



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:20 AM UTC

PDB ID : 6U4O / pdb_00006u4o
Title : Crystal structure of recombinant class II fumarase from *Schistosoma mansoni*
Authors : Cardoso, I.A.; Nonato, M.C.
Deposited on : 2019-08-26
Resolution : 1.85 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

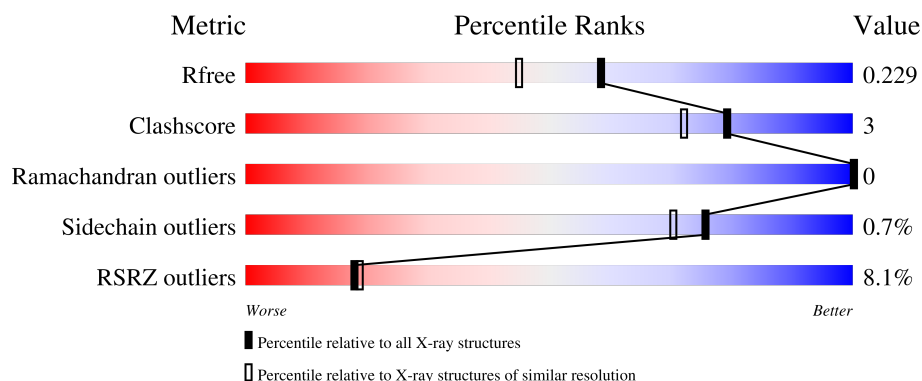
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	488	0% 92% 6%
1	B	488	5% 89% 9%
1	C	488	11% 91% 7%
1	D	488	15% 91% 6%

2 Entry composition [i](#)

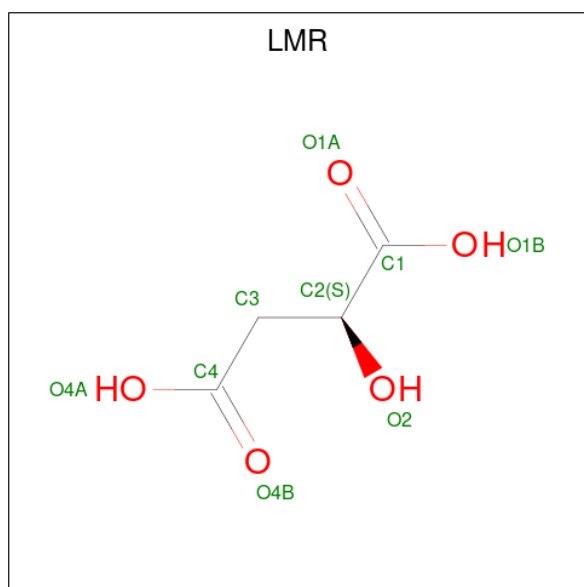
There are 5 unique types of molecules in this entry. The entry contains 29877 atoms, of which 14505 are hydrogens and 0 are deuteriums.

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 Fumarate hydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	477	Total	C	H	N	O	S	245	4	0
			7157	2247	3577	620	678	35			
1	A	479	Total	C	H	N	O	S	224	0	0
			7364	2296	3711	633	690	34			
1	D	478	Total	C	H	N	O	S	252	3	0
			7093	2225	3531	619	683	35			
1	B	478	Total	C	H	N	O	S	241	2	0
			7227	2262	3626	623	684	32			

- Molecule 2 is (2S)-2-hydroxybutanedioic acid (CCD ID: LMR) (formula: C₄H₆O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	H	O	1	0
			13	4	4	5		
2	A	1	Total	C	H	O	1	0
			13	4	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	H	O	1	0
			13	4	4	5		
2	B	1	Total	C	H	O	1	0
			13	4	4	5		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	H	O	2	0
			14	3	8	3		
3	A	1	Total	C	H	O	2	0
			14	3	8	3		
3	A	1	Total	C	H	O	2	0
			14	3	8	3		
3	B	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			7	2	3	2		
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	D	1	Total	C	H	O	0	0
			7	2	3	2		
4	B	1	Total	C	H	O	0	0
			7	2	3	2		

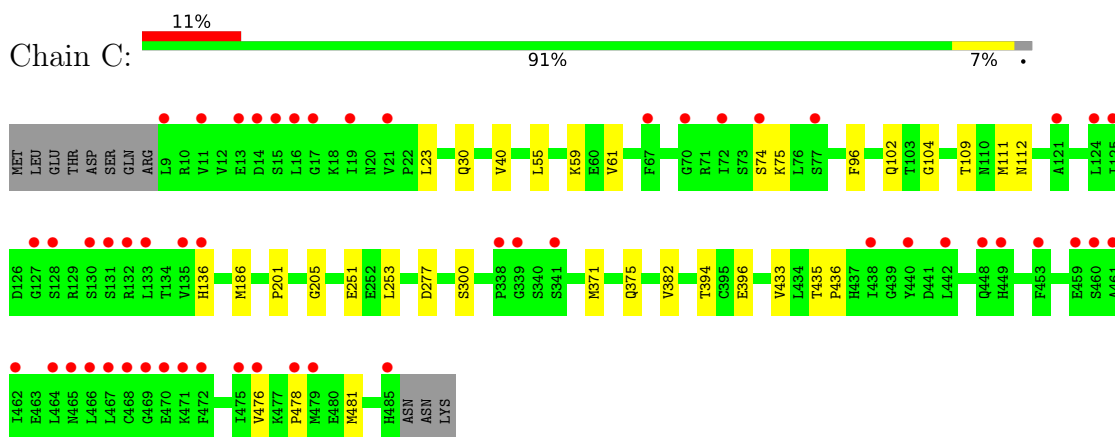
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	193	Total	O	0	1
			194	194		
5	A	284	Total	O	0	4
			288	288		
5	D	191	Total	O	0	1
			192	192		
5	B	225	Total	O	0	1
			226	226		

