



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:30 AM UTC

PDB ID : 4CAD / pdb_00004cad
Title : Mechanism of farnesylated CAAX protein processing by the integral membrane protease Rce1
Authors : Kulkarni, K.; Manolaridis, I.; Dodd, R.B.; Cronin, N.; Ogasawara, S.; Iwata, S.; Barford, D.
Deposited on : 2013-10-08
Resolution : 2.50 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

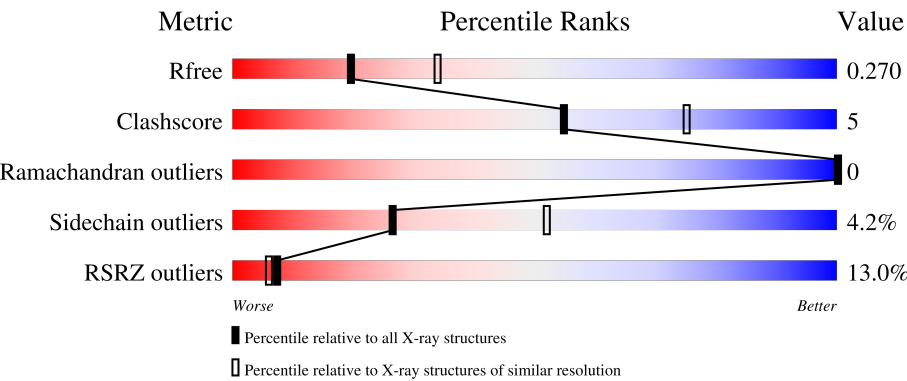
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



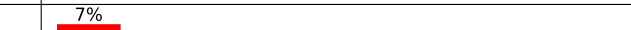
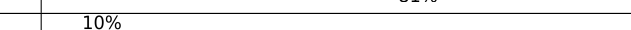
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	214	7% 90% 8% .
1	D	214	7% 86% 11% ..
1	G	214	10% 89% 10% .
1	J	214	10% 86% 13% .

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Mol	Chain	Length	Quality of chain
2	B	227	 7% 90% 7%
2	E	227	 9% 83% 13%
2	H	227	 7% 81% 15%
2	K	227	 10% 85% 12%
3	C	271	 20% 72% 17% 7%
3	F	271	 23% 76% 15% 8%
3	I	271	 17% 79% 14% 6%
3	L	271	 17% 78% 13% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21755 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 ANTIBODY FAB FRAGMENT LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1642	1028	280	329	5			
1	D	211	Total	C	N	O	S	0	0	0
			1642	1028	280	329	5			
1	G	212	Total	C	N	O	S	0	0	0
			1647	1030	280	332	5			
1	J	212	Total	C	N	O	S	0	0	0
			1650	1032	281	332	5			

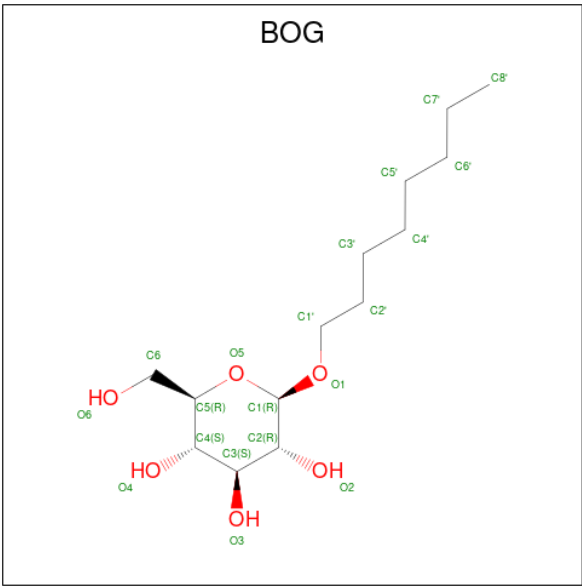
- Molecule 2 is a protein called ANTIBODY FAB FRAGMENT HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	221	Total	C	N	O	S	0	0	0
			1666	1057	270	331	8			
2	E	220	Total	C	N	O	S	0	0	0
			1663	1056	269	330	8			
2	H	221	Total	C	N	O	S	0	0	0
			1668	1059	270	331	8			
2	K	221	Total	C	N	O	S	0	0	0
			1668	1059	270	331	8			

- Molecule 3 is a protein called RAS AND A-FACTOR CONVERTING ENZYME 1, RCE1.

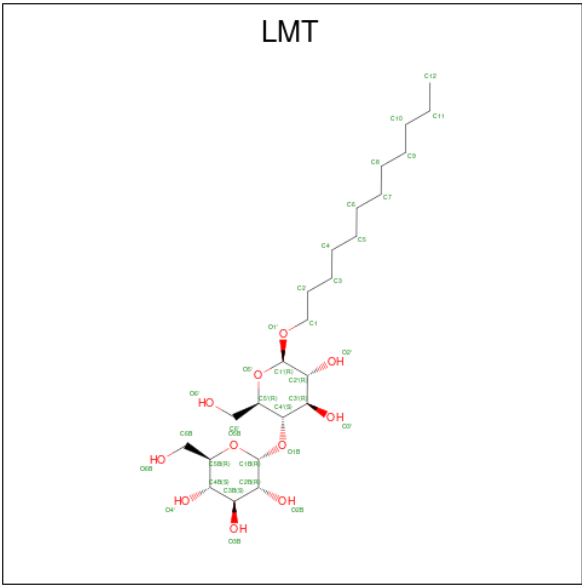
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	251	Total	C	N	O	S	0	0	0
			2020	1386	293	333	8			
3	F	250	Total	C	N	O	S	0	0	0
			2011	1381	290	332	8			
3	I	254	Total	C	N	O	S	0	0	0
			2040	1397	297	339	7			
3	L	253	Total	C	N	O	S	0	0	0
			2041	1398	297	338	8			

- Molecule 4 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			13	7	6		
4	F	1	Total	C	O	0	0
			13	7	6		

- Molecule 5 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	I	1	Total	C	O	0	0
			25	14	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			23	12	11		

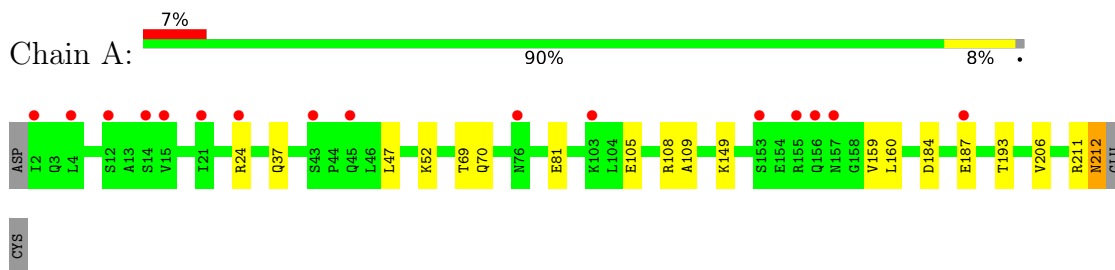
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	39	Total	O	0	0
			39	39		
6	B	46	Total	O	0	0
			46	46		
6	C	7	Total	O	0	0
			7	7		
6	D	37	Total	O	0	0
			37	37		
6	E	51	Total	O	0	0
			51	51		
6	F	7	Total	O	0	0
			7	7		
6	G	32	Total	O	0	0
			32	32		
6	H	33	Total	O	0	0
			33	33		
6	I	2	Total	O	0	0
			2	2		
6	J	31	Total	O	0	0
			31	31		
6	K	36	Total	O	0	0
			36	36		
6	L	2	Total	O	0	0
			2	2		

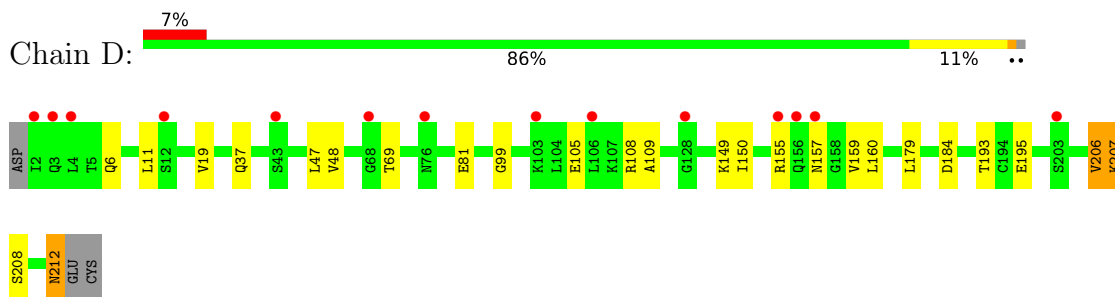
3 Residue-property plots [i](#)

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.

