Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:25 AM UTC

PDB ID	:	6HLU / pdb_00006hlu
Title	:	Crystal structure of the LRR-Roc-COR domain of the Chlorobium tepidum Roco protein
Authors	:	Deyaert, E.; Versees, W.; Singh, R.
Deposited on	:	2018-09-11
Resolution	:	3.29 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:

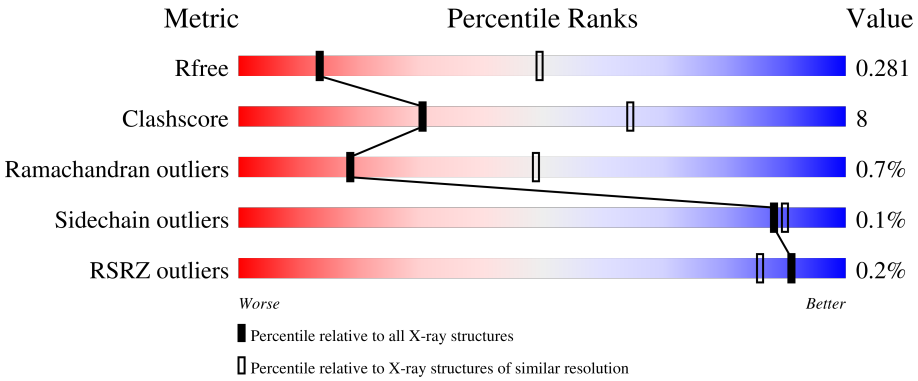
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 <=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	974	76% 17% 7%
1	B	974	72% 19% 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 13681 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 Rab family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	908	Total	C	N	O	S	0	0	0
			6890	4379	1117	1372	22			
1	B	896	Total	C	N	O	S	0	0	0
			6791	4306	1103	1361	21			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP Q8KC98
A	-26	SER	-	expression tag	UNP Q8KC98
A	-25	TYR	-	expression tag	UNP Q8KC98
A	-24	TYR	-	expression tag	UNP Q8KC98
A	-23	HIS	-	expression tag	UNP Q8KC98
A	-22	HIS	-	expression tag	UNP Q8KC98
A	-21	HIS	-	expression tag	UNP Q8KC98
A	-20	HIS	-	expression tag	UNP Q8KC98
A	-19	HIS	-	expression tag	UNP Q8KC98
A	-18	HIS	-	expression tag	UNP Q8KC98
A	-17	ASP	-	expression tag	UNP Q8KC98
A	-16	TYR	-	expression tag	UNP Q8KC98
A	-15	ASP	-	expression tag	UNP Q8KC98
A	-14	ILE	-	expression tag	UNP Q8KC98
A	-13	PRO	-	expression tag	UNP Q8KC98
A	-12	THR	-	expression tag	UNP Q8KC98
A	-11	THR	-	expression tag	UNP Q8KC98
A	-10	GLU	-	expression tag	UNP Q8KC98
A	-9	ASN	-	expression tag	UNP Q8KC98
