



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:42 AM UTC

PDB ID : 2XJZ / pdb_00002xjz
Title : Crystal structure of the LMO2:LDB1-LID complex, C2 crystal form
Authors : El Omari, K.; Karia, D.; Porcher, C.; Mancini, E.J.
Deposited on : 2010-07-06
Resolution : 2.80 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

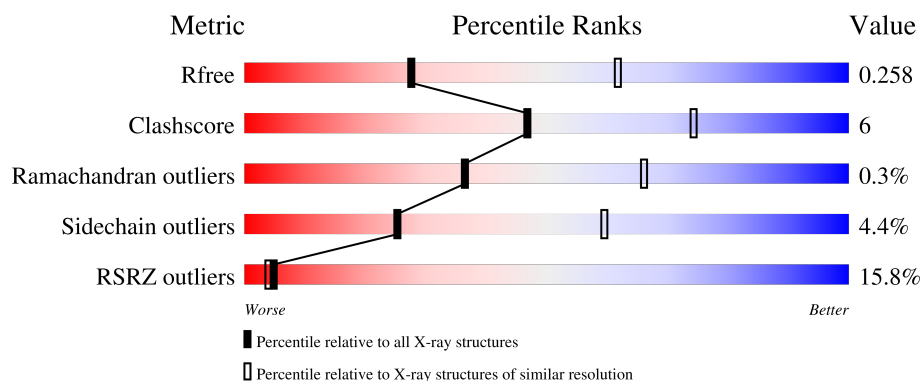
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	131	14% 80% 12% • 5%
1	B	131	8% 75% 17% • 7%
1	C	131	21% 74% 10% • 15%
1	D	131	11% 84% 14% • •
1	E	131	17% 80% 15% • • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	36	8% 69% 8% 19%
2	J	36	28% 61% 22% 14%
2	K	36	11% 50% 8% 42%
2	L	36	11% 64% 17% 19%
2	M	36	19% 58% 14% 28%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6166 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 RHOMBOTIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			1029	645	187	182	15			
1	B	122	Total	C	N	O	S	0	0	0
			1011	634	184	177	16			
1	C	112	Total	C	N	O	S	0	0	0
			920	575	168	162	15			
1	D	129	Total	C	N	O	S	0	0	0
			1056	663	190	187	16			
1	E	127	Total	C	N	O	S	0	0	0
			1039	650	189	184	16			

- Molecule 2 is a protein called LIM DOMAIN-BINDING PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	29	Total	C	N	O	S	0	0	0
			223	136	36	49	2			
2	J	31	Total	C	N	O	S	0	0	0
			230	139	38	51	2			
2	K	21	Total	C	N	O	S	0	0	0
			157	95	24	36	2			
2	L	29	Total	C	N	O	S	0	0	0
			223	136	36	49	2			
2	M	26	Total	C	N	O	S	0	0	0
			199	123	32	42	2			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	333	SER	-	expression tag	UNP Q86U70
J	333	SER	-	expression tag	UNP Q86U70
K	333	SER	-	expression tag	UNP Q86U70
L	333	SER	-	expression tag	UNP Q86U70
M	333	SER	-	expression tag	UNP Q86U70

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	Zn 4	0	0
3	B	4	Total 4	Zn 4	0	0
3	C	4	Total 4	Zn 4	0	0
3	D	4	Total 4	Zn 4	0	0
3	E	4	Total 4	Zn 4	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0

