Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 07:30 pm BST

PDB ID	:	6HLU
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)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.29 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.
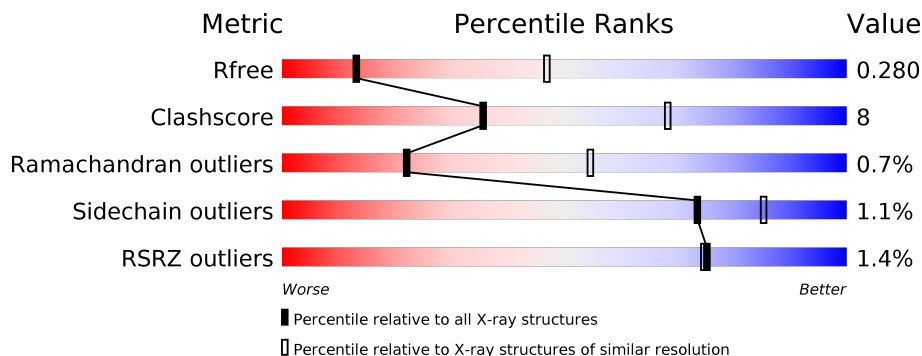
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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	73% 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 6890	C 4379	N 1117	O 1372	S 22	0	0	0
1	B	896	Total 6791	C 4306	N 1103	O 1361	S 21	0	0	0