A	-8	LEU	-	expression tag	UNP Q8KC98
A	-7	TYR	-	expression tag	UNP Q8KC98
A	-6	PHE	-	expression tag	UNP Q8KC98
A	-5	GLN	-	expression tag	UNP Q8KC98
A	-4	GLY	-	expression tag	UNP Q8KC98
A	-3	ALA	-	expression tag	UNP Q8KC98

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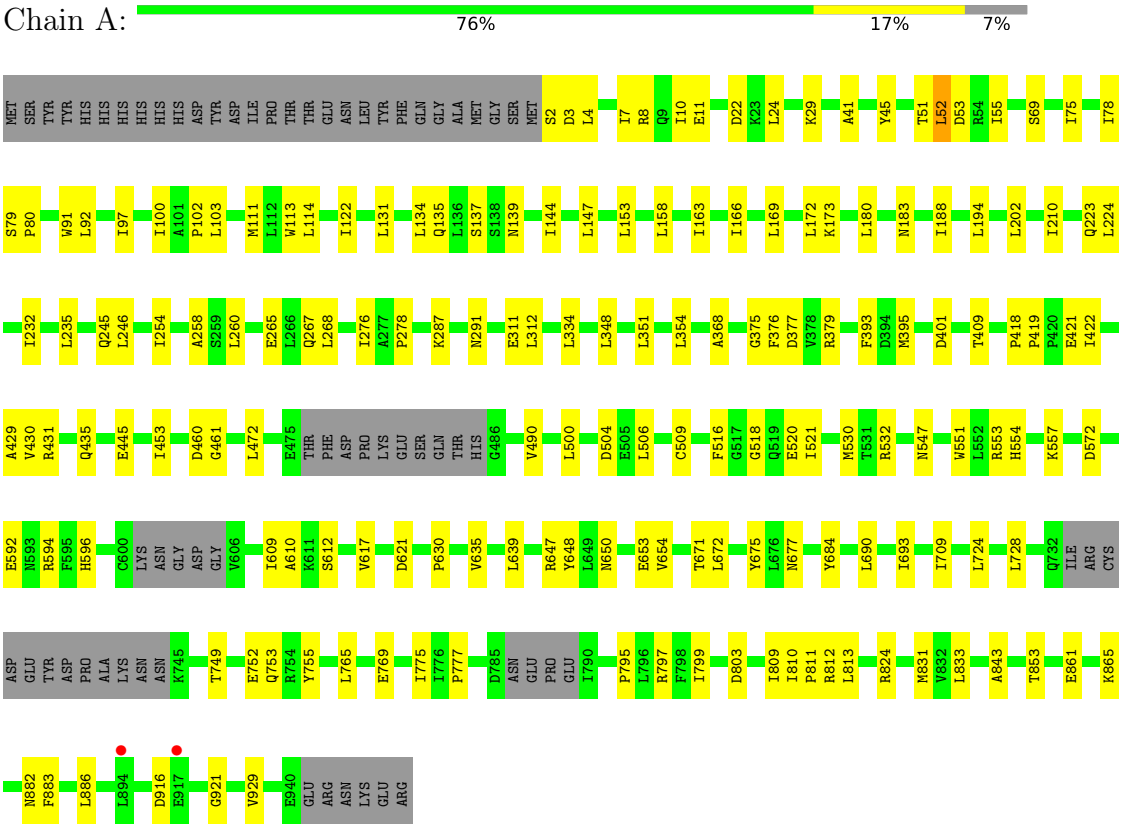
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP Q8KC98
A	-1	GLY	-	expression tag	UNP Q8KC98
A	0	SER	-	expression tag	UNP Q8KC98
B	-27	MET	-	initiating methionine	UNP Q8KC98
B	-26	SER	-	expression tag	UNP Q8KC98
B	-25	TYR	-	expression tag	UNP Q8KC98
B	-24	TYR	-	expression tag	UNP Q8KC98
B	-23	HIS	-	expression tag	UNP Q8KC98
B	-22	HIS	-	expression tag	UNP Q8KC98
B	-21	HIS	-	expression tag	UNP Q8KC98
B	-20	HIS	-	expression tag	UNP Q8KC98
B	-19	HIS	-	expression tag	UNP Q8KC98
B	-18	HIS	-	expression tag	UNP Q8KC98
B	-17	ASP	-	expression tag	UNP Q8KC98
B	-16	TYR	-	expression tag	UNP Q8KC98
B	-15	ASP	-	expression tag	UNP Q8KC98
B	-14	ILE	-	expression tag	UNP Q8KC98
B	-13	PRO	-	expression tag	UNP Q8KC98
B	-12	THR	-	expression tag	UNP Q8KC98
B	-11	THR	-	expression tag	UNP Q8KC98
B	-10	GLU	-	expression tag	UNP Q8KC98
B	-9	ASN	-	expression tag	UNP Q8KC98
B	-8	LEU	-	expression tag	UNP Q8KC98
B	-7	TYR	-	expression tag	UNP Q8KC98
B	-6	PHE	-	expression tag	UNP Q8KC98
B	-5	GLN	-	expression tag	UNP Q8KC98
B	-4	GLY	-	expression tag	UNP Q8KC98
B	-3	ALA	-	expression tag	UNP Q8KC98
B	-2	MET	-	expression tag	UNP Q8KC98
B	-1	GLY	-	expression tag	UNP Q8KC98
B	0	SER	-	expression tag	UNP Q8KC98

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.

