



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:22 AM UTC

PDB ID : 5HCJ / pdb_00005hcj
Title : Cationic Ligand-Gated Ion Channel
Authors : Shahsavar, A.; Sauguet, L.; Delarue, M.
Deposited on : 2016-01-04
Resolution : 2.95 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

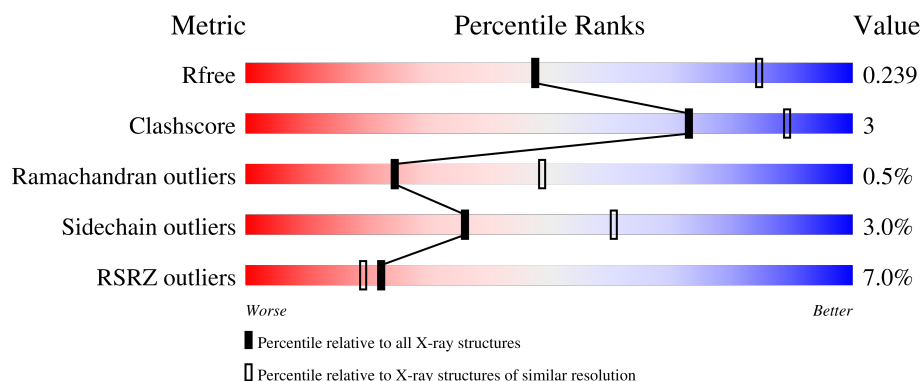
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	317	7% 87% 11% .
1	B	317	4% 87% 10% ..
1	C	317	7% 84% 13% ..
1	D	317	10% 84% 14% .
1	E	317	7% 86% 11% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NA	A	403	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12743 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 Proton-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	1	0
			2525	1663	402	455	5			
1	B	311	Total	C	N	O	S	0	1	0
			2525	1663	402	455	5			
1	C	311	Total	C	N	O	S	0	1	0
			2525	1663	402	455	5			
1	D	311	Total	C	N	O	S	0	0	0
			2516	1655	402	454	5			
1	E	311	Total	C	N	O	S	0	1	0
			2525	1663	402	455	5			

There are 20 discrepancies between the modelled and reference sequences:

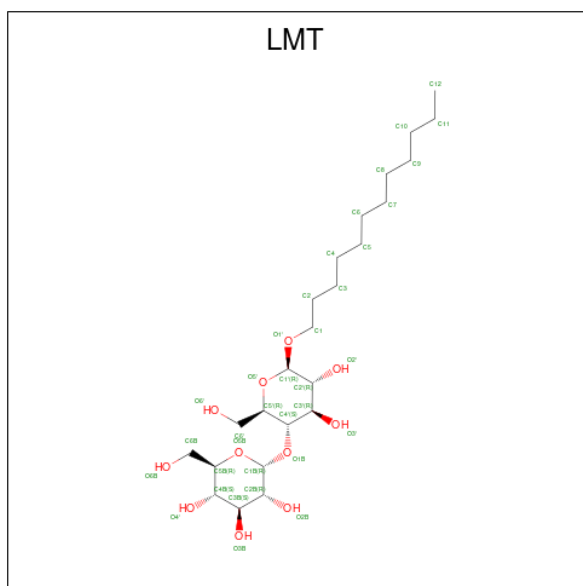
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP Q7NDN8
A	27	SER	CYS	engineered mutation	UNP Q7NDN8
A	33	CYS	LYS	engineered mutation	UNP Q7NDN8
A	246	CYS	LEU	engineered mutation	UNP Q7NDN8
B	1	ALA	-	expression tag	UNP Q7NDN8
B	27	SER	CYS	engineered mutation	UNP Q7NDN8
B	33	CYS	LYS	engineered mutation	UNP Q7NDN8
B	246	CYS	LEU	engineered mutation	UNP Q7NDN8
C	1	ALA	-	expression tag	UNP Q7NDN8
C	27	SER	CYS	engineered mutation	UNP Q7NDN8
C	33	CYS	LYS	engineered mutation	UNP Q7NDN8
C	246	CYS	LEU	engineered mutation	UNP Q7NDN8
D	1	ALA	-	expression tag	UNP Q7NDN8
D	27	SER	CYS	engineered mutation	UNP Q7NDN8
D	33	CYS	LYS	engineered mutation	UNP Q7NDN8
D	246	CYS	LEU	engineered mutation	UNP Q7NDN8
E	1	ALA	-	expression tag	UNP Q7NDN8
E	27	SER	CYS	engineered mutation	UNP Q7NDN8
E	33	CYS	LYS	engineered mutation	UNP Q7NDN8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	246	CYS	LEU	engineered mutation	UNP Q7NDN8