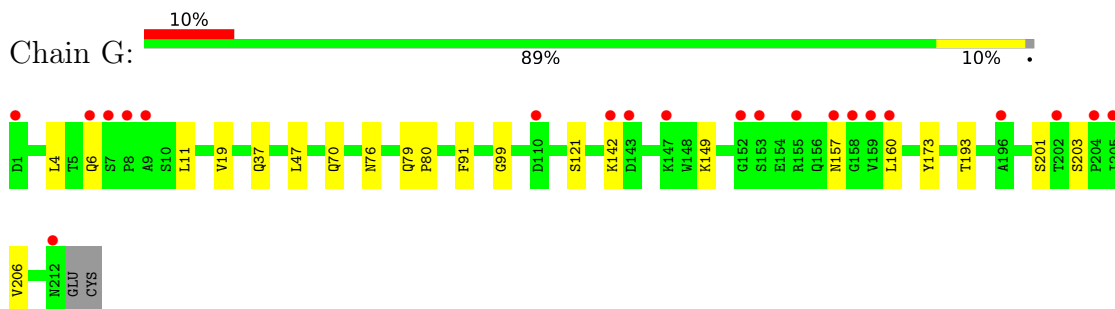
- Molecule 1: ANTIBODY FAB FRAGMENT LIGHT CHAIN



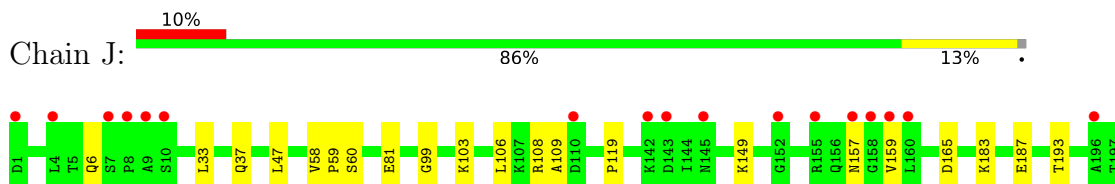
- Molecule 1: ANTIBODY FAB FRAGMENT LIGHT CHAIN



- Molecule 1: ANTIBODY FAB FRAGMENT LIGHT CHAIN

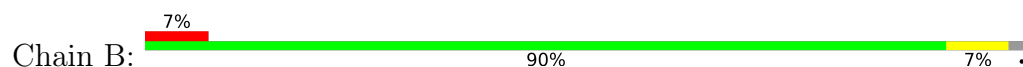


- Molecule 1: ANTIBODY FAB FRAGMENT LIGHT CHAIN

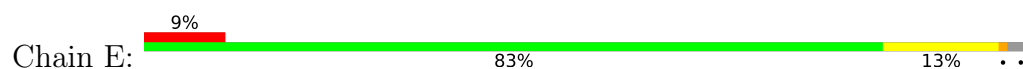




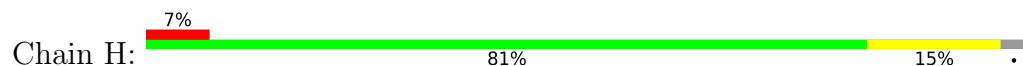
• Molecule 2: ANTIBODY FAB FRAGMENT HEAVY CHAIN



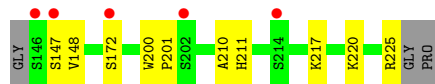
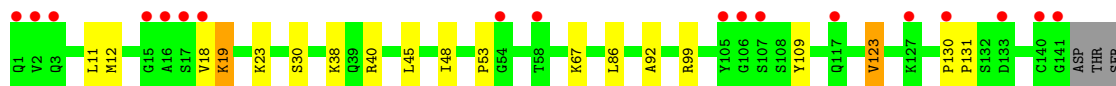
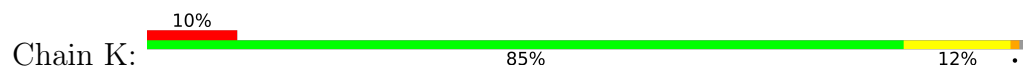
• Molecule 2: ANTIBODY FAB FRAGMENT HEAVY CHAIN



• Molecule 2: ANTIBODY FAB FRAGMENT HEAVY CHAIN

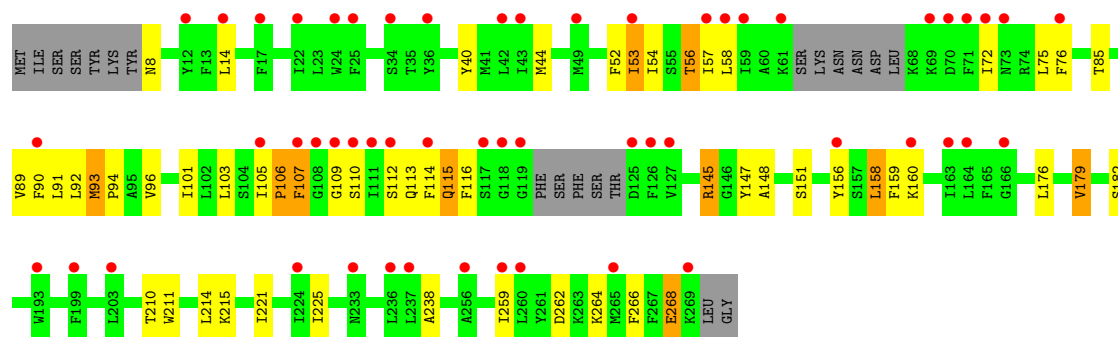


• Molecule 2: ANTIBODY FAB FRAGMENT HEAVY CHAIN

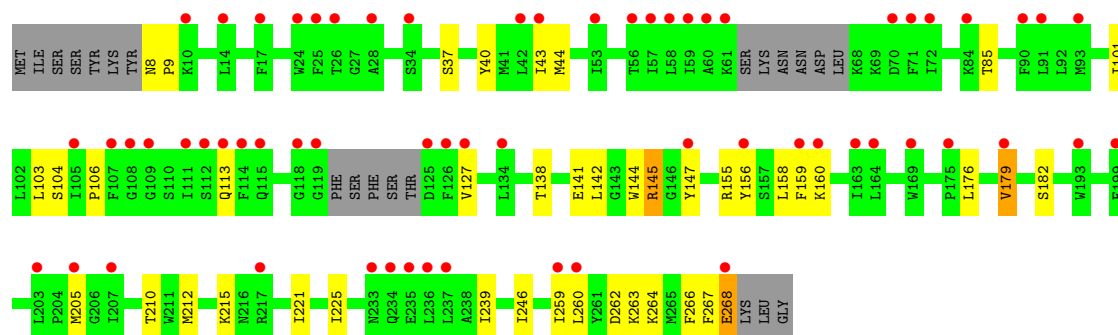
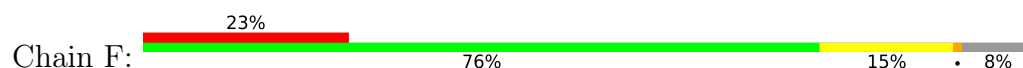


• Molecule 3: RAS AND A-FACTOR CONVERTING ENZYME 1, RCE1

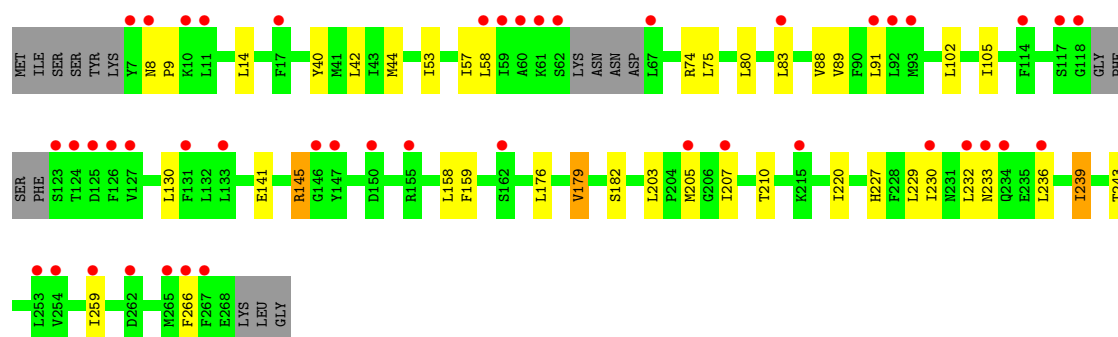
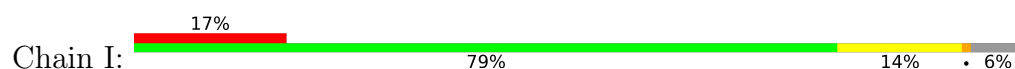




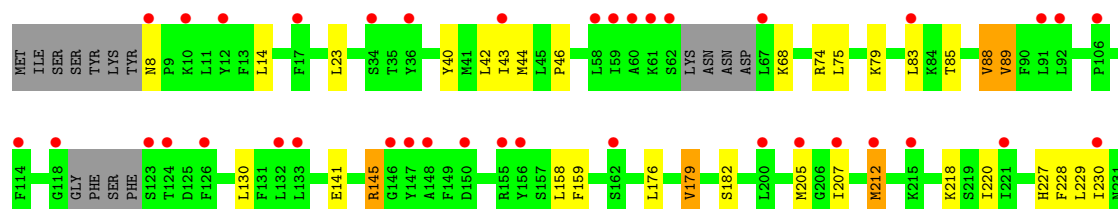
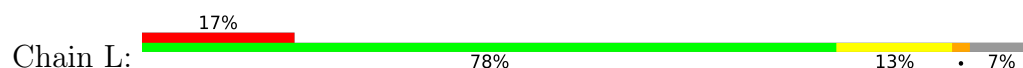
• Molecule 3: RAS AND A-FACTOR CONVERTING ENZYME 1, RCE1

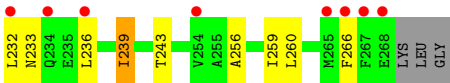


• Molecule 3: RAS AND A-FACTOR CONVERTING ENZYME 1, RCE1



• Molecule 3: RAS AND A-FACTOR CONVERTING ENZYME 1, RCE1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	113.06Å 90.09Å 99.30Å 89.06° 102.29° 90.00°	Depositor
Resolution (Å)	42.34 – 2.50 42.34 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (42.34-2.50) 97.8 (42.34-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.226 , 0.267 0.231 , 0.270	Depositor DCC
R_{free} test set	6543 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.085 for -h,k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21755	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 99.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9210e-12. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: LMT, BOG