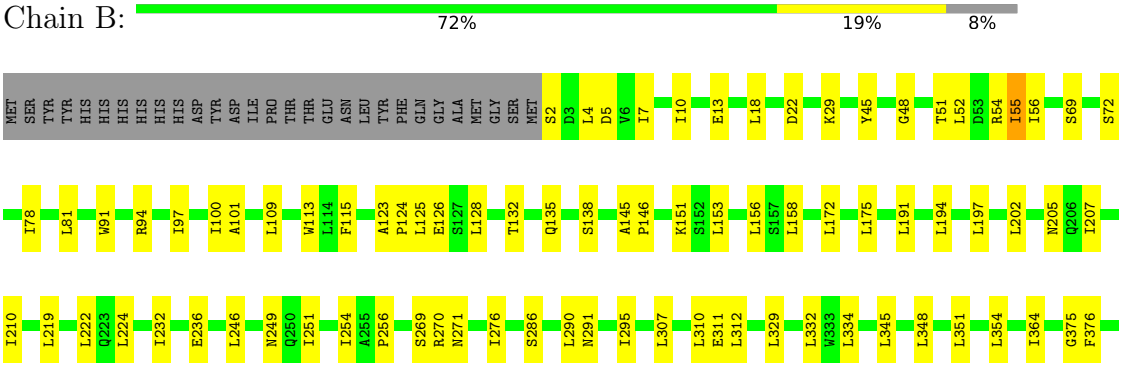
• Molecule 1: Rab family protein

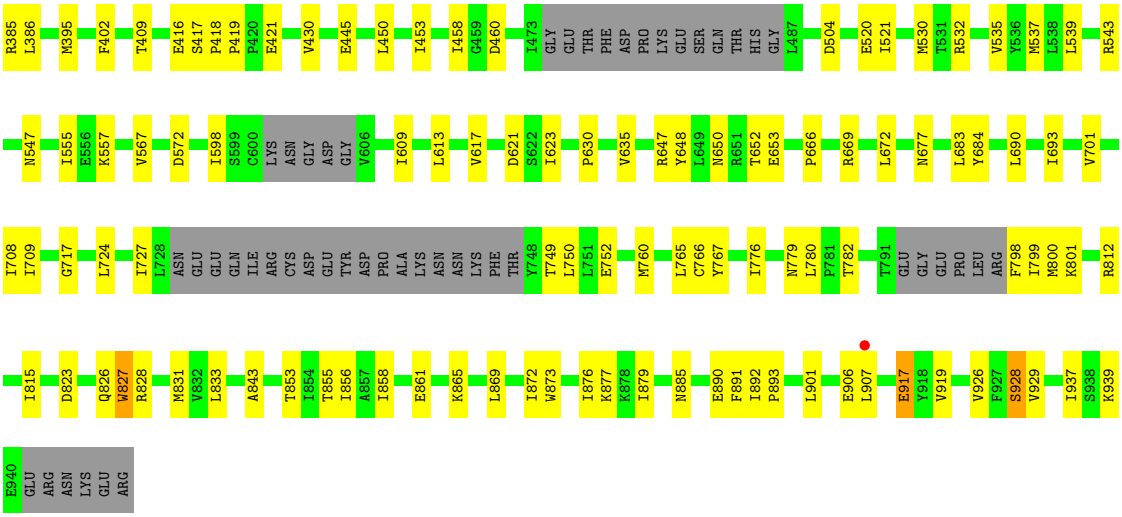
Chain A:



• Molecule 1: Rab family protein

Chain B:




R385 L386 M395 F402 T409 E416 S417 P418 P419 P420 E421 V430 E445 L450 I453 I458 G459 D460 I473 GLY GLU THR PHE ASP PRO LYS GLU SER GLN THR HIS GLY L487 D504 E520 I521 M530 T531 R532 V535 Y536 M537 L538 L539 R543
N547 I555 E556 K557 V567 D572 I598 S599 C600 LYS ASN GLY ASP GLY V606 I609 L613 V617 D621 S622 I623 P630 V635 R647 Y648 L649 N650 R651 T652 E653 P666 R669 L672 N677 L683 Y684 L690 I693 V701
I708 I709 G717 L724 I727 L728 ASN GLU GLU GLN ILE ARG CYS ASP GLU TYR ASP PRO ALA LYS ASN ASN LYS PHE THR Y748 T749 L750 L751 E752 M760 L765 C766 Y767 I776 N779 L780 P781 T782 T791 GLU GLY GLU PRO LEU ARG F798 I799 M800 K801 R812
I815 D823 Q826 W827 R828 M831 V832 L833 A843 T853 I854 T855 I856 A857 I858 E861 K866 L869 I872 W873 I876 K877 K878 I879 N885 E890 F891 I892 P893 L901 E906 L907 E917 Y918 V919 V926 F927 S928 V929 I937 S938 K939
E940 GLU ARG ASN LYS GLU ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.59Å 129.76Å 179.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.85 – 3.29 44.85 – 3.29	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.85-3.29) 99.1 (44.85-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.230 , 0.281 0.230 , 0.281	Depositor DCC
R_{free} test set	1686 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	85.1	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 63.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13681	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.09	0/7010	0.28	0/9556
1	B	0.10	0/6906	0.30	0/9419
All	All	0.09	0/13916	0.29	0/18975

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	6890	0	6658	112	0
1	B	6791	0	6584	118	0
All	All	13681	0	13242	227	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 8.

