



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:46 AM UTC

PDB ID : 3U7D / pdb_00003u7d
Title : Crystal structure of the KRIT1/CCM1 FERM domain in complex with the heart of glass (HEG1) cytoplasmic tail
Authors : Gingras, A.R.; Liu, J.J.; Ginsberg, M.H.; Assembly, Dynamics and Evolution of Cell-Cell and Cell-Matrix Adhesions (CELLMAT)
Deposited on : 2011-10-13
Resolution : 2.49 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

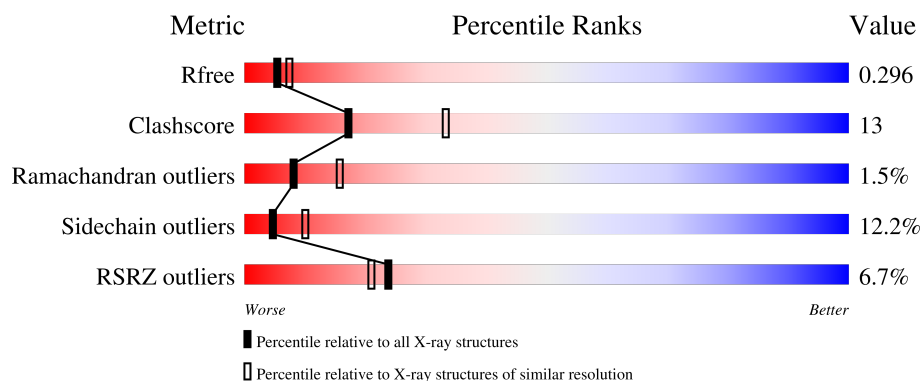
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

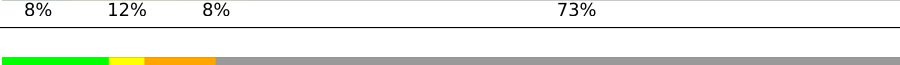
The reported resolution of this entry is 2.49 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	322	
1	C	322	
2	B	26	
2	D	26	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5136 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	305	Total	C	N	O	S	0	0	0
			2493	1608	427	444	14			
1	C	305	Total	C	N	O	S	0	1	0
			2499	1612	427	446	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	415	GLY	-	expression tag	UNP O00522
A	416	ALA	-	expression tag	UNP O00522
C	415	GLY	-	expression tag	UNP O00522
C	416	ALA	-	expression tag	UNP O00522

- Molecule 2 is a protein called Protein HEG homolog 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	0	0	0
			70	43	16	11			
2	D	6	Total	C	N	O	0	0	0
			64	40	15	9			

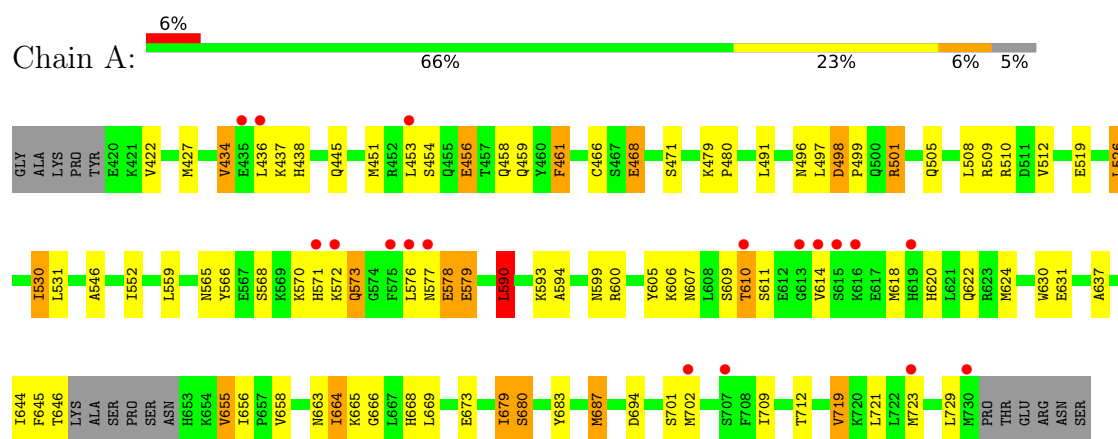
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		
3	C	2	Total	O	0	0
			2	2		