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	0.30	0/1683	0.69	0/2288
1	D	0.34	0/1683	0.68	0/2288
1	G	0.34	2/1688 (0.1%)	0.70	2/2296 (0.1%)
1	J	0.32	1/1691 (0.1%)	0.69	0/2299
2	B	0.29	0/1712	0.70	2/2334 (0.1%)
2	E	0.56	6/1709 (0.4%)	0.86	7/2330 (0.3%)
2	H	0.34	1/1714 (0.1%)	0.75	2/2337 (0.1%)
2	K	0.30	0/1714	0.71	2/2337 (0.1%)
3	C	0.43	4/2079 (0.2%)	0.80	7/2830 (0.2%)
3	F	0.33	0/2070	0.72	0/2818
3	I	0.36	2/2099 (0.1%)	0.74	2/2859 (0.1%)
3	L	0.32	0/2100	0.71	0/2858
All	All	0.36	16/21942 (0.1%)	0.73	24/29874 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	129	THR	C-N	6.33	1.40	1.33
2	E	130	PRO	C-N	5.50	1.40	1.33
2	E	130	PRO	N-CD	5.37	1.55	1.47
1	J	204	PRO	N-CD	5.34	1.55	1.47
2	E	135	PRO	N-CD	5.28	1.55	1.47
3	I	9	PRO	N-CD	5.25	1.55	1.47
3	C	105	ILE	C-N	5.24	1.41	1.34
1	G	80	PRO	N-CD	5.22	1.55	1.47
3	C	106	PRO	N-CD	5.15	1.54	1.47
3	I	8	ASN	C-N	5.12	1.41	1.34
3	C	94	PRO	N-CD	5.10	1.54	1.47
1	G	79	GLN	C-N	5.09	1.41	1.34
3	C	93	MET	C-N	5.08	1.40	1.34
2	H	161	PRO	N-CD	5.06	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	161	PRO	N-CD	5.03	1.54	1.47
2	E	131	PRO	N-CD	5.02	1.54	1.47

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	160	GLU	C-N-CD	8.64	139.60	120.60
2	E	160	GLU	C-N-CD	8.43	139.15	120.60
2	E	129	THR	CA-C-N	-6.64	113.54	120.38
2	E	129	THR	C-N-CA	-6.64	113.54	120.38
2	E	130	PRO	CA-C-N	-6.56	113.22	119.85
2	E	130	PRO	C-N-CA	-6.56	113.22	119.85
3	C	90	PHE	N-CA-C	6.10	118.01	111.36
2	E	133	ASP	N-CA-C	5.84	118.72	109.50
3	C	105	ILE	O-C-N	5.76	124.16	120.07
2	H	161	PRO	CA-N-CD	-5.71	103.50	111.50
2	B	211	HIS	CA-C-N	5.67	125.35	119.05
2	B	211	HIS	C-N-CA	5.67	125.35	119.05
3	C	105	ILE	CA-C-N	-5.63	112.81	119.05
3	C	105	ILE	C-N-CA	-5.63	112.81	119.05
2	E	161	PRO	CA-N-CD	-5.50	103.80	111.50
2	K	211	HIS	CA-C-N	5.36	125.68	119.47
2	K	211	HIS	C-N-CA	5.36	125.68	119.47
3	I	8	ASN	CA-C-N	-5.31	113.16	119.05
3	I	8	ASN	C-N-CA	-5.31	113.16	119.05
3	C	93	MET	CA-C-N	-5.19	113.29	119.05
3	C	93	MET	C-N-CA	-5.19	113.29	119.05
3	C	93	MET	O-C-N	5.11	124.42	120.38
1	G	79	GLN	CA-C-N	-5.10	113.39	119.05
1	G	79	GLN	C-N-CA	-5.10	113.39	119.05

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	1642	0	1567	8	0
1	D	1642	0	1567	13	0
1	G	1647	0	1565	11	0
1	J	1650	0	1574	10	0
2	B	1666	0	1594	9	0
2	E	1663	0	1593	12	0
2	H	1668	0	1598	19	0
2	K	1668	0	1598	20	0
3	C	2020	0	2052	38	0
3	F	2011	0	2046	29	0
3	I	2040	0	2073	18	0
3	L	2041	0	2087	23	0
4	C	13	0	11	0	0
4	F	13	0	11	0	0
5	I	25	0	23	2	0
5	L	23	0	21	3	0
6	A	39	0	0	0	0
6	B	46	0	0	0	0
6	C	7	0	0	0	0
6	D	37	0	0	0	0
6	E	51	0	0	0	0
6	F	7	0	0	0	0
6	G	32	0	0	1	0
6	H	33	0	0	0	0
6	I	2	0	0	0	0
6	J	31	0	0	0	0
6	K	36	0	0	1	0
6	L	2	0	0	0	0
All	All	21755	0	20980	203	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 5.