All (227) 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:557:LYS:NZ	1:B:885:ASN:O	2.10	0.83
1:A:769:GLU:OE2	1:A:824:ARG:NH1	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ARG:NH1	1:A:621:ASP:O	2.14	0.80
1:B:109:LEU:HD11	1:B:128:LEU:HD23	1.63	0.80
1:A:29:LYS:NZ	1:A:45:TYR:O	2.15	0.79
1:B:329:LEU:HD13	1:B:332:LEU:HD11	1.69	0.75
1:B:29:LYS:NZ	1:B:45:TYR:O	2.20	0.74
1:A:122:ILE:HD11	1:A:144:ILE:HA	1.72	0.71
1:B:385:ARG:HG2	1:B:417:SER:HB3	1.72	0.71
1:B:708:ILE:HG22	1:B:727:ILE:HD12	1.72	0.70
1:B:126:GLU:HB2	1:B:146:PRO:HB3	1.74	0.69
1:B:269:SER:O	1:B:271:ASN:N	2.22	0.69
1:B:892:ILE:HD12	1:B:893:PRO:HD2	1.74	0.69
1:A:521:ILE:HG23	1:A:765:LEU:HD11	1.74	0.68
1:B:418:PRO:HG3	1:B:430:VAL:HG13	1.74	0.68
1:A:188:ILE:HD11	1:A:210:ILE:HA	1.74	0.67
1:B:800:MET:HE1	1:B:876:ILE:HG21	1.75	0.67
1:A:8:ARG:NH1	1:A:11:GLU:OE2	2.29	0.66
1:A:431:ARG:NH1	1:A:435:GLN:OE1	2.29	0.66
1:A:69:SER:HA	1:A:91:TRP:HB2	1.78	0.65
1:A:291:ASN:HB3	1:A:311:GLU:OE2	1.96	0.64
1:B:132:THR:HA	1:B:153:LEU:HA	1.78	0.64
1:B:385:ARG:NH1	1:B:416:GLU:OE1	2.30	0.64
1:B:635:VAL:HG21	1:B:672:LEU:HD21	1.80	0.64
1:B:826:GLN:HA	1:B:831:MET:HA	1.80	0.64
1:A:422:ILE:HD11	1:A:675:TYR:CD1	2.34	0.63
1:B:153:LEU:HD11	1:B:172:LEU:HD13	1.78	0.63
1:B:453:ILE:HG12	1:B:535:VAL:HG23	1.80	0.63
1:A:24:LEU:HD22	1:A:41:ALA:HB1	1.81	0.62
1:B:799:ILE:HG12	1:B:891:PHE:HB2	1.81	0.62
1:A:592:GLU:OE1	1:A:594:ARG:NH2	2.32	0.62
1:B:123:ALA:HA	1:B:146:PRO:HG2	1.82	0.61
1:B:683:LEU:HD12	1:B:701:VAL:HG11	1.81	0.61
1:B:10:ILE:HA	1:B:55:ILE:HD11	1.82	0.61
1:A:52:LEU:H	1:A:55:ILE:HG22	1.66	0.60
1:A:445:GLU:HB3	1:A:630:PRO:HG2	1.83	0.60
1:A:749:THR:N	1:A:752:GLU:OE2	2.23	0.60
1:A:921:GLY:N	1:B:906:GLU:OE2	2.34	0.60
1:B:749:THR:N	1:B:752:GLU:OE2	2.22	0.60
1:B:799:ILE:HD13	1:B:901:LEU:HD22	1.82	0.60
1:A:144:ILE:HB	1:A:147:LEU:HD12	1.84	0.59
1:A:254:ILE:HD11	1:A:276:ILE:HA	1.83	0.59
1:A:180:LEU:HD23	1:A:183:ASN:HD22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LEU:HD22	1:B:207:ILE:HD13	1.85	0.59
1:A:113:TRP:HA	1:A:135:GLN:HB3	1.83	0.59
1:B:54:ARG:O	1:B:56:ILE:N	2.35	0.59
1:B:798:PHE:HB3	1:B:856:ILE:HG23	1.84	0.59
1:B:532:ARG:NH1	1:B:621:ASP:O	2.34	0.59
1:B:419:PRO:HB2	1:B:421:GLU:OE2	2.04	0.58
1:B:458:ILE:HD12	1:B:555:ILE:HG12	1.84	0.58