- Molecule 2 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 12 12	0	0

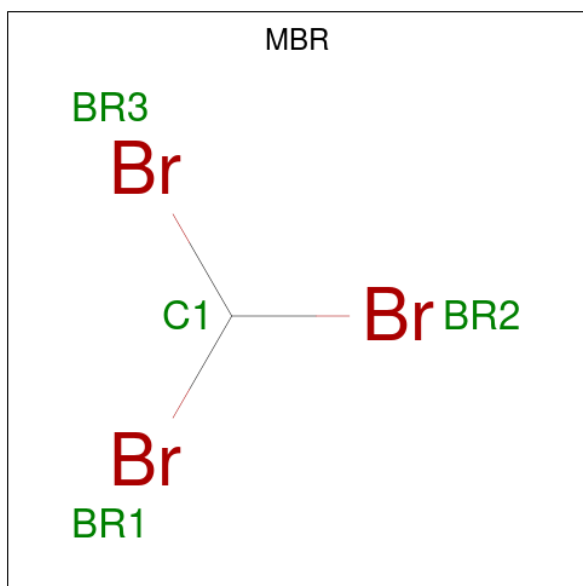
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is TRIBROMOMETHANE (CCD ID: MBR) (formula: CHBr_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	Br	C	0	0
			4	3	1		

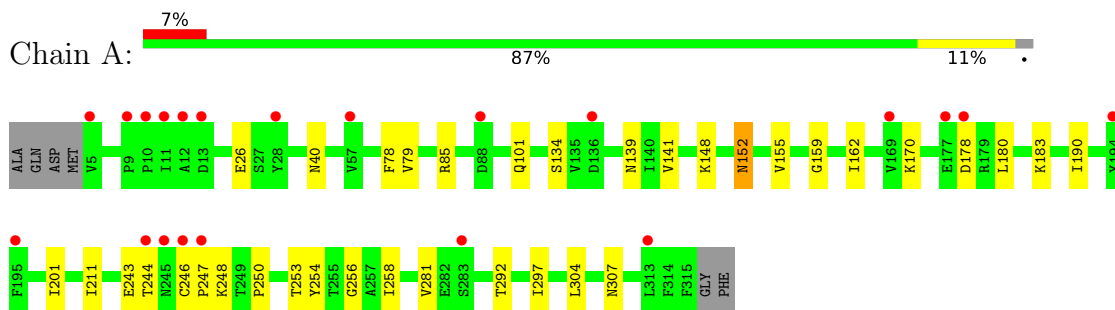
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	23	Total	O	0	0
			23	23		
6	B	25	Total	O	0	0
			25	25		
6	C	22	Total	O	0	0
			22	22		
6	D	15	Total	O	0	0
			15	15		
6	E	20	Total	O	0	0
			20	20		

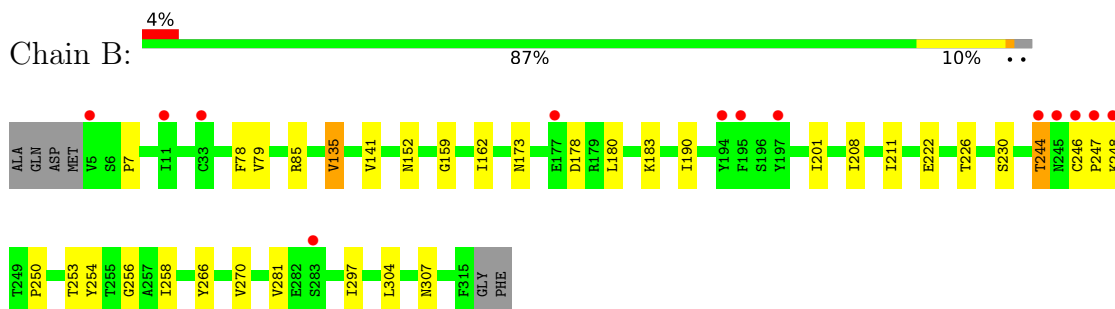
3 Residue-property plots

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.

