



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:41 PM UTC

PDB ID : 7MJ2 / pdb_00007mj2
Title : LarB, a carboxylase/hydrolase involved in synthesis of the cofactor for lactate racemase, in complex with Zn
Authors : Chatterjee, S.; Rankin, J.A.; Lagishetty, S.; Hu, J.; Hausinger, R.P.
Deposited on : 2021-04-19
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:

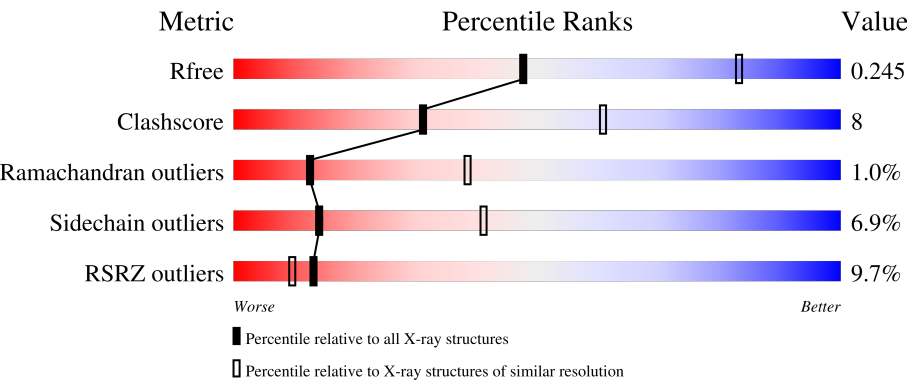
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance i

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	256	2% 61%16%•19%
1	B	256	2% 66%11%•21%
1	C	256	2% 66%12%•21%
1	D	256	5% 67%11%•20%
1	E	256	16% 54%20%•21%

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Mol	Chain	Length	Quality of chain
1	F	256	18% 60% 18% • 21%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8787 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 Pyridinium-3,5-biscarboxylic acid mononucleotide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1484	942	250	284	8			
1	B	201	Total	C	N	O	S	0	0	0
			1427	906	243	270	8			
1	C	201	Total	C	N	O	S	0	0	0
			1440	915	243	274	8			
1	D	205	Total	C	N	O	S	0	0	0
			1446	916	247	275	8			
1	E	201	Total	C	N	O	S	0	0	0
			1405	891	240	266	8			
1	F	201	Total	C	N	O	S	0	0	0
			1413	896	241	269	7			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	247	ALA	-	expression tag	UNP F9UST0
A	248	SER	-	expression tag	UNP F9UST0
A	249	TRP	-	expression tag	UNP F9UST0
A	250	SER	-	expression tag	UNP F9UST0
A	251	HIS	-	expression tag	UNP F9UST0
A	252	PRO	-	expression tag	UNP F9UST0
A	253	GLN	-	expression tag	UNP F9UST0
A	254	PHE	-	expression tag	UNP F9UST0
A	255	GLU	-	expression tag	UNP F9UST0
A	256	LYS	-	expression tag	UNP F9UST0
B	247	ALA	-	expression tag	UNP F9UST0
B	248	SER	-	expression tag	UNP F9UST0
B	249	TRP	-	expression tag	UNP F9UST0
B	250	SER	-	expression tag	UNP F9UST0
B	251	HIS	-	expression tag	UNP F9UST0
B	252	PRO	-	expression tag	UNP F9UST0
B	253	GLN	-	expression tag	UNP F9UST0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	254	PHE	-	expression tag	UNP F9UST0
B	255	GLU	-	expression tag	UNP F9UST0
B	256	LYS	-	expression tag	UNP F9UST0
C	247	ALA	-	expression tag	UNP F9UST0
C	248	SER	-	expression tag	UNP F9UST0
C	249	TRP	-	expression tag	UNP F9UST0
C	250	SER	-	expression tag	UNP F9UST0
C	251	HIS	-	expression tag	UNP F9UST0
C	252	PRO	-	expression tag	UNP F9UST0
C	253	GLN	-	expression tag	UNP F9UST0
C	254	PHE	-	expression tag	UNP F9UST0
C	255	GLU	-	expression tag	UNP F9UST0
C	256	LYS	-	expression tag	UNP F9UST0
D	247	ALA	-	expression tag	UNP F9UST0
D	248	SER	-	expression tag	UNP F9UST0
D	249	TRP	-	expression tag	UNP F9UST0
D	250	SER	-	expression tag	UNP F9UST0
D	251	HIS	-	expression tag	UNP F9UST0
D	252	PRO	-	expression tag	UNP F9UST0
D	253	GLN	-	expression tag	UNP F9UST0
D	254	PHE	-	expression tag	UNP F9UST0
D	255	GLU	-	expression tag	UNP F9UST0
D	256	LYS	-	expression tag	UNP F9UST0
E	247	ALA	-	expression tag	UNP F9UST0
E	248	SER	-	expression tag	UNP F9UST0
E	249	TRP	-	expression tag	UNP F9UST0
E	250	SER	-	expression tag	UNP F9UST0
E	251	HIS	-	expression tag	UNP F9UST0
E	252	PRO	-	expression tag	UNP F9UST0
E	253	GLN	-	expression tag	UNP F9UST0
E	254	PHE	-	expression tag	UNP F9UST0
E	255	GLU	-	expression tag	UNP F9UST0
E	256	LYS	-	expression tag	UNP F9UST0
F	247	ALA	-	expression tag	UNP F9UST0
F	248	SER	-	expression tag	UNP F9UST0
F	249	TRP	-	expression tag	UNP F9UST0
F	250	SER	-	expression tag	UNP F9UST0
F	251	HIS	-	expression tag	UNP F9UST0
F	252	PRO	-	expression tag	UNP F9UST0
F	253	GLN	-	expression tag	UNP F9UST0
F	254	PHE	-	expression tag	UNP F9UST0
F	255	GLU	-	expression tag	UNP F9UST0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	256	LYS	-	expression tag	UNP F9UST0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0

