



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:31 AM UTC

PDB ID : 6LOH / pdb_00006loh
Title : Crystal structure of the catalytic domain of human ubiquitin ligase AREL1
Authors : Chen, Z.Z.; Li, Z.H.; Shang, G.H.
Deposited on : 2020-01-05
Resolution : 3.21 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

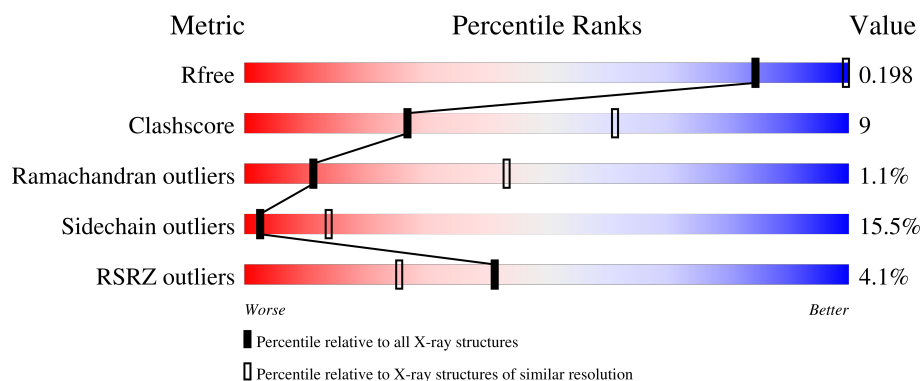
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	389	3% 71% 21% . .
1	B	389	3% 66% 27% . .
1	C	389	5% 62% 27% 7% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8990 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 Apoptosis-resistant E3 ubiquitin protein ligase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			3003	1921	517	551	14			
1	B	375	Total	C	N	O	S	0	0	0
			3002	1927	514	546	15			
1	C	372	Total	C	N	O	S	0	0	0
			2979	1907	509	548	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	423	HIS	-	expression tag	UNP O15033
A	424	HIS	-	expression tag	UNP O15033
A	425	HIS	-	expression tag	UNP O15033
A	426	HIS	-	expression tag	UNP O15033
A	427	HIS	-	expression tag	UNP O15033
A	428	HIS	-	expression tag	UNP O15033
A	429	GLU	-	expression tag	UNP O15033
A	430	ASN	-	expression tag	UNP O15033
A	431	LEU	-	expression tag	UNP O15033
A	432	TYR	-	expression tag	UNP O15033
A	433	PHE	-	expression tag	UNP O15033
A	434	GLN	-	expression tag	UNP O15033
B	423	HIS	-	expression tag	UNP O15033
B	424	HIS	-	expression tag	UNP O15033
B	425	HIS	-	expression tag	UNP O15033
B	426	HIS	-	expression tag	UNP O15033
B	427	HIS	-	expression tag	UNP O15033
B	428	HIS	-	expression tag	UNP O15033
B	429	GLU	-	expression tag	UNP O15033
B	430	ASN	-	expression tag	UNP O15033
B	431	LEU	-	expression tag	UNP O15033
B	432	TYR	-	expression tag	UNP O15033
B	433	PHE	-	expression tag	UNP O15033

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Chain	Residue	Modelled	Actual	Comment	Reference
B	434	GLN	-	expression tag	UNP O15033
C	423	HIS	-	expression tag	UNP O15033
C	424	HIS	-	expression tag	UNP O15033
C	425	HIS	-	expression tag	UNP O15033
C	426	HIS	-	expression tag	UNP O15033
C	427	HIS	-	expression tag	UNP O15033
C	428	HIS	-	expression tag	UNP O15033
C	429	GLU	-	expression tag	UNP O15033
C	430	ASN	-	expression tag	UNP O15033
C	431	LEU	-	expression tag	UNP O15033
C	432	TYR	-	expression tag	UNP O15033
C	433	PHE	-	expression tag	UNP O15033
C	434	GLN	-	expression tag	UNP O15033