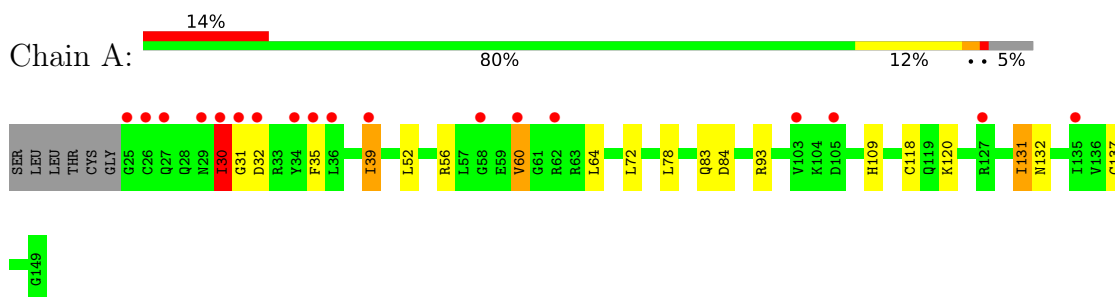
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total 7	O 7	0	0
5	B	15	Total 15	O 15	0	0
5	C	10	Total 10	O 10	0	0
5	D	11	Total 11	O 11	0	0
5	E	4	Total 4	O 4	0	0
5	I	2	Total 2	O 2	0	0
5	J	3	Total 3	O 3	0	0
5	K	1	Total 1	O 1	0	0
5	L	1	Total 1	O 1	0	0
5	M	3	Total 3	O 3	0	0

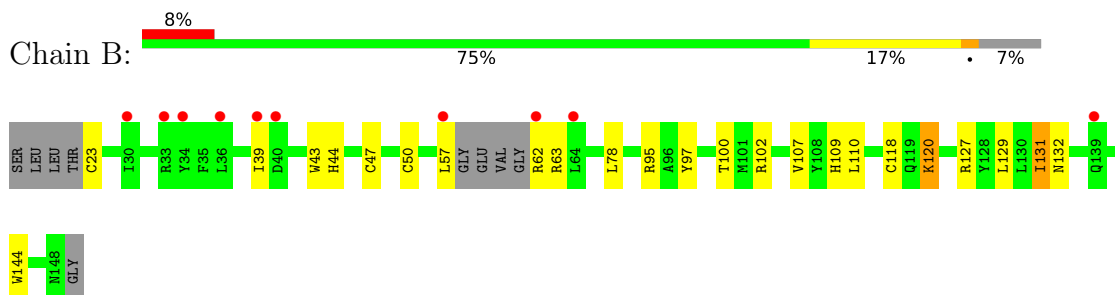
3 Residue-property plots [i](#)

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.