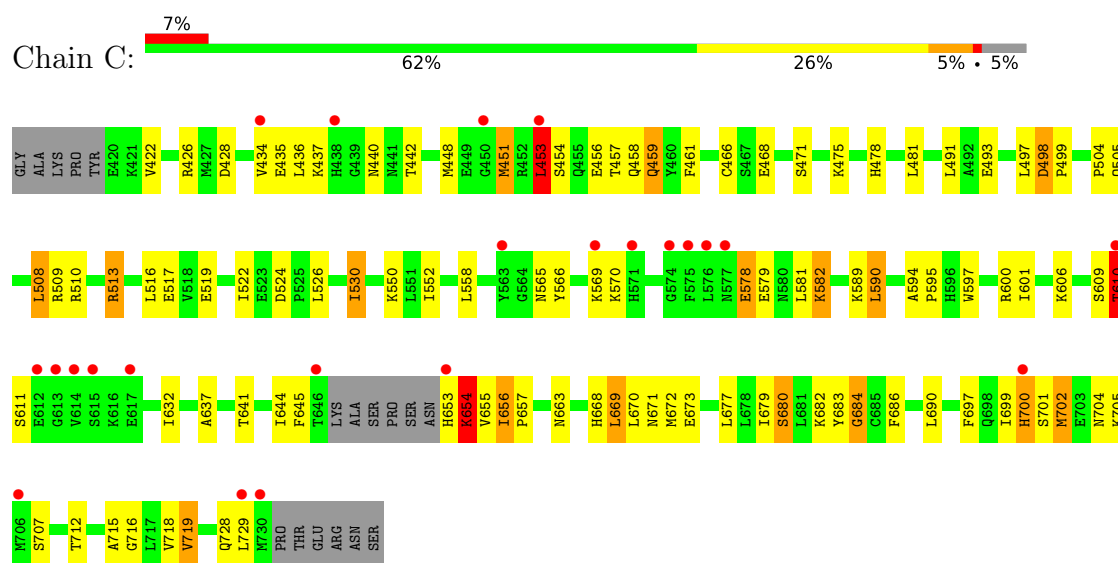
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Krev interaction trapped protein 1



• Molecule 1: Krev interaction trapped protein 1



• Molecule 2: Protein HEG homolog 1



SER	ARG	HIS	SER	CYS	ILE	PHE	PRO	GLY	GLN	TYR	ASN	PRO	SER	PHE	ILE	SER	ASP	GLU	S1376	R1376	R1377	R1378	F1381
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● Molecule 2: Protein HEG homolog 1



SER	ARG	HIS	SER	CYS	ILE	PHE	PRO	GLY	GLN	TYR	ASN	PRO	SER	PHE	ILE	SER	ASP	GLU	SER	R1376	R1377	R1378	F1381
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.05Å 76.82Å 79.18Å 90.00° 113.62° 90.00°	Depositor
Resolution (Å)	72.55 – 2.49 72.55 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.3 (72.55-2.49) 98.3 (72.55-2.49)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.234 , 0.309 0.227 , 0.296	Depositor DCC
R_{free} test set	1407 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.1	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	5136	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.06% 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

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	0.97	0/2549	1.12	9/3445 (0.3%)
1	C	0.97	0/2558	1.15	12/3457 (0.3%)
2	B	0.84	0/71	1.09	0/92
2	D	0.99	0/65	1.13	0/84
All	All	0.97	0/5243	1.13	21/7078 (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	C	0	1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	498	ASP	CA-C-N	8.79	130.83	119.84
1	A	498	ASP	C-N-CA	8.79	130.83	119.84
1	C	524	ASP	CA-C-N	8.78	129.32	119.32
1	C	524	ASP	C-N-CA	8.78	129.32	119.32
1	C	498	ASP	CA-C-N	7.68	129.44	119.84
1	C	498	ASP	C-N-CA	7.68	129.44	119.84
1	A	546	ALA	N-CA-C	-7.27	101.68	108.22
1	C	453	LEU	N-CA-C	6.47	119.24	108.96
1	C	684	GLY	N-CA-C	-6.37	106.90	114.48
1	C	569	LYS	N-CA-C	6.11	118.02	111.36
1	A	658	VAL	N-CA-C	5.56	117.41	108.85
1	A	453	LEU	N-CA-C	5.52	118.46	108.69
1	A	590	LEU	N-CA-C	5.50	118.20	111.82
1	C	632	ILE	CB-CA-C	5.39	116.88	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	594	ALA	CA-C-N	-5.34	113.16	119.84
1	A	594	ALA	C-N-CA	-5.34	113.16	119.84
1	C	716	GLY	N-CA-C	-5.26	106.04	112.77
1	C	656	ILE	CA-C-N	-5.19	114.45	119.90
1	C	656	ILE	C-N-CA	-5.19	114.45	119.90
1	A	422	VAL	N-CA-C	5.07	115.05	108.35
1	C	589	LYS	N-CA-C	-5.05	107.07	114.39