All (203) 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)
3:C:158:LEU:HD23	3:C:266:PHE:HA	1.08	1.07
3:C:93:MET:HA	3:C:93:MET:HE2	1.39	1.03
3:C:158:LEU:HD23	3:C:266:PHE:CA	2.00	0.90
1:D:160:LEU:HD11	2:E:183:GLN:HB3	1.55	0.88
2:K:18:VAL:HG23	2:K:86:LEU:HD11	1.60	0.83
2:K:12:MET:HG3	2:K:18:VAL:CG2	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:11:LEU:O	2:K:12:MET:HE2	1.84	0.78
3:C:158:LEU:CD2	3:C:266:PHE:HA	2.04	0.77
2:K:12:MET:HG3	2:K:18:VAL:HG21	1.68	0.75
3:F:8:ASN:N	3:F:147:TYR:HH	1.82	0.75
3:L:228:PHE:CZ	3:L:232:LEU:HD11	2.22	0.74
2:E:155:LYS:NZ	2:E:183:GLN:OE1	2.22	0.72
3:F:145:ARG:N	3:F:145:ARG:HD2	2.05	0.69
3:F:9:PRO:HG2	3:F:155:ARG:HD2	1.74	0.69
3:L:89:VAL:HG23	3:L:212:MET:HE3	1.75	0.69
1:A:108:ARG:NH1	1:A:109:ALA:O	2.25	0.69
3:C:93:MET:HE2	3:C:93:MET:CA	2.15	0.69
2:B:18:VAL:HG13	2:B:86:LEU:HD21	1.74	0.68
3:C:93:MET:HA	3:C:93:MET:CE	2.20	0.68
2:E:18:VAL:HG13	2:E:86:LEU:HD21	1.75	0.68
1:A:160:LEU:HD11	2:B:183:GLN:HB3	1.75	0.67
3:C:8:ASN:N	3:C:147:TYR:HH	1.94	0.66
1:D:155:ARG:NE	1:D:157:ASN:O	2.27	0.66
2:K:12:MET:SD	2:K:18:VAL:HG22	2.36	0.65
3:F:113:GLN:HE21	3:F:239:ILE:HG22	1.62	0.65
3:L:130:LEU:HD22	3:L:232:LEU:HD21	1.79	0.65
3:I:158:LEU:HB3	3:I:266:PHE:HA	1.80	0.64
2:E:182:LEU:HD13	2:E:187:TYR:CE1	2.33	0.63
3:L:229:LEU:O	3:L:233:ASN:ND2	2.29	0.62
3:L:179:VAL:HG22	3:L:182:SER:HB3	1.81	0.62
2:B:38:LYS:HE2	2:B:40:ARG:HD2	1.81	0.61
3:L:233:ASN:OD1	5:L:301:LMT:O4'	2.18	0.61
2:H:133:ASP:HA	2:H:153:LEU:O	2.01	0.60
3:F:113:GLN:NE2	3:F:239:ILE:HG22	2.18	0.59
2:H:50:GLU:HG2	2:H:59:ASN:HB2	1.85	0.59
3:I:179:VAL:HG22	3:I:182:SER:HB3	1.84	0.58
1:J:183:LYS:NZ	1:J:187:GLU:OE2	2.36	0.57
1:G:121:SER:OG	2:H:134:TYR:HB3	2.05	0.57
1:J:103:LYS:NZ	1:J:165:ASP:OD1	2.36	0.57
3:F:85:THR:HB	3:F:212:MET:HE1	1.86	0.56
3:C:159:PHE:HE1	3:C:259:ILE:HD13	1.69	0.56
3:L:158:LEU:HB3	3:L:266:PHE:HA	1.88	0.56
3:L:23:LEU:HD13	3:L:46:PRO:HB2	1.87	0.56
3:C:107:PHE:CD1	3:C:107:PHE:N	2.74	0.56
3:I:205:MET:HE2	3:I:230:ILE:HD13	1.88	0.56
3:I:141:GLU:OE2	3:I:227:HIS:ND1	2.37	0.55
3:F:156:TYR:HB3	3:F:160:LYS:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:11:LEU:O	2:H:12:MET:HE2	2.06	0.55
2:E:38:LYS:HE2	2:E:40:ARG:HD2	1.88	0.55
3:F:263:LYS:O	3:F:267:PHE:HD2	1.90	0.54
2:K:210:ALA:HB2	2:K:217:LYS:HD3	1.89	0.54
2:B:155:LYS:NZ	2:B:183:GLN:OE1	2.41	0.54
2:E:184:SER:OG	2:E:185:ASP:N	2.37	0.54
1:G:160:LEU:HD11	2:H:181:VAL:HG11	1.90	0.53
3:F:264:LYS:O	3:F:268:GLU:HB2	2.08	0.53
1:D:108:ARG:NH1	1:D:109:ALA:O	2.38	0.53
3:C:114:PHE:O	3:C:116:PHE:CD2	2.62	0.53
1:D:149:LYS:HB2	1:D:193:THR:HB	1.90	0.53
3:I:130:LEU:HD22	3:I:232:LEU:HD11	1.91	0.53
3:F:144:TRP:HE3	3:F:144:TRP:HA	1.74	0.52
3:C:52:PHE:O	3:C:56:THR:OG1	2.28	0.51
3:F:144:TRP:HA	3:F:144:TRP:CE3	2.45	0.51
3:L:233:ASN:CG	5:L:301:LMT:O4'	2.53	0.51
1:G:37:GLN:HB2	1:G:47:LEU:HD11	1.92	0.51
2:K:12:MET:CG	2:K:18:VAL:CG2	2.88	0.51
2:K:40:ARG:HG2	2:K:92:ALA:HB2	1.93	0.50
1:G:201:SER:OG	1:G:203:SER:O	2.26	0.50
3:L:205:MET:HE2	3:L:230:ILE:HD13	1.92	0.50
1:A:187:GLU:O	1:A:211:ARG:NH2	2.44	0.50
3:C:112:SER:O	3:C:115:GLN:HB2	2.11	0.50
3:C:159:PHE:CE1	3:C:259:ILE:HD13	2.46	0.50
3:I:233:ASN:ND2	5:I:301:LMT:O4'	2.43	0.50
2:H:140:CYS:HB3	2:H:225:ARG:HB2	1.92	0.50
2:K:38:LYS:HE2	2:K:40:ARG:HD2	1.94	0.50
2:H:18:VAL:HG12	2:H:83:LEU:HB2	1.93	0.50
1:J:37:GLN:HB2	1:J:47:LEU:HD11	1.94	0.49
3:C:145:ARG:NH2	3:C:210:THR:OG1	2.45	0.49
3:C:156:TYR:HB3	3:C:160:LYS:HG2	1.95	0.49
2:H:38:LYS:HE2	2:H:40:ARG:HD2	1.93	0.49
3:C:107:PHE:N	3:C:107:PHE:HD1	2.10	0.49
2:H:131:PRO:HB3	2:H:157:TYR:HB3	1.95	0.49
1:D:37:GLN:HB2	1:D:47:LEU:HD11	1.93	0.49
3:C:53:ILE:O	3:C:57:ILE:HG12	2.12	0.49
3:L:85:THR:HB	3:L:212:MET:HE1	1.94	0.49
1:J:193:THR:HG23	1:J:208:SER:HB2	1.95	0.48
3:I:176:LEU:HA	3:I:179:VAL:HG13	1.95	0.48
2:K:30:SER:HA	2:K:53:PRO:HB2	1.94	0.48
3:C:109:GLY:O	3:C:110:SER:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:144:TRP:C	3:F:145:ARG:HD2	2.38	0.48
1:G:149:LYS:HB2	1:G:193:THR:HB	1.94	0.48
3:F:179:VAL:HG22	3:F:182:SER:HB3	1.95	0.48
1:G:70:GLN:NE2	6:G:2019:HOH:O	2.39	0.48
3:C:93:MET:CA	3:C:93:MET:CE	2.87	0.48
3:F:176:LEU:HA	3:F:179:VAL:HG13	1.96	0.48
5:L:301:LMT:O5B	5:L:301:LMT:O6'	2.23	0.48
2:K:67:LYS:NZ	6:K:2020:HOH:O	2.47	0.48
2:B:217:LYS:NZ	2:B:219:ASP:OD1	2.47	0.48
2:B:18:VAL:HG22	2:B:83:LEU:HB2	1.96	0.48
3:C:148:ALA:O	3:C:151:SER:OG	2.28	0.48
3:L:74:ARG:HD2	3:L:218:LYS:HB3	1.95	0.48
1:G:6:GLN:HG3	1:G:99:GLY:HA3	1.95	0.47
1:D:157:ASN:N	1:D:157:ASN:OD1	2.44	0.47
2:H:157:TYR:CE2	2:H:162:VAL:HG13	2.50	0.47
3:L:176:LEU:HA	3:L:179:VAL:HG13	1.96	0.47
2:H:133:ASP:OD1	2:H:133:ASP:N	2.46	0.47
3:I:53:ILE:O	3:I:57:ILE:HG12	2.15	0.47
3:L:141:GLU:OE2	3:L:227:HIS:ND1	2.37	0.47
3:C:101:ILE:HG23	3:C:110:SER:OG	2.15	0.47
2:H:99:ARG:HD2	2:H:109:TYR:O	2.14	0.46
1:J:108:ARG:NH1	1:J:109:ALA:O	2.45	0.46
3:C:176:LEU:HA	3:C:179:VAL:HG13	1.96	0.46
1:J:149:LYS:HB2	1:J:193:THR:HB	1.98	0.46
1:D:150:ILE:HD11	1:D:179:LEU:HD21	1.98	0.46
1:D:207:LYS:HD3	1:D:207:LYS:HA	1.56	0.46
2:H:29:PHE:CD2	2:H:77:ASN:HA	2.51	0.46
2:H:40:ARG:HG2	2:H:92:ALA:HB2	1.97	0.46
3:I:40:TYR:O	3:I:44:MET:HG2	2.16	0.46
1:A:212:ASN:OD1	1:A:212:ASN:N	2.47	0.45
3:C:158:LEU:CD1	3:C:214:LEU:HD11	2.47	0.45
3:F:141:GLU:O	3:F:145:ARG:HB2	2.16	0.45
2:H:210:ALA:HB2	2:H:217:LYS:HE3	1.98	0.45
1:A:149:LYS:HB2	1:A:193:THR:HB	1.98	0.45
3:I:229:LEU:O	3:I:233:ASN:ND2	2.40	0.45
1:A:70:GLN:HE22	2:H:128:THR:HB	1.82	0.45
3:F:145:ARG:NH2	3:F:210:THR:OG1	2.50	0.45
3:C:72:ILE:O	3:C:76:PHE:HD2	1.99	0.45
1:D:11:LEU:HD21	1:D:19:VAL:HB	1.99	0.45
3:L:40:TYR:O	3:L:44:MET:HG2	2.17	0.44
3:F:221:ILE:O	3:F:225:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:159:PHE:HE1	3:I:259:ILE:HD13	1.83	0.44
2:K:200:TRP:CG	2:K:201:PRO:HA	2.52	0.44
3:L:232:LEU:O	3:L:236:LEU:HB2	2.18	0.44
2:B:40:ARG:HG2	2:B:92:ALA:HB2	2.00	0.44
1:D:160:LEU:HD11	2:E:183:GLN:CB	2.37	0.44
3:F:8:ASN:N	3:F:147:TYR:OH	2.45	0.44
3:L:43:ILE:O	3:L:46:PRO:HD2	2.17	0.44
2:K:220:LYS:HD3	2:K:220:LYS:HA	1.75	0.44
3:I:102:LEU:HA	3:I:105:ILE:HD12	2.00	0.44
1:J:198:HIS:ND1	1:J:200:THR:OG1	2.35	0.44
1:A:24:ARG:CZ	1:A:70:GLN:HG2	2.47	0.43
1:G:11:LEU:HD21	1:G:19:VAL:HB	1.99	0.43
2:K:130:PRO:HA	2:K:131:PRO:HD3	1.84	0.43
3:C:103:LEU:O	3:C:106:PRO:HD2	2.18	0.43
2:E:200:TRP:CG	2:E:201:PRO:HA	2.53	0.43
3:C:264:LYS:O	3:C:268:GLU:HB2	2.17	0.43
2:K:18:VAL:HG23	2:K:86:LEU:CD1	2.39	0.43
3:F:113:GLN:HE21	3:F:239:ILE:HA	1.83	0.43
2:E:18:VAL:HG22	2:E:83:LEU:HB2	2.00	0.43
3:F:40:TYR:O	3:F:44:MET:HG2	2.18	0.43
1:G:142:LYS:HB3	1:G:173:TYR:CE1	2.53	0.43
1:J:119:PRO:HG2	2:K:225:ARG:CZ	2.48	0.43
3:L:159:PHE:HE1	3:L:259:ILE:HD13	1.84	0.43
2:E:157:TYR:CE2	2:E:162:VAL:HG13	2.54	0.43
3:L:88:VAL:HG22	3:L:212:MET:HE2	2.01	0.42
3:F:158:LEU:HD23	3:F:266:PHE:HA	2.01	0.42
2:K:38:LYS:HB2	2:K:48:ILE:HD11	2.01	0.42
2:K:12:MET:O	2:K:123:VAL:HA	2.19	0.42
3:C:103:LEU:C	3:C:106:PRO:HD2	2.44	0.42
3:I:141:GLU:O	3:I:145:ARG:HB2	2.19	0.42
3:C:211:TRP:O	3:C:215:LYS:HG2	2.19	0.42
2:B:200:TRP:CG	2:B:201:PRO:HA	2.54	0.42
3:C:40:TYR:O	3:C:44:MET:HG2	2.19	0.42
3:F:103:LEU:O	3:F:106:PRO:HD2	2.19	0.42
3:I:74:ARG:HB3	3:I:220:ILE:HG13	2.01	0.42
3:I:239:ILE:HG13	3:I:243:THR:HB	2.01	0.42
3:L:256:ALA:O	3:L:260:LEU:HG	2.20	0.42
3:C:158:LEU:HD13	3:C:214:LEU:HD11	2.01	0.42
1:D:195:GLU:HG3	1:D:206:VAL:HG12	2.00	0.42
1:A:37:GLN:HB2	1:A:47:LEU:HD11	2.01	0.42
3:C:53:ILE:HG13	3:C:54:ILE:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:101:ILE:O	3:F:104:SER:OG	2.35	0.42
3:C:221:ILE:O	3:C:225:ILE:HG12	2.20	0.42
3:C:85:THR:O	3:C:89:VAL:HG23	2.20	0.41
3:C:113:GLN:O	3:C:114:PHE:C	2.63	0.41
3:C:179:VAL:HG22	3:C:182:SER:HB3	2.02	0.41
1:D:212:ASN:OD1	1:D:212:ASN:N	2.53	0.41
2:E:206:THR:HG23	2:E:220:LYS:C	2.46	0.41
2:H:200:TRP:CG	2:H:201:PRO:HA	2.54	0.41
3:F:104:SER:HB3	3:F:246:ILE:HD12	2.01	0.41
3:F:138:THR:O	3:F:142:LEU:HG	2.20	0.41
1:J:58:VAL:HA	1:J:59:PRO:HD3	1.94	0.41
2:B:103:TYR:CD1	3:C:238:ALA:HB1	2.56	0.41
3:C:92:LEU:O	3:C:96:VAL:HG23	2.20	0.41
3:F:37:SER:O	3:F:40:TYR:HD1	2.04	0.41
3:I:207:ILE:HD13	3:I:259:ILE:HD11	2.02	0.41
5:I:301:LMT:H1B	5:I:301:LMT:H5'	1.34	0.41
2:K:19:LYS:HE2	2:K:19:LYS:HB3	1.88	0.41
3:L:239:ILE:HG13	3:L:243:THR:HB	2.02	0.41
3:F:215:LYS:HD3	3:F:215:LYS:HA	1.85	0.41
1:D:6:GLN:HG3	1:D:99:GLY:HA3	2.02	0.41
3:F:159:PHE:HE1	3:F:259:ILE:HD13	1.86	0.41
3:I:232:LEU:O	3:I:236:LEU:HB2	2.21	0.41
1:J:6:GLN:HG3	1:J:99:GLY:HA3	2.02	0.41
3:L:145:ARG:HB3	3:L:220:ILE:HG12	2.03	0.41
3:C:109:GLY:O	3:C:110:SER:CB	2.68	0.41
3:F:205:MET:HA	3:F:205:MET:HE3	2.03	0.41
3:I:159:PHE:HA	3:I:266:PHE:HD1	1.86	0.40
2:H:30:SER:HA	2:H:53:PRO:HB2	2.03	0.40
3:L:207:ILE:HD13	3:L:259:ILE:HD11	2.02	0.40
2:E:223:GLU:HA	2:E:224:PRO:HD3	1.99	0.40
1:G:91:PHE:CZ	2:H:99:ARG:HD3	2.56	0.40
1:G:142:LYS:HB3	1:G:173:TYR:CD1	2.57	0.40
2:K:99:ARG:HD2	2:K:109:TYR:O	2.21	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	209/214 (98%)	205 (98%)	4 (2%)	0	100	100
1	D	209/214 (98%)	205 (98%)	4 (2%)	0	100	100
1	G	210/214 (98%)	207 (99%)	3 (1%)	0	100	100
1	J	210/214 (98%)	206 (98%)	4 (2%)	0	100	100
2	B	217/227 (96%)	214 (99%)	3 (1%)	0	100	100
2	E	216/227 (95%)	213 (99%)	3 (1%)	0	100	100
2	H	217/227 (96%)	214 (99%)	3 (1%)	0	100	100
2	K	217/227 (96%)	212 (98%)	5 (2%)	0	100	100
3	C	245/271 (90%)	242 (99%)	3 (1%)	0	100	100
3	F	244/271 (90%)	242 (99%)	2 (1%)	0	100	100
3	I	248/271 (92%)	244 (98%)	4 (2%)	0	100	100
3	L	247/271 (91%)	245 (99%)	2 (1%)	0	100	100
All	All	2689/2848 (94%)	2649 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	185/188 (98%)	177 (96%)	8 (4%)	26	51
1	D	185/188 (98%)	175 (95%)	10 (5%)	20	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	185/188 (98%)	181 (98%)	4 (2%)	45	73
1	J	186/188 (99%)	178 (96%)	8 (4%)	26	51
2	B	185/192 (96%)	182 (98%)	3 (2%)	55	79
2	E	185/192 (96%)	178 (96%)	7 (4%)	29	56
2	H	185/192 (96%)	179 (97%)	6 (3%)	34	62
2	K	185/192 (96%)	178 (96%)	7 (4%)	29	56
3	C	216/244 (88%)	203 (94%)	13 (6%)	17	36
3	F	216/244 (88%)	209 (97%)	7 (3%)	34	62
3	I	220/244 (90%)	206 (94%)	14 (6%)	16	33
3	L	222/244 (91%)	209 (94%)	13 (6%)	18	37
All	All	2355/2496 (94%)	2255 (96%)	100 (4%)	26	52