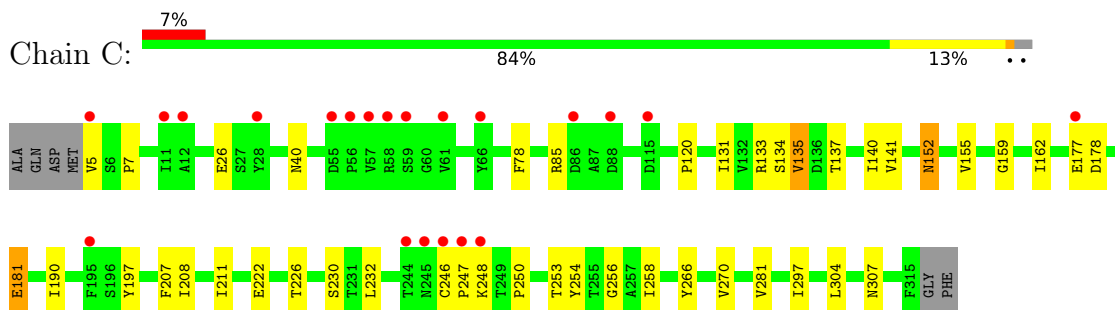
- Molecule 1: Proton-gated ion channel



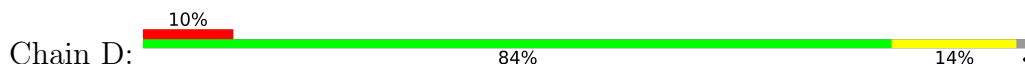
- Molecule 1: Proton-gated ion channel

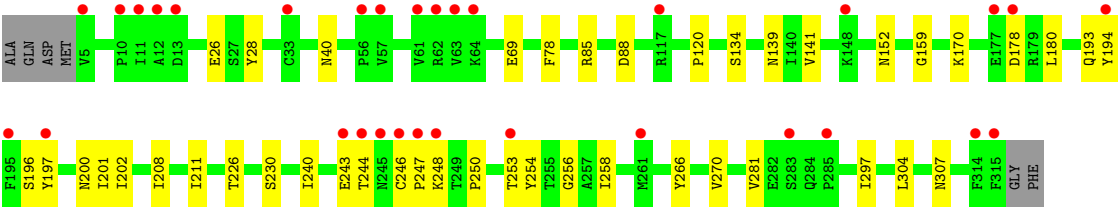


- Molecule 1: Proton-gated ion channel

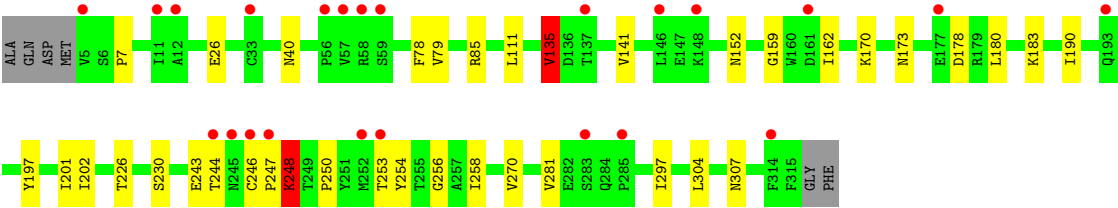
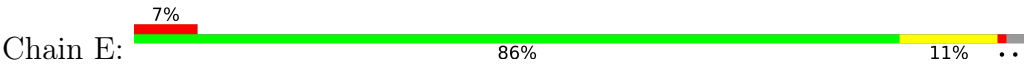


- Molecule 1: Proton-gated ion channel





● Molecule 1: Proton-gated ion channel



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.94Å 133.37Å 159.34Å 90.00° 102.34° 90.00°	Depositor
Resolution (Å)	20.00 – 2.95 20.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.95) 99.2 (20.00-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.213 , 0.218 0.234 , 0.239	Depositor DCC
R_{free} test set	3930 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	83.1	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12743	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: MBR, LMT, NA, 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	0.76	0/2597	1.21	1/3553 (0.0%)
1	B	0.75	0/2597	1.22	3/3553 (0.1%)
1	C	0.74	0/2597	1.20	1/3553 (0.0%)
1	D	0.75	0/2584	1.20	2/3535 (0.1%)
1	E	0.75	0/2597	1.22	5/3553 (0.1%)
All	All	0.75	0/12972	1.21	12/17747 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	152	ASN	CA-CB-CG	6.45	119.05	112.60
1	E	152	ASN	CA-CB-CG	6.26	118.86	112.60
1	B	152	ASN	CA-CB-CG	6.18	118.78	112.60
1	A	152	ASN	CA-CB-CG	5.99	118.59	112.60
1	E	135	VAL	CA-C-N	5.98	128.54	120.65
1	E	135	VAL	C-N-CA	5.98	128.54	120.65
1	B	135	VAL	CA-C-N	5.87	128.95	120.79
1	B	135	VAL	C-N-CA	5.87	128.95	120.79
1	D	152	ASN	CA-CB-CG	5.86	118.46	112.60
1	D	69	GLU	CB-CG-CD	5.20	121.44	112.60
1	E	248	LYS	CA-C-N	5.06	127.67	120.49
1	E	248	LYS	C-N-CA	5.06	127.67	120.49