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	654	LYS	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	2493	0	2530	51	0
1	C	2499	0	2536	68	0
2	B	70	0	65	7	0
2	D	64	0	60	8	0
3	A	8	0	0	1	0
3	C	2	0	0	0	0
All	All	5136	0	5191	130	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 13.

All (130) 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)
2:D:1377:ARG:HH11	2:D:1377:ARG:HG2	1.25	0.97
2:D:1376:ARG:HG3	2:D:1376:ARG:HH11	1.31	0.94
1:A:456:GLU:O	1:A:459:GLN:HG2	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:701:SER:HB2	1:C:704:ASN:HB3	1.55	0.89
2:B:1377:ARG:HG2	2:B:1377:ARG:HH21	1.38	0.87
1:A:552:ILE:HG21	1:A:600:ARG:HG2	1.57	0.86
2:B:1376:ARG:HG2	2:B:1376:ARG:HH11	1.41	0.86
1:A:620:HIS:O	1:A:624:MET:HG3	1.79	0.81
1:A:668:HIS:HD2	1:A:680:SER:OG	1.67	0.77
1:A:526:LEU:O	1:A:530:ILE:HD12	1.86	0.76
1:C:491:LEU:HD22	1:C:497:LEU:HD12	1.66	0.75
1:A:498:ASP:HB3	1:A:501:ARG:HG3	1.70	0.74
1:A:573:GLN:NE2	1:A:599:ASN:OD1	2.22	0.72
1:A:427:MET:SD	1:A:509:ARG:HD2	2.31	0.70
1:A:590:LEU:O	1:A:590:LEU:HD22	1.91	0.70
1:C:451:MET:HB2	1:C:453:LEU:HD22	1.74	0.70
1:C:700:HIS:CD2	1:C:700:HIS:N	2.60	0.69
1:C:448:MET:HE2	1:C:458:GLN:HG2	1.74	0.69
1:A:510:ARG:NH2	1:A:519:GLU:OE1	2.26	0.68
2:B:1376:ARG:HG2	2:B:1376:ARG:NH1	2.00	0.68
2:B:1377:ARG:HG2	2:B:1377:ARG:NH2	2.09	0.67
1:A:454:SER:O	1:A:458:GLN:HG3	1.94	0.66
1:C:671:ASN:OD1	1:C:673:GLU:N	2.28	0.66
1:A:578:GLU:O	1:A:579:GLU:HB2	1.97	0.65
1:C:701:SER:CB	1:C:704:ASN:HB3	2.26	0.65
1:A:468:GLU:H	1:A:468:GLU:CD	2.06	0.64
1:C:663:ASN:OD1	1:C:668:HIS:HE1	1.82	0.63
2:B:1376:ARG:HH11	2:B:1376:ARG:CG	2.09	0.63
2:D:1376:ARG:HH11	2:D:1376:ARG:CG	2.08	0.62
1:C:579:GLU:HA	1:C:579:GLU:OE1	2.00	0.62
1:C:448:MET:CE	1:C:458:GLN:HG2	2.30	0.61
1:C:701:SER:HB2	1:C:704:ASN:CB	2.30	0.60
1:A:644:ILE:HG22	1:A:709:ILE:O	2.02	0.58
1:C:475:LYS:H	1:C:478:HIS:HD2	1.50	0.58
1:A:456:GLU:O	1:A:459:GLN:CG	2.48	0.58
2:D:1377:ARG:HG2	2:D:1377:ARG:NH1	2.00	0.57
1:C:641:THR:HG22	1:C:672:MET:HE2	1.86	0.57
1:C:475:LYS:H	1:C:478:HIS:CD2	2.22	0.57
1:C:700:HIS:N	1:C:700:HIS:HD2	2.03	0.57
1:C:668:HIS:HD2	1:C:680:SER:OG	1.88	0.57
1:C:701:SER:CB	1:C:704:ASN:CB	2.83	0.56