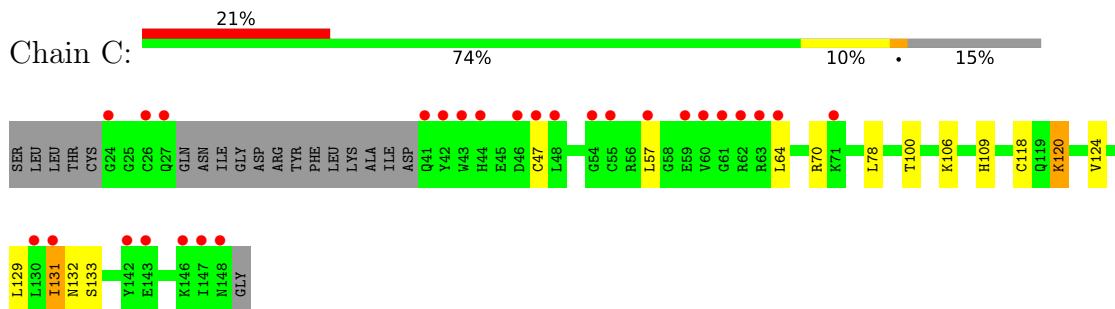
• Molecule 1: RHOMBOTIN-2



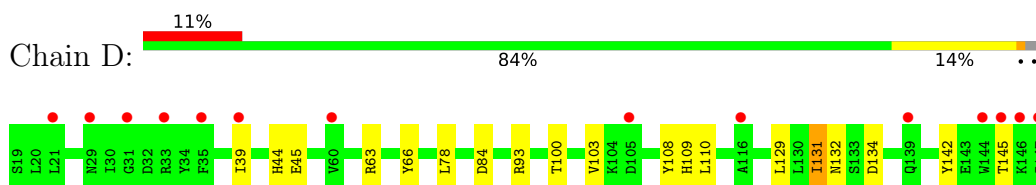
• Molecule 1: RHOMBOTIN-2



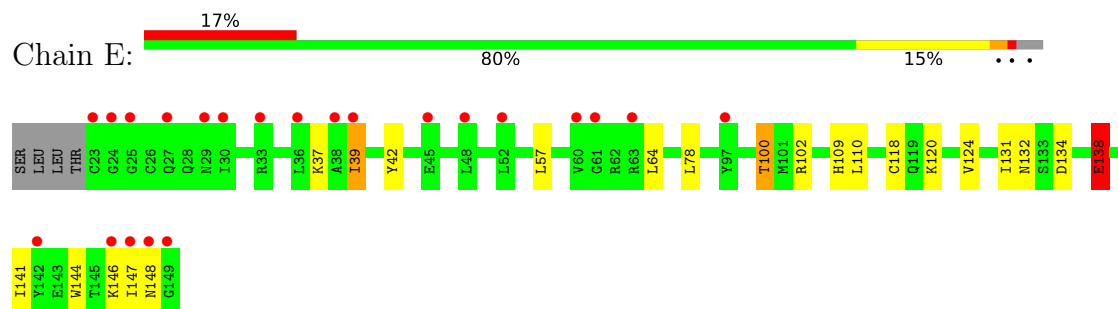
• Molecule 1: RHOMBOTIN-2



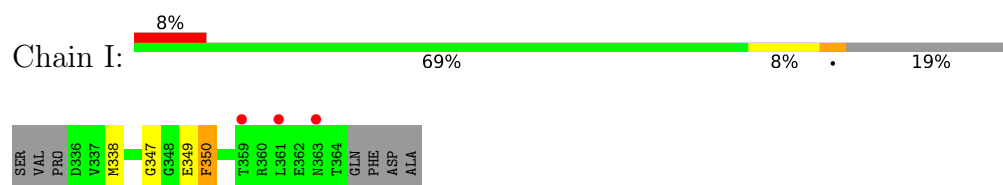
• Molecule 1: RHOMBOTIN-2



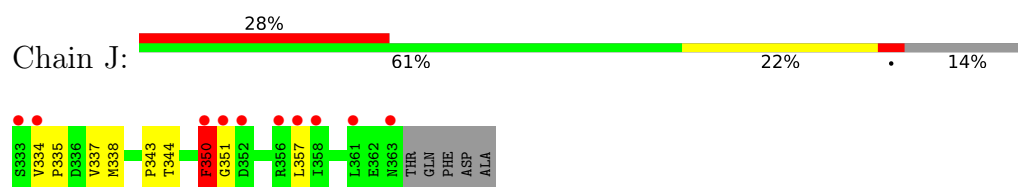
- Molecule 1: RHOMBOTIN-2



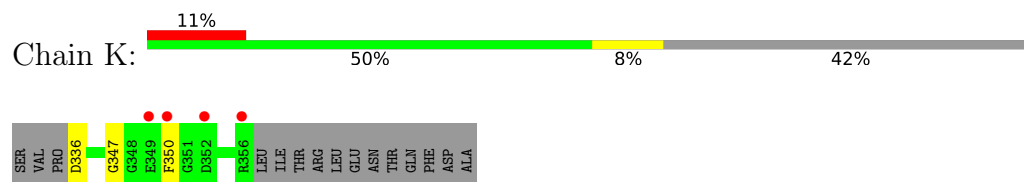
- Molecule 2: LIM DOMAIN-BINDING PROTEIN 1



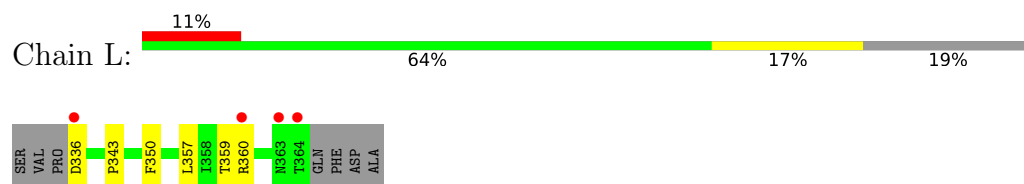
- Molecule 2: LIM DOMAIN-BINDING PROTEIN 1