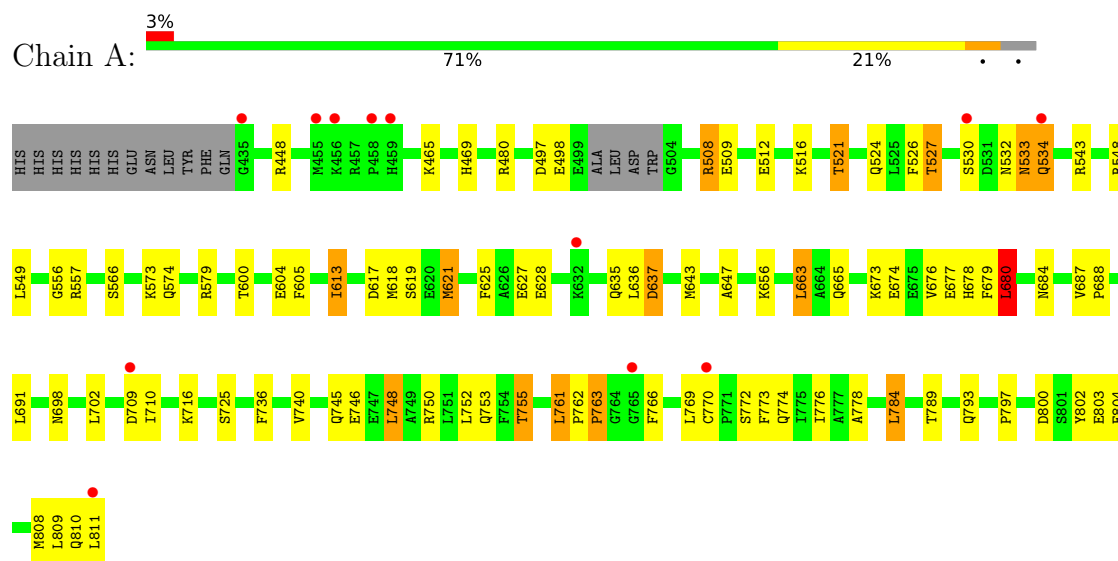
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total O 3 3	0	0
2	B	3	Total O 3 3	0	0

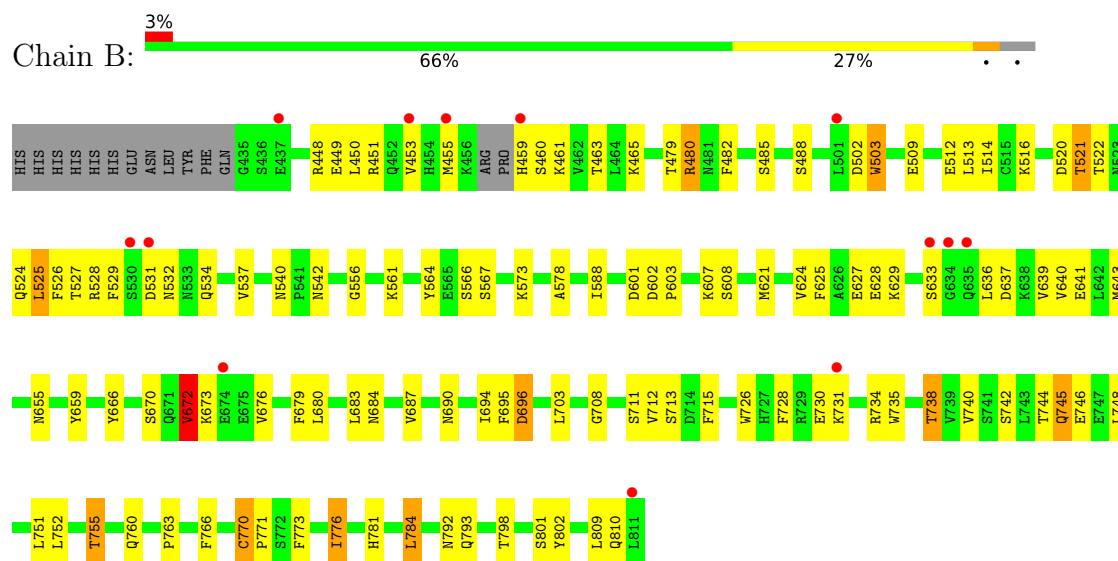
3 Residue-property plots

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.