1:B:919:VAL:HG12	1:B:926:VAL:HG12	1.86	0.58
1:A:557:LYS:HZ1	1:A:803:ASP:CG	2.10	0.58
1:B:232:ILE:HD11	1:B:254:ILE:HA	1.85	0.57
1:B:812:ARG:HD2	1:B:879:ILE:HB	1.86	0.57
1:A:418:PRO:HG3	1:A:430:VAL:HG13	1.86	0.57
1:B:69:SER:HA	1:B:91:TRP:HB2	1.86	0.56
1:B:332:LEU:HD23	1:B:334:LEU:HD11	1.87	0.56
1:A:419:PRO:HB2	1:A:421:GLU:OE2	2.06	0.56
1:A:557:LYS:HZ3	1:A:886:LEU:HA	1.70	0.56
1:B:450:LEU:HD23	1:B:623:ILE:HD12	1.87	0.56
1:B:52:LEU:HD11	1:B:81:LEU:HD23	1.88	0.56
1:B:345:LEU:HA	1:B:348:LEU:HD13	1.87	0.55
1:B:254:ILE:HD11	1:B:276:ILE:HA	1.88	0.55
1:B:709:ILE:O	1:B:779:ASN:ND2	2.39	0.55
1:B:521:ILE:HG23	1:B:765:LEU:HD11	1.89	0.55
1:A:169:LEU:HD23	1:A:172:LEU:HD13	1.88	0.54
1:B:310:LEU:HD12	1:B:329:LEU:HD11	1.88	0.54
1:B:782:THR:HG23	1:B:828:ARG:HB3	1.90	0.54
1:A:557:LYS:NZ	1:A:803:ASP:OD2	2.31	0.54
1:A:472:LEU:H	1:A:472:LEU:HD23	1.72	0.54
1:A:547:ASN:HB2	1:B:547:ASN:HB2	1.89	0.54
1:A:833:LEU:HB2	1:A:843:ALA:HB3	1.88	0.54
1:B:917:GLU:HA	1:B:928:SER:HA	1.90	0.54
1:B:2:SER:O	1:B:4:LEU:N	2.40	0.53
1:B:291:ASN:HB3	1:B:311:GLU:OE2	2.08	0.53
1:A:520:GLU:HB3	1:A:530:MET:HE3	1.90	0.53
1:B:113:TRP:HA	1:B:135:GLN:HB3	1.91	0.53
1:A:354:LEU:HB3	1:A:376:PHE:HB2	1.90	0.53
1:A:223:GLN:OE1	1:A:245:GLN:NE2	2.42	0.53
1:B:798:PHE:HE1	1:B:890:GLU:HB3	1.75	0.52
1:A:137:SER:O	1:A:139:ASN:ND2	2.42	0.52
1:A:8:ARG:HD3	1:A:11:GLU:OE2	2.09	0.52
1:B:537:MET:HE1	1:B:613:LEU:HD11	1.92	0.52
1:A:635:VAL:HG21	1:A:672:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LYS:HA	1:A:194:LEU:HD23	1.92	0.52
1:A:639:LEU:HD21	1:A:654:VAL:HG23	1.92	0.51
1:B:375:GLY:N	1:B:395:MET:SD	2.83	0.51
1:A:2:SER:OG	1:A:3:ASP:N	2.38	0.51
1:A:312:LEU:HB2	1:A:334:LEU:HD23	1.92	0.51
1:A:375:GLY:N	1:A:395:MET:SD	2.83	0.51
1:B:78:ILE:HD13	1:B:97:ILE:HD13	1.93	0.51
1:B:598:ILE:HD11	1:B:609:ILE:HD11	1.91	0.51
1:A:134:LEU:HD12	1:A:153:LEU:HD11	1.93	0.51
1:B:246:LEU:HD13	1:B:251:ILE:HG13	1.93	0.51
1:A:166:ILE:HD11	1:A:188:ILE:HA	1.93	0.51
1:B:749:THR:HG22	1:B:750:LEU:H	1.76	0.51
1:B:650:ASN:OD1	1:B:652:THR:OG1	2.27	0.51
1:B:312:LEU:HB2	1:B:334:LEU:HD23	1.93	0.50
1:A:813:LEU:HB3	1:A:831:MET:HE1	1.93	0.50
1:B:520:GLU:HB3	1:B:530:MET:HE3	1.93	0.50
1:A:677:ASN:ND2	1:A:684:TYR:O	2.45	0.50
1:A:557:LYS:NZ	1:A:886:LEU:HA	2.26	0.50
1:B:650:ASN:ND2	1:B:653:GLU:OE1	2.45	0.50