1:A:630:TRP:O	1:A:665:LYS:NZ	2.39	0.56
1:A:644:ILE:HG13	1:A:656:ILE:HB	1.87	0.56
1:C:461:PHE:CZ	1:C:530:ILE:HD13	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:ASN:OD1	1:A:668:HIS:HE1	1.89	0.55
1:C:456:GLU:O	1:C:459:GLN:HG3	2.06	0.55
1:C:461:PHE:HB2	1:C:509:ARG:O	2.07	0.54
1:A:669:LEU:HD12	1:A:679:ILE:HG22	1.90	0.54
1:A:668:HIS:CD2	1:A:680:SER:OG	2.57	0.53
1:C:637:ALA:HA	1:C:663:ASN:HB3	1.91	0.52
1:A:437:LYS:HE3	1:A:438:HIS:CE1	2.44	0.52
1:A:607:ASN:O	1:A:611:SER:HB2	2.11	0.51
1:C:517[B]:GLU:H	1:C:517[B]:GLU:CD	2.16	0.51
1:C:510:ARG:NH2	1:C:519:GLU:OE1	2.42	0.51
1:A:606:LYS:O	1:A:610:THR:HB	2.11	0.50
1:C:552:ILE:HG21	1:C:600:ARG:HG2	1.94	0.50
1:A:572:LYS:O	1:A:573:GLN:HB2	2.12	0.50
1:C:597:TRP:O	1:C:601:ILE:HG13	2.11	0.49
2:D:1376:ARG:HG3	2:D:1376:ARG:NH1	2.12	0.49
1:A:496:ASN:HB3	1:C:657:PRO:HG3	1.93	0.49
1:A:566:TYR:H	1:A:609:SER:CB	2.25	0.49
1:C:457:THR:C	1:C:459:GLN:H	2.20	0.49
1:A:719:VAL:HG13	1:A:723:MET:HE3	1.95	0.49
1:C:697:PHE:CZ	1:C:718:VAL:HG11	2.48	0.49
1:C:526:LEU:O	1:C:530:ILE:HD12	2.13	0.48
1:C:466:CYS:SG	1:C:471:SER:HB3	2.54	0.48
1:C:609:SER:O	1:C:611:SER:N	2.47	0.48
1:C:684:GLY:O	1:C:702:MET:HE3	2.14	0.48
2:B:1375:SER:HB3	2:B:1376:ARG:NH1	2.29	0.48
1:C:582:LYS:HB3	1:C:590:LEU:HD11	1.96	0.47
1:A:434:VAL:HG21	1:A:451:MET:HG2	1.96	0.47
1:C:456:GLU:O	1:C:459:GLN:CG	2.62	0.47
1:A:618:MET:HG3	1:A:622:GLN:NE2	2.29	0.47
1:A:646:THR:HG22	1:A:656:ILE:HD11	1.95	0.47
1:C:641:THR:HG22	1:C:672:MET:CE	2.44	0.47
1:A:577:ASN:O	1:A:579:GLU:N	2.48	0.47
1:A:687:MET:HE2	1:A:687:MET:HB3	1.73	0.47
1:C:436:LEU:HB3	1:C:442:THR:OG1	2.15	0.47
1:A:607:ASN:HA	1:A:610:THR:HG22	1.96	0.47
1:A:479:LYS:HA	1:A:480:PRO:HD2	1.73	0.46
1:A:559:LEU:HD13	1:A:605:TYR:CD2	2.50	0.46
1:C:699:ILE:O	1:C:707:SER:HA	2.15	0.46
1:A:491:LEU:HD22	1:A:497:LEU:HD12	1.98	0.46
1:A:501:ARG:CZ	1:C:468:GLU:O	2.64	0.46
1:C:565:ASN:HD22	1:C:609:SER:CA	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:581:LEU:HB3	1:C:590:LEU:HD21	1.96	0.46
1:A:645:PHE:CE2	1:A:655:VAL:HG13	2.51	0.45
1:C:645:PHE:CE2	1:C:655:VAL:HG22	2.52	0.45
1:C:516:LEU:HD12	1:C:516:LEU:HA	1.86	0.45
1:A:721:LEU:HD13	2:B:1381:PHE:HB3	1.98	0.45
