



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 02:31 am BST

PDB ID : 5A5C  
Title : Structure of an engineered neuronal LRRTM2 adhesion molecule  
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tunen, H.; Kajander, T.  
Deposited on : 2015-06-17  
Resolution : 2.10 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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

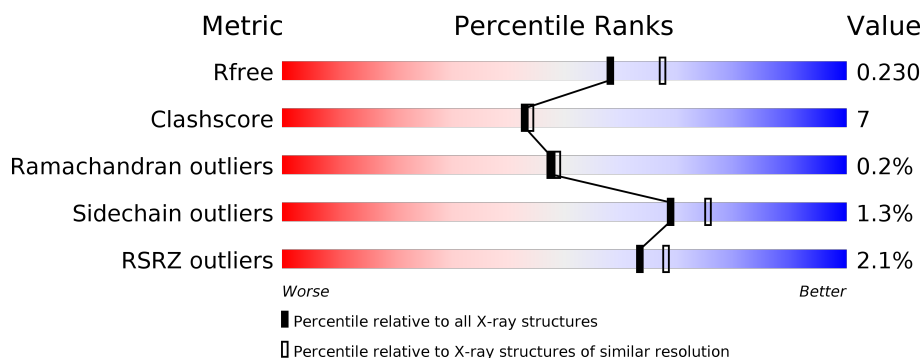
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	357	<div> <div>6%</div> <div>80% 11% 8%</div> </div>
1	B	357	<div> <div>80% 13% 7%</div> </div>
1	C	357	<div> <div>82% 9% 8%</div> </div>
1	D	357	<div> <div>6% 80% 11% 8%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20811 atoms, of which 10133 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 LRRTM.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	330	Total	C	H	N	O	S	0	0	0
			5140	1638	2563	444	487	8			
1	B	332	Total	C	H	N	O	S	0	0	0
			5159	1650	2566	442	492	9			
1	C	329	Total	C	H	N	O	S	0	0	0
			5062	1619	2514	437	484	8			
1	D	329	Total	C	H	N	O	S	0	0	0
			5029	1614	2490	432	484	9			

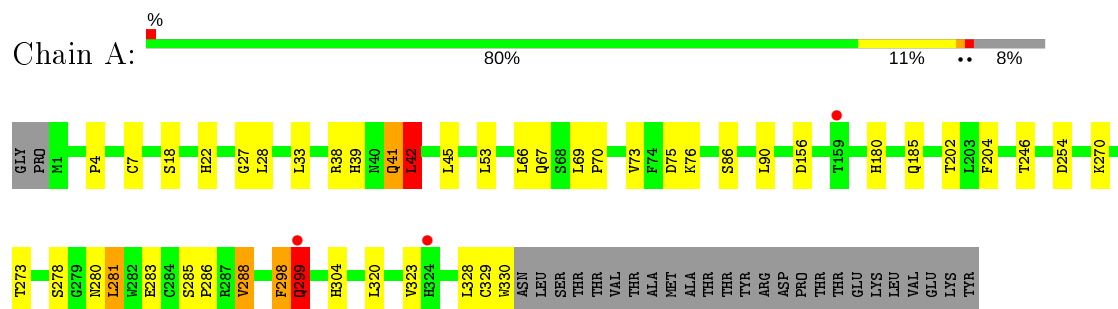
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	133	Total	O	0	0
			133	133		
2	B	139	Total	O	0	0
			139	139		
2	C	104	Total	O	0	0
			104	104		
2	D	45	Total	O	0	0
			45	45		

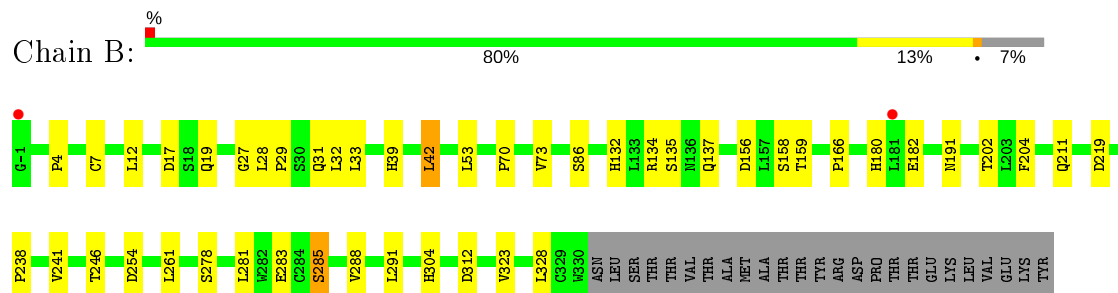
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