1:B:156:LEU:HD21	1:B:158:LEU:HD13	1.94	0.49
1:A:78:ILE:HD13	1:A:97:ILE:HD13	1.94	0.49
1:B:873:TRP:CZ2	1:B:877:LYS:HD2	2.47	0.49
1:A:100:ILE:HB	1:A:103:LEU:HD12	1.93	0.49
1:B:801:LYS:HA	1:B:853:THR:HG22	1.94	0.49
1:A:377:ASP:OD1	1:A:409:THR:OG1	2.31	0.49
1:A:777:PRO:HB2	1:A:811:PRO:HB3	1.95	0.49
1:A:419:PRO:HG2	1:A:422:ILE:HG12	1.93	0.49
1:A:158:LEU:HD22	1:A:163:ILE:HD11	1.93	0.49
1:A:131:LEU:HD13	1:A:134:LEU:HG	1.94	0.48
1:B:799:ILE:HD13	1:B:901:LEU:CD2	2.43	0.48
1:A:812:ARG:NH1	1:A:882:ASN:OD1	2.44	0.48
1:A:916:ASP:HA	1:A:929:VAL:HG22	1.96	0.48
1:A:210:ILE:HD11	1:A:232:ILE:HA	1.95	0.48
1:A:422:ILE:CD1	1:A:675:TYR:HB2	2.44	0.48
1:B:54:ARG:C	1:B:56:ILE:H	2.22	0.48
1:B:799:ILE:CG1	1:B:891:PHE:HB2	2.43	0.47
1:A:429:ALA:HA	1:A:671:THR:HG21	1.96	0.47
1:B:766:CYS:HB3	1:B:776:ILE:HD13	1.95	0.47
1:B:354:LEU:HB3	1:B:376:PHE:HB2	1.95	0.47
1:A:504:ASP:OD1	1:A:504:ASP:N	2.48	0.47
1:B:2:SER:N	1:B:5:ASP:OD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLN:HG3	1:A:267:GLN:HB2	1.96	0.47
1:A:709:ILE:HD11	1:A:765:LEU:HD13	1.96	0.47
1:B:504:ASP:OD1	1:B:504:ASP:N	2.47	0.47
1:A:500:LEU:HD22	1:A:610:ALA:HB1	1.95	0.47
1:B:219:LEU:HD21	1:B:222:LEU:HD13	1.95	0.47
1:B:861:GLU:O	1:B:865:LYS:N	2.48	0.47
1:B:100:ILE:O	1:B:124:PRO:HG2	2.15	0.47
1:B:760:MET:HE2	1:B:760:MET:HB3	1.80	0.46
1:A:4:LEU:O	1:A:7:ILE:HG13	2.14	0.46
1:A:650:ASN:ND2	1:A:653:GLU:OE1	2.48	0.46
1:B:7:ILE:HD13	1:B:10:ILE:HD12	1.96	0.46
1:A:92:LEU:HB2	1:A:114:LEU:HD12	1.97	0.46
1:A:728:LEU:HD12	1:A:753:GLN:HG2	1.97	0.46
1:A:596:HIS:CD2	1:A:609:ILE:HG22	2.50	0.46
1:B:833:LEU:HB2	1:B:843:ALA:HB3	1.98	0.46
1:A:461:GLY:H	1:B:543:ARG:HB3	1.80	0.46
1:A:10:ILE:HA	1:A:55:ILE:HD11	1.97	0.46
1:A:422:ILE:HD11	1:A:675:TYR:CG	2.50	0.46
1:B:175:LEU:HB3	1:B:197:LEU:HD21	1.98	0.46
1:A:180:LEU:HD23	1:A:183:ASN:ND2	2.30	0.46
1:A:202:LEU:HB2	1:A:224:LEU:HD12	1.98	0.46
1:A:460:ASP:HB3	1:A:551:TRP:HE1	1.81	0.45
1:B:666:PRO:HA	1:B:669:ARG:HG2	1.97	0.45
1:B:539:LEU:HD23	1:B:567:VAL:HG13	1.99	0.45
1:B:125:LEU:HA	1:B:128:LEU:HD13	1.98	0.45
1:B:191:LEU:HA	1:B:194:LEU:HD23	1.98	0.45
1:B:246:LEU:O	1:B:249:ASN:ND2	2.47	0.45
1:A:509:CYS:SG	1:A:617:VAL:HG11	2.57	0.45
1:A:883:PHE:HB2	1:A:886:LEU:HD23	1.99	0.45
1:B:872:ILE:O	1:B:876:ILE:HG13	2.17	0.45