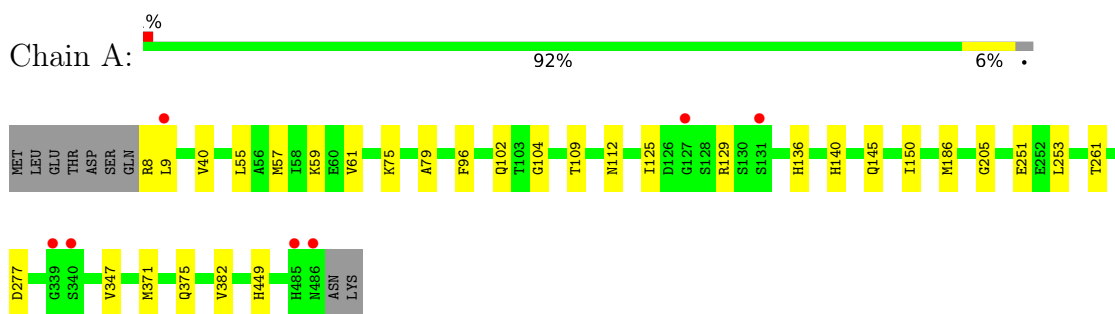
3 Residue-property plots [i](#)

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.

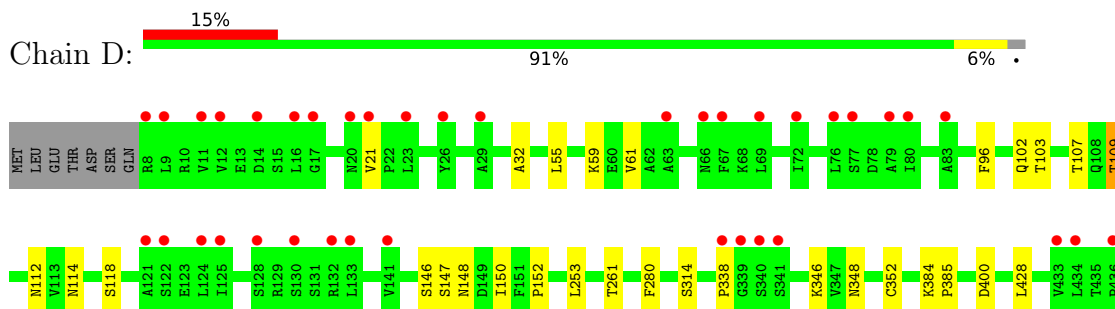
- Molecule 1: Fumarate hydratase

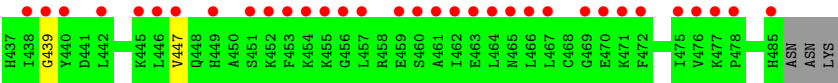


- Molecule 1: Fumarate hydratase

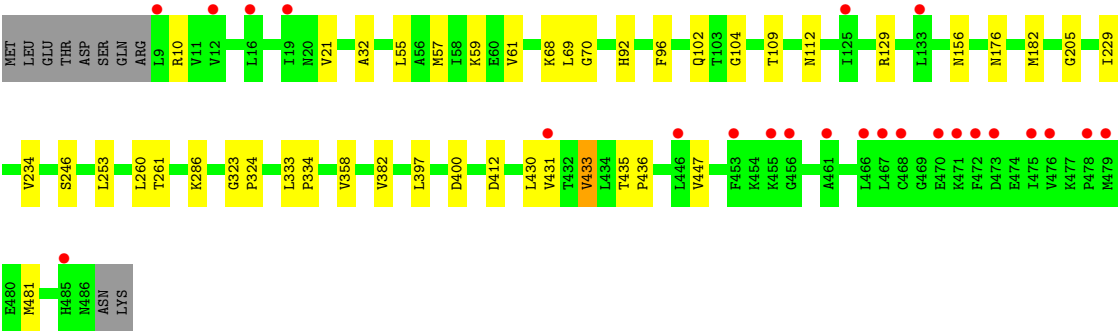
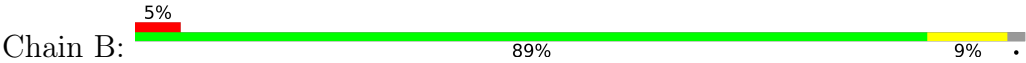


- Molecule 1: Fumarate hydratase





● Molecule 1: Fumarate hydratase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	180.65Å 67.86Å 187.27Å 90.00° 118.61° 90.00°	Depositor
Resolution (Å)	46.93 – 1.85 46.93 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.93-1.85) 98.5 (46.93-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.192 , 0.227 0.194 , 0.229	Depositor DCC
R_{free} test set	8368 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	29877	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACT, LMR