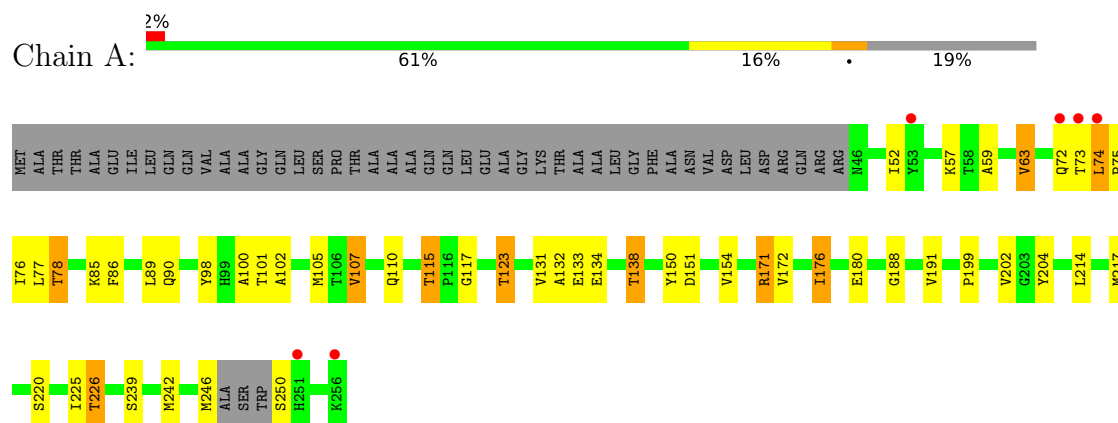
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	48	Total O 48 48	0	0
4	B	44	Total O 44 44	0	0
4	C	40	Total O 40 40	0	0
4	D	26	Total O 26 26	0	0
4	E	5	Total O 5 5	0	0
4	F	4	Total O 4 4	0	0

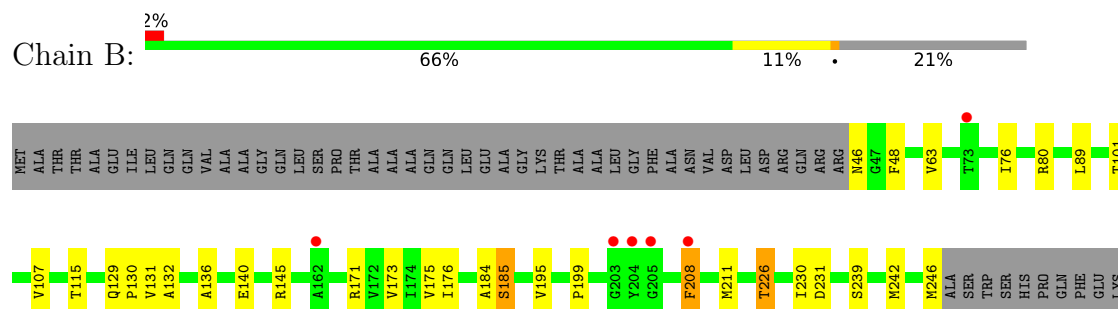
3 Residue-property plots [i](#)

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.

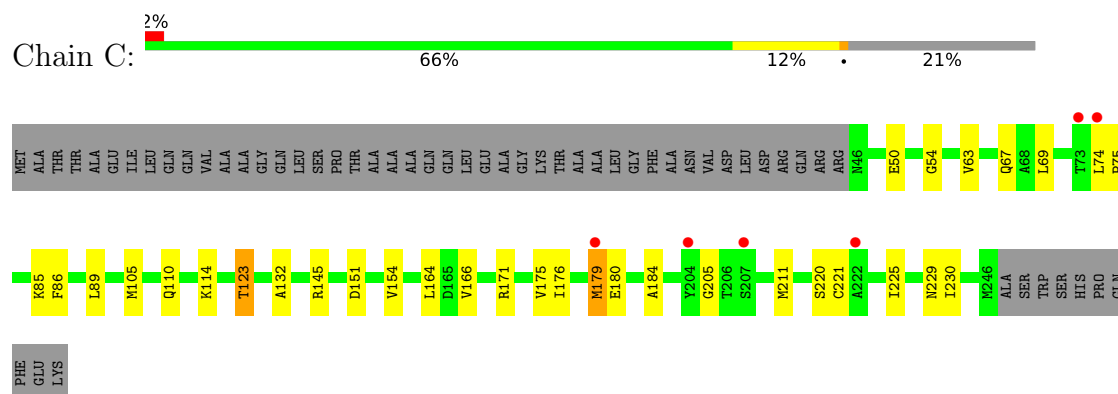
- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase



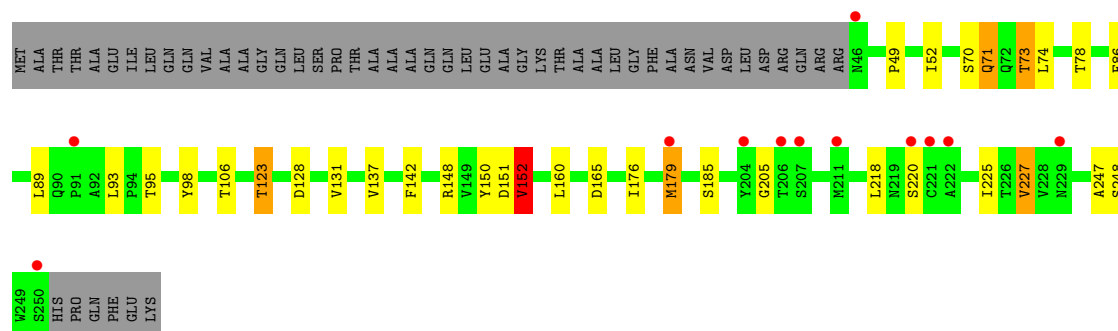
- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase



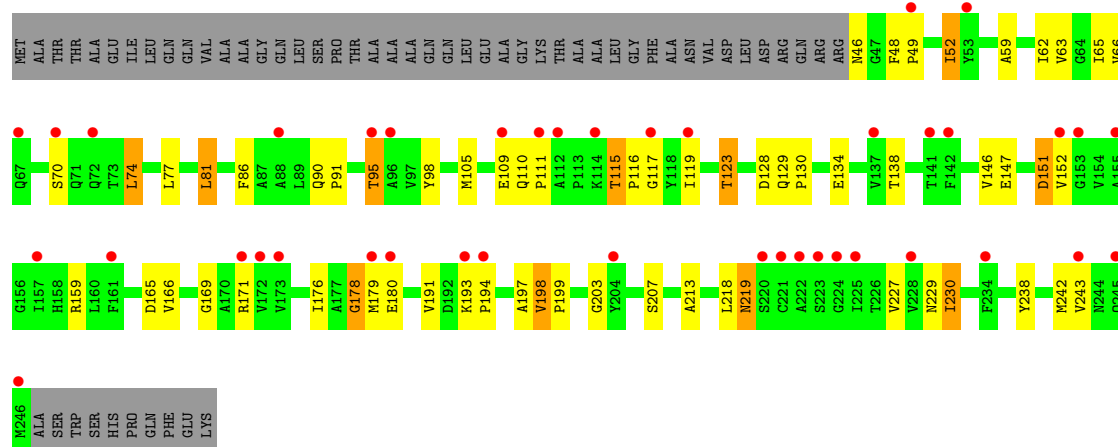
- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase



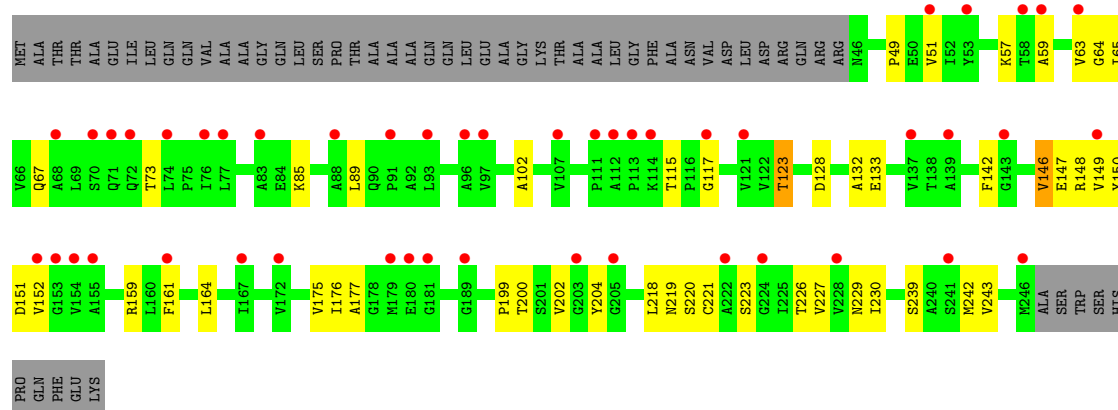
• Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase



• Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase



• Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.10Å 120.10Å 212.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.98 – 2.80 33.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.98-2.80) 99.3 (33.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.210 , 0.244 0.212 , 0.245	Depositor DCC
R_{free} test set	1921 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8787	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.67% 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, MG

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	0.50	0/1508	0.73	0/2057
1	B	0.44	0/1449	0.60	0/1980
1	C	0.46	0/1463	0.65	1/1999 (0.1%)
1	D	0.46	0/1469	0.63	1/2009 (0.0%)
1	E	0.20	0/1426	0.49	2/1951 (0.1%)
1	F	0.19	0/1435	0.45	1/1964 (0.1%)
All	All	0.40	0/8750	0.60	5/11960 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	151	ASP	N-CA-C	9.33	124.34	111.74
1	C	179	MET	CB-CA-C	-6.25	109.35	116.54
1	D	179	MET	N-CA-C	-5.95	106.05	113.55
1	E	152	VAL	N-CA-CB	-5.50	102.15	111.23
1	F	204	TYR	CB-CA-C	-5.01	102.58	114.16