1:B:724:LEU:HA	1:B:727:ILE:HD11	1.99	0.45
1:A:258:ALA:HB2	1:A:278:PRO:HB3	1.98	0.45
1:A:52:LEU:HD21	1:A:75:ILE:HG21	2.00	0.44
1:A:799:ILE:HG23	1:A:853:THR:OG1	2.17	0.44
1:B:798:PHE:CE1	1:B:890:GLU:HB3	2.51	0.44
1:A:52:LEU:HD23	1:A:75:ILE:HD13	1.99	0.44
1:B:286:SER:HA	1:B:307:LEU:HA	2.00	0.44
1:B:151:LYS:HA	1:B:172:LEU:HD22	2.00	0.44
1:B:52:LEU:HA	1:B:52:LEU:HD23	1.72	0.44
1:B:210:ILE:HG12	1:B:224:LEU:HD21	2.00	0.44
1:B:290:LEU:HD22	1:B:295:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:SER:OG	1:A:80:PRO:HD3	2.18	0.43
1:B:207:ILE:HD12	1:B:210:ILE:HD13	1.99	0.43
1:B:690:LEU:HD23	1:B:693:ILE:H	1.83	0.43
1:B:826:GLN:HG2	1:B:827:TRP:H	1.83	0.43
1:A:235:LEU:O	1:A:260:LEU:HD21	2.18	0.43
1:A:810:ILE:HG23	1:A:831:MET:HE2	1.98	0.43
1:A:861:GLU:O	1:A:865:LYS:N	2.51	0.43
1:B:717:GLY:HA2	1:B:779:ASN:HB2	2.00	0.43
1:A:232:ILE:HD11	1:A:254:ILE:HA	2.01	0.43
1:B:7:ILE:HG23	1:B:18:LEU:HD12	2.00	0.43
1:A:775:ILE:O	1:A:777:PRO:HD3	2.19	0.43
1:B:22:ASP:N	1:B:22:ASP:OD1	2.52	0.43
1:B:572:ASP:N	1:B:572:ASP:OD1	2.51	0.43
1:A:79:SER:HA	1:A:102:PRO:HG2	2.01	0.43
1:A:572:ASP:OD1	1:A:572:ASP:N	2.50	0.43
1:B:202:LEU:HD23	1:B:205:ASN:ND2	2.34	0.43
1:B:402:PHE:O	1:B:409:THR:HG21	2.18	0.43
1:A:379:ARG:HH11	1:A:401:ASP:C	2.27	0.43
1:A:553:ARG:O	1:A:557:LYS:HG2	2.19	0.43
1:B:780:LEU:O	1:B:828:ARG:HB2	2.19	0.43
1:A:22:ASP:OD1	1:A:22:ASP:N	2.52	0.42
1:B:236:GLU:HG2	1:B:256:PRO:HB3	2.00	0.42
1:A:724:LEU:HD13	1:A:753:GLN:HB3	2.01	0.42
1:B:332:LEU:HD13	1:B:351:LEU:HD13	2.00	0.42
1:B:445:GLU:HB3	1:B:630:PRO:HG2	2.01	0.42
1:B:648:TYR:CE2	1:B:693:ILE:HG12	2.54	0.42
1:A:795:PRO:HB3	1:A:797:ARG:NH1	2.34	0.42
1:B:858:ILE:HD11	1:B:869:LEU:HD23	2.01	0.42
1:A:100:ILE:HD11	1:A:122:ILE:HA	2.02	0.42
1:B:613:LEU:O	1:B:617:VAL:HG12	2.20	0.42
1:A:516:PHE:O	1:A:518:GLY:N	2.47	0.42
1:B:72:SER:HA	1:B:94:ARG:O	2.20	0.42
1:A:180:LEU:HB3	1:A:202:LEU:HD23	2.02	0.41
1:A:348:LEU:HB3	1:A:351:LEU:HB2	2.02	0.41
1:A:594:ARG:HD3	1:A:612:SER:HB3	2.01	0.41
1:A:51:THR:O	1:A:52:LEU:HG	2.20	0.41
1:A:51:THR:O	1:A:53:ASP:N	2.46	0.41
1:A:246:LEU:HB2	1:A:268:LEU:HD23	2.01	0.41
1:A:551:TRP:HA	1:A:554:HIS:HB3	2.03	0.41
1:A:265:GLU:HG3	1:A:287:LYS:HD3	2.02	0.41
1:B:51:THR:O	1:B:55:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:PHE:O	1:B:138:SER:HB3	2.21	0.41