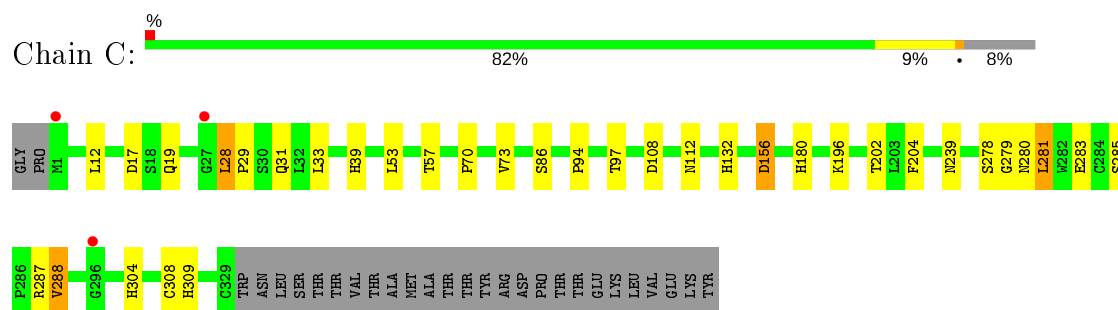
#### • Molecule 1: LRRTM



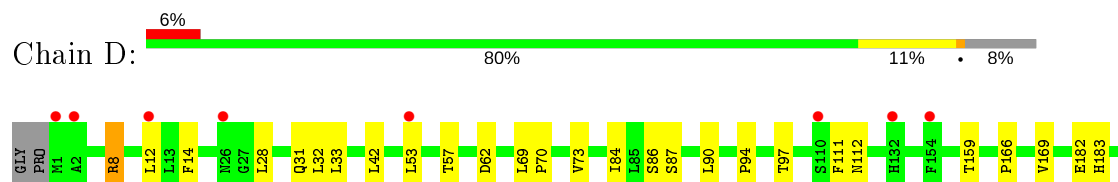
#### • Molecule 1: LRRTM

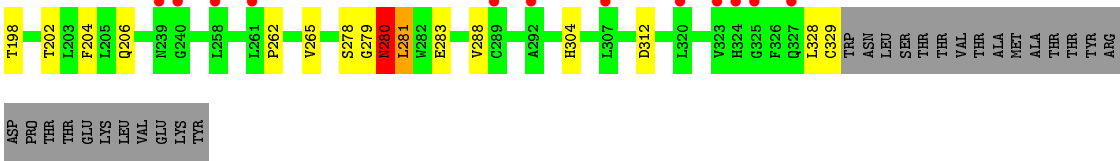


#### • Molecule 1: LRRTM



#### • Molecule 1: LRRTM





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	235.99Å 57.32Å 144.45Å 90.00° 115.49° 90.00°	Depositor
Resolution (Å)	44.74 – 2.10 44.74 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.74-2.10) 99.6 (44.74-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 2.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.195 , 0.236 0.192 , 0.230	Depositor DCC
$R_{free}$ test set	5080 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.1	Xtriage
Anisotropy	0.690	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	20811	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.73	0/2631	0.85	8/3583 (0.2%)
1	B	0.72	0/2650	0.80	6/3612 (0.2%)
1	C	0.68	1/2601 (0.0%)	0.77	3/3546 (0.1%)
1	D	0.63	0/2593	0.78	6/3538 (0.2%)
All	All	0.69	1/10475 (0.0%)	0.80	23/14279 (0.2%)

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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	308	CYS	CB-SG	-5.79	1.72	1.81