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	1484	0	1490	29	0
1	B	1427	0	1447	19	0
1	C	1440	0	1463	22	0
1	D	1446	0	1455	17	0
1	E	1405	0	1416	37	0
1	F	1413	0	1414	28	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	48	0	0	3	0
4	B	44	0	0	2	0
4	C	40	0	0	3	0
4	D	26	0	0	1	0
4	E	5	0	0	0	0
4	F	4	0	0	2	0
All	All	8787	0	8685	142	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 (142) 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:242:MET:SD	4:A:444:HOH:O	2.22	0.97
1:A:134:GLU:O	1:A:138:THR:HG23	1.77	0.84
1:F:161:PHE:HA	1:F:164:LEU:HB2	1.59	0.83
1:B:211:MET:SD	4:B:344:HOH:O	2.39	0.79
1:C:123:THR:HG22	1:C:151:ASP:H	1.47	0.79
1:E:151:ASP:OD1	1:E:151:ASP:O	2.04	0.74
1:A:123:THR:HG22	1:A:151:ASP:H	1.51	0.74
1:A:63:VAL:HG23	1:A:89:LEU:HD22	1.70	0.72
1:E:110:GLN:NE2	1:E:111:PRO:O	2.24	0.71
1:B:46:ASN:HB3	1:B:48:PHE:H	1.57	0.69
1:E:49:PRO:HD3	1:E:74:LEU:HD11	1.76	0.68
1:E:117:GLY:HA3	1:E:171:ARG:HD2	1.76	0.66
1:F:115:THR:HG22	1:F:117:GLY:H	1.59	0.66
1:F:200:THR:HG22	1:F:202:VAL:H	1.62	0.65
1:B:101:THR:HG22	1:B:130:PRO:HA	1.79	0.64
1:E:194:PRO:HG3	1:F:242:MET:HB2	1.80	0.64
1:C:63:VAL:HG23	1:C:89:LEU:HD23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:GLU:N	4:F:301:HOH:O	2.22	0.64
1:D:220:SER:CB	1:D:225:ILE:HD12	2.27	0.64
1:B:80:ARG:NH2	1:B:231:ASP:O	2.30	0.63
1:C:171:ARG:NH2	1:D:247:ALA:O	2.32	0.63
1:A:132:ALA:HA	1:A:176:ILE:HD12	1.81	0.62
1:F:199:PRO:HG2	1:F:230:ILE:HA	1.80	0.62
1:E:52:ILE:HD12	1:E:65:ILE:HD11	1.80	0.62
1:C:86:PHE:HA	1:C:89:LEU:HD12	1.81	0.62
1:C:89:LEU:HD13	1:C:105:MET:HE1	1.81	0.62
1:D:152:VAL:HG22	1:D:160:LEU:HA	1.82	0.61
1:F:133:GLU:OE2	1:F:148:ARG:NH1	2.33	0.61
1:E:151:ASP:OD1	1:E:159:ARG:NH1	2.34	0.61
1:B:208:PHE:HB3	1:B:211:MET:HB3	1.83	0.60
1:F:49:PRO:HD2	1:F:142:PHE:CE2	2.36	0.60
1:A:102:ALA:HB2	1:A:133:GLU:HB3	1.83	0.60
1:E:199:PRO:HG2	1:E:230:ILE:HA	1.84	0.59
1:B:76:ILE:HB	1:B:107:VAL:HG23	1.83	0.59
1:F:64:GLY:HA2	1:F:67:GLN:HB2	1.85	0.59
1:A:226:THR:OG1	1:B:226:THR:HG23	2.03	0.58
1:C:211:MET:HE2	1:C:230:ILE:HD11	1.84	0.58
1:A:72:GLN:O	1:A:73:THR:OG1	2.19	0.58
1:A:123:THR:HB	1:A:150:TYR:HA	1.84	0.58
1:A:86:PHE:HD1	1:A:105:MET:HE3	1.68	0.57
1:A:199:PRO:HD3	1:A:217:MET:HE1	1.86	0.57
1:A:115:THR:HG23	1:A:117:GLY:H	1.68	0.57
1:D:123:THR:HG22	1:D:151:ASP:H	1.68	0.57
1:E:134:GLU:O	1:E:138:THR:OG1	2.21	0.57
1:D:52:ILE:HB	1:D:78:THR:HG23	1.87	0.56
1:A:246:MET:HE3	1:B:171:ARG:CZ	2.35	0.56
1:D:218:LEU:HD23	1:D:227:VAL:HG21	1.87	0.56
1:E:95:THR:O	1:E:95:THR:OG1	2.22	0.56
1:E:46:ASN:HB3	1:E:48:PHE:HD2	1.70	0.56
1:C:63:VAL:O	1:C:67:GLN:HG2	2.06	0.55
1:A:188:GLY:HA3	1:A:225:ILE:HD11	1.89	0.54
1:F:123:THR:HG22	1:F:151:ASP:H	1.72	0.53
1:F:218:LEU:HG	1:F:227:VAL:HG11	1.90	0.53
1:A:199:PRO:CD	1:A:217:MET:HE1	2.38	0.53
1:E:147:GLU:HG2	1:E:166:VAL:HG11	1.90	0.52
1:C:229:ASN:OD1	1:C:230:ILE:N	2.39	0.52
1:C:50:GLU:HG2	1:C:69:LEU:HD22	1.92	0.52
1:C:166:VAL:HG23	4:C:430:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:VAL:HG12	1:F:159:ARG:HB3	1.93	0.51
1:A:86:PHE:CD1	1:A:105:MET:HE3	2.45	0.50
1:E:243:VAL:HG13	1:F:243:VAL:HG13	1.93	0.50
1:E:59:ALA:O	1:E:63:VAL:HG12	2.11	0.50
1:E:176:ILE:HG13	1:E:198:VAL:HG13	1.93	0.50
1:B:145:ARG:NH2	1:C:166:VAL:HG22	2.26	0.50
1:D:220:SER:HB3	1:D:225:ILE:HD12	1.93	0.50
1:A:220:SER:O	1:A:225:ILE:HD12	2.12	0.50
1:D:128:ASP:HB3	1:D:176:ILE:HG22	1.93	0.49
1:D:218:LEU:HD23	1:D:227:VAL:CG2	2.42	0.49
1:B:63:VAL:HG23	1:B:89:LEU:HD22	1.94	0.49
1:A:74:LEU:CB	1:A:75:PRO:HD3	2.41	0.49
1:F:123:THR:HB	1:F:150:TYR:HA	1.95	0.49
1:E:115:THR:HG22	1:E:116:PRO:HD2	1.95	0.49
1:E:178:GLY:O	1:E:213:ALA:HB2	2.13	0.49
1:A:59:ALA:O	1:A:89:LEU:HD21	2.13	0.48
1:C:74:LEU:HB3	1:C:75:PRO:CD	2.43	0.48
1:F:123:THR:HG23	1:F:128:ASP:HB2	1.95	0.48
1:B:185:SER:HB2	4:B:325:HOH:O	2.14	0.48
1:E:238:TYR:CZ	1:E:242:MET:HE3	2.49	0.48
1:E:179:MET:HE1	1:E:203:GLY:HA2	1.95	0.48
1:F:146:VAL:HG13	4:F:301:HOH:O	2.13	0.48
1:D:165:ASP:N	1:D:165:ASP:OD1	2.46	0.47
1:F:132:ALA:HA	1:F:176:ILE:HD13	1.96	0.47
1:D:148:ARG:HG2	1:D:150:TYR:CZ	2.49	0.47
1:E:191:VAL:HG12	1:E:193:LYS:H	1.80	0.47
1:A:52:ILE:HB	1:A:78:THR:HG23	1.96	0.47
1:B:173:VAL:HB	1:B:195:VAL:HG22	1.96	0.47
1:F:63:VAL:HG23	1:F:89:LEU:HD22	1.97	0.47
1:C:74:LEU:O	1:C:75:PRO:C	2.58	0.47
1:F:219:ASN:O	1:F:221:CYS:N	2.46	0.47
1:F:59:ALA:HB1	1:F:89:LEU:HD21	1.96	0.46
1:A:110:GLN:HB2	4:A:409:HOH:O	2.15	0.46
1:B:132:ALA:HA	1:B:176:ILE:HD13	1.96	0.46
1:E:117:GLY:HA3	1:E:171:ARG:CD	2.45	0.46
1:E:52:ILE:HD11	1:E:62:ILE:HG12	1.98	0.46
1:F:149:VAL:HG12	1:F:152:VAL:HG21	1.98	0.46
1:F:128:ASP:OD2	1:F:177:ALA:HA	2.16	0.46
1:A:171:ARG:HB3	1:B:246:MET:HE1	1.98	0.46
1:F:102:ALA:HB2	1:F:133:GLU:HB3	1.98	0.45
1:F:57:LYS:HD3	1:F:65:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:THR:HG23	1:E:128:ASP:HB2	1.99	0.45
1:C:221:CYS:HA	1:C:225:ILE:HB	1.98	0.45
1:C:132:ALA:HA	1:C:176:ILE:HD13	2.00	0.44
1:E:62:ILE:O	1:E:66:VAL:HG23	2.16	0.44
1:F:57:LYS:O	1:F:85:LYS:NZ	2.35	0.44
1:E:86:PHE:CD1	1:E:98:TYR:HB2	2.51	0.44
1:C:145:ARG:NE	4:C:401:HOH:O	2.25	0.44
1:D:152:VAL:HG13	1:D:160:LEU:HD13	2.00	0.44
1:D:70:SER:O	1:D:71:GLN:C	2.61	0.43
1:C:164:LEU:HA	1:C:164:LEU:HD12	1.75	0.43
1:E:77:LEU:HD21	1:E:138:THR:HG23	2.01	0.43
1:A:98:TYR:CE2	1:A:100:ALA:HA	2.53	0.43
1:B:101:THR:HG21	1:B:129:GLN:HG2	2.00	0.43
1:A:214:LEU:HA	1:A:217:MET:HE2	2.01	0.43
1:E:81:LEU:HD21	1:E:105:MET:HB3	2.01	0.43
1:B:199:PRO:HG2	1:B:230:ILE:HA	2.00	0.43
1:E:219:ASN:HA	1:F:229:ASN:HD21	1.82	0.43
1:B:136:ALA:O	1:B:140:GLU:HG3	2.20	0.42
1:B:239:SER:HA	1:B:242:MET:HE3	2.00	0.42
1:E:165:ASP:O	1:E:169:GLY:N	2.51	0.42
1:C:145:ARG:NH2	4:C:401:HOH:O	2.48	0.42
1:E:119:ILE:O	1:E:146:VAL:HA	2.19	0.42
1:E:128:ASP:HB3	1:E:176:ILE:HG22	2.01	0.42
1:A:76:ILE:HB	1:A:107:VAL:HG22	2.00	0.42
1:C:50:GLU:HG2	1:C:69:LEU:HD13	2.01	0.42
1:E:90:GLN:N	1:E:91:PRO:HD2	2.35	0.42
1:E:129:GLN:HB3	1:E:130:PRO:HD3	2.02	0.42
1:E:197:ALA:O	1:E:227:VAL:HA	2.19	0.42
1:C:175:VAL:HG21	1:C:184:ALA:HA	2.02	0.42
1:C:54:GLY:O	1:C:85:LYS:NZ	2.53	0.41
1:D:73:THR:O	4:D:401:HOH:O	2.20	0.41
1:E:199:PRO:HG2	1:E:230:ILE:CA	2.50	0.41
1:D:86:PHE:CZ	1:D:98:TYR:HB2	2.56	0.41
1:E:86:PHE:CE1	1:E:98:TYR:HB2	2.56	0.41
1:A:77:LEU:CD2	1:A:138:THR:HB	2.51	0.41
1:A:86:PHE:CE1	1:A:98:TYR:HB2	2.55	0.41
1:A:239:SER:HA	4:A:444:HOH:O	2.19	0.41
1:C:171:ARG:HH21	1:D:248:SER:HA	1.85	0.41
1:A:57:LYS:O	1:A:85:LYS:NZ	2.35	0.41
1:E:229:ASN:ND2	1:F:219:ASN:OD1	2.53	0.41
1:B:175:VAL:HG11	1:B:184:ALA:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:PRO:HG2	1:D:142:PHE:CE1	2.56	0.40
1:F:239:SER:O	1:F:243:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	204/256 (80%)	194 (95%)	9 (4%)	1 (0%)	24	55
1	B	199/256 (78%)	189 (95%)	10 (5%)	0	100	100
1	C	199/256 (78%)	184 (92%)	14 (7%)	1 (0%)	24	55
1	D	203/256 (79%)	187 (92%)	12 (6%)	4 (2%)	6	21
1	E	199/256 (78%)	180 (90%)	14 (7%)	5 (2%)	4	16
1	F	199/256 (78%)	179 (90%)	19 (10%)	1 (0%)	24	55
All	All	1203/1536 (78%)	1113 (92%)	78 (6%)	12 (1%)	12	38