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	1.03	0/3714	1.38	0/5030
1	B	1.06	0/3662	1.41	0/4973
1	C	1.06	0/3642	1.48	3/4951 (0.1%)
1	D	1.08	0/3622	1.48	1/4922 (0.0%)
All	All	1.06	0/14640	1.44	4/19876 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	300	SER	CA-C-N	5.39	125.96	119.98
1	C	300	SER	C-N-CA	5.39	125.96	119.98
1	D	439	GLY	CA-C-O	-5.09	118.17	122.29
1	C	394	THR	CA-CB-OG1	-5.03	102.05	109.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3653	3711	3682	17	0
1	B	3601	3626	3567	25	0
1	C	3580	3577	3495	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3562	3531	3444	20	0
2	A	9	4	4	0	0
2	B	9	4	4	0	0
2	C	9	4	4	0	0
2	D	9	4	4	0	0
3	A	12	16	16	1	0
3	B	6	8	8	1	0
3	C	6	8	8	0	0
4	A	4	3	3	0	0
4	B	4	3	3	0	0
4	C	4	3	3	0	0
4	D	4	3	3	0	0
5	A	288	0	0	2	0
5	B	226	0	0	5	0
5	C	194	0	0	3	0
5	D	192	0	0	1	0
All	All	15372	14505	14248	77	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 (77) 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:102:GLN:HE22	1:B:109:THR:H	1.36	0.73
1:C:111:MET:HG2	5:C:775:HOH:O	1.90	0.71
1:D:102:GLN:HE22	1:D:109:THR:H	1.46	0.63
1:C:476:VAL:HG23	1:C:476:VAL:O	1.97	0.63
1:A:102:GLN:HE22	1:A:109:THR:H	1.45	0.63
1:D:261[A]:THR:HG23	5:D:633:HOH:O	1.98	0.63
1:B:96:PHE:HA	1:B:112:ASN:HD21	1.64	0.61
1:C:102:GLN:HE22	1:C:109:THR:H	1.49	0.60
1:A:96:PHE:HA	1:A:112:ASN:HD21	1.66	0.59
1:B:430:LEU:O	1:B:433:VAL:HG22	2.03	0.58
1:A:55:LEU:O	1:A:59:LYS:HG2	2.03	0.57
1:D:96:PHE:HA	1:D:112:ASN:HD21	1.70	0.57
1:C:75:LYS:O	5:C:601:HOH:O	2.17	0.57
1:D:55:LEU:O	1:D:59:LYS:HG2	2.07	0.55
1:C:96:PHE:HA	1:C:112:ASN:HD21	1.70	0.55
1:A:449:HIS:HD2	5:A:857:HOH:O	1.90	0.54
1:B:234:VAL:O	1:B:286:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:HIS:HD2	5:B:606:HOH:O	1.91	0.53
1:C:476:VAL:O	1:C:476:VAL:CG2	2.56	0.53
1:C:435:THR:N	1:C:436:PRO:HD2	2.24	0.53
1:D:346:LYS:NZ	1:D:348:ASN:HD21	2.08	0.52
1:B:176:ASN:ND2	5:B:604:HOH:O	2.40	0.51
1:A:79:ALA:HB2	1:A:125:ILE:HD11	1.92	0.51
1:B:10:ARG:NH1	5:B:612:HOH:O	2.44	0.51
1:A:104:GLY:HA3	1:A:382:VAL:O	2.10	0.50
1:B:57:MET:HE1	1:B:261:THR:HG22	1.93	0.50
1:B:334:PRO:HG3	1:B:412:ASP:HB2	1.93	0.50
1:A:57:MET:HE1	1:A:261:THR:HG22	1.94	0.49
1:C:186:MET:HA	1:C:205:GLY:HA3	1.95	0.48
1:C:371:MET:O	1:C:375:GLN:HG2	2.13	0.48
1:C:433:VAL:HG13	1:C:481:MET:HE3	1.95	0.48
1:D:114:ASN:O	1:D:118:SER:HB2	2.14	0.48
1:D:146:SER:O	1:D:150:ILE:HG22	2.14	0.48
1:D:147:SER:HA	1:D:150:ILE:HG22	1.96	0.47
1:D:21:VAL:HG12	1:D:32:ALA:HB2	1.97	0.47
1:A:40:VAL:HA	1:B:400:ASP:HB3	1.95	0.47
1:A:61:VAL:HG23	1:A:253:LEU:HG	1.95	0.47
1:B:70:GLY:HA2	5:B:653:HOH:O	2.14	0.47
1:B:260:LEU:HD12	5:B:782:HOH:O	2.14	0.47
1:C:55:LEU:O	1:C:59:LYS:HG2	2.15	0.46
1:C:104:GLY:HA3	1:C:382:VAL:O	2.14	0.46
1:B:104:GLY:HA3	1:B:382:VAL:O	2.16	0.46
1:C:40:VAL:HA	1:D:400:ASP:HB3	1.98	0.46
1:D:61:VAL:HG23	1:D:253:LEU:HG	1.98	0.46
1:A:186:MET:HA	1:A:205:GLY:HA3	1.98	0.45
1:D:428:LEU:HB3	1:D:447:VAL:HG23	1.98	0.45
1:A:8:ARG:C	1:A:9:LEU:HD22	2.42	0.45
1:A:251:GLU:HG2	5:A:863:HOH:O	2.16	0.45
1:D:346:LYS:HZ3	1:D:348:ASN:HD21	1.64	0.45
1:C:396:GLU:CD	5:C:694:HOH:O	2.59	0.45
1:C:201:PRO:HD2	1:C:481:MET:HE2	1.98	0.45
1:D:384:LYS:HB2	1:D:385:PRO:HD3	1.99	0.44
1:A:145:GLN:HB3	1:A:150:ILE:HG13	1.99	0.44
1:B:433:VAL:HG13	1:B:481:MET:HE3	1.98	0.44
1:A:75:LYS:HG2	1:A:125:ILE:HD12	2.00	0.44
1:D:21:VAL:CG1	1:D:32:ALA:HB2	2.47	0.44
1:D:148:ASN:O	1:D:152:PRO:HG2	2.18	0.43
1:B:435:THR:N	1:B:436:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314[A]:SER:OG	1:D:352:CYS:O	2.36	0.43
1:B:358:VAL:HG13	1:B:397:LEU:HB3	2.01	0.43
1:C:61:VAL:HG23	1:C:253:LEU:HG	2.01	0.43
1:B:55:LEU:O	1:B:59:LYS:HG2	2.18	0.43
1:B:21:VAL:HG12	1:B:32:ALA:HB2	2.01	0.42
1:D:261[A]:THR:HG21	1:D:280:PHE:HE2	1.84	0.42
1:C:30:GLN:HE22	1:D:338:PRO:HG2	1.85	0.42
1:C:136[A]:HIS:CD2	1:C:136[A]:HIS:N	2.88	0.41
1:D:103:THR:HG21	1:D:107:THR:HB	2.01	0.41
1:B:61:VAL:HG23	1:B:253:LEU:HG	2.02	0.41
1:A:371:MET:O	1:A:375:GLN:HG2	2.21	0.41
1:A:136:HIS:H	1:A:140:HIS:CD2	2.39	0.41
1:B:182:MET:HG3	1:B:205:GLY:O	2.21	0.41
1:B:323:GLY:HA3	1:B:324:PRO:HA	1.91	0.41
1:B:333:LEU:H	3:B:502:GOL:C1	2.33	0.41
1:B:69:LEU:HD13	1:B:246:SER:OG	2.21	0.41
1:A:347:VAL:O	3:A:502:GOL:H12	2.21	0.40
1:B:431:VAL:HG11	1:B:447:VAL:CG2	2.51	0.40
1:B:156:ASN:HB3	1:B:229[B]:ILE: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	477/488 (98%)	466 (98%)	11 (2%)	0	100	100
1	B	478/488 (98%)	464 (97%)	14 (3%)	0	100	100
1	C	479/488 (98%)	463 (97%)	16 (3%)	0	100	100
1	D	479/488 (98%)	461 (96%)	18 (4%)	0	100	100
All	All	1913/1952 (98%)	1854 (97%)	59 (3%)	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	412/428 (96%)	410 (100%)	2 (0%)	81	77
1	B	399/428 (93%)	396 (99%)	3 (1%)	73	67
1	C	389/428 (91%)	384 (99%)	5 (1%)	61	51
1	D	384/428 (90%)	383 (100%)	1 (0%)	86	85
All	All	1584/1712 (92%)	1573 (99%)	11 (1%)	76	70