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	69	THR
1	A	81	GLU
1	A	105	GLU
1	A	159	VAL
1	A	184	ASP
1	A	206	VAL
1	A	212	ASN
2	B	45	LEU
2	B	86	LEU
2	B	123	VAL
3	C	14	LEU
3	C	53	ILE
3	C	56	THR
3	C	58	LEU
3	C	75	LEU
3	C	91	LEU
3	C	107	PHE
3	C	115	GLN
3	C	145	ARG
3	C	158	LEU
3	C	179	VAL
3	C	262	ASP

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Mol	Chain	Res	Type
3	C	268	GLU
1	D	48	VAL
1	D	69	THR
1	D	81	GLU
1	D	105	GLU
1	D	159	VAL
1	D	184	ASP
1	D	206	VAL
1	D	207	LYS
1	D	208	SER
1	D	212	ASN
2	E	18	VAL
2	E	45	LEU
2	E	86	LEU
2	E	123	VAL
2	E	132	SER
2	E	172	SER
2	E	208	ASN
3	F	43	ILE
3	F	127	VAL
3	F	145	ARG
3	F	179	VAL
3	F	260	LEU
3	F	262	ASP
3	F	268	GLU
1	G	4	LEU
1	G	76	ASN
1	G	157	ASN
1	G	206	VAL
2	H	19	LYS
2	H	45	LEU
2	H	123	VAL
2	H	147	SER
2	H	172	SER
2	H	217	LYS
3	I	14	LEU
3	I	42	LEU
3	I	58	LEU
3	I	75	LEU
3	I	80	LEU
3	I	83	LEU
3	I	88	VAL

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Mol	Chain	Res	Type
3	I	89	VAL
3	I	91	LEU
3	I	145	ARG
3	I	179	VAL
3	I	203	LEU
3	I	210	THR
3	I	239	ILE
1	J	33	LEU
1	J	60	SER
1	J	81	GLU
1	J	106	LEU
1	J	157	ASN
1	J	159	VAL
1	J	203	SER
1	J	206	VAL
2	K	19	LYS
2	K	23	LYS
2	K	45	LEU
2	K	123	VAL
2	K	147	SER
2	K	148	VAL
2	K	172	SER
3	L	8	ASN
3	L	14	LEU
3	L	42	LEU
3	L	68	LYS
3	L	75	LEU
3	L	79	LYS
3	L	83	LEU
3	L	88	VAL
3	L	89	VAL
3	L	145	ARG
3	L	179	VAL
3	L	212	MET
3	L	239	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	190	ASN
1	A	210	ASN

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Mol	Chain	Res	Type
3	C	181	ASN
3	C	241	GLN
1	D	85	ASN
1	D	190	ASN
1	D	210	ASN
3	F	233	ASN
3	F	241	GLN
1	G	85	ASN
3	I	241	GLN
1	J	38	GLN
1	J	210	ASN
2	K	39	GLN
3	L	8	ASN
3	L	241	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	LMT	I	301	-	26,26,36	0.49	0	37,37,47	0.66	0
4	BOG	F	301	-	13,13,20	0.56	0	18,18,25	0.65	0
4	BOG	C	301	-	13,13,20	0.75	0	18,18,25	0.99	2 (11%)
5	LMT	L	301	-	24,24,36	0.37	0	35,35,47	1.99	4 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LMT	I	301	-	-	4/11/51/61	0/2/2/2
4	BOG	F	301	-	-	0/4/24/31	0/1/1/1
4	BOG	C	301	-	-	2/4/24/31	0/1/1/1
5	LMT	L	301	-	-	2/8/48/61	0/2/2/2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	301	LMT	C1B-O1B-C4'	-9.41	95.67	117.98
5	L	301	LMT	O1B-C1B-C2B	4.27	118.59	108.09
5	L	301	LMT	O1B-C4'-C3'	2.69	114.07	107.23
4	C	301	BOG	O5-C1-C2	2.68	115.87	110.37
5	L	301	LMT	O1B-C1B-O5B	2.65	117.67	110.69
4	C	301	BOG	C3-C4-C5	-2.05	106.52	110.23

There are no chirality outliers.