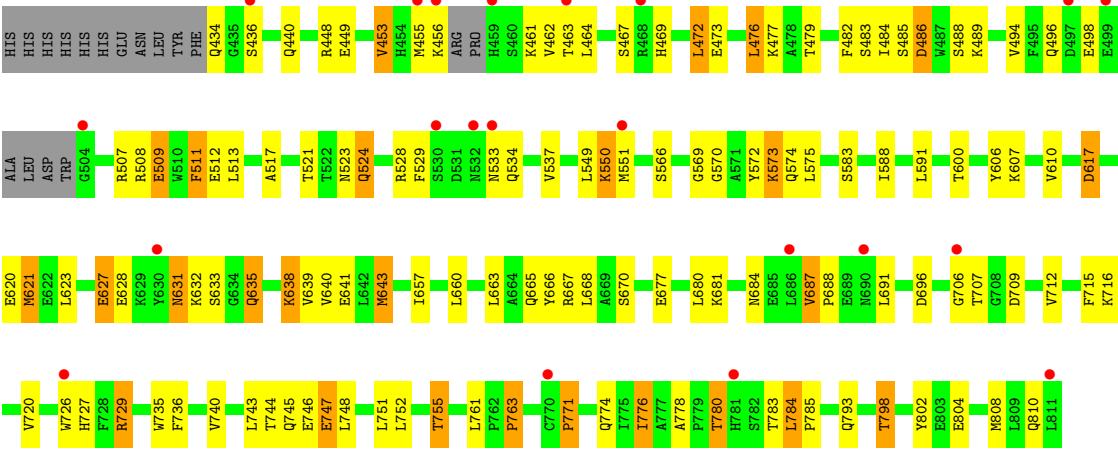
- Molecule 1: Apoptosis-resistant E3 ubiquitin protein ligase 1



- Molecule 1: Apoptosis-resistant E3 ubiquitin protein ligase 1



- Molecule 1: Apoptosis-resistant E3 ubiquitin protein ligase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	150.23Å 150.23Å 342.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.22 – 3.21 49.22 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.22-3.21) 99.8 (49.22-3.21)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.211 , 0.225 (Not available) , 0.198	Depositor DCC
R_{free} test set	1881 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	71.9	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 74.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8990	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 2.56% 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	1.04	0/3075	1.52	8/4158 (0.2%)
1	B	1.05	0/3075	1.49	6/4160 (0.1%)
1	C	1.09	2/3048 (0.1%)	1.55	18/4119 (0.4%)
All	All	1.06	2/9198 (0.0%)	1.52	32/12437 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	511	PHE	C-O	6.71	1.31	1.24
1	C	771	PRO	C-O	-5.90	1.16	1.24

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	525	LEU	N-CA-C	-7.47	102.28	111.40
1	C	607	LYS	CA-C-O	-7.26	112.79	120.63
1	C	727	HIS	N-CA-C	-7.22	103.34	111.07
1	B	637	ASP	N-CA-C	-7.14	102.91	111.69
1	A	680	LEU	N-CA-CB	6.12	119.65	110.53
1	C	696	ASP	CA-C-N	6.01	129.15	120.79
1	C	696	ASP	C-N-CA	6.01	129.15	120.79
1	C	606	TYR	CA-C-N	6.00	128.59	120.38
1	C	606	TYR	C-N-CA	6.00	128.59	120.38
1	C	569	GLY	CA-C-N	5.99	126.74	120.03
1	C	569	GLY	C-N-CA	5.99	126.74	120.03
1	B	672	VAL	CA-C-N	5.87	128.07	120.44
1	B	672	VAL	C-N-CA	5.87	128.07	120.44
1	C	453	VAL	N-CA-C	-5.86	104.80	110.42
1	B	608	SER	CA-C-O	-5.81	114.69	120.80
1	C	715	PHE	CA-C-O	-5.55	114.96	120.90
1	C	469	HIS	N-CA-C	-5.55	107.06	113.88
1	C	620	GLU	CA-C-N	5.52	127.99	120.54
1	C	620	GLU	C-N-CA	5.52	127.99	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	570	GLY	CA-C-N	5.46	127.59	120.28
1	C	570	GLY	C-N-CA	5.46	127.59	120.28
1	C	706	GLY	CA-C-O	-5.30	118.63	122.45
1	A	637	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	789	THR	CA-C-N	5.17	127.73	120.28
1	A	789	THR	C-N-CA	5.17	127.73	120.28
1	A	673	LYS	CA-C-N	5.13	127.11	120.44
1	A	673	LYS	C-N-CA	5.13	127.11	120.44
1	A	755	THR	CA-C-O	-5.08	113.50	119.24
1	B	738	THR	CB-CA-C	5.06	118.80	110.95
1	C	476	LEU	CA-C-N	5.06	127.06	120.28
1	C	476	LEU	C-N-CA	5.06	127.06	120.28
1	A	647	ALA	N-CA-C	-5.00	106.02	111.82