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	23	LEU
1	C	74	SER
1	C	251	GLU
1	C	277	ASP
1	C	478	PRO
1	A	129	ARG
1	A	277	ASP
1	D	109	THR
1	B	68	LYS
1	B	129	ARG
1	B	433	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	20	ASN
1	C	30	GLN
1	C	66	ASN
1	C	94	ASN
1	C	102	GLN
1	C	112	ASN

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Mol	Chain	Res	Type
1	C	195	HIS
1	C	293	HIS
1	C	304	ASN
1	C	351	GLN
1	C	361	GLN
1	A	30	GLN
1	A	66	ASN
1	A	89	HIS
1	A	91	GLN
1	A	94	ASN
1	A	102	GLN
1	A	112	ASN
1	A	140	HIS
1	A	195	HIS
1	A	293	HIS
1	A	336	ASN
1	A	361	GLN
1	A	375	GLN
1	A	377	GLN
1	A	449	HIS
1	A	465	ASN
1	D	30	GLN
1	D	92	HIS
1	D	94	ASN
1	D	102	GLN
1	D	112	ASN
1	D	216	GLN
1	D	231	HIS
1	D	304	ASN
1	D	348	ASN
1	D	375	GLN
1	D	390	ASN
1	D	449	HIS
1	B	66	ASN
1	B	92	HIS
1	B	94	ASN
1	B	102	GLN
1	B	112	ASN
1	B	195	HIS
1	B	390	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	$\# Z > 2$
4	ACT	B	503	-	3,3,3	1.25	0	3,3,3	0.99	0
2	LMR	A	501	-	8,8,8	1.18	1 (12%)	10,10,10	1.59	2 (20%)
2	LMR	C	501	-	8,8,8	1.18	1 (12%)	10,10,10	1.41	1 (10%)
4	ACT	C	503	-	3,3,3	1.41	0	3,3,3	0.52	0
2	LMR	D	501	-	8,8,8	1.09	0	10,10,10	1.81	3 (30%)
2	LMR	B	501	-	8,8,8	1.09	0	10,10,10	1.75	4 (40%)
4	ACT	D	502	-	3,3,3	1.33	0	3,3,3	0.96	0
3	GOL	A	502	-	5,5,5	0.09	0	5,5,5	0.24	0
3	GOL	C	502	-	5,5,5	0.12	0	5,5,5	0.33	0
3	GOL	A	503	-	5,5,5	0.11	0	5,5,5	0.31	0
3	GOL	B	502	-	5,5,5	0.05	0	5,5,5	0.34	0
4	ACT	A	504	-	3,3,3	1.49	1 (33%)	3,3,3	0.93	0