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	2525	0	2527	14	0
1	B	2525	0	2527	17	0
1	C	2525	0	2527	22	0
1	D	2516	0	2518	24	0
1	E	2525	0	2527	18	0
2	A	12	0	23	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	1	0	0	0	0
5	E	4	0	0	0	0
6	A	23	0	0	0	0
6	B	25	0	0	0	0
6	C	22	0	0	0	0
6	D	15	0	0	0	0
6	E	20	0	0	0	0
All	All	12743	0	12649	82	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 3.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:PRO:HG3	1:B:135:VAL:HG21	1.57	0.86
1:D:194:TYR:OH	1:E:248:LYS:CB	2.44	0.64
1:C:208:ILE:HG22	1:C:266:TYR:OH	2.01	0.59
1:D:194:TYR:CD2	1:D:197:TYR:HB2	2.39	0.58
1:C:253:THR:HG23	1:C:256:GLY:H	1.71	0.56
1:B:253:THR:HG23	1:B:256:GLY:H	1.71	0.56
1:D:193:GLN:O	1:D:193:GLN:HG2	2.06	0.55
1:E:253:THR:HG23	1:E:256:GLY:H	1.71	0.55
1:C:211:ILE:HG23	1:D:270:VAL:HG11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:HG23	1:A:256:GLY:H	1.71	0.54
1:D:120:PRO:HG3	1:D:197:TYR:CD2	2.42	0.54
1:A:159:GLY:HA2	1:B:250:PRO:HB3	1.89	0.53
2:A:401:LMT:H52	1:D:240:ILE:HG21	1.90	0.53
1:D:193:GLN:O	1:D:193:GLN:CG	2.57	0.52
1:C:7:PRO:HG3	1:C:135:VAL:HG21	1.91	0.52
1:E:246:CYS:HB3	1:E:247:PRO:HD2	1.91	0.52
1:D:253:THR:HG23	1:D:256:GLY:H	1.74	0.52
1:C:246:CYS:HB3	1:C:247:PRO:HD2	1.92	0.50
1:A:201:ILE:HG21	1:A:244:THR:HG21	1.93	0.50
1:C:159:GLY:HA2	1:D:250:PRO:HB3	1.94	0.49
1:D:120:PRO:HG3	1:D:197:TYR:CG	2.47	0.49
1:A:246:CYS:HB3	1:A:247:PRO:HD2	1.94	0.49
1:E:201:ILE:HG21	1:E:244:THR:HG21	1.94	0.49
1:B:246:CYS:HB3	1:B:247:PRO:HD2	1.94	0.48
1:E:78:PHE:CE2	1:E:85:ARG:HD3	2.49	0.48
1:E:254:TYR:CZ	1:E:258:ILE:HD11	2.48	0.48
1:B:201:ILE:HG21	1:B:244:THR:HG21	1.96	0.48
1:B:208:ILE:HG22	1:B:266:TYR:OH	2.14	0.47
1:E:162:ILE:HG13	1:E:190:ILE:HG22	1.97	0.47
1:D:196:SER:O	1:D:200:ASN:HB2	2.14	0.47
1:D:159:GLY:HA2	1:E:250:PRO:HB3	1.97	0.47
1:D:201:ILE:HG21	1:D:244:THR:HG21	1.96	0.47
1:B:78:PHE:CE2	1:B:85:ARG:HD3	2.49	0.47
1:B:222:GLU:HB3	1:C:222:GLU:OE2	2.15	0.47
1:A:78:PHE:CE2	1:A:85:ARG:HD3	2.50	0.47
1:C:254:TYR:CZ	1:C:258:ILE:HD11	2.49	0.47
1:D:246:CYS:HB3	1:D:247:PRO:HD2	1.95	0.47
1:E:197[B]:TYR:HD2	1:E:202:ILE:HD11	1.79	0.47
1:D:197:TYR:CE2	1:D:202:ILE:HD11	2.50	0.47
1:D:254:TYR:CZ	1:D:258:ILE:HD11	2.50	0.46
1:E:197[B]:TYR:HD2	1:E:202:ILE:CD1	2.29	0.46
1:A:254:TYR:CZ	1:A:258:ILE:HD11	2.50	0.46
1:E:173:ASN:HB3	1:E:180:LEU:HD11	1.97	0.46
1:B:254:TYR:CZ	1:B:258:ILE:HD11	2.50	0.46
1:C:78:PHE:CE2	1:C:85:ARG:HD3	2.51	0.46
1:D:78:PHE:CE2	1:D:85:ARG:HD3	2.51	0.46
1:C:131:ILE:HD11	1:C:181:GLU:HG2	1.98	0.45
1:A:134:SER:HB3	1:A:139:ASN:HA	1.98	0.45
1:B:79:VAL:HG21	1:B:183:LYS:HD2	1.98	0.45
1:D:201:ILE:HG12	1:D:244:THR:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ILE:HG13	1:C:190:ILE:HG22	1.99	0.44
1:B:211:ILE:HG23	1:C:270:VAL:HG11	2.00	0.44
1:D:26:GLU:HB2	1:D:40:ASN:HB3	2.00	0.44
1:B:159:GLY:HA2	1:C:250:PRO:HB3	1.99	0.43
1:C:120:PRO:HG3	1:C:197[B]:TYR:CD2	2.53	0.43
1:E:26:GLU:HB2	1:E:40:ASN:HB3	1.99	0.43
1:D:208:ILE:HG22	1:D:266:TYR:OH	2.18	0.43
1:E:79:VAL:HG21	1:E:183:LYS:HD2	2.01	0.43
1:B:162:ILE:HG13	1:B:190:ILE:HG22	2.01	0.43
1:A:162:ILE:HG13	1:A:190:ILE:HG22	2.01	0.43
1:A:101:GLN:HE21	1:A:148:LYS:HZ3	1.66	0.43
1:C:26:GLU:HB2	1:C:40:ASN:HB3	2.00	0.42
1:C:134:SER:HA	1:C:140:ILE:HD12	2.01	0.42
1:B:173:ASN:HB3	1:B:180:LEU:HD11	2.01	0.42
1:C:133:ARG:NH1	1:C:177:GLU:HB2	2.34	0.42
1:D:28:TYR:HB3	1:E:111:LEU:HD22	2.01	0.42
1:B:208:ILE:HG12	1:C:232:LEU:HD21	2.01	0.42
1:C:135:VAL:HG23	1:C:137:THR:H	1.84	0.42
1:A:26:GLU:HB2	1:A:40:ASN:HB3	2.01	0.42
1:D:226:THR:O	1:D:230:SER:HB2	2.20	0.42
1:C:226:THR:O	1:C:230:SER:HB2	2.20	0.41
1:A:211:ILE:HG23	1:B:270:VAL:HG11	2.01	0.41
1:C:152:ASN:HB3	1:C:155:VAL:HG23	2.02	0.41
1:E:226:THR:O	1:E:230:SER:HB2	2.21	0.41
1:A:79:VAL:HG21	1:A:183:LYS:HD2	2.03	0.41
1:E:7:PRO:HG3	1:E:135:VAL:HG21	2.02	0.41
1:A:250:PRO:HB3	1:E:159:GLY:HA2	2.01	0.41
1:B:226:THR:O	1:B:230:SER:HB2	2.21	0.41
1:D:211:ILE:HG23	1:E:270:VAL:HG11	2.03	0.41
1:C:207:PHE:O	1:C:211:ILE:HG13	2.21	0.41
1:A:152:ASN:HB3	1:A:155:VAL:HG23	2.03	0.40
1:D:134:SER:HB3	1:D:139:ASN:HA	2.04	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	310/317 (98%)	302 (97%)	6 (2%)	2 (1%)	21	45
1	B	310/317 (98%)	302 (97%)	7 (2%)	1 (0%)	36	59
1	C	310/317 (98%)	303 (98%)	6 (2%)	1 (0%)	36	59
1	D	309/317 (98%)	301 (97%)	6 (2%)	2 (1%)	21	45
1	E	310/317 (98%)	300 (97%)	8 (3%)	2 (1%)	21	45
All	All	1549/1585 (98%)	1508 (97%)	33 (2%)	8 (0%)	24	49