All (8) torsion outliers are listed below:

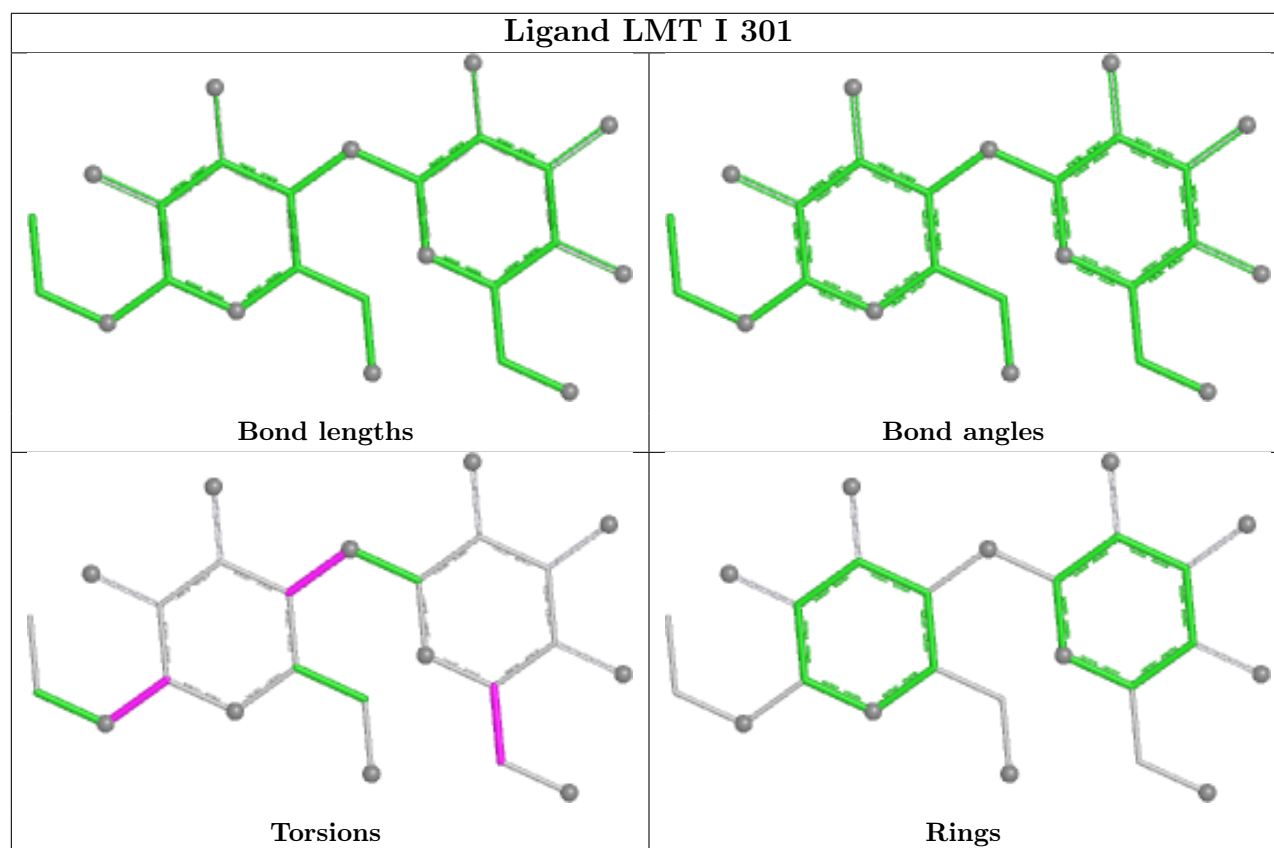
Mol	Chain	Res	Type	Atoms
5	I	301	LMT	O5'-C1'-O1'-C1
5	I	301	LMT	C5'-C4'-O1B-C1B
5	I	301	LMT	O5B-C5B-C6B-O6B
4	C	301	BOG	C2-C1-O1-C1'
5	L	301	LMT	C4B-C5B-C6B-O6B
5	I	301	LMT	C4B-C5B-C6B-O6B
5	L	301	LMT	O5B-C5B-C6B-O6B
4	C	301	BOG	O5-C5-C6-O6

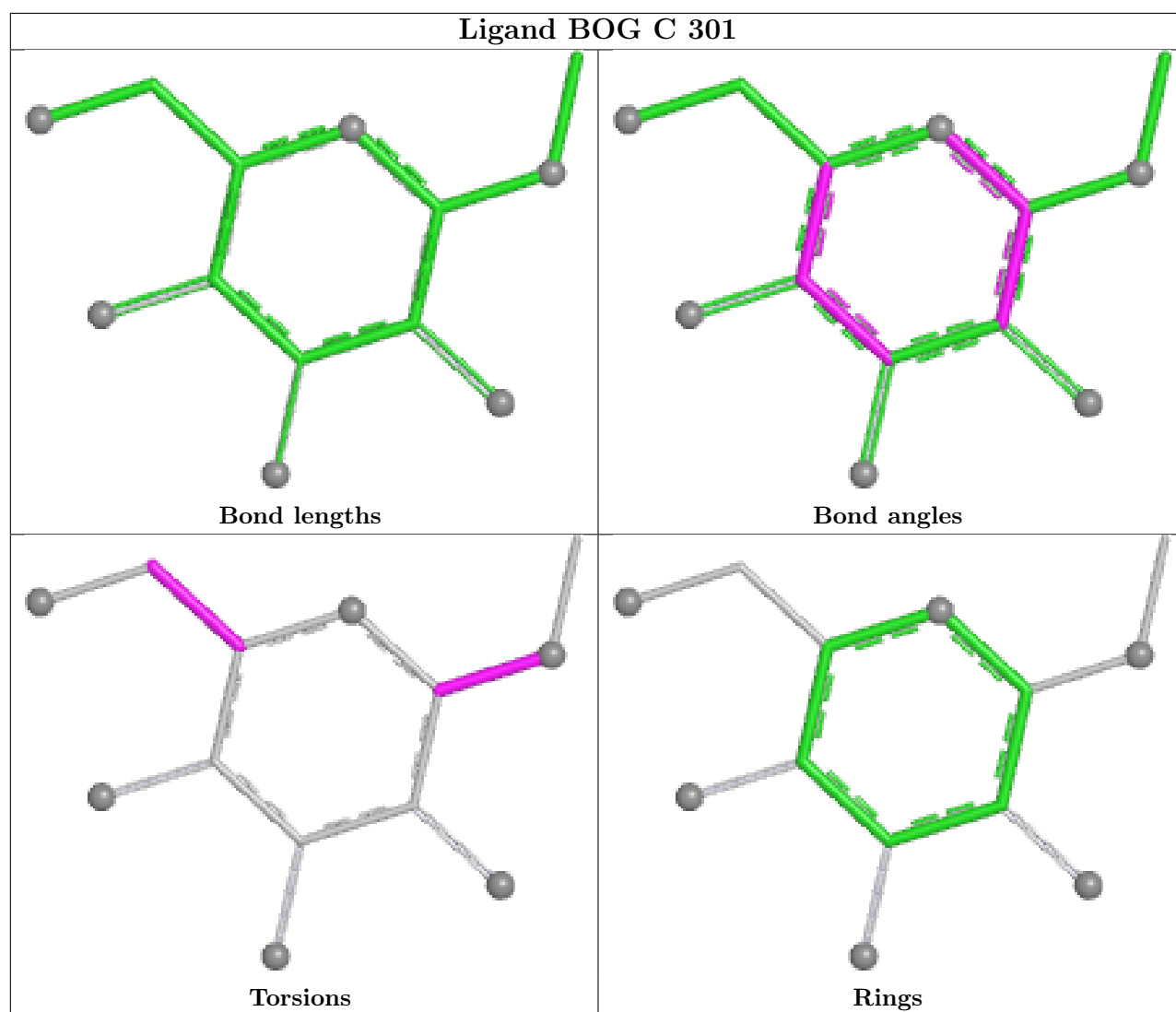
There are no ring outliers.

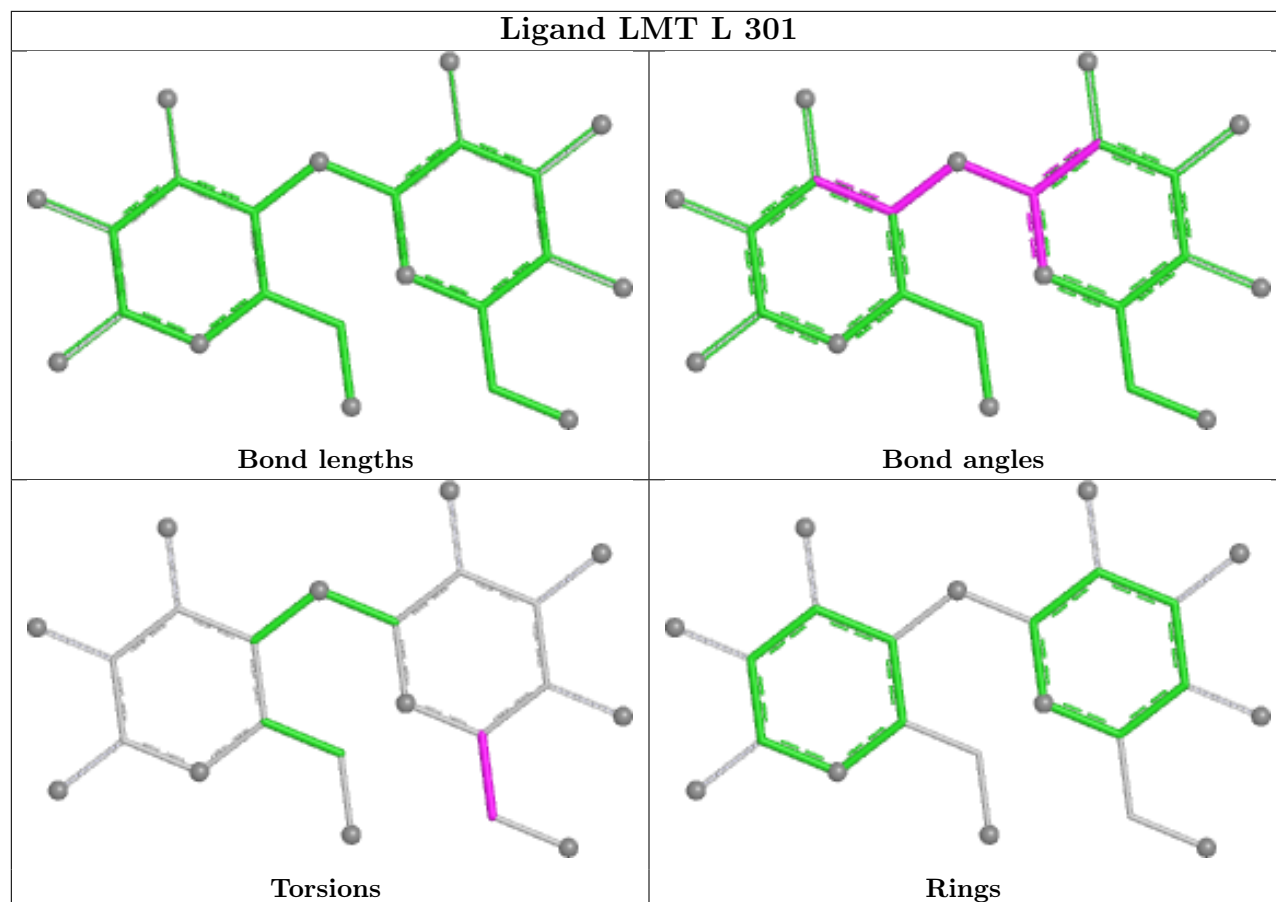
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	301	LMT	2	0
5	L	301	LMT	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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	211/214 (98%)	0.75	16 (7%) 20 17	36, 58, 88, 101	0
1	D	211/214 (98%)	0.82	14 (6%) 24 21	41, 56, 86, 107	0
1	G	212/214 (99%)	0.79	21 (9%) 13 11	43, 58, 96, 117	0
1	J	212/214 (99%)	0.81	21 (9%) 13 11	38, 60, 98, 122	0
2	B	221/227 (97%)	0.77	17 (7%) 19 17	38, 59, 81, 106	0
2	E	220/227 (96%)	0.81	21 (9%) 14 12	42, 57, 83, 109	0
2	H	221/227 (97%)	0.76	17 (7%) 19 17	41, 55, 81, 100	0
2	K	221/227 (97%)	0.76	23 (10%) 11 10	40, 57, 84, 109	0
3	C	251/271 (92%)	1.31	54 (21%) 2 2	50, 83, 133, 156	0
3	F	250/271 (92%)	1.33	62 (24%) 2 1	51, 83, 129, 152	0
3	I	254/271 (93%)	1.20	45 (17%) 4 3	51, 81, 127, 164	0
3	L	253/271 (93%)	1.12	46 (18%) 3 2	52, 82, 129, 159	0
All	All	2737/2848 (96%)	0.95	357 (13%) 7 6	36, 65, 111, 164	0