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	PHE	C-N-CA	7.66	140.86	121.70
1	A	27	GLY	N-CA-C	-7.40	94.61	113.10
1	D	280	ASN	C-N-CA	7.30	139.96	121.70
1	D	280	ASN	CA-C-N	6.87	132.31	117.20
1	A	41	GLN	N-CA-C	-6.83	92.57	111.00
1	A	298	PHE	CA-C-N	6.80	132.16	117.20
1	D	8	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	D	281	LEU	CA-CB-CG	-6.44	100.49	115.30
1	B	134	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	B	285	SER	N-CA-C	-6.15	94.39	111.00
1	B	42	LEU	CB-CG-CD2	-6.00	100.80	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	LEU	CB-CG-CD1	5.93	121.09	111.00
1	D	280	ASN	O-C-N	-5.81	113.41	122.70
1	B	27	GLY	N-CA-C	-5.79	98.62	113.10
1	A	299	GLN	N-CA-C	-5.79	95.37	111.00
1	C	281	LEU	CB-CG-CD1	5.60	120.51	111.00
1	D	8	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	281	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	A	281	LEU	CB-CG-CD2	-5.48	101.68	111.00
1	C	288	VAL	CB-CA-C	-5.26	101.40	111.40
1	A	298	PHE	O-C-N	-5.10	114.53	122.70
1	C	156	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	A	288	VAL	CB-CA-C	-5.02	101.86	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	280	ASN	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	2577	2563	2552	44	0
1	B	2593	2566	2555	38	0
1	C	2548	2514	2502	27	0
1	D	2539	2490	2479	36	0
2	A	133	0	0	6	0
2	B	139	0	0	7	0
2	C	104	0	0	3	0
2	D	45	0	0	1	0
All	All	10678	10133	10088	138	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 7.