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	LYS
1	B	248	LYS
1	C	248	LYS
1	D	248	LYS
1	A	243	GLU
1	D	243	GLU
1	E	243	GLU
1	E	248	LYS

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	280/284 (99%)	271 (97%)	9 (3%)	34	59
1	B	280/284 (99%)	273 (98%)	7 (2%)	42	66
1	C	280/284 (99%)	271 (97%)	9 (3%)	34	59
1	D	279/284 (98%)	270 (97%)	9 (3%)	34	59
1	E	280/284 (99%)	272 (97%)	8 (3%)	37	61
All	All	1399/1420 (98%)	1357 (97%)	42 (3%)	36	60

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	VAL
1	A	170	LYS
1	A	178	ASP
1	A	180	LEU
1	A	281	VAL
1	A	292	THR
1	A	297	ILE
1	A	304	LEU
1	A	307	ASN
1	B	141	VAL
1	B	178	ASP
1	B	244	THR
1	B	281	VAL
1	B	297	ILE
1	B	304	LEU
1	B	307	ASN
1	C	5	VAL
1	C	135	VAL
1	C	141	VAL
1	C	178	ASP
1	C	181	GLU
1	C	281	VAL
1	C	297	ILE
1	C	304	LEU
1	C	307	ASN
1	D	88	ASP
1	D	141	VAL
1	D	170	LYS
1	D	178	ASP
1	D	180	LEU
1	D	281	VAL
1	D	297	ILE
1	D	304	LEU
1	D	307	ASN
1	E	135	VAL
1	E	141	VAL
1	E	170	LYS
1	E	178	ASP
1	E	281	VAL
1	E	297	ILE
1	E	304	LEU
1	E	307	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	193	GLN
1	A	239	ASN
1	A	277	HIS
1	A	307	ASN
1	B	101	GLN
1	B	239	ASN
1	B	277	HIS
1	B	307	ASN
1	C	83	ASN
1	C	239	ASN
1	C	277	HIS
1	C	307	ASN
1	D	101	GLN
1	D	277	HIS
1	D	307	ASN
1	E	193	GLN
1	E	239	ASN
1	E	276	GLN
1	E	277	HIS
1	E	307	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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
2	LMT	A	401	-	11,11,36	0.29	0	10,10,47	0.81	0
5	MBR	E	402	-	3,3,3	0.57	0	3,3,3	1.66	1 (33%)

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
2	LMT	A	401	-	-	4/9/9/61	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	402	MBR	BR3-C1-BR2	-2.16	104.92	111.12

There are no chirality outliers.

All (4) torsion outliers are listed below:

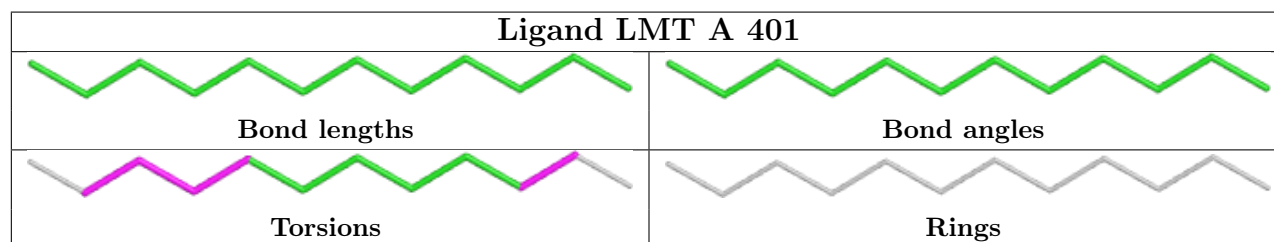
Mol	Chain	Res	Type	Atoms
2	A	401	LMT	C1-C2-C3-C4
2	A	401	LMT	C11-C10-C9-C8
2	A	401	LMT	C7-C8-C9-C10
2	A	401	LMT	C9-C10-C11-C12