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	3003	0	2935	39	0
1	B	3002	0	2924	61	0
1	C	2979	0	2900	63	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
All	All	8990	0	8759	163	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (163) 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:770:CYS:CB	1:B:771:PRO:HD3	1.71	1.16
1:B:776:ILE:HD11	1:B:793:GLN:OE1	1.56	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:ILE:CD1	1:B:793:GLN:OE1	2.13	0.97
1:C:804:GLU:O	1:C:808:MET:HG2	1.72	0.89
1:B:770:CYS:CB	1:B:771:PRO:CD	2.52	0.84
1:A:676:VAL:O	1:A:680:LEU:CD2	2.26	0.83
1:C:785:PRO:HD3	1:C:808:MET:HE3	1.64	0.78
1:A:676:VAL:O	1:A:680:LEU:HD23	1.88	0.74
1:A:533:ASN:O	1:A:533:ASN:ND2	2.21	0.74
1:B:520:ASP:O	1:B:522:THR:N	2.26	0.68
1:A:508:ARG:HD3	1:A:574:GLN:HE22	1.63	0.63
1:B:776:ILE:HD11	1:B:793:GLN:CD	2.23	0.63
1:C:524:GLN:HE21	1:C:524:GLN:HA	1.64	0.62
1:C:784:LEU:HA	1:C:808:MET:CE	2.29	0.62
1:C:784:LEU:HD12	1:C:808:MET:HE1	1.82	0.62
1:B:460:SER:C	1:B:461:LYS:HD3	2.26	0.61
1:B:751:LEU:O	1:B:755:THR:HG23	2.00	0.61
1:A:684:ASN:HA	1:A:687:VAL:O	2.01	0.61
1:A:534:GLN:HG2	1:A:534:GLN:O	1.99	0.61
1:B:684:ASN:HA	1:B:687:VAL:O	2.01	0.60
1:A:804:GLU:O	1:A:808:MET:HG2	2.02	0.60
1:A:512:GLU:O	1:A:516:LYS:HG3	2.01	0.59
1:B:532:ASN:C	1:B:534:GLN:H	2.11	0.59
1:C:550:LYS:HE3	1:C:550:LYS:H	1.67	0.59
1:C:534:GLN:O	1:C:534:GLN:HG2	2.02	0.59
1:C:810:GLN:HE21	1:C:810:GLN:HA	1.66	0.58
1:C:631:ASN:C	1:C:633:SER:H	2.11	0.58
1:C:684:ASN:HA	1:C:687:VAL:O	2.04	0.58
1:B:728:PHE:CD1	1:B:798:THR:HG22	2.39	0.58
1:B:603:PRO:O	1:B:607:LYS:HG3	2.04	0.58
1:C:810:GLN:HA	1:C:810:GLN:NE2	2.19	0.58
1:B:802:TYR:CD2	1:B:802:TYR:C	2.81	0.58
1:C:533:ASN:OD1	1:C:763:PRO:HG2	2.04	0.58
1:B:695:PHE:CZ	1:B:703:LEU:HD22	2.39	0.57
1:A:521:THR:OG1	1:A:526:PHE:O	2.20	0.56
1:B:459:HIS:O	1:B:461:LYS:NZ	2.38	0.56
1:C:778:ALA:O	1:C:798:THR:HG22	2.05	0.56
1:A:534:GLN:HG3	1:A:762:PRO:CG	2.36	0.56
1:A:676:VAL:O	1:A:680:LEU:HD22	2.06	0.55
1:C:588:ILE:HA	1:C:680:LEU:HD11	1.88	0.55
1:B:672:VAL:HG13	1:B:676:VAL:HG23	1.87	0.55
1:C:483:SER:OG	1:C:484:ILE:N	2.40	0.54
1:C:550:LYS:H	1:C:550:LYS:CE	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:ILE:O	1:A:656:LYS:HD2	2.07	0.54
1:C:785:PRO:HD3	1:C:808:MET:CE	2.37	0.54
1:C:583:SER:OG	1:C:668:LEU:HB3	2.08	0.54
1:C:712:VAL:HG13	1:C:740:VAL:HG12	1.89	0.54
1:B:449:GLU:O	1:B:453:VAL:HG23	2.08	0.53
1:C:631:ASN:HD21	1:C:635:GLN:HG2	1.72	0.53
1:C:524:GLN:HA	1:C:524:GLN:NE2	2.23	0.53
1:C:802:TYR:CD2	1:C:802:TYR:C	2.87	0.53