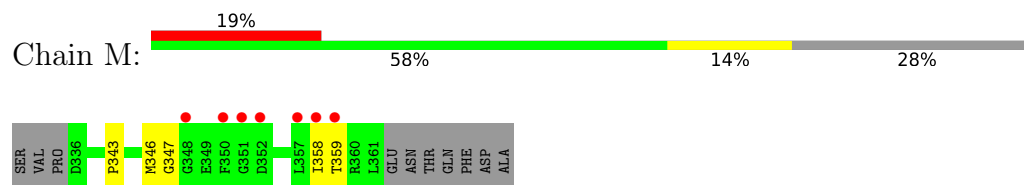
- Molecule 2: LIM DOMAIN-BINDING PROTEIN 1



- Molecule 2: LIM DOMAIN-BINDING PROTEIN 1



- Molecule 2: LIM DOMAIN-BINDING PROTEIN 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.92Å 55.53Å 114.71Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	48.32 – 2.80 48.32 – 2.81	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.32-2.80) 96.4 (48.32-2.81)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.228 , 0.244 0.239 , 0.258	Depositor DCC
R_{free} test set	1376 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 83.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6166	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 4.92% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CL

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	0.77	0/1048	1.30	3/1402 (0.2%)
1	B	0.80	0/1029	1.28	4/1375 (0.3%)
1	C	0.82	0/936	1.30	2/1250 (0.2%)
1	D	0.77	0/1075	1.26	5/1439 (0.3%)
1	E	0.78	0/1058	1.27	3/1415 (0.2%)
2	I	0.88	0/224	1.40	4/301 (1.3%)
2	J	0.85	0/231	1.26	3/309 (1.0%)
2	K	0.82	0/158	1.47	3/211 (1.4%)
2	L	0.79	0/224	1.24	1/301 (0.3%)
2	M	0.78	0/200	1.24	2/268 (0.7%)
All	All	0.79	0/6183	1.29	30/8271 (0.4%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	ILE	N-CA-C	13.39	123.12	110.53
1	C	47	CYS	N-CA-C	8.93	121.10	111.36
1	D	142	TYR	N-CA-C	7.35	118.93	111.07
1	D	84	ASP	CA-CB-CG	7.26	119.86	112.60
2	I	350	PHE	N-CA-C	7.26	121.40	112.54
1	A	84	ASP	CA-CB-CG	6.97	119.57	112.60
1	D	44	HIS	N-CA-C	-6.28	101.65	110.50
2	J	350	PHE	N-CA-C	6.14	117.64	111.07
1	D	109	HIS	N-CA-C	-6.00	101.52	110.23
1	A	109	HIS	N-CA-C	-5.87	101.72	110.23
1	E	109	HIS	N-CA-C	-5.77	101.75	110.28
2	L	350	PHE	N-CA-C	5.76	120.45	112.90
2	K	347	GLY	CA-C-N	5.54	127.07	120.14
2	K	347	GLY	C-N-CA	5.54	127.07	120.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	350	PHE	N-CA-C	5.54	120.15	112.90
1	C	109	HIS	N-CA-C	-5.53	102.21	110.23
1	E	100	THR	N-CA-C	5.48	117.51	109.24
2	M	347	GLY	CA-C-N	5.39	127.07	120.22
2	M	347	GLY	C-N-CA	5.39	127.07	120.22
1	B	109	HIS	N-CA-C	-5.39	102.42	110.23
1	D	134	ASP	CA-CB-CG	5.25	117.85	112.60
1	E	138	GLU	CB-CG-CD	5.21	121.45	112.60
2	I	349	GLU	CA-C-N	5.18	129.37	120.72
2	I	349	GLU	C-N-CA	5.18	129.37	120.72
2	J	357	LEU	N-CA-C	5.16	117.38	109.07
1	B	62	ARG	CA-C-N	5.14	128.64	121.24
1	B	62	ARG	C-N-CA	5.14	128.64	121.24
2	J	337	VAL	N-CA-CB	5.08	116.64	110.95
1	B	63	ARG	N-CA-C	5.06	117.03	109.59
2	I	338	MET	N-CA-C	5.01	117.48	109.81