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	LEU
1	C	205	GLY
1	D	74	LEU
1	E	70	SER
1	E	178	GLY
1	E	219	ASN
1	D	71	GLN
1	D	152	VAL
1	D	205	GLY
1	F	220	SER

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Mol	Chain	Res	Type
1	E	109	GLU
1	E	218	LEU

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	152/191 (80%)	133 (88%)	19 (12%)	4	15
1	B	145/191 (76%)	140 (97%)	5 (3%)	32	68
1	C	148/191 (78%)	141 (95%)	7 (5%)	23	57
1	D	146/191 (76%)	134 (92%)	12 (8%)	10	33
1	E	141/191 (74%)	131 (93%)	10 (7%)	13	39
1	F	141/191 (74%)	134 (95%)	7 (5%)	22	54
All	All	873/1146 (76%)	813 (93%)	60 (7%)	14	41

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	VAL
1	A	78	THR
1	A	90	GLN
1	A	101	THR
1	A	107	VAL
1	A	115	THR
1	A	123	THR
1	A	131	VAL
1	A	138	THR
1	A	154	VAL
1	A	171	ARG
1	A	172	VAL
1	A	176	ILE
1	A	180	GLU
1	A	191	VAL
1	A	202	VAL

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Mol	Chain	Res	Type
1	A	204	TYR
1	A	226	THR
1	A	250	SER
1	B	115	THR
1	B	131	VAL
1	B	185	SER
1	B	208	PHE
1	B	226	THR
1	C	110	GLN
1	C	114	LYS
1	C	123	THR
1	C	154	VAL
1	C	179	MET
1	C	180	GLU
1	C	220	SER
1	D	73	THR
1	D	89	LEU
1	D	93	LEU
1	D	95	THR
1	D	106	THR
1	D	123	THR
1	D	131	VAL
1	D	137	VAL
1	D	152	VAL
1	D	179	MET
1	D	185	SER
1	D	227	VAL
1	E	52	ILE
1	E	74	LEU
1	E	81	LEU
1	E	95	THR
1	E	115	THR
1	E	123	THR
1	E	180	GLU
1	E	198	VAL
1	E	207	SER
1	E	230	ILE
1	F	51	VAL
1	F	73	THR
1	F	123	THR
1	F	146	VAL
1	F	175	VAL