1:C:565:ASN:HD22	1:C:609:SER:HA	1.81	0.45
1:A:637:ALA:HA	1:A:663:ASN:HB3	1.98	0.45
1:C:508:LEU:HA	1:C:508:LEU:HD12	1.67	0.45
1:A:666:GLY:HA2	1:A:683:TYR:CZ	2.52	0.45
1:C:457:THR:C	1:C:459:GLN:N	2.75	0.45
1:C:686:PHE:O	1:C:702:MET:HE2	2.17	0.45
1:A:461:PHE:CD1	1:A:461:PHE:N	2.85	0.44
1:C:565:ASN:ND2	1:C:609:SER:HA	2.32	0.44
1:C:670:LEU:CD2	1:C:677:LEU:HD12	2.48	0.44
2:D:1376:ARG:CG	2:D:1376:ARG:NH1	2.75	0.44
2:D:1377:ARG:NH1	2:D:1377:ARG:CG	2.77	0.44
1:C:669:LEU:C	1:C:670:LEU:HD23	2.43	0.44
1:A:593:LYS:HD2	1:A:593:LYS:N	2.32	0.43
1:C:498:ASP:HA	1:C:499:PRO:HD2	1.51	0.43
1:C:654:LYS:HD2	1:C:655:VAL:H	1.83	0.43
1:A:645:PHE:O	1:A:646:THR:C	2.61	0.43
1:C:428:ASP:OD1	1:C:428:ASP:C	2.62	0.43
1:C:558:LEU:HD23	1:C:558:LEU:HA	1.87	0.43
1:C:682:LYS:O	1:C:683:TYR:C	2.61	0.43
1:C:606:LYS:O	1:C:610:THR:HB	2.18	0.43
1:C:440:ASN:HB2	1:C:481:LEU:HB2	2.01	0.42
1:C:513:ARG:HE	1:C:513:ARG:HB2	1.50	0.42
1:C:491:LEU:CD2	1:C:497:LEU:HD12	2.44	0.42
1:C:700:HIS:CD2	1:C:700:HIS:H	2.34	0.42
1:C:668:HIS:CD2	1:C:680:SER:OG	2.71	0.42
1:C:700:HIS:HD2	1:C:700:HIS:H	1.66	0.41
1:C:715:ALA:O	1:C:719:VAL:HB	2.20	0.41
1:A:498:ASP:HA	1:A:499:PRO:HD2	1.54	0.41
1:A:526:LEU:HD12	1:A:530:ILE:CD1	2.50	0.41
1:C:654:LYS:HD2	1:C:655:VAL:N	2.35	0.41
1:C:504:PRO:O	1:C:505:GLN:HG3	2.19	0.41
1:C:594:ALA:N	1:C:595:PRO:CD	2.84	0.41
1:C:609:SER:C	1:C:611:SER:N	2.78	0.41
1:A:466:CYS:SG	1:A:471:SER:HB3	2.61	0.41
1:C:566:TYR:H	1:C:609:SER:CB	2.33	0.41
1:A:664:ILE:HG13	3:A:2:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:LEU:O	1:A:530:ILE:CD1	2.62	0.41
1:A:637:ALA:CA	1:A:663:ASN:HB3	2.51	0.40
1:C:493:GLU:OE1	2:D:1378:ARG:NH1	2.53	0.40
1:A:497:LEU:O	1:A:499:PRO:HD3	2.21	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	301/322 (94%)	280 (93%)	16 (5%)	5 (2%)	7	13
1	C	302/322 (94%)	269 (89%)	29 (10%)	4 (1%)	9	18
2	B	5/26 (19%)	4 (80%)	1 (20%)	0	100	100
2	D	4/26 (15%)	3 (75%)	1 (25%)	0	100	100
All	All	612/696 (88%)	556 (91%)	47 (8%)	9 (2%)	8	16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	578	GLU
1	A	579	GLU
1	C	610	THR
1	C	705	LYS
1	A	571	HIS
1	C	578	GLU
1	A	573	GLN
1	A	664	ILE
1	C	437	LYS