1:C:524:GLN:HE21	1:C:524:GLN:CA	2.21	0.53
1:A:680:LEU:HD23	1:A:680:LEU:H	1.72	0.53
1:B:485:SER:O	1:B:488:SER:OG	2.25	0.53
1:C:627:GLU:OE2	1:C:667:ARG:NH1	2.42	0.52
1:C:521:THR:O	1:C:521:THR:HG22	2.10	0.52
1:C:529:PHE:N	1:C:529:PHE:CD2	2.77	0.52
1:C:707:THR:HB	1:C:746:GLU:HA	1.91	0.51
1:B:728:PHE:HD1	1:B:798:THR:HG22	1.75	0.51
1:A:549:LEU:HB3	1:A:678:HIS:CD2	2.46	0.51
1:A:618:MET:HA	1:A:621:MET:HG3	1.92	0.51
1:C:566:SER:HA	1:C:573:LYS:HA	1.93	0.51
1:B:521:THR:HG22	1:B:524:GLN:NE2	2.25	0.50
1:A:698:ASN:HB3	1:A:753:GLN:CD	2.36	0.50
1:B:527:THR:HG22	1:B:540:ASN:HA	1.94	0.50
1:B:566:SER:HA	1:B:573:LYS:HA	1.94	0.50
1:B:776:ILE:CG1	1:B:793:GLN:OE1	2.60	0.50
1:C:726:TRP:HA	1:C:729:ARG:HG3	1.94	0.50
1:A:761:LEU:HD21	1:A:766:PHE:CD2	2.46	0.49
1:C:747:GLU:OE2	1:C:810:GLN:NE2	2.45	0.49
1:B:520:ASP:C	1:B:522:THR:H	2.18	0.49
1:C:610:VAL:HG13	1:C:660:LEU:HD22	1.95	0.49
1:B:521:THR:HG22	1:B:524:GLN:HE22	1.78	0.49
1:B:655:ASN:OD1	1:B:655:ASN:C	2.56	0.48
1:B:521:THR:CG2	1:B:524:GLN:HE22	2.26	0.48
1:A:566:SER:HA	1:A:573:LYS:HA	1.95	0.48
1:C:740:VAL:HA	1:C:743:LEU:HD12	1.95	0.48
1:C:621:MET:HE2	1:C:621:MET:CA	2.43	0.48
1:C:688:PRO:HD2	1:C:691:LEU:HD12	1.95	0.48
1:C:785:PRO:CD	1:C:808:MET:HE3	2.39	0.48
1:B:532:ASN:C	1:B:534:GLN:N	2.71	0.48
1:B:712:VAL:HG13	1:B:740:VAL:HG12	1.96	0.47
1:A:534:GLN:HG3	1:A:762:PRO:HG3	1.96	0.47
1:A:521:THR:O	1:A:521:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:736:PHE:O	1:C:740:VAL:HG23	2.14	0.47
1:B:771:PRO:HD2	1:B:792:ASN:ND2	2.29	0.47
1:C:631:ASN:ND2	1:C:635:GLN:HG2	2.30	0.47
1:B:521:THR:O	1:B:522:THR:C	2.57	0.47
1:C:621:MET:HE2	1:C:621:MET:N	2.30	0.47
1:A:710:ILE:H	1:A:745:GLN:HE22	1.62	0.46
1:C:479:THR:HA	1:C:482:PHE:CD1	2.50	0.46
1:B:479:THR:HA	1:B:482:PHE:CD1	2.50	0.46
1:B:773:PHE:C	1:B:773:PHE:CD1	2.94	0.46
1:C:709:ASP:OD2	1:C:709:ASP:N	2.47	0.46
1:B:588:ILE:HA	1:B:680:LEU:HD21	1.97	0.46
1:A:625:PHE:CG	1:A:643:MET:HE2	2.51	0.46
1:A:556:GLY:HA3	1:A:679:PHE:O	2.16	0.45
1:B:556:GLY:HA3	1:B:679:PHE:O	2.16	0.45
1:A:605:PHE:HZ	1:A:663:LEU:HD21	1.81	0.45
1:B:509:GLU:O	1:B:513:LEU:HG	2.15	0.45
1:C:641:GLU:HB3	1:C:643:MET:O	2.17	0.45
1:B:521:THR:HA	1:B:526:PHE:O	2.16	0.45
1:C:709:ASP:HA	1:C:745:GLN:NE2	2.31	0.45
1:A:530:SER:C	1:A:532:ASN:H	2.24	0.45
1:A:784:LEU:HD12	1:A:784:LEU:HA	1.88	0.45
1:B:715:PHE:CD1	1:B:766:PHE:CE1	3.05	0.45
1:C:617:ASP:OD1	1:C:617:ASP:C	2.59	0.45
1:A:736:PHE:CD1	1:A:809:LEU:HD21	2.52	0.44
1:B:527:THR:CG2	1:B:540:ASN:HA	2.48	0.44
1:C:666:TYR:HA	1:C:670:SER:HB2	1.98	0.44