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	LMR	A	501	-	-	3/8/8/8	-
2	LMR	C	501	-	-	3/8/8/8	-
2	LMR	D	501	-	-	4/8/8/8	-
2	LMR	B	501	-	-	4/8/8/8	-
3	GOL	A	502	-	-	0/4/4/4	-
3	GOL	C	502	-	-	4/4/4/4	-
3	GOL	A	503	-	-	1/4/4/4	-
3	GOL	B	502	-	-	4/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	LMR	O1A-C1	2.04	1.28	1.22
4	A	504	ACT	OXT-C	-2.02	1.21	1.30
2	A	501	LMR	O1A-C1	2.01	1.28	1.22

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	LMR	O1B-C1-C2	3.13	119.35	112.74
2	B	501	LMR	O1B-C1-C2	3.01	119.11	112.74
2	D	501	LMR	O1B-C1-C2	2.98	119.04	112.74
2	C	501	LMR	O1B-C1-C2	2.94	118.95	112.74
2	D	501	LMR	O4A-C4-C3	2.79	122.68	114.00
2	A	501	LMR	O1B-C1-O1A	-2.52	118.36	124.08
2	D	501	LMR	C3-C2-C1	-2.47	104.45	110.53
2	B	501	LMR	O4A-C4-C3	2.46	121.66	114.00
2	B	501	LMR	O1A-C1-C2	-2.12	118.37	122.60
2	B	501	LMR	C3-C2-C1	-2.02	105.58	110.53

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	LMR	O1A-C1-C2-O2
2	A	501	LMR	O1B-C1-C2-O2
3	C	502	GOL	O1-C1-C2-O2
3	C	502	GOL	O1-C1-C2-C3
3	C	502	GOL	C1-C2-C3-O3

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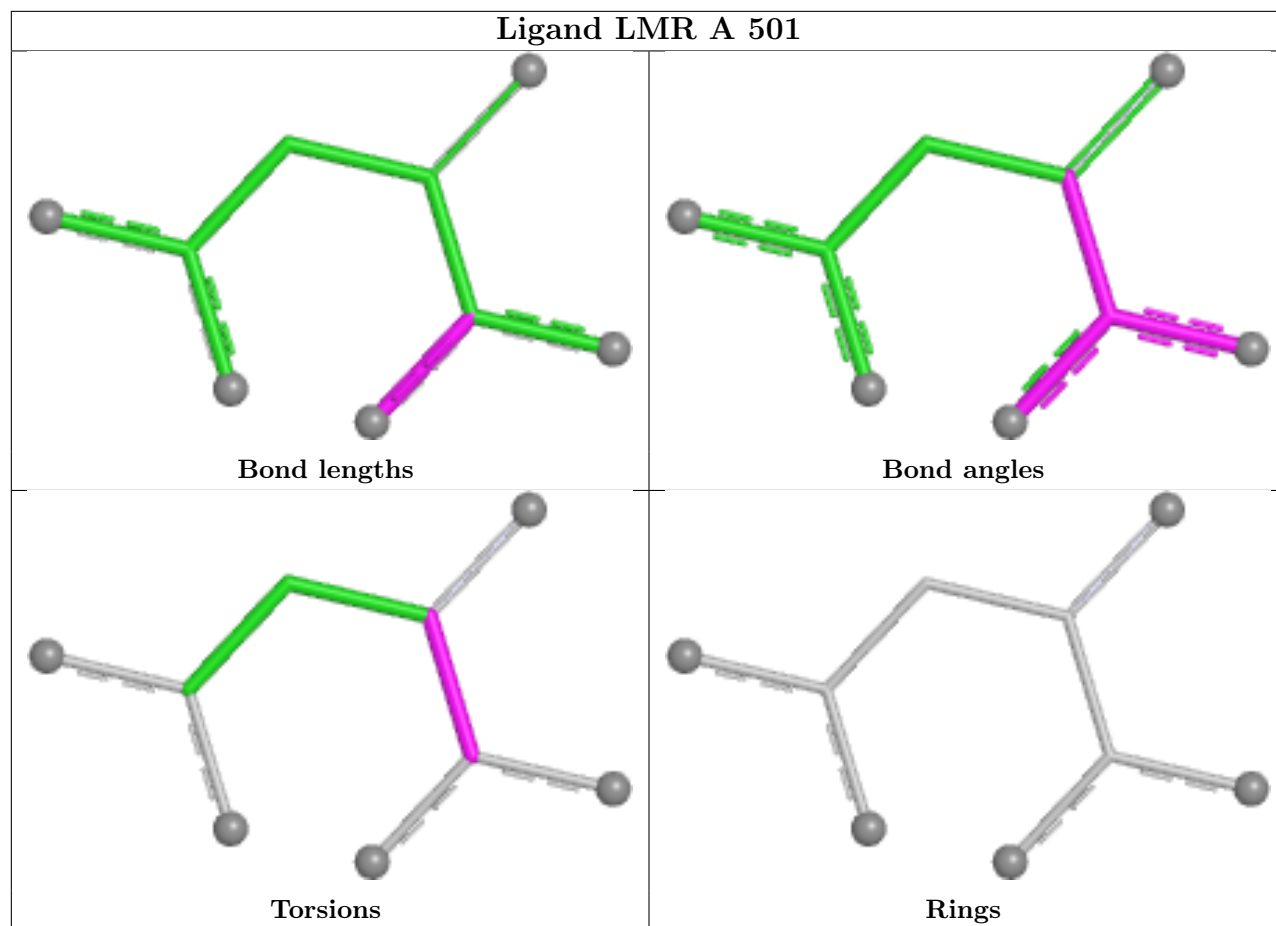
Mol	Chain	Res	Type	Atoms
3	B	502	GOL	C1-C2-C3-O3
3	B	502	GOL	O1-C1-C2-C3
3	B	502	GOL	O1-C1-C2-O2
3	C	502	GOL	O2-C2-C3-O3
2	C	501	LMR	O1A-C1-C2-O2
2	C	501	LMR	O1B-C1-C2-O2
2	B	501	LMR	O1B-C1-C2-O2
2	B	501	LMR	O1A-C1-C2-O2
2	B	501	LMR	C2-C3-C4-O4A
3	B	502	GOL	O2-C2-C3-O3
2	D	501	LMR	C2-C3-C4-O4A
2	B	501	LMR	C2-C3-C4-O4B
2	D	501	LMR	C2-C3-C4-O4B
2	D	501	LMR	O1A-C1-C2-O2
2	C	501	LMR	O1A-C1-C2-C3
2	A	501	LMR	O1A-C1-C2-C3
3	A	503	GOL	O1-C1-C2-C3
2	D	501	LMR	O1B-C1-C2-O2