All (357) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	54	GLY	7.5
3	I	67	LEU	7.4
3	L	67	LEU	6.5
3	C	236	LEU	6.4
2	B	54	GLY	6.2
1	J	158	GLY	6.1
3	F	236	LEU	6.0
3	F	119	GLY	5.8
2	H	146	SER	5.7
2	H	54	GLY	5.5
3	I	7	TYR	5.4

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Mol	Chain	Res	Type	RSRZ
3	F	114	PHE	5.4
3	F	70	ASP	5.4
1	G	158	GLY	5.3
1	J	204	PRO	5.3
3	C	114	PHE	5.1
1	J	7	SER	5.0
3	L	118	GLY	5.0
3	C	70	ASP	5.0
1	G	7	SER	5.0
3	F	111	ILE	4.7
3	C	269	LYS	4.7
3	L	265	MET	4.6
3	I	62	SER	4.6
3	I	123	SER	4.6
3	L	8	ASN	4.5
3	F	25	PHE	4.5
2	K	54	GLY	4.4
3	I	114	PHE	4.4
2	K	146	SER	4.3
3	C	72	ILE	4.2
2	H	15	GLY	4.2
3	I	230	ILE	4.2
3	F	72	ILE	4.1
3	I	118	GLY	4.1
2	B	105	TYR	4.1
3	L	230	ILE	4.1
3	L	114	PHE	4.1
1	D	3	GLN	4.0
2	B	141	GLY	4.0
3	C	53	ILE	4.0
2	H	18	VAL	3.9
3	I	8	ASN	3.9
3	L	267	PHE	3.9
3	I	146	GLY	3.9
3	C	111	ILE	3.9
3	C	193	TRP	3.8
3	L	59	ILE	3.8
3	I	234	GLN	3.8
3	C	25	PHE	3.8
3	C	112	SER	3.8
2	K	141	GLY	3.8
1	J	143	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
3	C	14	LEU	3.7
1	J	202	THR	3.7
2	K	130	PRO	3.7
3	F	193	TRP	3.6
3	C	22	ILE	3.6
1	D	12	SER	3.6
3	I	124	THR	3.6
1	D	2	ILE	3.6
3	F	109	GLY	3.6
1	G	204	PRO	3.6
3	F	57	ILE	3.6
3	I	17	PHE	3.6
1	G	205	ILE	3.5
1	D	76	ASN	3.5
3	I	233	ASN	3.5
2	B	74	THR	3.5
3	C	260	LEU	3.5
1	J	152	GLY	3.5
3	L	147	TYR	3.5
3	F	17	PHE	3.5
3	L	146	GLY	3.5
1	A	14	SER	3.4
3	F	53	ILE	3.4
2	H	172	SER	3.4
1	D	156	GLN	3.4
1	A	2	ILE	3.4
3	I	162	SER	3.4
3	I	147	TYR	3.3
2	E	74	THR	3.3
2	K	18	VAL	3.3
2	K	3	GLN	3.3
1	D	4	LEU	3.3
3	I	126	PHE	3.3
3	L	61	LYS	3.3
2	K	133	ASP	3.3
3	C	57	ILE	3.3
3	C	17	PHE	3.3
3	I	91	LEU	3.3
2	H	41	PRO	3.2
2	H	140	CYS	3.2
3	F	91	LEU	3.2
3	C	125	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
3	F	14	LEU	3.2
3	F	260	LEU	3.2
2	B	25	THR	3.2
2	E	3	GLN	3.2
2	H	133	ASP	3.2
1	G	152	GLY	3.2
2	K	2	VAL	3.2
3	L	92	LEU	3.1
3	C	73	ASN	3.1
3	C	118	GLY	3.1
1	D	155	ARG	3.1
3	I	92	LEU	3.1
2	E	140	CYS	3.1
2	K	15	GLY	3.1
3	L	234	GLN	3.1
2	H	130	PRO	3.1
3	I	133	LEU	3.1
1	D	157	ASN	3.1
1	J	157	ASN	3.1
1	J	155	ARG	3.1
2	H	105	TYR	3.0
1	G	143	ASP	3.0
3	C	110	SER	3.0
1	A	24	ARG	3.0
2	E	181	VAL	3.0
3	L	232	LEU	3.0
3	C	107	PHE	3.0
2	H	17	SER	3.0
3	F	61	LYS	3.0
3	C	109	GLY	3.0
3	C	127	VAL	3.0
3	F	127	VAL	3.0
3	F	126	PHE	3.0
3	I	207	ILE	3.0
3	C	265	MET	3.0
3	I	267	PHE	3.0
3	L	150	ASP	3.0
2	K	140	CYS	3.0
1	G	142	LYS	2.9
2	E	105	TYR	2.9
3	F	164	LEU	2.9
1	G	157	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	8	PRO	2.9
3	C	61	LYS	2.9
3	I	236	LEU	2.9
3	L	62	SER	2.9
3	I	265	MET	2.9
3	F	217	ARG	2.9
3	L	10	LYS	2.9
3	L	205	MET	2.9
3	L	207	ILE	2.9
3	L	200	LEU	2.9
2	E	66	GLY	2.9
1	A	21	ILE	2.8
1	A	76	ASN	2.8
2	H	147	SER	2.8
3	L	221	ILE	2.8
1	G	159	VAL	2.8
1	A	4	LEU	2.8
3	F	203	LEU	2.8
3	F	113	GLN	2.8
3	F	107	PHE	2.8
3	L	155	ARG	2.8
1	J	212	ASN	2.8
3	C	59	ILE	2.8
2	H	3	GLN	2.8
2	K	17	SER	2.8
3	F	112	SER	2.8
3	L	162	SER	2.8
3	L	212	MET	2.8
3	F	10	LYS	2.8
1	A	12	SER	2.7
1	A	43	SER	2.7
1	D	203	SER	2.7
3	F	125	ASP	2.7
2	E	172	SER	2.7
1	A	103	LYS	2.7
1	D	103	LYS	2.7
3	L	148	ALA	2.7
2	H	141	GLY	2.7
3	C	71	PHE	2.7
3	C	90	PHE	2.7
3	C	119	GLY	2.7
3	F	108	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	142	LYS	2.7
2	B	181	VAL	2.7
3	C	117	SER	2.7
3	I	61	LYS	2.7
3	L	133	LEU	2.7
2	B	169	GLY	2.7
1	J	160	LEU	2.7
3	C	58	LEU	2.7
3	I	150	ASP	2.6
1	D	128	GLY	2.6
1	J	205	ILE	2.6
2	B	130	PRO	2.6
3	F	233	ASN	2.6
3	I	155	ARG	2.6
3	I	205	MET	2.6
3	F	24	TRP	2.6
3	C	108	GLY	2.6
1	G	196	ALA	2.6
2	E	25	THR	2.6
3	L	91	LEU	2.6
2	B	3	GLN	2.6
2	K	172	SER	2.6
3	C	34	SER	2.6
1	G	9	ALA	2.6
1	J	196	ALA	2.6
1	G	155	ARG	2.6
1	D	106	LEU	2.6
1	J	4	LEU	2.6
3	C	42	LEU	2.6
2	B	55	SER	2.6
2	H	16	ALA	2.6
3	C	24	TRP	2.5
1	J	8	PRO	2.5
3	C	43	ILE	2.5
3	C	199	PHE	2.5
3	F	58	LEU	2.5
2	H	2	VAL	2.5
1	J	9	ALA	2.5
2	K	214	SER	2.5
3	C	224	ILE	2.5
3	C	259	ILE	2.5
3	C	126	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	59	ILE	2.5
3	I	59	ILE	2.5
3	F	90	PHE	2.5
1	A	157	ASN	2.5
2	E	55	SER	2.5
3	C	69	LYS	2.5
3	I	83	LEU	2.5
1	A	153	SER	2.5
2	B	185	ASP	2.4
3	C	105	ILE	2.4
3	F	147	TYR	2.4
3	L	156	TYR	2.4
1	J	10	SER	2.4
3	F	43	ILE	2.4
3	F	105	ILE	2.4
3	C	203	LEU	2.4
3	F	237	LEU	2.4
2	E	18	VAL	2.4
2	E	130	PRO	2.4
2	K	105	TYR	2.4
1	J	159	VAL	2.4
1	J	145	ASN	2.4
3	F	26	THR	2.3
2	E	125	SER	2.3
2	E	2	VAL	2.3
3	F	235	GLU	2.3
2	K	147	SER	2.3
2	K	106	GLY	2.3
2	K	117	GLN	2.3
3	L	83	LEU	2.3
3	I	125	ASP	2.3
1	A	15	VAL	2.3
3	C	156	TYR	2.3
3	I	254	VAL	2.3
1	G	212	ASN	2.3
1	A	45	GLN	2.3
3	F	34	SER	2.3
3	C	163	ILE	2.3
3	C	164	LEU	2.3
3	F	163	ILE	2.3
3	L	58	LEU	2.3
3	L	124	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	6	GLN	2.3
2	B	56	GLY	2.3
2	E	132	SER	2.3
1	G	110	ASP	2.3
2	B	133	ASP	2.3
3	I	10	LYS	2.3
3	L	17	PHE	2.3
1	A	155	ARG	2.3
3	L	106	PRO	2.3
3	C	256	ALA	2.2
3	F	60	ALA	2.2
2	K	1	GLN	2.2
3	I	232	LEU	2.2
1	J	1	ASP	2.2
3	F	156	TYR	2.2
1	G	202	THR	2.2
2	B	145	GLY	2.2
3	F	205	MET	2.2
3	I	11	LEU	2.2
2	B	132	SER	2.2
2	E	185	ASP	2.2
2	E	65	LYS	2.2
2	K	58	THR	2.2
2	B	66	GLY	2.2
2	H	106	GLY	2.2
3	C	166	GLY	2.2
3	F	118	GLY	2.2
3	I	58	LEU	2.2
3	L	236	LEU	2.2
3	F	169	TRP	2.2
3	I	127	VAL	2.2
3	F	84	LYS	2.2
3	I	60	ALA	2.2
3	F	42	LEU	2.2
3	F	268	GLU	2.2
3	F	160	LYS	2.2
1	A	156	GLN	2.1
3	F	115	GLN	2.1
2	E	56	GLY	2.1
2	B	62	GLU	2.1
3	L	268	GLU	2.1
2	E	215	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	I	117	SER	2.1
3	L	123	SER	2.1
3	I	131	PHE	2.1
3	I	266	PHE	2.1
3	L	126	PHE	2.1
3	L	266	PHE	2.1
3	F	207	ILE	2.1
1	G	1	ASP	2.1
3	L	34	SER	2.1
3	C	160	LYS	2.1
3	C	49	MET	2.1
3	F	71	PHE	2.1
3	F	199	PHE	2.1
3	L	254	VAL	2.1
2	E	26	GLY	2.1
3	C	237	LEU	2.1
3	I	253	LEU	2.1
3	F	56	THR	2.1
3	I	259	ILE	2.1
3	C	12	TYR	2.1
3	L	12	TYR	2.1
1	J	110	ASP	2.1
2	K	202	SER	2.1
3	I	262	ASP	2.1
3	C	76	PHE	2.1
3	F	159	PHE	2.1
3	F	234	GLN	2.1
3	F	179	VAL	2.1
3	L	60	ALA	2.1
3	F	259	ILE	2.1
2	K	127	LYS	2.1
2	K	107	SER	2.1
3	F	93	MET	2.1
1	G	160	LEU	2.0
3	C	233	ASN	2.0
3	F	134	LEU	2.0
1	A	187	GLU	2.0
1	D	68	GLY	2.0
1	G	147	LYS	2.0
3	I	215	LYS	2.0
3	L	43	ILE	2.0
3	L	215	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
3	L	36	TYR	2.0
1	D	43	SER	2.0
1	G	153	SER	2.0
3	I	93	MET	2.0
2	K	16	ALA	2.0
3	F	28	ALA	2.0
3	L	132	LEU	2.0
2	E	57	ASN	2.0
3	F	175	PRO	2.0
3	C	36	TYR	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](#)