All (138) 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:A:41:GLN:O	1:A:42:LEU:HB2	1.48	1.07
1:A:298:PHE:HA	1:A:299:GLN:HG2	1.49	0.93
1:A:298:PHE:CD1	1:A:299:GLN:HG2	2.10	0.87
1:D:279:GLY:HA2	1:D:280:ASN:HB2	1.56	0.86
1:A:298:PHE:CD1	1:A:299:GLN:CG	2.58	0.85
1:D:202:THR:CG2	1:D:204:PHE:CE2	2.65	0.80
1:A:298:PHE:HD1	1:A:299:GLN:HG2	1.45	0.80
1:A:75:ASP:O	1:A:76:LYS:HB2	1.80	0.79
1:C:202:THR:CG2	1:C:204:PHE:CE2	2.67	0.77
1:A:67:GLN:O	2:A:2026:HOH:O	2.02	0.77
1:B:70:PRO:HD2	1:B:73:VAL:HG11	1.66	0.76
1:C:283:GLU:O	1:C:288:VAL:CG1	2.33	0.76
1:A:298:PHE:HD1	1:A:299:GLN:CG	1.97	0.75
1:B:283:GLU:O	1:B:288:VAL:CG1	2.36	0.74
1:B:132:HIS:HD2	2:B:2047:HOH:O	1.69	0.73
1:D:262:PRO:O	1:D:265:VAL:HG23	1.89	0.73
1:D:283:GLU:O	1:D:288:VAL:HG13	1.88	0.73
1:D:70:PRO:HB2	1:D:73:VAL:HG13	1.71	0.72
1:B:202:THR:CG2	1:B:204:PHE:CE2	2.73	0.72
1:C:283:GLU:O	1:C:288:VAL:HG13	1.89	0.72
1:D:70:PRO:HD2	1:D:73:VAL:HG11	1.71	0.71
1:D:328:LEU:O	1:D:329:CYS:HB2	1.89	0.71
1:A:41:GLN:O	1:A:42:LEU:CB	2.31	0.71
1:C:70:PRO:HB2	1:C:73:VAL:HG13	1.73	0.71
1:A:298:PHE:CD1	1:A:299:GLN:HG3	2.27	0.70
1:D:70:PRO:HB2	1:D:73:VAL:CG1	2.23	0.69
1:B:254:ASP:OD2	1:B:278:SER:HB3	1.92	0.69
1:A:75:ASP:O	1:A:76:LYS:CB	2.39	0.68
2:A:2091:HOH:O	1:B:211:GLN:OE1	2.11	0.68
1:A:53:LEU:HD12	1:A:53:LEU:N	2.09	0.68
1:A:283:GLU:O	1:A:288:VAL:HG13	1.94	0.66
1:B:70:PRO:HB2	1:B:73:VAL:CG1	2.26	0.65
1:C:70:PRO:HD2	1:C:73:VAL:HG11	1.78	0.65
1:B:12:LEU:HB2	2:B:2006:HOH:O	1.97	0.65
1:B:283:GLU:O	1:B:288:VAL:HG13	1.97	0.64
1:A:202:THR:CG2	1:A:204:PHE:CE2	2.81	0.64
1:A:283:GLU:O	1:A:288:VAL:CG1	2.46	0.64
1:D:202:THR:HG21	1:D:204:PHE:CE2	2.33	0.63
1:A:53:LEU:CD1	1:A:53:LEU:N	2.61	0.63
1:A:246:THR:HG23	1:A:270:LYS:HD3	1.81	0.62
1:D:328:LEU:O	1:D:329:CYS:CB	2.42	0.62
1:D:262:PRO:HD2	1:D:265:VAL:HG21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:SER:OG	1:A:304:HIS:HB2	2.00	0.61
1:A:70:PRO:HB2	1:A:73:VAL:HG13	1.83	0.60
1:A:70:PRO:HB2	1:A:73:VAL:CG1	2.32	0.60
1:C:202:THR:HG21	1:C:204:PHE:CE2	2.37	0.60
1:C:278:SER:OG	1:C:304:HIS:HB2	2.02	0.60
1:D:283:GLU:O	1:D:288:VAL:CG1	2.49	0.60
1:D:94:PRO:HG2	1:D:97:THR:OG1	2.01	0.59
1:C:12:LEU:HD23	1:C:31:GLN:O	2.03	0.59
1:B:166:PRO:HD3	2:B:2063:HOH:O	2.03	0.58
1:D:12:LEU:HD23	1:D:31:GLN:O	2.03	0.58
1:A:298:PHE:CA	1:A:299:GLN:HG2	2.29	0.57
1:D:33:LEU:O	1:D:57:THR:HG22	2.04	0.56
1:A:280:ASN:O	1:A:281:LEU:HD12	2.07	0.55
1:B:219:ASP:O	2:B:2100:HOH:O	2.17	0.54
1:C:285:SER:O	1:C:288:VAL:HG22	2.09	0.53
1:B:70:PRO:HB2	1:B:73:VAL:HG13	1.88	0.53
1:A:38:ARG:CZ	1:D:159:THR:HG22	2.39	0.53
1:B:246:THR:HG22	1:B:246:THR:O	2.09	0.53
1:B:70:PRO:CD	1:B:73:VAL:HG11	2.37	0.52
1:B:202:THR:HG21	1:B:204:PHE:CE2	2.44	0.52
1:B:156:ASP:HA	1:B:180:HIS:HB2	1.90	0.52
1:A:69:LEU:HD13	1:A:90:LEU:HD21	1.92	0.51
1:A:329:CYS:O	1:A:330:TRP:CB	2.58	0.51
1:C:94:PRO:HG2	1:C:97:THR:OG1	2.10	0.51
2:A:2072:HOH:O	1:D:8:ARG:NH2	2.38	0.50
1:D:70:PRO:CD	1:D:73:VAL:HG11	2.39	0.50
1:B:288:VAL:HG12	2:B:2117:HOH:O	2.11	0.50
1:C:239:ASN:OD1	2:C:2082:HOH:O	2.20	0.49
1:D:198:THR:OG1	2:D:2027:HOH:O	2.20	0.49
1:D:262:PRO:HB2	1:D:265:VAL:CG2	2.42	0.49
1:B:238:PRO:HG2	1:B:241:VAL:HB	1.95	0.49