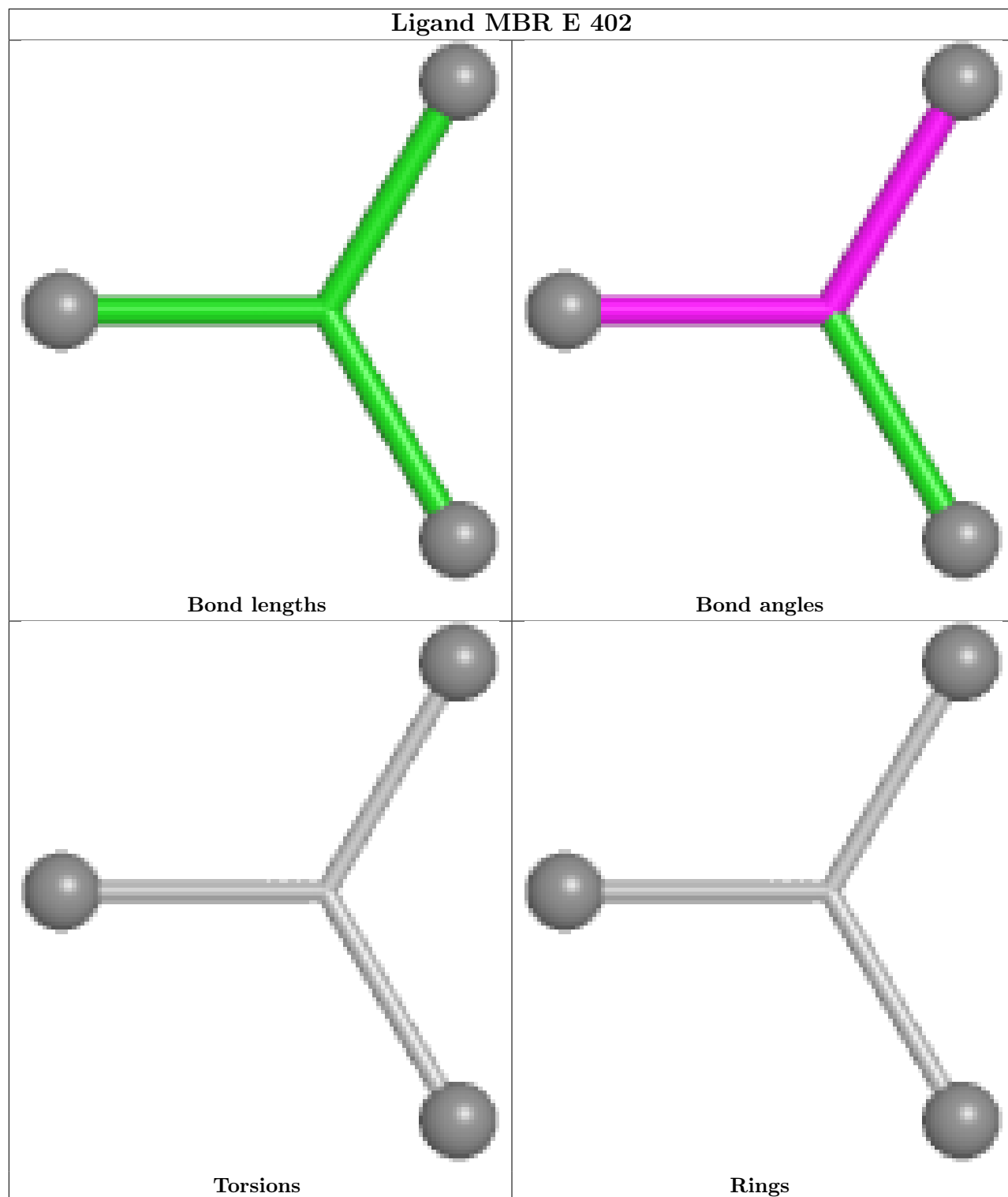
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	LMT	1	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