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	277/293 (94%)	245 (88%)	32 (12%)	5	11
1	C	278/293 (95%)	246 (88%)	32 (12%)	5	11
2	B	7/25 (28%)	4 (57%)	3 (43%)	0	0
2	D	6/25 (24%)	4 (67%)	2 (33%)	0	0
All	All	568/636 (89%)	499 (88%)	69 (12%)	5	10

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	434	VAL
1	A	436	LEU
1	A	445	GLN
1	A	456	GLU
1	A	461	PHE
1	A	468	GLU
1	A	501	ARG
1	A	505	GLN
1	A	508	LEU
1	A	512	VAL
1	A	526	LEU
1	A	530	ILE
1	A	531	LEU
1	A	565	ASN
1	A	568	SER
1	A	570	LYS
1	A	576	LEU
1	A	590	LEU
1	A	610	THR
1	A	614	VAL
1	A	631	GLU
1	A	655	VAL
1	A	673	GLU
1	A	679	ILE

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Mol	Chain	Res	Type
1	A	680	SER
1	A	687	MET
1	A	694	ASP
1	A	701	SER
1	A	702	MET
1	A	712	THR
1	A	719	VAL
1	A	729	LEU
2	B	1376	ARG
2	B	1377	ARG
2	B	1378	ARG
1	C	422	VAL
1	C	426	ARG
1	C	434	VAL
1	C	435	GLU
1	C	451	MET
1	C	453	LEU
1	C	454	SER
1	C	459	GLN
1	C	508	LEU
1	C	513	ARG
1	C	522	ILE
1	C	530	ILE
1	C	550	LYS
1	C	570	LYS
1	C	578	GLU
1	C	582	LYS
1	C	590	LEU
1	C	610	THR
1	C	644	ILE
1	C	653	HIS
1	C	654	LYS
1	C	656	ILE
1	C	669	LEU
1	C	679	ILE
1	C	680	SER
1	C	690	LEU
1	C	700	HIS
1	C	702	MET
1	C	712	THR
1	C	719	VAL
1	C	728	GLN

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Mol	Chain	Res	Type
1	C	729	LEU
2	D	1376	ARG
2	D	1377	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	483	HIS
1	A	496	ASN
1	A	560	GLN
1	A	565	ASN
1	A	577	ASN
1	A	580	ASN
1	A	622	GLN
1	A	668	HIS
1	A	700	HIS
1	A	711	HIS
1	C	440	ASN
1	C	478	HIS
1	C	496	ASN
1	C	500	GLN
1	C	560	GLN
1	C	565	ASN
1	C	571	HIS
1	C	668	HIS
1	C	689	GLN
1	C	698	GLN
1	C	700	HIS
1	C	704	ASN
1	C	711	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 [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	305/322 (94%)	0.39	18 (5%) 28 24	26, 45, 82, 92	0
1	C	305/322 (94%)	0.43	23 (7%) 20 18	23, 46, 82, 100	1 (0%)
2	B	7/26 (26%)	0.58	1 (14%) 6 5	40, 53, 71, 71	0
2	D	6/26 (23%)	0.97	0 100 100	45, 59, 73, 76	0
All	All	623/696 (89%)	0.41	42 (6%) 24 21	23, 46, 82, 100	1 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	575	PHE	6.0
1	A	730	MET	5.8
1	A	614	VAL	5.3
1	A	615	SER	4.4
1	C	575	PHE	4.2
1	A	435	GLU	4.0
1	C	574	GLY	3.9
1	C	614	VAL	3.9
1	C	610	THR	3.7
1	C	613	GLY	3.5
1	A	436	LEU	3.2
1	C	653	HIS	3.2
1	A	577	ASN	3.2
1	C	646	THR	3.2
1	A	616	LYS	3.1
1	A	707	SER	3.1
1	C	612	GLU	3.0
1	C	577	ASN	3.0
1	A	613	GLY	3.0
1	C	450	GLY	3.0
1	C	576	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	730	MET	2.8
1	A	576	LEU	2.8
1	C	700	HIS	2.7
1	A	571	HIS	2.6
2	B	1375	SER	2.6
1	C	569	LYS	2.5
1	A	572	LYS	2.4
1	C	571	HIS	2.4
1	C	563	TYR	2.4
1	C	434	VAL	2.3
1	A	610	THR	2.3
1	C	729	LEU	2.3
1	A	702	MET	2.2
1	C	615	SER	2.1
1	A	453	LEU	2.1
1	C	453	LEU	2.1
1	A	619	HIS	2.1
1	A	723	MET	2.1
1	C	706	MET	2.1
1	C	438	HIS	2.1
1	C	617	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.