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	1029	0	997	11	0
1	B	1011	0	979	15	0
1	C	920	0	891	6	0
1	D	1056	0	1029	14	0
1	E	1039	0	1004	17	0
2	I	223	0	211	2	0
2	J	230	0	210	8	0
2	K	157	0	139	0	0
2	L	223	0	211	6	0
2	M	199	0	192	3	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	4	0	0	0	0
3	E	4	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	7	0	0	0	0
5	B	15	0	0	1	0
5	C	10	0	0	0	0
5	D	11	0	0	0	0
5	E	4	0	0	0	0
5	I	2	0	0	0	0
5	J	3	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	3	0	0	0	0
All	All	6166	0	5863	68	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 6.

All (68) 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:56:ARG:O	1:A:60:VAL:HG23	1.50	1.08
2:J:350:PHE:HD2	2:J:351:GLY:N	1.57	1.02
2:J:350:PHE:CD2	2:J:351:GLY:N	2.36	0.92
2:J:350:PHE:CD2	2:J:350:PHE:C	2.46	0.92
1:A:30:ILE:HG13	1:A:31:GLY:N	1.94	0.81
1:A:56:ARG:O	1:A:60:VAL:CG2	2.30	0.79
1:D:39:ILE:HD11	1:D:66:TYR:CD1	2.20	0.75
1:E:37:LYS:HE2	1:E:42:TYR:HE2	1.52	0.74
1:D:39:ILE:CD1	1:D:66:TYR:CD1	2.70	0.74
1:D:39:ILE:HG22	1:D:39:ILE:O	1.87	0.74
1:B:97:TYR:O	1:C:70:ARG:NH2	2.22	0.72
1:A:118:CYS:SG	1:A:120:LYS:HB3	2.35	0.67
1:E:118:CYS:SG	1:E:120:LYS:HB3	2.35	0.66
1:B:118:CYS:SG	1:B:120:LYS:HB3	2.35	0.66
1:C:118:CYS:SG	1:C:120:LYS:HB3	2.39	0.62
1:D:45:GLU:HG2	2:L:360:ARG:HH22	1.66	0.59
1:D:39:ILE:HD13	1:D:66:TYR:CD1	2.37	0.58
1:D:39:ILE:HD13	1:D:66:TYR:CE1	2.39	0.57
1:E:131:ILE:HD11	1:E:144:TRP:HE1	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ILE:O	1:D:39:ILE:CG2	2.55	0.54
1:E:147:ILE:HG21	2:L:357:LEU:HB3	1.90	0.53
1:E:147:ILE:HD12	1:E:148:ASN:HB2	1.89	0.53
1:B:100:THR:CG2	1:B:107:VAL:HG22	2.39	0.53
1:B:95:ARG:NH1	5:B:2007:HOH:O	2.42	0.53
1:A:30:ILE:HD13	1:A:35:PHE:HB3	1.91	0.52
1:A:39:ILE:HD11	1:A:64:LEU:HD11	1.92	0.52
1:B:129:LEU:HD23	1:B:131:ILE:HD11	1.92	0.52
1:E:131:ILE:HG13	1:E:134:ASP:HB2	1.93	0.50
1:D:129:LEU:HD12	2:L:336:ASP:O	2.11	0.49
1:A:52:LEU:HD23	1:A:72:LEU:HD21	1.95	0.49
1:B:50:CYS:HB2	1:B:57:LEU:HD21	1.96	0.48
2:J:350:PHE:CD2	2:J:351:GLY:CA	2.97	0.48
1:A:30:ILE:HG13	1:A:32:ASP:H	1.80	0.47