1:C:486:ASP:OD1	1:C:486:ASP:N	2.51	0.44
1:B:625:PHE:CZ	1:B:659:TYR:HB2	2.53	0.44
1:C:751:LEU:O	1:C:755:THR:HG23	2.17	0.44
1:A:762:PRO:HD3	1:A:769:LEU:HD21	2.00	0.44
1:C:780:THR:HG21	1:C:783:THR:CG2	2.48	0.44
1:C:449:GLU:OE1	1:C:449:GLU:HA	2.17	0.44
1:B:641:GLU:HB3	1:B:643:MET:O	2.18	0.43
1:C:631:ASN:C	1:C:633:SER:N	2.76	0.43
1:C:660:LEU:O	1:C:663:LEU:HB3	2.18	0.43
1:A:774:GLN:CG	1:A:793:GLN:HG3	2.48	0.43
1:C:638:LYS:HD2	1:C:640:VAL:HG22	1.99	0.43
1:A:534:GLN:O	1:A:579:ARG:NH1	2.50	0.43
1:C:509:GLU:O	1:C:513:LEU:HG	2.18	0.43
1:C:517:ALA:O	1:C:523:ASN:ND2	2.52	0.43
1:B:695:PHE:CE2	1:B:703:LEU:HD22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:MET:HA	1:C:455:MET:HE2	2.00	0.43
1:A:617:ASP:OD1	1:A:619:SER:OG	2.33	0.43
1:B:529:PHE:HB3	1:B:602:ASP:CG	2.44	0.43
1:B:666:TYR:HA	1:B:670:SER:HB2	2.01	0.42
1:C:440:GLN:HA	1:C:440:GLN:OE1	2.18	0.42
1:A:521:THR:OG1	1:A:527:THR:HA	2.20	0.42
1:A:778:ALA:HB3	1:A:797:PRO:HA	2.01	0.42
1:B:514:ILE:HD12	1:B:514:ILE:HA	1.91	0.42
1:B:726:TRP:CD1	1:B:726:TRP:C	2.98	0.42
1:C:751:LEU:O	1:C:755:THR:CG2	2.66	0.42
1:C:472:LEU:HG	1:C:551:MET:HE1	2.01	0.42
1:B:784:LEU:HD12	1:B:784:LEU:HA	1.83	0.42
1:B:696:ASP:OD1	1:B:696:ASP:C	2.63	0.42
1:C:776:ILE:HD11	1:C:793:GLN:CG	2.50	0.42
1:A:774:GLN:HG2	1:A:793:GLN:HG3	2.02	0.42
1:B:450:LEU:HD12	1:B:450:LEU:HA	1.92	0.42
1:A:688:PRO:HD2	1:A:691:LEU:HD12	2.01	0.42
1:A:773:PHE:CD1	1:A:773:PHE:C	2.97	0.42
1:B:448:ARG:HG2	1:B:451:ARG:HH21	1.85	0.42
1:B:708:GLY:O	1:B:745:GLN:NE2	2.54	0.41
1:B:625:PHE:CE2	1:B:659:TYR:HA	2.55	0.41
1:B:735:TRP:CZ3	1:B:801:SER:C	2.98	0.41
1:B:564:TYR:O	1:B:567:SER:OG	2.30	0.41
1:B:728:PHE:HB2	1:B:798:THR:HG22	2.03	0.41
1:C:720:VAL:O	1:C:774:GLN:HA	2.21	0.41
1:A:762:PRO:CD	1:A:769:LEU:CD2	2.98	0.41
1:B:480:ARG:HH11	1:B:480:ARG:CB	2.34	0.41
1:B:503:TRP:HA	1:B:503:TRP:CE3	2.55	0.41
1:B:525:LEU:HD12	1:B:525:LEU:HA	1.81	0.41
1:B:730:GLU:OE1	1:B:734:ARG:NH2	2.54	0.41
1:C:496:GLN:OE1	1:C:496:GLN:N	2.53	0.41
1:C:511:PHE:CD2	1:C:574:GLN:HG3	2.56	0.40
1:C:784:LEU:HA	1:C:808:MET:HE3	2.03	0.40
1:A:802:TYR:CD2	1:A:802:TYR:C	3.00	0.40
1:B:578:ALA:O	1:B:760:GLN:NE2	2.52	0.40
1:C:735:TRP:O	1:C:736:PHE:C	2.64	0.40
1:A:710:ILE:HB	1:A:748:LEU:HD12	2.03	0.40
1:B:529:PHE:HD2	1:B:601:ASP:O	2.04	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	369/389 (95%)	336 (91%)	29 (8%)	4 (1%)	11	43
1	B	371/389 (95%)	338 (91%)	28 (8%)	5 (1%)	9	40
1	C	366/389 (94%)	337 (92%)	26 (7%)	3 (1%)	16	50
All	All	1106/1167 (95%)	1011 (91%)	83 (8%)	12 (1%)	11	43