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Mol	Chain	Res	Type
1	F	223	SER
1	F	226	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	244	ASN
1	A	245	GLN
1	B	144	ASN
1	B	244	ASN
1	B	245	GLN
1	D	99	HIS
1	D	244	ASN
1	E	90	GLN
1	E	144	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	208/256 (81%)	-0.17	6 (2%) 53 43	16, 37, 88, 125	0
1	B	201/256 (78%)	-0.06	6 (2%) 52 42	18, 41, 89, 110	0
1	C	201/256 (78%)	-0.27	6 (2%) 52 42	12, 34, 81, 134	0
1	D	205/256 (80%)	0.30	12 (5%) 28 21	21, 60, 110, 140	0
1	E	201/256 (78%)	1.25	41 (20%) 3 2	96, 124, 174, 200	0
1	F	201/256 (78%)	1.47	47 (23%) 2 1	108, 143, 178, 204	0
All	All	1217/1536 (79%)	0.42	118 (9%) 13 10	12, 64, 160, 204	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	91	PRO	5.7
1	D	204	TYR	4.8
1	F	112	ALA	4.2
1	D	221	CYS	4.2
1	E	221	CYS	4.1
1	F	88	ALA	4.0
1	F	114	LYS	4.0
1	F	72	GLN	3.9
1	E	246	MET	3.8
1	A	251	HIS	3.7
1	D	222	ALA	3.6
1	F	241	SER	3.6
1	F	179	MET	3.6
1	F	53	TYR	3.4
1	D	220	SER	3.4
1	E	152	VAL	3.3
1	B	203	GLY	3.3
1	F	76	ILE	3.2
1	A	74	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	72	GLN	3.1
1	D	250	SER	3.1
1	E	172	VAL	3.1
1	E	220	SER	3.1
1	D	206	THR	3.0
1	B	162	ALA	3.0
1	E	112	ALA	2.9
1	F	203	GLY	2.9
1	F	77	LEU	2.9
1	E	204	TYR	2.8
1	C	179	MET	2.8
1	E	67	GLN	2.8
1	F	137	VAL	2.8
1	E	53	TYR	2.8
1	F	172	VAL	2.8
1	E	180	GLU	2.7
1	E	222	ALA	2.7
1	E	49	PRO	2.7
1	F	68	ALA	2.7
1	F	70	SER	2.7
1	F	107	VAL	2.7
1	E	224	GLY	2.7
1	E	228	VAL	2.7
1	E	243	VAL	2.7
1	E	193	LYS	2.6
1	F	111	PRO	2.6
1	F	143	GLY	2.6
1	F	181	GLY	2.6
1	E	173	VAL	2.6
1	F	59	ALA	2.6
1	F	167	ILE	2.6
1	E	137	VAL	2.6
1	E	96	ALA	2.6
1	A	256	LYS	2.5
1	C	74	LEU	2.5
1	F	113	PRO	2.5
1	F	205	GLY	2.5
1	D	207	SER	2.5
1	F	96	ALA	2.4
1	F	222	ALA	2.4
1	B	205	GLY	2.4
1	E	245	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	73	THR	2.4
1	E	70	SER	2.4
1	E	109	GLU	2.4
1	F	161	PHE	2.4
1	F	180	GLU	2.4
1	C	222	ALA	2.4
1	F	121	VAL	2.4
1	E	114	LYS	2.4
1	E	141	THR	2.4
1	D	91	PRO	2.4
1	F	154	VAL	2.3
1	E	223	SER	2.3
1	A	73	THR	2.3
1	E	225	ILE	2.3
1	E	95	THR	2.3
1	E	194	PRO	2.3
1	E	155	ALA	2.3
1	F	155	ALA	2.3
1	F	71	GLN	2.3
1	E	119	ILE	2.3
1	A	53	TYR	2.3
1	E	111	PRO	2.3
1	F	83	ALA	2.2
1	F	228	VAL	2.2
1	B	204	TYR	2.2
1	E	153	GLY	2.2
1	F	153	GLY	2.2
1	E	88	ALA	2.2
1	A	72	GLN	2.2
1	E	171	ARG	2.2
1	F	63	VAL	2.2
1	E	179	MET	2.2
1	F	74	LEU	2.2
1	F	58	THR	2.2
1	F	189	GLY	2.2
1	B	73	THR	2.2
1	B	208	PHE	2.2
1	E	161	PHE	2.2
1	F	149	VAL	2.1
1	D	179	MET	2.1
1	D	211	MET	2.1
1	F	117	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	139	ALA	2.1
1	C	207	SER	2.1
1	E	157	ILE	2.1
1	F	152	VAL	2.1
1	C	204	TYR	2.1
1	F	97	VAL	2.1
1	D	229	ASN	2.1
1	E	234	PHE	2.1
1	F	93	LEU	2.0
1	E	117	GLY	2.0
1	E	142	PHE	2.0
1	D	46	ASN	2.0
1	F	224	GLY	2.0
1	F	246	MET	2.0
1	F	51	VAL	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.

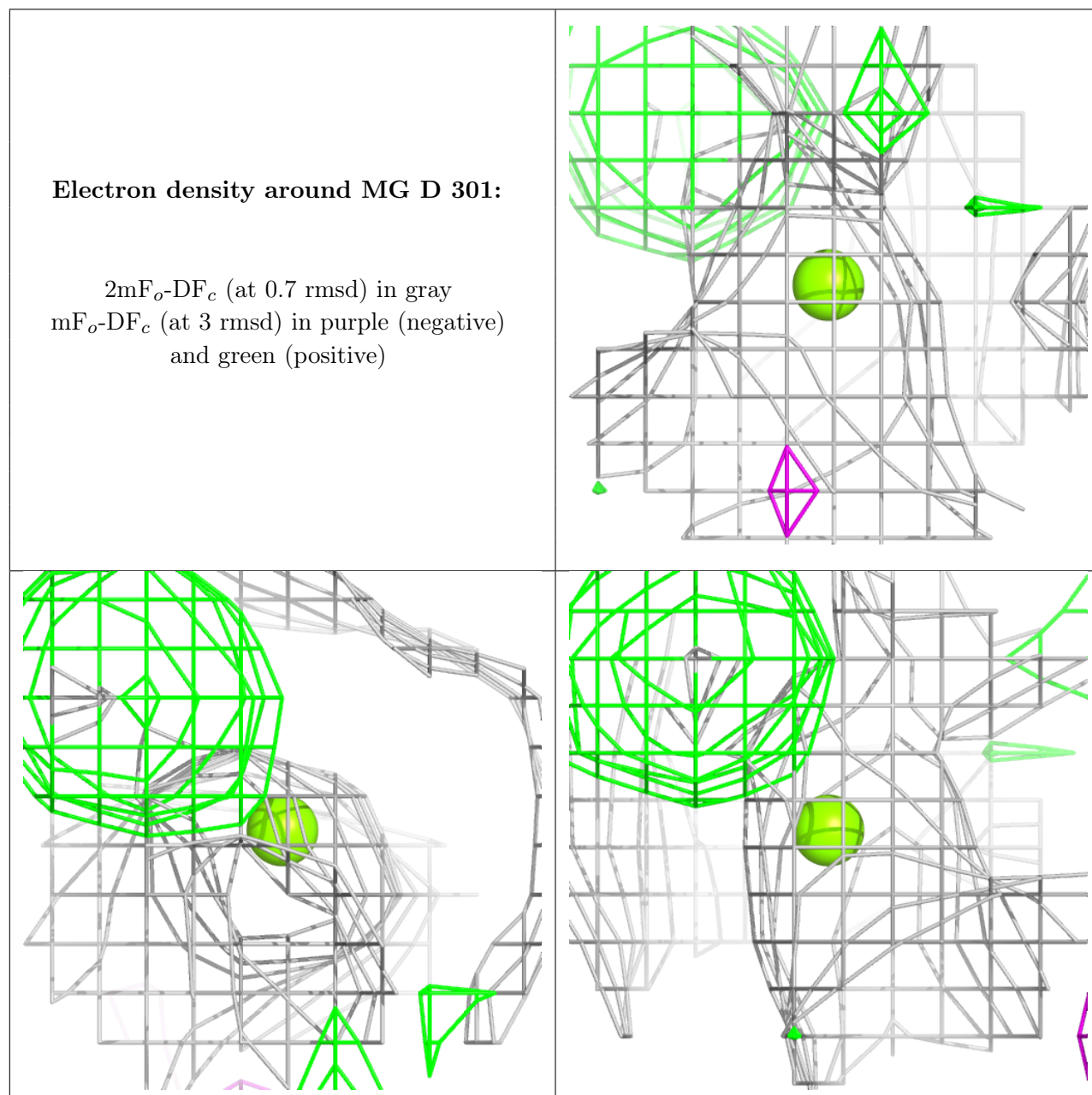
6.4 Ligands [i](#)