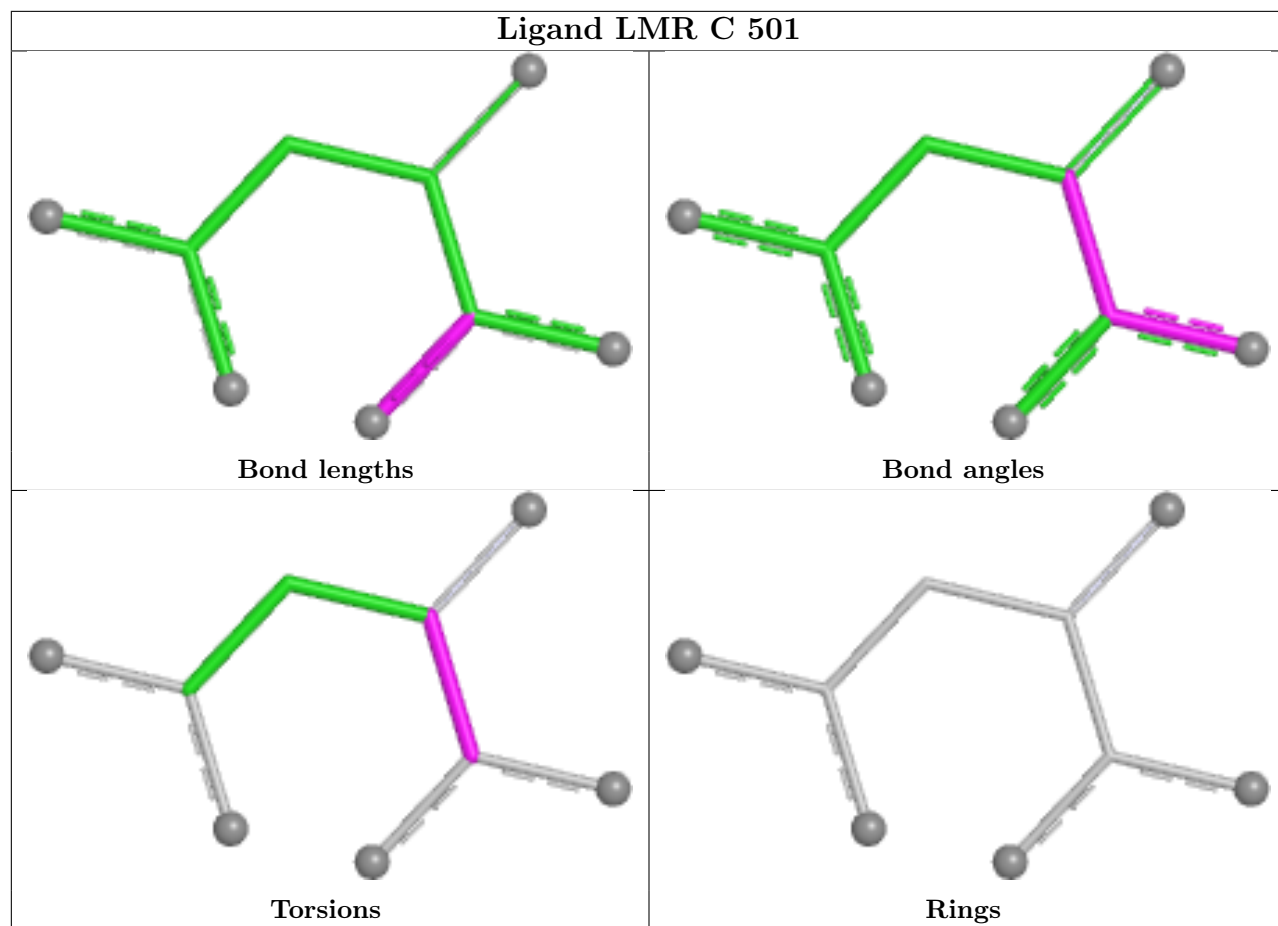
There are no ring outliers.