1:A:70:PRO:HD2	1:A:73:VAL:HG11	1.95	0.49
1:D:166:PRO:HG2	1:D:169:VAL:HB	1.95	0.48
1:B:323:VAL:HA	1:B:328:LEU:HD12	1.95	0.48
1:C:281:LEU:HG	1:C:309:HIS:CD2	2.48	0.48
1:A:18:SER:HA	1:A:39:HIS:O	2.14	0.48
1:C:202:THR:HG21	1:C:204:PHE:HE2	1.77	0.48
1:D:12:LEU:N	1:D:12:LEU:HD12	2.29	0.47
1:C:287:ARG:NH2	2:C:2103:HOH:O	2.37	0.47
1:A:39:HIS:HE1	1:D:112:ASN:O	1.97	0.47
1:A:69:LEU:HD13	1:A:90:LEU:CD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LEU:N	1:C:53:LEU:CD1	2.77	0.47
1:B:261:LEU:HD12	1:B:291:LEU:HD13	1.95	0.47
1:B:29:PRO:HD2	1:B:32:LEU:HG	1.97	0.46
2:A:2105:HOH:O	1:B:238:PRO:HD3	2.14	0.46
1:C:279:GLY:O	1:C:280:ASN:HB2	2.15	0.46
1:C:53:LEU:HD12	1:C:53:LEU:N	2.30	0.46
1:D:53:LEU:CD1	1:D:53:LEU:N	2.78	0.46
1:D:53:LEU:N	1:D:53:LEU:HD12	2.31	0.46
1:A:4:PRO:HB2	1:A:7:CYS:SG	2.56	0.46
1:B:39:HIS:HE1	1:C:112:ASN:O	1.98	0.46
1:A:246:THR:O	1:A:246:THR:HG22	2.15	0.46
1:B:246:THR:O	1:B:246:THR:CG2	2.64	0.46
1:B:53:LEU:N	1:B:53:LEU:HD12	2.31	0.46
1:A:246:THR:CG2	1:A:270:LYS:HD3	2.46	0.45
1:D:70:PRO:CB	1:D:73:VAL:CG1	2.94	0.45
1:B:12:LEU:HD13	1:B:31:GLN:O	2.16	0.45
1:D:202:THR:HG21	1:D:204:PHE:HE2	1.78	0.45
1:A:22:HIS:C	1:A:42:LEU:HD12	2.36	0.45
1:B:278:SER:HB2	1:B:304:HIS:HB2	1.99	0.44
1:B:17:ASP:O	1:B:19:GLN:HG2	2.18	0.44
2:A:2005:HOH:O	1:D:183:HIS:HD2	2.00	0.44
1:B:53:LEU:N	1:B:53:LEU:CD1	2.80	0.44
1:D:69:LEU:HD13	1:D:90:LEU:CD2	2.48	0.44
1:B:135:SER:OG	1:C:39:HIS:HE1	2.01	0.44
1:D:87:SER:HA	1:D:111:PHE:O	2.19	0.43
1:A:254:ASP:OD2	1:A:278:SER:HB2	2.19	0.43
1:D:14:PHE:CD1	1:D:32:LEU:HD21	2.54	0.43
1:A:45:LEU:CD2	1:A:66:LEU:CD2	2.97	0.43
1:B:191:ASN:ND2	2:B:2088:HOH:O	2.52	0.43
1:B:135:SER:HA	1:B:159:THR:O	2.19	0.42
1:A:156:ASP:HA	1:A:180:HIS:HB2	2.01	0.42
1:A:323:VAL:HA	1:A:328:LEU:HD12	2.01	0.42
1:D:62:ASP:HB3	1:D:84:ILE:HG22	2.00	0.42
1:C:17:ASP:O	1:C:19:GLN:HG2	2.19	0.42
1:A:185:GLN:HG2	1:D:8:ARG:NH2	2.35	0.42
1:C:28:LEU:HA	1:C:29:PRO:HD3	1.86	0.42
1:A:45:LEU:CD2	1:A:66:LEU:HD22	2.50	0.42
1:B:132:HIS:CD2	2:B:2047:HOH:O	2.56	0.42
1:C:33:LEU:O	1:C:57:THR:HG22	2.19	0.42
1:A:285:SER:O	1:A:288:VAL:HG22	2.20	0.41
1:B:70:PRO:CB	1:B:73:VAL:CG1	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:PRO:HB2	1:B:7:CYS:SG	2.60	0.41
1:A:273:THR:OG1	2:A:2119:HOH:O	2.22	0.41
1:B:285:SER:O	1:B:288:VAL:HG22	2.20	0.41
1:D:182:GLU:HB2	1:D:206:GLN:HG2	2.02	0.41
1:C:196:LYS:NZ	2:C:2063:HOH:O	2.36	0.41
1:A:285:SER:HB2	1:A:286:PRO:CD	2.51	0.41
1:C:108:ASP:HA	1:C:132:HIS:HB2	2.01	0.41
1:C:70:PRO:CB	1:C:73:VAL:HG13	2.48	0.41
1:B:158:SER:HB2	1:B:182:GLU:HG2	2.02	0.41
1:B:137:GLN:HE21	1:C:39:HIS:CD2	2.39	0.41
1:A:38:ARG:NE	1:D:159:THR:CG2	2.84	0.41
1:A:320:LEU:HA	1:A:320:LEU:HD23	1.92	0.40
1:D:278:SER:OG	1:D:304:HIS:HB2	2.20	0.40
1:C:156:ASP:HA	1:C:180:HIS:HB2	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	328/357 (92%)	304 (93%)	22 (7%)	2 (1%)	25	21
1	B	330/357 (92%)	311 (94%)	19 (6%)	0	100	100
1	C	327/357 (92%)	305 (93%)	22 (7%)	0	100	100
1	D	327/357 (92%)	306 (94%)	20 (6%)	1 (0%)	41	41
All	All	1312/1428 (92%)	1226 (93%)	83 (6%)	3 (0%)	47	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	LEU