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	498	GLU
1	B	521	THR
1	B	633	SER
1	B	636	LEU
1	A	636	LEU
1	C	632	LYS
1	A	763	PRO
1	C	436	SER
1	C	771	PRO
1	B	770	CYS
1	B	763	PRO
1	A	770	CYS

5.3.2 Protein sidechains [i](#)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	326/346 (94%)	279 (86%)	47 (14%)	3 16
1	B	321/346 (93%)	279 (87%)	42 (13%)	4 19
1	C	321/346 (93%)	260 (81%)	61 (19%)	1 9
All	All	968/1038 (93%)	818 (84%)	150 (16%)	2 14

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	448	ARG
1	A	465	LYS
1	A	469	HIS
1	A	480	ARG
1	A	497	ASP
1	A	508	ARG
1	A	509	GLU
1	A	521	THR
1	A	524	GLN
1	A	527	THR
1	A	533	ASN
1	A	534	GLN
1	A	543	ARG
1	A	548	ARG
1	A	557	ARG
1	A	600	THR
1	A	604	GLU
1	A	613	ILE
1	A	621	MET
1	A	627	GLU
1	A	628	GLU
1	A	635	GLN
1	A	637	ASP
1	A	663	LEU
1	A	665	GLN
1	A	674	GLU
1	A	677	GLU
1	A	680	LEU
1	A	702	LEU
1	A	709	ASP
1	A	716	LYS

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Mol	Chain	Res	Type
1	A	725	SER
1	A	740	VAL
1	A	746	GLU
1	A	748	LEU
1	A	750	ARG
1	A	752	LEU
1	A	755	THR
1	A	761	LEU
1	A	763	PRO
1	A	772	SER
1	A	776	ILE
1	A	784	LEU
1	A	800	ASP
1	A	803	GLU
1	A	810	GLN
1	A	811	LEU
1	B	455	MET
1	B	463	THR
1	B	465	LYS
1	B	480	ARG
1	B	502	ASP
1	B	503	TRP
1	B	512	GLU
1	B	516	LYS
1	B	528	ARG
1	B	531	ASP
1	B	537	VAL
1	B	542	ASN
1	B	561	LYS
1	B	621	MET
1	B	624	VAL
1	B	627	GLU
1	B	628	GLU
1	B	629	LYS
1	B	639	VAL
1	B	640	VAL
1	B	672	VAL
1	B	673	LYS
1	B	683	LEU
1	B	690	ASN
1	B	694	ILE
1	B	696	ASP