1:B:131:ILE:HD13	1:B:144:TRP:CZ3	2.49	0.47
1:C:57:LEU:HG	1:C:64:LEU:HD13	1.95	0.47
1:B:100:THR:HG21	1:B:107:VAL:HG22	1.97	0.47
1:A:83:GLN:HB3	2:I:350:PHE:CD1	2.50	0.47
1:D:39:ILE:HD11	1:D:66:TYR:HD1	1.78	0.47
1:B:100:THR:HG21	1:B:107:VAL:CG2	2.45	0.45
1:D:63:ARG:HE	2:L:357:LEU:HD21	1.81	0.45
1:D:103:VAL:CG1	1:D:108:TYR:HE2	2.29	0.45
1:E:131:ILE:O	1:E:132:ASN:HB2	2.16	0.45
1:E:37:LYS:HE2	1:E:42:TYR:CE2	2.42	0.45
1:B:131:ILE:O	1:B:132:ASN:HB2	2.16	0.45
1:E:131:ILE:CD1	1:E:144:TRP:HE1	2.30	0.44
1:E:146:LYS:HB3	2:L:359:THR:HG23	1.98	0.44
1:C:131:ILE:O	1:C:132:ASN:HB2	2.16	0.44
1:A:30:ILE:CD1	1:A:35:PHE:HB3	2.48	0.44
1:E:64:LEU:HB2	2:M:358:ILE:HD11	1.99	0.44
1:A:131:ILE:O	1:A:132:ASN:HB2	2.17	0.43
1:B:110:LEU:HD13	2:J:343:PRO:HB3	1.99	0.43
1:C:106:LYS:NZ	1:C:133:SER:HB3	2.33	0.43
1:B:102:ARG:HD2	2:J:344:THR:HG21	2.01	0.43
1:E:110:LEU:HD13	2:M:343:PRO:HB3	1.99	0.43
1:E:39:ILE:HD11	1:E:64:LEU:HD21	2.00	0.43
2:J:350:PHE:HD2	2:J:351:GLY:CA	2.29	0.42
1:B:23:CYS:SG	1:B:43:TRP:HA	2.60	0.42
1:C:129:LEU:HD23	1:C:131:ILE:HD11	2.01	0.42
1:D:110:LEU:HD13	2:L:343:PRO:HB3	2.02	0.42
1:B:44:HIS:H	1:B:47:CYS:HB2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:LYS:HG2	1:E:42:TYR:CD2	2.55	0.42
1:E:57:LEU:HD13	1:E:64:LEU:HD13	2.02	0.41
1:E:102:ARG:NH2	2:M:346:MET:O	2.42	0.41
1:E:138:GLU:HA	1:E:141:ILE:CD1	2.50	0.41
1:B:127:ARG:HA	2:J:338:MET:O	2.21	0.41
2:I:347:GLY:HA2	2:I:350:PHE:HD1	1.85	0.41
1:D:129:LEU:HD23	1:D:131:ILE:HD11	2.03	0.40
1:D:131:ILE:O	1:D:132:ASN:HB2	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	123/131 (94%)	113 (92%)	10 (8%)	0	100	100
1	B	118/131 (90%)	111 (94%)	7 (6%)	0	100	100
1	C	108/131 (82%)	99 (92%)	9 (8%)	0	100	100
1	D	127/131 (97%)	121 (95%)	6 (5%)	0	100	100
1	E	125/131 (95%)	117 (94%)	8 (6%)	0	100	100
2	I	27/36 (75%)	25 (93%)	2 (7%)	0	100	100
2	J	29/36 (81%)	27 (93%)	0	2 (7%)	1	2
2	K	19/36 (53%)	18 (95%)	1 (5%)	0	100	100
2	L	27/36 (75%)	25 (93%)	2 (7%)	0	100	100
2	M	24/36 (67%)	24 (100%)	0	0	100	100
All	All	727/835 (87%)	680 (94%)	45 (6%)	2 (0%)	36	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	335	PRO
2	J	334	VAL