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Mol	Chain	Res	Type
1	D	281	LEU
1	A	299	GLN

### 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	299/330 (91%)	295 (99%)	4 (1%)	69	75
1	B	301/330 (91%)	296 (98%)	5 (2%)	60	67
1	C	293/330 (89%)	291 (99%)	2 (1%)	84	88
1	D	292/330 (88%)	288 (99%)	4 (1%)	67	73
All	All	1185/1320 (90%)	1170 (99%)	15 (1%)	69	75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	33	LEU
1	A	42	LEU
1	A	86	SER
1	B	28	LEU
1	B	33	LEU
1	B	42	LEU
1	B	86	SER
1	B	312	ASP
1	C	28	LEU
1	C	86	SER
1	D	28	LEU
1	D	42	LEU
1	D	86	SER
1	D	312	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	183	HIS
1	C	39	HIS
1	C	309	HIS

### 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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	330/357 (92%)	0.00	3 (0%) 84 86	29, 50, 73, 95	0
1	B	332/357 (92%)	-0.06	2 (0%) 89 91	30, 47, 71, 82	0
1	C	329/357 (92%)	-0.16	3 (0%) 84 86	33, 51, 76, 94	0
1	D	329/357 (92%)	0.32	20 (6%) 21 26	40, 63, 87, 108	0
All	All	1320/1428 (92%)	0.03	28 (2%) 63 68	29, 52, 80, 108	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	4.3
1	D	325	GLY	4.0
1	B	-1	GLY	3.9
1	D	323	VAL	3.7
1	D	324	HIS	3.4
1	D	239	ASN	3.1
1	D	26	ASN	2.9
1	D	261	LEU	2.8
1	D	320	LEU	2.8
1	D	240	GLY	2.7
1	C	1	MET	2.7
1	D	154	PHE	2.6
1	D	292	ALA	2.6
1	C	296	GLY	2.5
1	B	181	LEU	2.4
1	D	110	SER	2.4
1	D	327	GLN	2.4
1	D	258	LEU	2.3
1	D	307	LEU	2.3
1	A	299	GLN	2.2
1	D	132	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	159	THR	2.2
1	D	53	LEU	2.1
1	D	289	CYS	2.1
1	C	27	GLY	2.1
1	D	12	LEU	2.1
1	D	2	ALA	2.1
1	A	324	HIS	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.