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Mol	Chain	Res	Type
1	B	711	SER
1	B	713	SER
1	B	731	LYS
1	B	738	THR
1	B	742	SER
1	B	744	THR
1	B	745	GLN
1	B	746	GLU
1	B	748	LEU
1	B	752	LEU
1	B	755	THR
1	B	776	ILE
1	B	781	HIS
1	B	784	LEU
1	B	809	LEU
1	B	810	GLN
1	C	434	GLN
1	C	448	ARG
1	C	453	VAL
1	C	456	LYS
1	C	461	LYS
1	C	462	VAL
1	C	463	THR
1	C	464	LEU
1	C	467	SER
1	C	472	LEU
1	C	473	GLU
1	C	476	LEU
1	C	477	LYS
1	C	485	SER
1	C	486	ASP
1	C	488	SER
1	C	489	LYS
1	C	494	VAL
1	C	498	GLU
1	C	507	ARG
1	C	508	ARG
1	C	509	GLU
1	C	512	GLU
1	C	524	GLN
1	C	528	ARG
1	C	537	VAL

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Mol	Chain	Res	Type
1	C	549	LEU
1	C	550	LYS
1	C	572	TYR
1	C	573	LYS
1	C	575	LEU
1	C	591	LEU
1	C	600	THR
1	C	617	ASP
1	C	621	MET
1	C	623	LEU
1	C	627	GLU
1	C	628	GLU
1	C	631	ASN
1	C	635	GLN
1	C	638	LYS
1	C	639	VAL
1	C	643	MET
1	C	657	ILE
1	C	665	GLN
1	C	677	GLU
1	C	681	LYS
1	C	687	VAL
1	C	716	LYS
1	C	729	ARG
1	C	744	THR
1	C	747	GLU
1	C	748	LEU
1	C	752	LEU
1	C	755	THR
1	C	761	LEU
1	C	763	PRO
1	C	776	ILE
1	C	780	THR
1	C	784	LEU
1	C	798	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	GLN
1	A	452	GLN
1	A	481	ASN

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Mol	Chain	Res	Type
1	A	524	GLN
1	A	574	GLN
1	A	635	GLN
1	A	678	HIS
1	A	684	ASN
1	A	698	ASN
1	A	727	HIS
1	A	745	GLN
1	A	792	ASN
1	B	459	HIS
1	B	524	GLN
1	B	631	ASN
1	B	648	GLN
1	B	774	GLN
1	B	781	HIS
1	B	792	ASN
1	B	806	HIS
1	C	452	GLN
1	C	524	GLN
1	C	542	ASN
1	C	546	HIS
1	C	635	GLN
1	C	678	HIS
1	C	727	HIS
1	C	792	ASN
1	C	793	GLN
1	C	806	HIS
1	C	810	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	373/389 (95%)	0.09	12 (3%)	50	31	41, 64, 112, 141	0
1	B	375/389 (96%)	0.15	13 (3%)	47	29	44, 69, 113, 146	0
1	C	372/389 (95%)	0.32	21 (5%)	30	19	40, 74, 128, 174	0
All	All	1120/1167 (95%)	0.19	46 (4%)	41	25	40, 69, 121, 174	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	811	LEU	6.2
1	C	811	LEU	5.8
1	C	726	TRP	3.9
1	A	435	GLY	3.6
1	C	459	HIS	3.5
1	A	534	GLN	3.3
1	C	497	ASP	3.3
1	C	532	ASN	3.2
1	B	459	HIS	3.0
1	C	504	GLY	3.0
1	B	531	ASP	2.9
1	B	674	GLU	2.9
1	C	630	TYR	2.9
1	C	436	SER	2.8
1	C	530	SER	2.8
1	C	781	HIS	2.8
1	B	633	SER	2.8
1	A	458	PRO	2.7
1	B	634	GLY	2.6
1	C	690	ASN	2.6
1	C	463	THR	2.6
1	A	709	ASP	2.6
1	A	456	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	706	GLY	2.5
1	B	453	VAL	2.5
1	A	455	MET	2.5
1	B	455	MET	2.5
1	A	811	LEU	2.4
1	C	770	CYS	2.3
1	A	632	LYS	2.3
1	C	455	MET	2.3
1	B	731	LYS	2.2
1	C	499	GLU	2.2
1	B	501	LEU	2.2
1	C	456	LYS	2.2
1	B	437	GLU	2.2
1	A	765	GLY	2.2
1	A	770	CYS	2.2
1	A	459	HIS	2.1
1	B	530	SER	2.1
1	C	468	ARG	2.1
1	A	530	SER	2.1
1	C	551	MET	2.1
1	C	686	LEU	2.1
1	B	635	GLN	2.1
1	C	533	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.