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	110/115 (96%)	103 (94%)	7 (6%)	16	44
1	B	109/115 (95%)	105 (96%)	4 (4%)	30	65
1	C	99/115 (86%)	94 (95%)	5 (5%)	21	54
1	D	114/115 (99%)	109 (96%)	5 (4%)	25	59
1	E	111/115 (96%)	106 (96%)	5 (4%)	24	58
2	I	25/31 (81%)	25 (100%)	0	100	100
2	J	25/31 (81%)	24 (96%)	1 (4%)	28	63
2	K	17/31 (55%)	16 (94%)	1 (6%)	18	48
2	L	25/31 (81%)	25 (100%)	0	100	100
2	M	22/31 (71%)	21 (96%)	1 (4%)	24	58
All	All	657/730 (90%)	628 (96%)	29 (4%)	25	59

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ILE
1	A	39	ILE
1	A	60	VAL
1	A	78	LEU
1	A	93	ARG
1	A	131	ILE
1	A	137	CYS
1	B	39	ILE
1	B	78	LEU
1	B	120	LYS
1	B	131	ILE
1	C	78	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	100	THR
1	C	120	LYS
1	C	124	VAL
1	C	131	ILE
1	D	78	LEU
1	D	93	ARG
1	D	100	THR
1	D	131	ILE
1	D	145	THR
1	E	39	ILE
1	E	78	LEU
1	E	100	THR
1	E	124	VAL
1	E	138	GLU
2	J	350	PHE
2	K	336	ASP
2	M	359	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	119	GLN
1	A	121	HIS
1	B	41	GLN
1	B	119	GLN
1	B	148	ASN
1	C	41	GLN
1	C	121	HIS
1	D	41	GLN
1	D	121	HIS
1	E	41	GLN
1	E	121	HIS
1	E	139	GLN
1	E	148	ASN