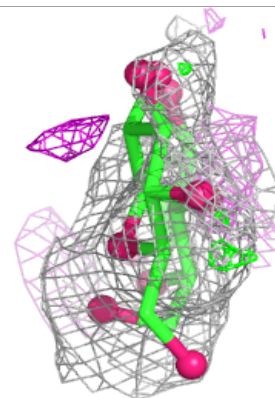
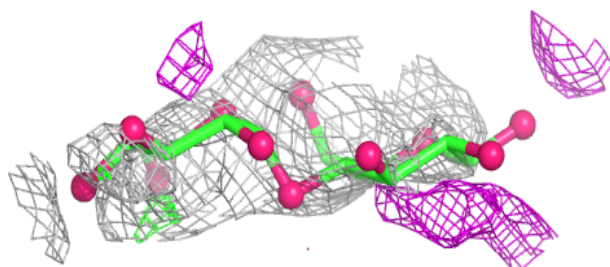
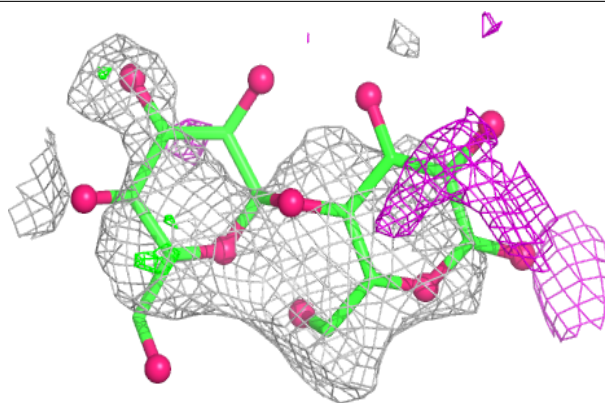
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	LMT	L	301	23/35	0.67	0.27	147,154,160,165	0
4	BOG	C	301	13/20	0.73	0.22	127,132,136,136	0
4	BOG	F	301	13/20	0.74	0.25	124,128,133,136	0
5	LMT	I	301	25/35	0.76	0.24	153,158,163,165	0

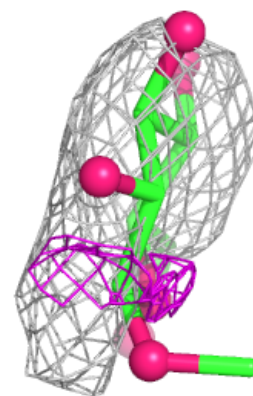
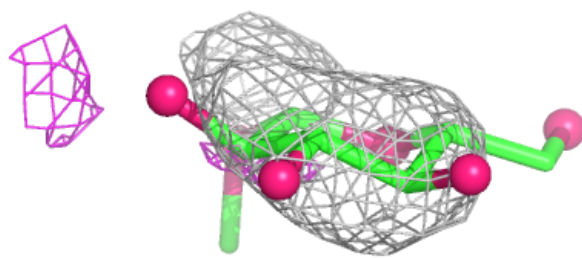
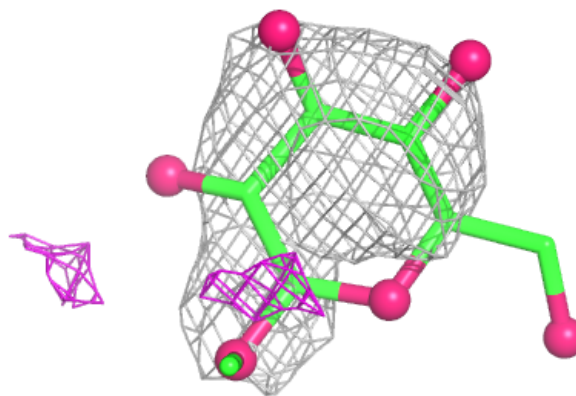
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LMT L 301:

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

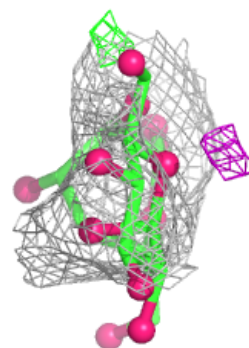
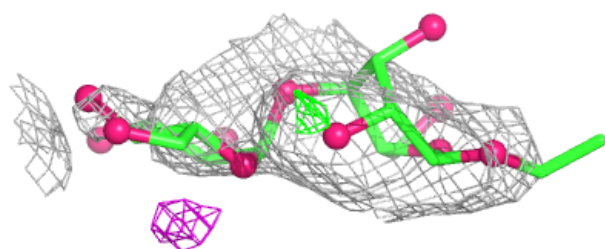
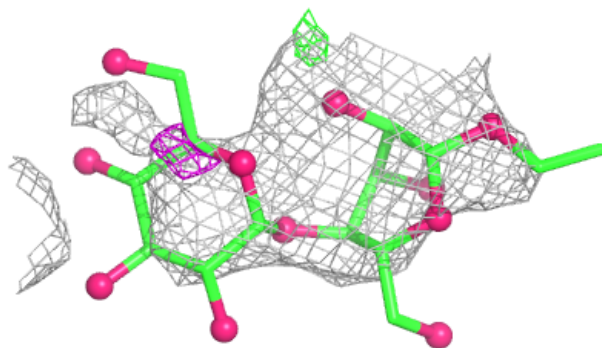
**Electron density around BOG C 301:**

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



Electron density around LMT I 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.