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
2	MG	D	301	1/1	0.86	0.12	30,30,30,30	1
2	MG	C	301	1/1	0.90	0.15	30,30,30,30	1
3	ZN	C	302	1/1	0.91	0.08	57,57,57,57	0
2	MG	A	301	1/1	0.93	0.08	40,40,40,40	0
3	ZN	A	302	1/1	0.99	0.03	57,57,57,57	0

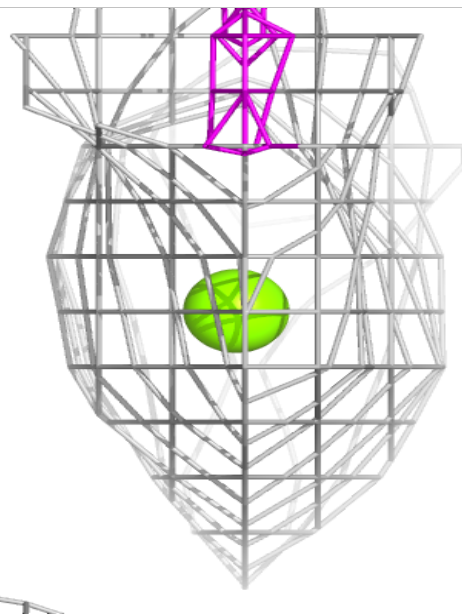
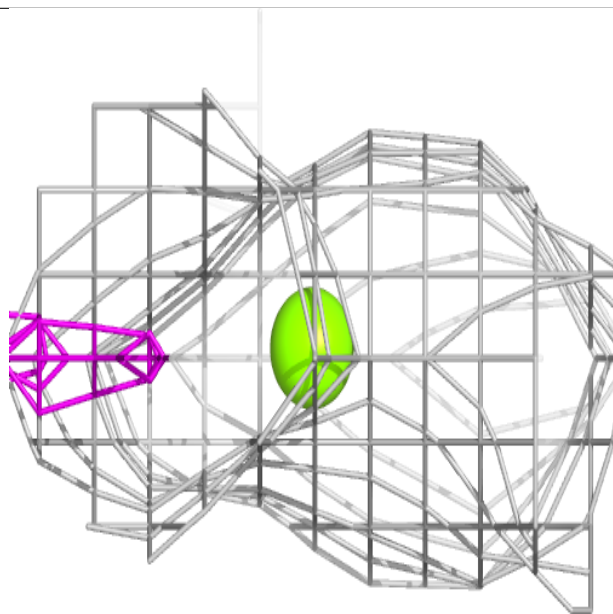
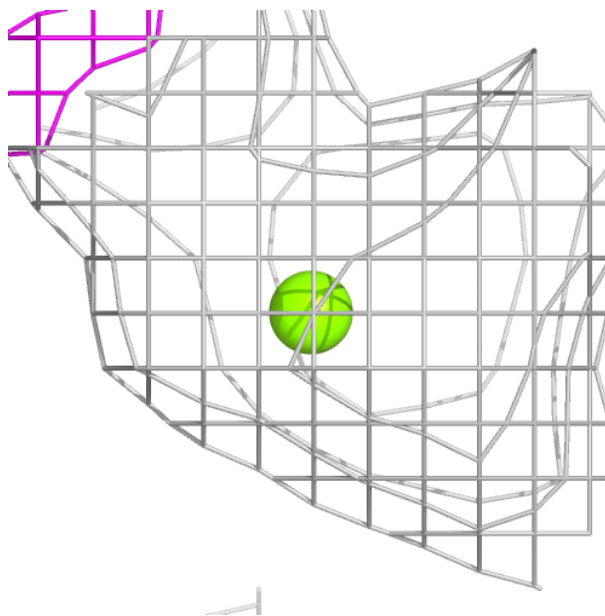
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



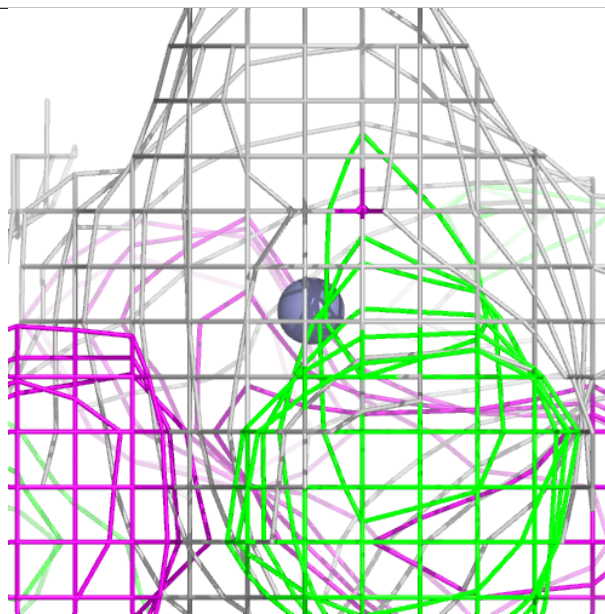
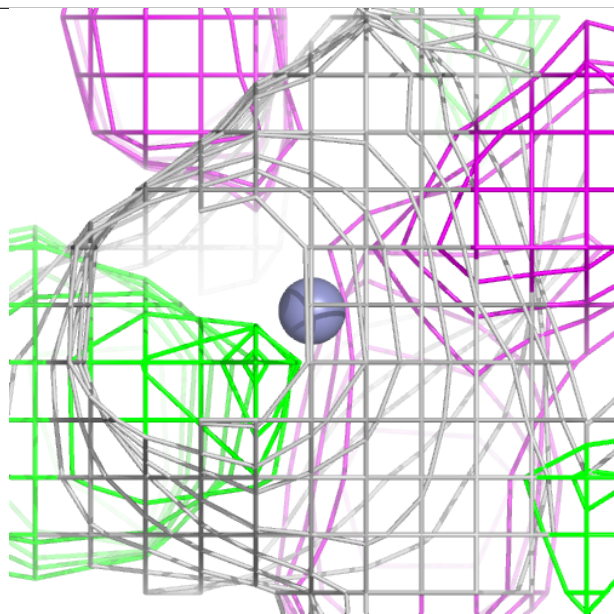
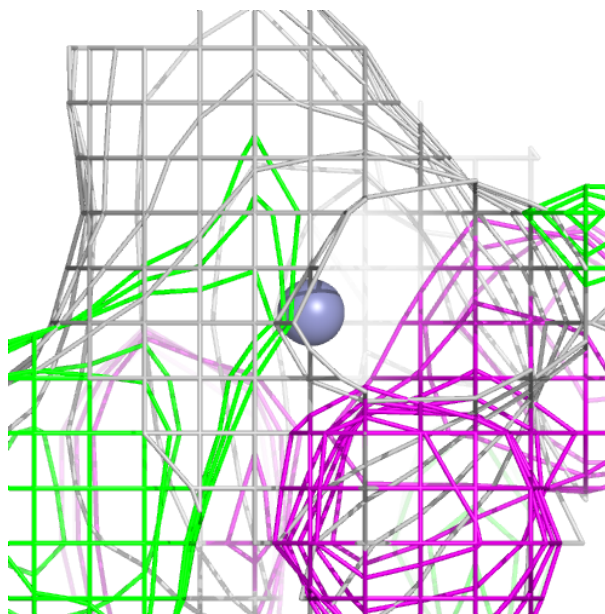
Electron density around MG C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