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 ⓘ

Of 22 ligands modelled in this entry, 22 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	125/131 (95%)	0.82	18 (14%) 6 5	42, 74, 186, 213	0
1	B	122/131 (93%)	0.40	10 (8%) 17 13	29, 61, 144, 166	0
1	C	112/131 (85%)	0.95	27 (24%) 2 1	31, 72, 171, 190	0
1	D	129/131 (98%)	0.67	14 (10%) 10 8	41, 84, 142, 161	0
1	E	127/131 (96%)	0.93	22 (17%) 4 3	39, 78, 196, 208	0
2	I	29/36 (80%)	0.65	3 (10%) 12 9	37, 78, 148, 149	0
2	J	31/36 (86%)	1.31	10 (32%) 1 1	37, 94, 137, 147	0
2	K	21/36 (58%)	1.06	4 (19%) 3 2	46, 73, 128, 141	0
2	L	29/36 (80%)	0.63	4 (13%) 6 5	40, 76, 133, 178	0
2	M	26/36 (72%)	1.27	7 (26%) 1 1	47, 102, 130, 148	0
All	All	751/835 (89%)	0.79	119 (15%) 5 4	29, 76, 161, 213	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	44	HIS	6.2
1	E	147	ILE	5.7
2	J	358	ILE	5.3
1	C	60	VAL	4.7
1	C	43	TRP	4.6
2	J	334	VAL	4.5
1	A	25	GLY	4.4
1	C	48	LEU	4.3
2	J	351	GLY	4.1
1	D	147	ILE	4.0
1	E	48	LEU	3.9
1	C	148	ASN	3.7
1	C	147	ILE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	47	CYS	3.7
2	L	364	THR	3.6
1	E	39	ILE	3.5
1	C	64	LEU	3.5
1	A	31	GLY	3.5
2	M	348	GLY	3.5
1	D	146	LYS	3.4
1	B	62	ARG	3.3
1	B	57	LEU	3.3
1	A	105	ASP	3.3
1	C	57	LEU	3.3
1	A	34	TYR	3.2
1	E	30	ILE	3.2
1	D	116	ALA	3.2
1	C	41	GLN	3.1
2	K	356	ARG	3.1
2	J	357	LEU	3.1
1	A	27	GLN	3.1
2	M	358	ILE	3.0
1	C	55	CYS	3.0
1	D	33	ARG	3.0
1	B	33	ARG	2.9
1	E	36	LEU	2.9
1	C	71	LYS	2.9
2	M	357	LEU	2.9
1	C	42	TYR	2.9
1	D	145	THR	2.9
1	D	21	LEU	2.9
1	C	24	GLY	2.8
1	C	142	TYR	2.8
1	E	33	ARG	2.8
1	A	135	ILE	2.8
2	J	356	ARG	2.8
1	A	35	PHE	2.8
1	D	29	ASN	2.7
1	C	54	GLY	2.7
1	E	63	ARG	2.7
1	E	25	GLY	2.7
1	D	144	TRP	2.7
1	E	146	LYS	2.7
1	A	30	ILE	2.7
1	E	149	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	I	359	THR	2.7
2	I	363	ASN	2.7
1	C	27	GLN	2.7
1	A	103	VAL	2.6
1	D	39	ILE	2.6
2	J	350	PHE	2.6
1	E	29	ASN	2.6
2	J	352	ASP	2.6
2	J	361	LEU	2.5
2	K	350	PHE	2.5
1	C	61	GLY	2.5
1	B	139	GLN	2.5
1	D	105	ASP	2.5
1	D	139	GLN	2.5
1	B	36	LEU	2.4
1	C	46	ASP	2.4
1	E	61	GLY	2.4
1	A	32	ASP	2.4
1	C	143	GLU	2.4
1	A	39	ILE	2.4
2	J	363	ASN	2.4
1	E	24	GLY	2.4
1	C	59	GLU	2.4
2	M	359	THR	2.4
1	B	64	LEU	2.4
1	E	148	ASN	2.3
1	E	38	ALA	2.3
2	K	349	GLU	2.3
1	D	31	GLY	2.3
1	C	26	CYS	2.3
1	C	130	LEU	2.3
1	E	97	TYR	2.3
2	J	333	SER	2.3
1	A	127	ARG	2.3
1	B	39	ILE	2.3
1	E	142	TYR	2.3
2	M	351	GLY	2.3
1	A	29	ASN	2.2
1	E	27	GLN	2.2
2	K	352	ASP	2.2
2	L	336	ASP	2.2
1	E	23	CYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	60	VAL	2.2
2	I	361	LEU	2.2
1	B	30	ILE	2.2
1	B	34	TYR	2.2
1	A	26	CYS	2.2
2	M	350	PHE	2.2
1	C	62	ARG	2.1
1	B	40	ASP	2.1
2	M	352	ASP	2.1
1	C	146	LYS	2.1
1	A	36	LEU	2.1
1	A	62	ARG	2.1
1	E	45	GLU	2.1
1	A	60	VAL	2.1
1	A	58	GLY	2.1
1	D	35	PHE	2.1
2	L	360	ARG	2.1
1	D	60	VAL	2.0
1	E	52	LEU	2.0
2	L	363	ASN	2.0
1	C	63	ARG	2.0
1	C	131	ILE	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	E	204	1/1	0.88	0.12	215,215,215,215	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	B	1149	1/1	0.88	0.14	109,109,109,109	0
3	ZN	A	204	1/1	0.89	0.14	152,152,152,152	0
4	CL	D	1148	1/1	0.92	0.14	82,82,82,82	0
3	ZN	C	204	1/1	0.93	0.19	149,149,149,149	0
3	ZN	A	201	1/1	0.94	0.10	87,87,87,87	0
3	ZN	B	204	1/1	0.94	0.09	189,189,189,189	0
3	ZN	D	203	1/1	0.95	0.13	73,73,73,73	0
3	ZN	E	202	1/1	0.95	0.12	64,64,64,64	0
3	ZN	E	203	1/1	0.95	0.08	113,113,113,113	0
3	ZN	C	202	1/1	0.95	0.15	62,62,62,62	0
3	ZN	B	202	1/1	0.95	0.12	61,61,61,61	0
3	ZN	D	201	1/1	0.95	0.12	113,113,113,113	0
3	ZN	D	204	1/1	0.96	0.10	119,119,119,119	0
3	ZN	D	202	1/1	0.96	0.10	96,96,96,96	0
3	ZN	A	203	1/1	0.96	0.13	91,91,91,91	0
3	ZN	E	201	1/1	0.97	0.14	92,92,92,92	0
3	ZN	B	203	1/1	0.97	0.08	89,89,89,89	0
3	ZN	C	203	1/1	0.98	0.09	129,129,129,129	0
3	ZN	C	201	1/1	0.98	0.13	94,94,94,94	0
3	ZN	B	201	1/1	0.98	0.09	83,83,83,83	0
3	ZN	A	202	1/1	0.99	0.07	78,78,78,78	0

6.5 Other polymers

There are no such residues in this entry.