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 ⓘ

These plots are drawn for all protein, RNA and DNA 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
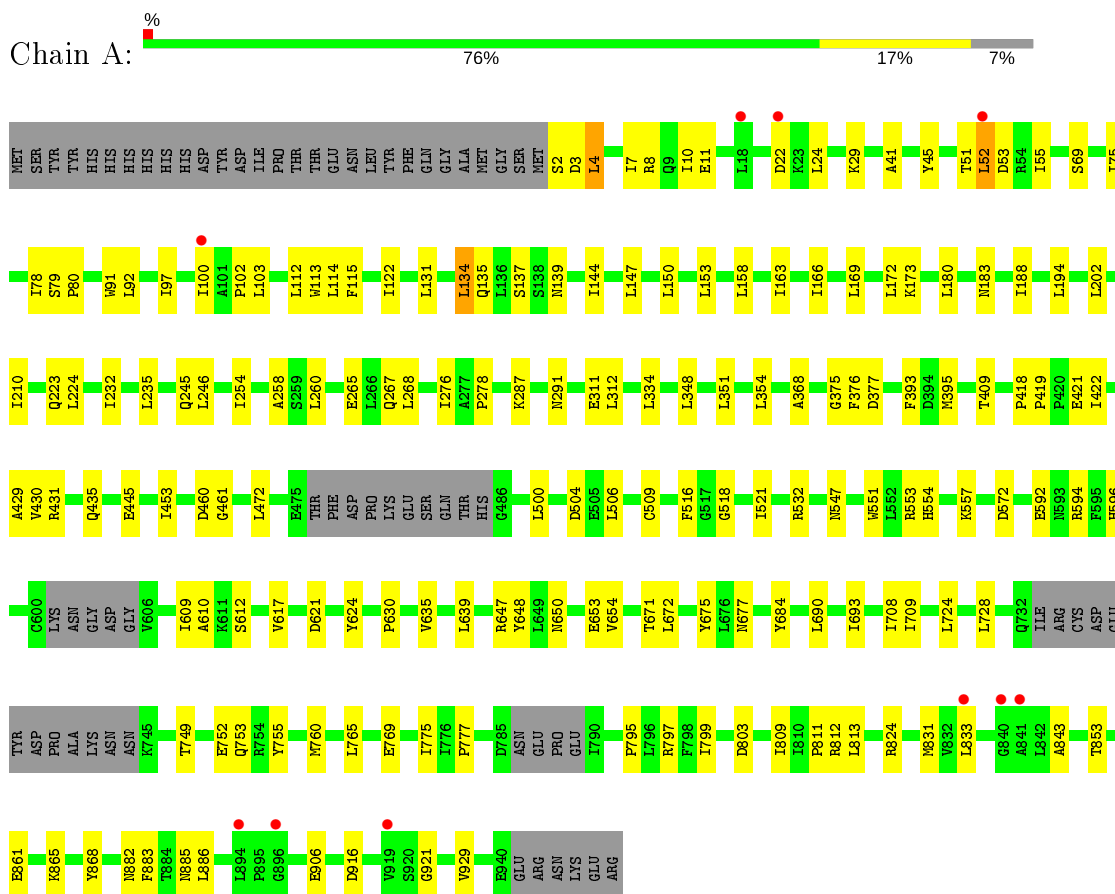
- Molecule 1: Rab family protein
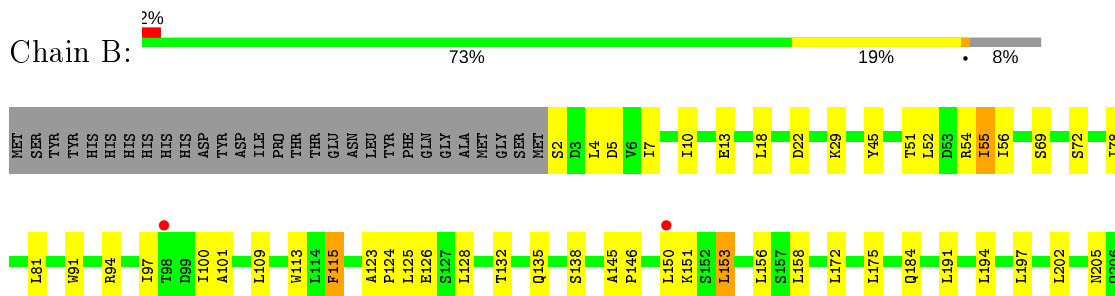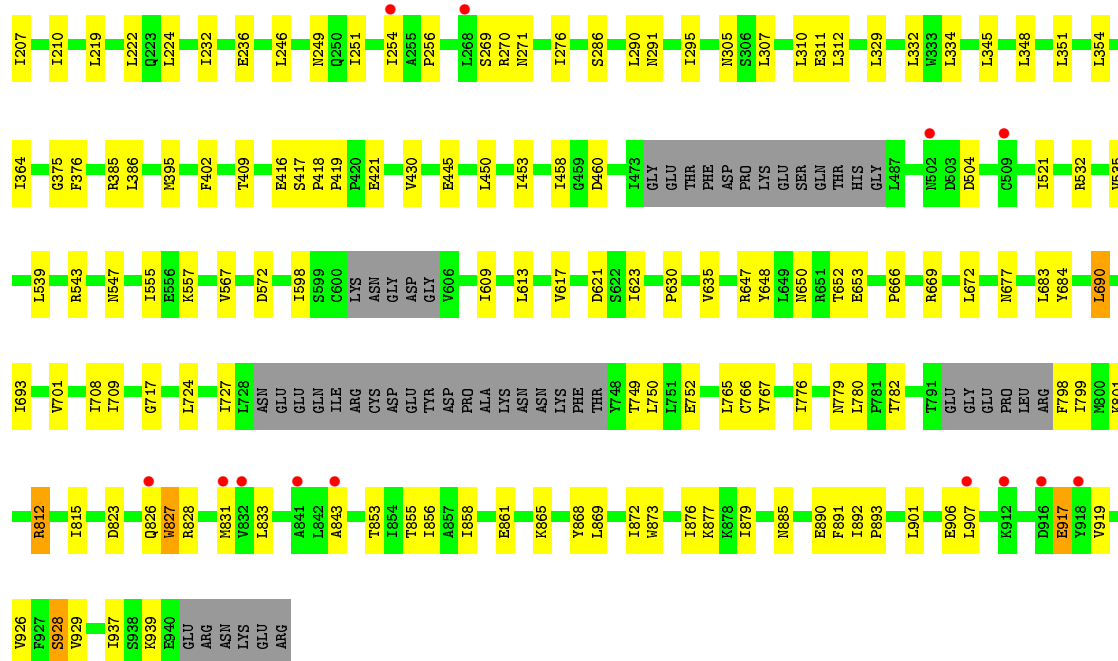
4 Data and refinement statistics (i)

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	Depositor
	47.23 – 3.29	EDS
% Data completeness	99.2 (44.85-3.29)	Depositor
(in resolution range)	99.2 (47.23-3.29)	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	Depositor
	0.229 , 0.280	DCC
R_{free} test set	1686 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å²)	85.1	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.29 , 63.4	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	0.92	EDS
Total number of atoms	13681	wwPDB-VP
Average B, all atoms (Å²)	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.*