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	311/317 (98%)	0.52	21 (6%)	23	20	50, 102, 151, 201	1 (0%)
1	B	311/317 (98%)	0.42	13 (4%)	40	33	52, 97, 129, 149	1 (0%)
1	C	311/317 (98%)	0.48	21 (6%)	23	20	52, 99, 139, 184	1 (0%)
1	D	311/317 (98%)	0.52	31 (9%)	12	11	73, 103, 149, 194	0
1	E	311/317 (98%)	0.52	23 (7%)	20	18	50, 100, 140, 180	1 (0%)
All	All	1555/1585 (98%)	0.49	109 (7%)	22	19	50, 100, 142, 201	4 (0%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	247	PRO	6.8
1	D	247	PRO	6.1
1	E	247	PRO	5.9
1	B	247	PRO	5.5
1	A	247	PRO	5.2
1	D	5	VAL	4.5
1	B	5	VAL	4.5
1	B	246	CYS	4.5
1	D	246	CYS	4.4
1	E	246	CYS	4.4
1	E	57	VAL	4.4
1	B	11	ILE	4.3
1	B	244	THR	4.3
1	D	244	THR	4.3
1	E	5	VAL	4.2
1	C	57	VAL	4.2
1	A	5	VAL	4.1
1	A	194	TYR	4.1
1	A	244	THR	4.1
1	C	56	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	197	TYR	4.0
1	A	11	ILE	4.0
1	C	245	ASN	4.0
1	C	59	SER	4.0
1	C	244	THR	3.9
1	B	195	PHE	3.9
1	B	245	ASN	3.8
1	A	245	ASN	3.8
1	C	11	ILE	3.7
1	A	10	PRO	3.7
1	A	283	SER	3.6
1	A	246	CYS	3.4
1	B	194	TYR	3.4
1	E	245	ASN	3.4
1	A	195	PHE	3.4
1	D	245	ASN	3.3
1	C	5	VAL	3.2
1	B	177	GLU	3.2
1	E	58	ARG	3.1
1	C	58	ARG	3.1
1	E	59	SER	3.1
1	D	56	PRO	3.1
1	D	117	ARG	3.0
1	E	56	PRO	3.0
1	D	285	PRO	3.0
1	A	28	TYR	3.0
1	D	283	SER	2.9
1	D	57	VAL	2.9
1	D	314	PHE	2.9
1	C	61	VAL	2.9
1	E	283	SER	2.9
1	C	115	ASP	2.8
1	A	177	GLU	2.8
1	E	177	GLU	2.8
1	E	11	ILE	2.8
1	D	61	VAL	2.7
1	E	244	THR	2.7
1	C	195	PHE	2.7
1	C	246	CYS	2.7
1	D	195	PHE	2.7
1	E	285	PRO	2.7
1	A	88	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	248	LYS	2.6
1	D	248	LYS	2.6
1	D	12	ALA	2.6
1	B	197[A]	TYR	2.6
1	C	28	TYR	2.6
1	B	33	CYS	2.6
1	E	193	GLN	2.6
1	C	177	GLU	2.5
1	E	253	THR	2.5
1	D	11	ILE	2.5
1	A	12	ALA	2.5
1	A	13	ASP	2.5
1	D	253	THR	2.5
1	E	137	THR	2.5
1	E	252	MET	2.5
1	D	33	CYS	2.5
1	A	57	VAL	2.4
1	D	63	VAL	2.4
1	D	177	GLU	2.4
1	B	283	SER	2.4
1	E	148	LYS	2.4
1	E	314	PHE	2.4
1	D	178	ASP	2.4
1	E	12	ALA	2.3
1	A	169	VAL	2.3
1	D	10	PRO	2.3
1	A	136	ASP	2.2
1	A	178	ASP	2.2
1	C	88	ASP	2.2
1	A	9	PRO	2.2
1	E	161	ASP	2.2
1	C	248	LYS	2.2
1	C	66	TYR	2.2
1	D	194	TYR	2.2
1	D	62	ARG	2.1
1	D	64	LYS	2.1
1	E	146	LEU	2.1
1	E	33	CYS	2.1
1	C	86	ASP	2.1
1	C	12	ALA	2.1
1	A	313	LEU	2.0
1	D	315	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	55	ASP	2.0
1	D	13	ASP	2.0
1	D	261	MET	2.0
1	D	148	LYS	2.0
1	D	243	GLU	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](#)

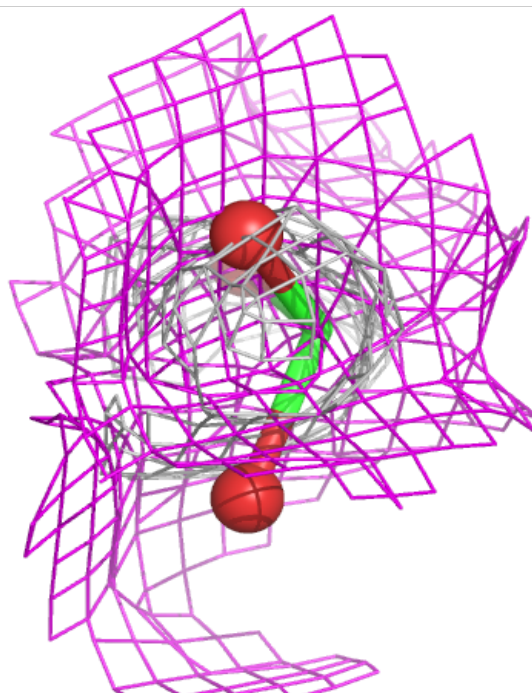
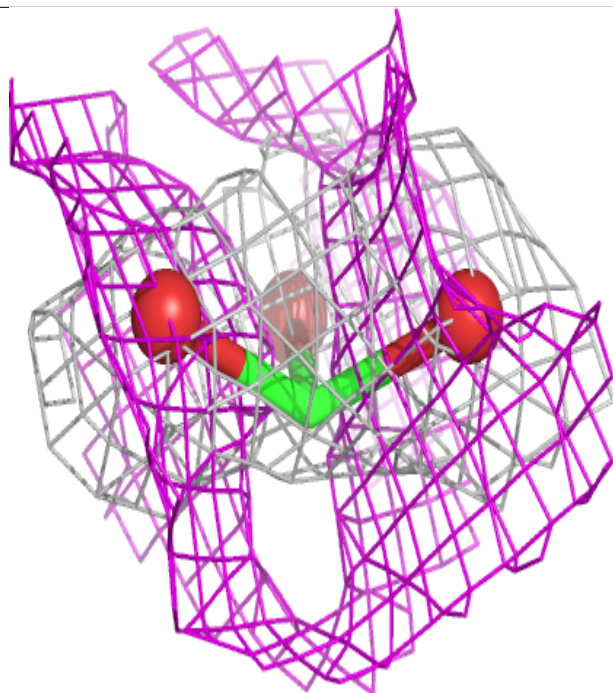
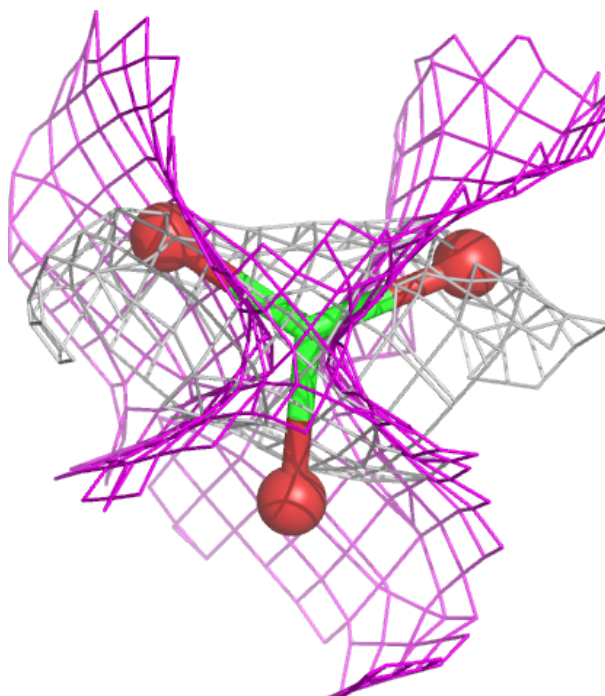
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