1:A:368:ALA:HA	1:A:393:PHE:CZ	2.56	0.41
1:A:648:TYR:CE2	1:A:693:ILE:HG12	2.55	0.41
1:A:506:LEU:HB2	1:A:509:CYS:HB2	2.02	0.41
1:A:690:LEU:HD22	1:A:755:TYR:HD1	1.85	0.41
1:A:111:MET:HE3	1:A:111:MET:HB3	1.92	0.41
1:A:724:LEU:HD23	1:A:724:LEU:HA	1.95	0.41
1:A:795:PRO:HB3	1:A:797:ARG:HH12	1.86	0.41
1:B:13:GLU:O	1:B:54:ARG:NH1	2.53	0.41
1:B:48:GLY:O	1:B:51:THR:OG1	2.29	0.41
1:B:364:ILE:HD11	1:B:386:LEU:HD22	2.03	0.41
1:B:460:ASP:OD1	1:B:460:ASP:N	2.39	0.41
1:B:677:ASN:ND2	1:B:684:TYR:O	2.54	0.41
1:B:799:ILE:HG22	1:B:855:THR:HB	2.03	0.41
1:A:453:ILE:HG21	1:A:617:VAL:HG22	2.02	0.40
1:A:809:ILE:HD13	1:A:809:ILE:HA	1.92	0.40
1:B:767:TYR:HD1	1:B:815:ILE:HG22	1.85	0.40
1:A:422:ILE:CD1	1:A:675:TYR:CD1	3.03	0.40
1:B:826:GLN:HG2	1:B:827:TRP:N	2.36	0.40
1:B:907:LEU:HB2	1:B:929:VAL:HG23	2.03	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	898/974 (92%)	806 (90%)	90 (10%)	2 (0%)	43 71
1	B	886/974 (91%)	785 (89%)	90 (10%)	11 (1%)	10 37
All	All	1784/1948 (92%)	1591 (89%)	180 (10%)	13 (1%)	18 49

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101	ALA
1	B	145	ALA
1	B	270	ARG
1	B	937	ILE
1	B	55	ILE
1	A	647	ARG
1	B	647	ARG
1	B	823	ASP
1	B	827	TRP
1	B	928	SER
1	B	939	LYS
1	A	52	LEU
1	B	917	GLU

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	745/886 (84%)	744 (100%)	1 (0%)	88 90
1	B	750/886 (85%)	750 (100%)	0	100 100
All	All	1495/1772 (84%)	1494 (100%)	1 (0%)	88 90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	490	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	135	GLN
1	A	139	ASN
1	A	245	GLN
1	A	283	ASN

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Mol	Chain	Res	Type
1	A	413	ASN
1	A	496	ASN
1	A	549	HIS
1	A	581	GLN
1	A	593	ASN
1	A	818	GLN
1	A	819	HIS
1	A	826	GLN
1	A	897	HIS
1	B	135	GLN
1	B	139	ASN
1	B	245	GLN
1	B	451	GLN
1	B	762	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, 95^{th} 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	908/974 (93%)	-0.23	2 (0%)	91	86	41, 79, 116, 140	0
1	B	896/974 (91%)	-0.12	1 (0%)	92	90	57, 90, 126, 157	0
All	All	1804/1948 (92%)	-0.18	3 (0%)	91	86	41, 85, 122, 157	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	907	LEU	3.4
1	A	917	GLU	2.4
1	A	894	LEU	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.