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[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 (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	0.24	0/7010	0.44	0/9556
1	B	0.24	0/6906	0.45	0/9419
All	All	0.24	0/13916	0.44	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 (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	6890	0	6658	109	0
1	B	6791	0	6584	113	0
All	All	13681	0	13242	219	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 (219) 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: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
1:B:202:LEU:HD22	1:B:207:ILE:HD13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2:SER:OG	1:A:3:ASP:N	2.38	0.57
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:HD23	1:A:472:LEU:H	1.72	0.54
1:A:833:LEU:HB2	1:A:843:ALA:HB3	1.88	0.54
1:A:547:ASN:HB2	1:B:547:ASN:HB2	1.89	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:557:LYS:HZ1	1:A:803:ASP:CG	2.10	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:A:635:VAL:HG21	1:A:672:LEU:HD21	1.91	0.52
1:A:813:LEU:HD23	1:A:831:MET:HE3	1.92	0.52
1:A:173:LYS:HA	1:A:194:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:598:ILE:HD11	1:B:609:ILE:HD11	1.91	0.51
1:B:78:ILE:HD13	1:B:97:ILE:HD13	1.93	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:312:LEU:HB2	1:B:334:LEU:HD23	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: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:504:ASP:OD1	1:B:504:ASP:N	2.47	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ILE:O	1:B:124:PRO:HG2	2.15	0.47
1:A:650:ASN:ND2	1:A:653:GLU:OE1	2.48	0.46
1:A:4:LEU:O	1:A:7:ILE:HG13	2.14	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:210:ILE:HG12	1:B:224:LEU:HD21	2.00	0.44
1:B:52:LEU:HD23	1:B:52:LEU:HA	1.72	0.44
1:B:290:LEU:HD22	1:B:295:ILE:HD11	1.99	0.44
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:861:GLU:O	1:A:865:LYS:N	2.51	0.43
1:B:650:ASN:OD1	1:B:652:THR:OG1	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:54:ARG:C	1:B:56:ILE:H	2.22	0.43
1:A:775:ILE:O	1:A:777:PRO:HD3	2.19	0.43
1:B:22:ASP:OD1	1:B:22:ASP:N	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:N	1:A:572:ASP:OD1	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: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:115:PHE:O	1:B:138:SER:HB3	2.21	0.41
1:B:51:THR:O	1:B:55:ILE:HG22	2.20	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:795:PRO:HB3	1:A:797:ARG:HH12	1.86	0.41
1:B:460:ASP:OD1	1:B:460:ASP:N	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:ASN:ND2	1:B:684:TYR:O	2.54	0.41
1:A:724:LEU:HA	1:A:724:LEU:HD23	1.95	0.41
1:B:13:GLU:O	1:B:54:ARG:NH1	2.53	0.41
1:B:364:ILE:HD11	1:B:386:LEU:HD22	2.03	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:708:ILE:HG21	1:A:760:MET:HE1	2.03	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%)	47	77
1	B	886/974 (91%)	785 (89%)	90 (10%)	11 (1%)	13	42
All	All	1784/1948 (92%)	1591 (89%)	180 (10%)	13 (1%)	22	54

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

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Mol	Chain	Res	Type
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%)	736 (99%)	9 (1%)	71	83
1	B	750/886 (85%)	742 (99%)	8 (1%)	73	85
All	All	1495/1772 (84%)	1478 (99%)	17 (1%)	73	85

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	112	LEU
1	A	115	PHE
1	A	134	LEU
1	A	150	LEU
1	A	624	TYR
1	A	868	TYR
1	A	885	ASN
1	A	906	GLU
1	B	115	PHE
1	B	150	LEU
1	B	153	LEU
1	B	184	GLN
1	B	305	ASN
1	B	690	LEU
1	B	812	ARG

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Mol	Chain	Res	Type
1	B	868	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	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 carbohydrates 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	908/974 (93%)	-0.04	10 (1%)	80	81	41, 79, 116, 140	0
1	B	896/974 (91%)	0.02	15 (1%)	70	68	57, 90, 126, 157	0
All	All	1804/1948 (92%)	-0.01	25 (1%)	75	75	41, 85, 122, 157	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	254	ILE	4.2
1	B	907	LEU	4.1
1	B	843	ALA	3.6
1	A	894	LEU	3.1
1	B	98	THR	3.1
1	B	509	CYS	3.0
1	B	268	LEU	2.8
1	B	831	MET	2.8
1	A	919	VAL	2.7
1	A	18	LEU	2.6
1	A	840	GLY	2.5
1	B	150	LEU	2.5
1	B	826	GLN	2.5
1	A	841	ALA	2.4
1	B	916	ASP	2.4
1	B	841	ALA	2.3
1	B	918	TYR	2.3
1	B	832	VAL	2.3
1	A	52	LEU	2.2
1	A	833	LEU	2.2
1	B	502	ASN	2.2
1	B	912	LYS	2.2
1	A	100	ILE	2.1
1	A	22	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	896	GLY	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 carbohydrates 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.