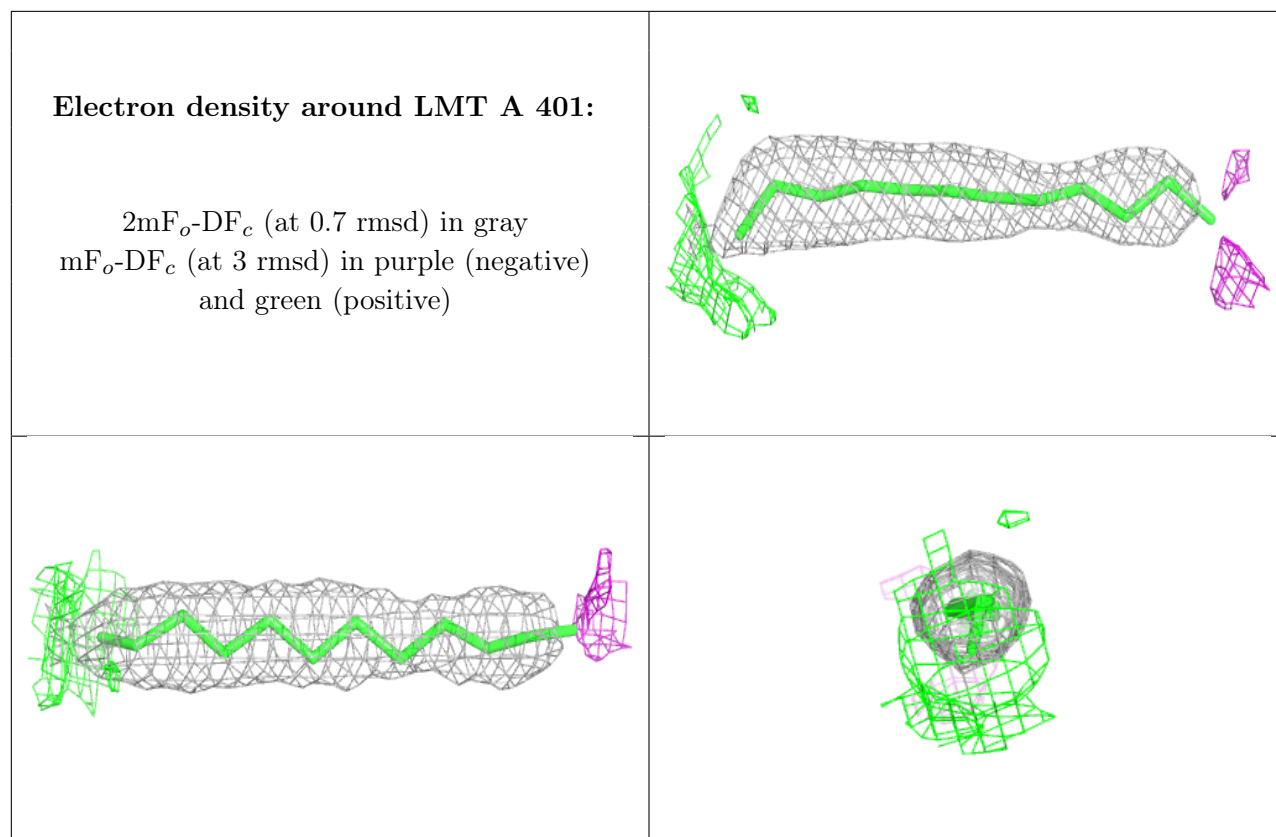
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NA	A	403	1/1	0.69	0.58	112,112,112,112	0
5	MBR	E	402	4/4	0.77	0.19	289,290,290,292	0
2	LMT	A	401	12/35	0.90	0.16	51,59,68,71	0
3	CL	B	401	1/1	0.96	0.06	88,88,88,88	0
3	CL	D	401	1/1	0.97	0.05	80,80,80,80	0
3	CL	E	401	1/1	0.98	0.09	90,90,90,90	0
3	CL	C	401	1/1	0.98	0.05	93,93,93,93	0
3	CL	A	402	1/1	0.98	0.04	84,84,84,84	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 MBR E 402:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.