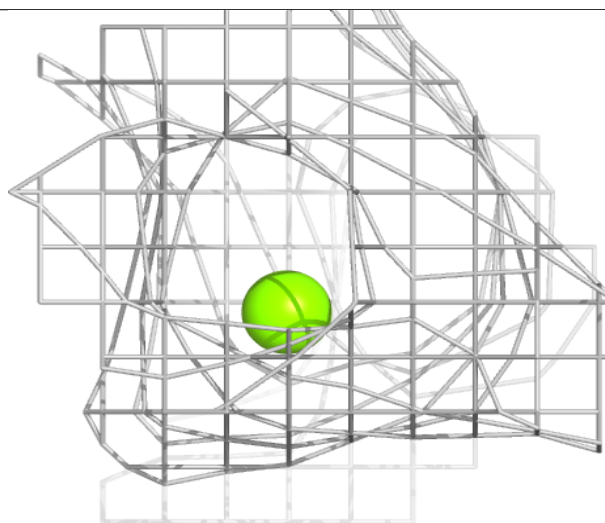
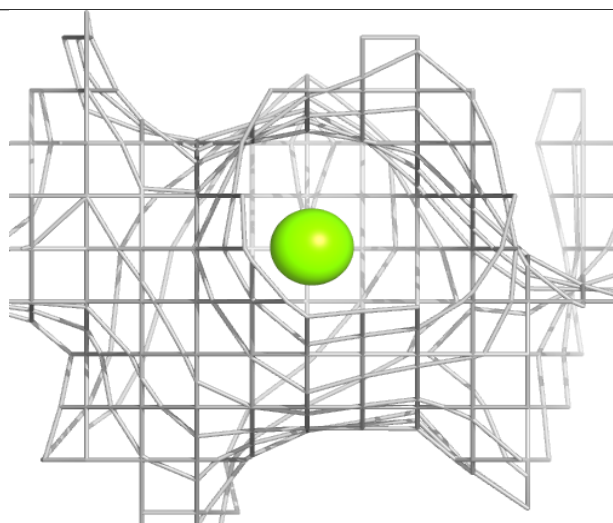
Electron density around ZN C 302:

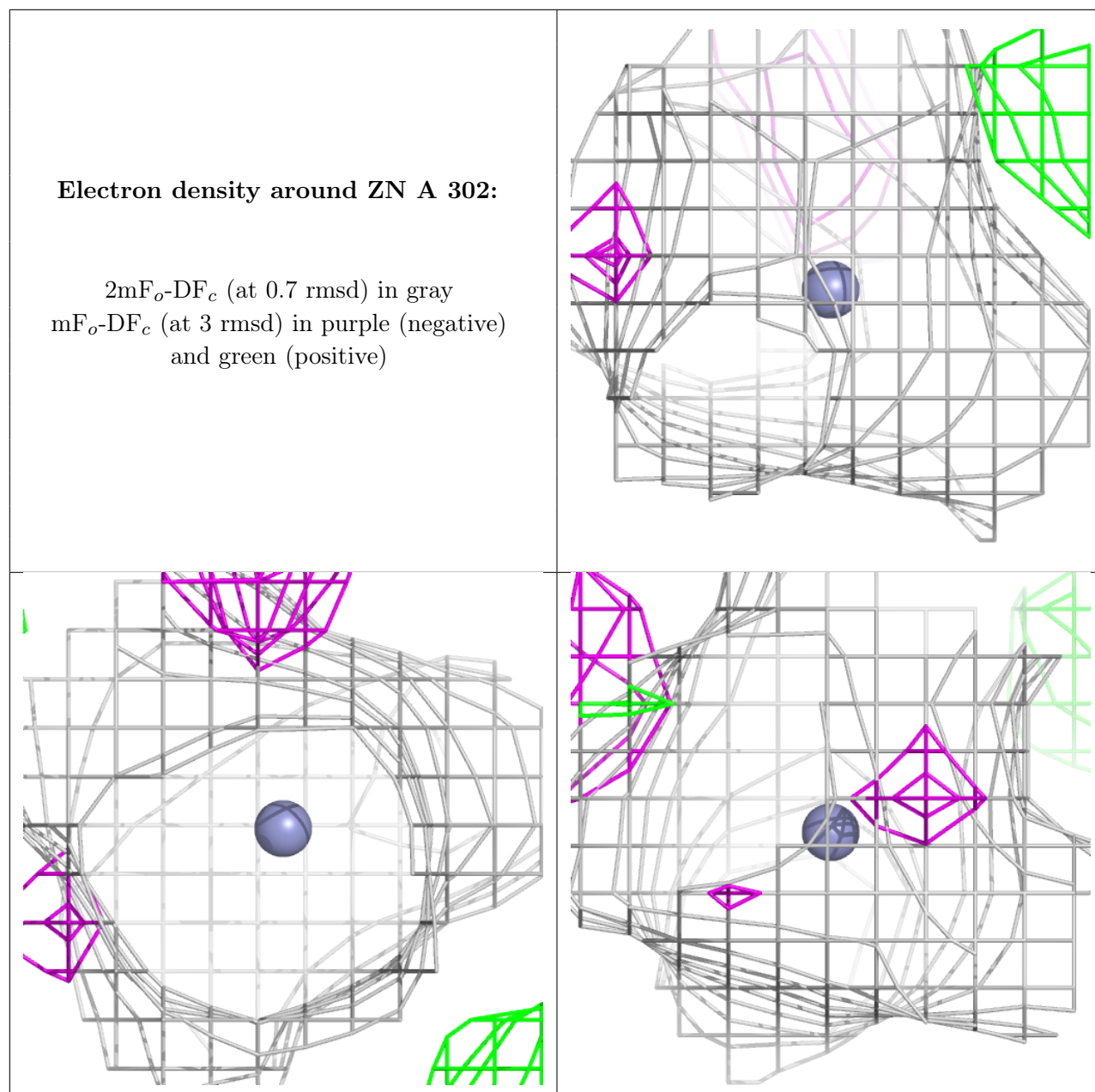
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG A 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.