
1	B	437/486 (89%)	0.30	26 (5%) 28 22	23, 42, 87, 125	0
1	C	431/486 (88%)	0.24	20 (4%) 37 29	23, 41, 83, 134	0
All	All	1301/1458 (89%)	0.24	67 (5%) 33 26	21, 41, 84, 134	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	615	SER	4.8
1	B	646	THR	4.4
1	C	610	THR	3.8
1	C	646	THR	3.7
1	A	730	MET	3.6
1	C	654	LYS	3.4
1	B	288	ASP	3.4
1	A	572	LYS	3.3
1	A	702	MET	3.3
1	C	700	HIS	3.3
1	C	705	LYS	3.2
1	C	704	ASN	3.2
1	B	616	LYS	3.2
1	C	569	LYS	3.2
1	A	703	GLU	3.2
1	A	615	SER	3.0
1	A	705	LYS	3.0
1	A	646	THR	2.9
1	B	693	THR	2.9
1	C	703	GLU	2.8
1	C	415	ILE	2.8
1	A	573	GLN	2.7
1	C	592	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	352	ASN	2.7
1	A	647	LYS	2.7
1	A	574	GLY	2.7
1	B	610	THR	2.6
1	B	302	GLU	2.6
1	C	615	SER	2.6
1	C	631	GLU	2.6
1	B	692	ASP	2.5
1	A	568	SER	2.5
1	B	706	MET	2.5
1	C	706	MET	2.5
1	B	388	GLN	2.5
1	B	573	GLN	2.5
1	A	457	THR	2.4
1	C	416	ASN	2.4
1	B	592	SER	2.4
1	B	571	HIS	2.4
1	B	579	GLU	2.4
1	B	736	SER	2.4
1	C	609	SER	2.3
1	B	413	GLU	2.3
1	A	654	LYS	2.3
1	B	695	THR	2.3
1	B	352	ASN	2.3
1	A	571	HIS	2.2
1	B	574	GLY	2.2
1	B	569	LYS	2.2
1	C	616	LYS	2.2
1	C	414	ALA	2.2
1	A	459	GLN	2.2
1	B	701	SER	2.2
1	B	452	ARG	2.2
1	C	701	SER	2.2
1	B	398	GLU	2.2
1	C	390	ARG	2.1
1	B	705	LYS	2.1
1	B	416	ASN	2.1
1	C	352	ASN	2.1
1	A	415	ILE	2.1
1	A	575	PHE	2.1
1	A	694	ASP	2.1
1	A	354	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	570	LYS	2.0
1	A	704	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.