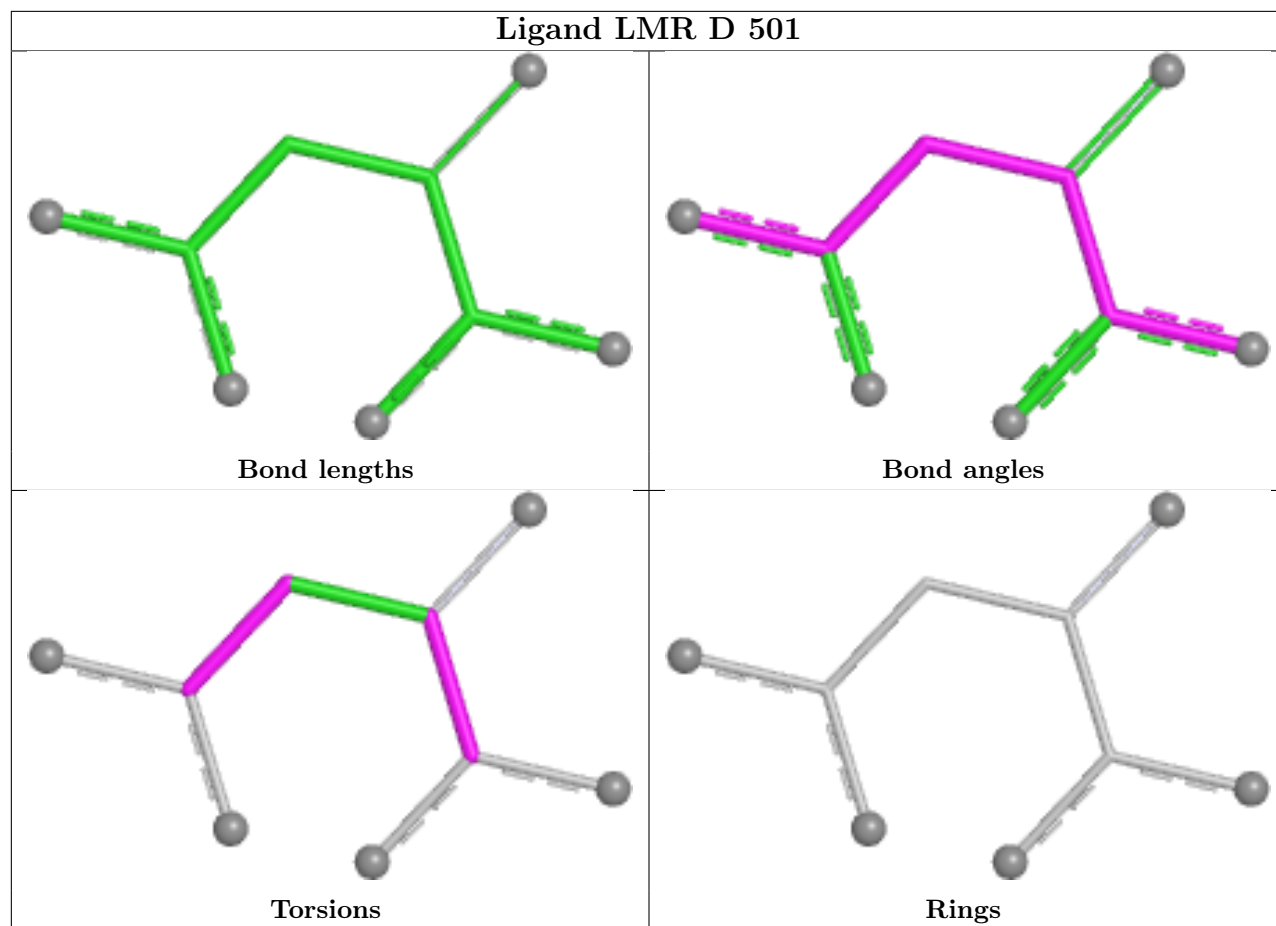
2 monomers are involved in 2 short contacts:

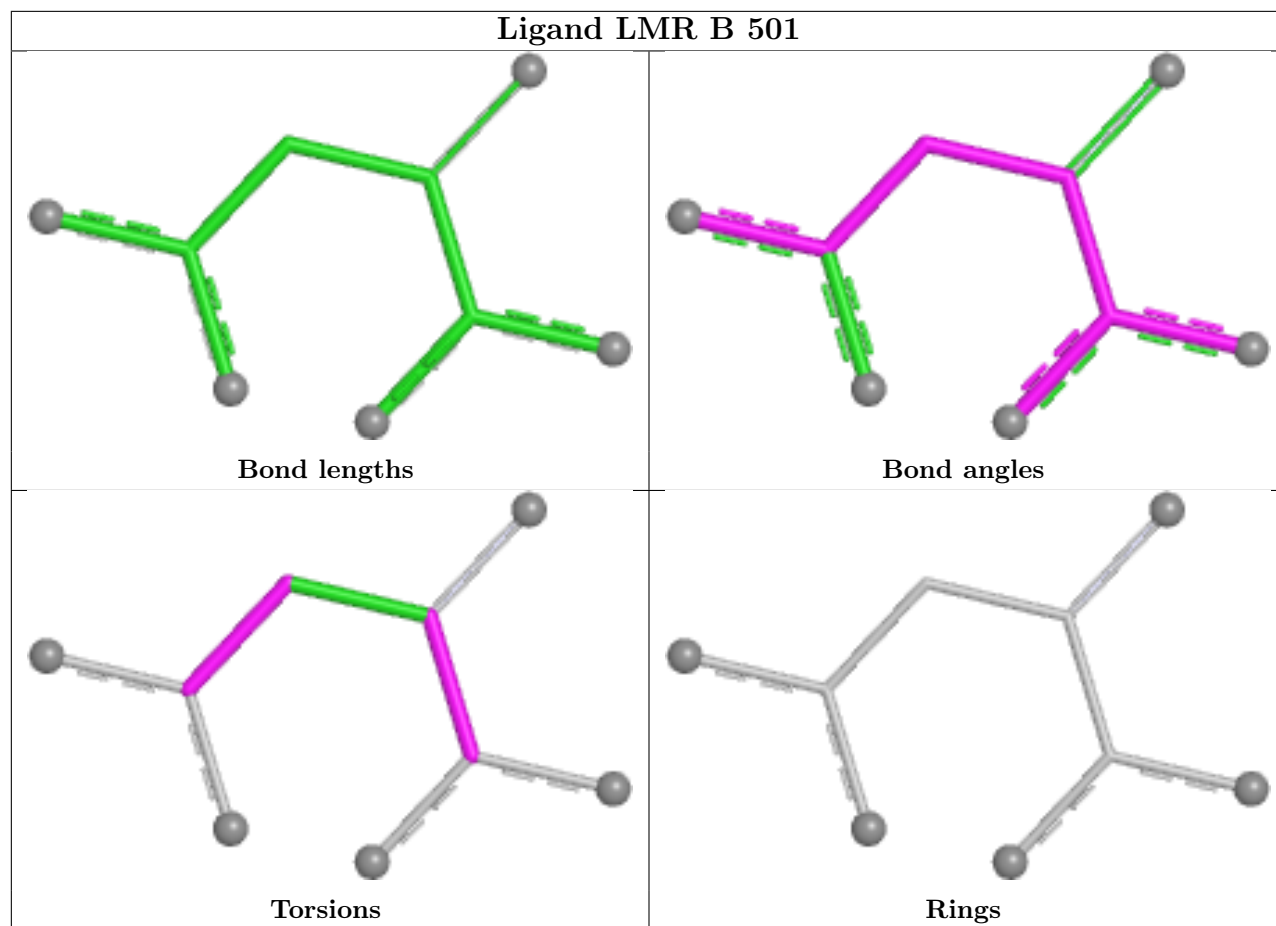
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	GOL	1	0
3	B	502	GOL	1	0

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 [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	479/488 (98%)	-0.13	7 (1%) 72 76	14, 25, 45, 70	0
1	B	478/488 (97%)	0.12	24 (5%) 34 37	10, 26, 55, 69	2 (0%)
1	C	477/488 (97%)	0.40	52 (10%) 10 10	10, 29, 64, 82	5 (1%)
1	D	478/488 (97%)	0.50	71 (14%) 5 5	11, 29, 69, 90	3 (0%)
All	All	1912/1952 (97%)	0.22	154 (8%) 18 19	10, 27, 61, 90	10 (0%)

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	486	ASN	6.3
1	C	468	CYS	5.9
1	D	467	LEU	5.6
1	D	475	ILE	5.3
1	D	12	VAL	4.7
1	C	16	LEU	4.7
1	D	476	VAL	4.5
1	C	467	LEU	4.5
1	D	338	PRO	4.5
1	D	11	VAL	4.5
1	C	9	LEU	4.4
1	D	466	LEU	4.4
1	D	339	GLY	4.4
1	D	462	ILE	4.4
1	B	468	CYS	4.3
1	A	339	GLY	4.2
1	C	466	LEU	4.2
1	B	467	LEU	4.1
1	D	14	ASP	4.0
1	D	464	LEU	3.9
1	D	453	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	16	LEU	3.9
1	D	124	LEU	3.9
1	D	457	LEU	3.8
1	B	9	LEU	3.8
1	C	485	HIS	3.7
1	D	471	LYS	3.7
1	D	461	ALA	3.7
1	D	8	ARG	3.6
1	D	434	LEU	3.6
1	D	485	HIS	3.5
1	D	478	PRO	3.5
1	D	23	LEU	3.5
1	D	133	LEU	3.5
1	D	447	VAL	3.5
1	D	472	PHE	3.4
1	C	14	ASP	3.4
1	C	440	TYR	3.4
1	C	136[A]	HIS	3.4
1	D	72	ILE	3.4
1	C	471	LYS	3.3
1	A	131	SER	3.3
1	C	464	LEU	3.3
1	C	15	SER	3.3
1	D	341	SER	3.3
1	D	121	ALA	3.3
1	D	469	GLY	3.2
1	C	461	ALA	3.1
1	C	21	VAL	3.1
1	C	472	PHE	3.1
1	D	21	VAL	3.1
1	C	128	SER	3.1
1	D	440	TYR	3.0
1	C	465	ASN	3.0
1	D	459	GLU	3.0
1	D	454	LYS	3.0
1	D	438	ILE	3.0
1	A	485	HIS	2.9
1	B	453	PHE	2.9
1	C	125	ILE	2.9
1	C	460	SER	2.9
1	C	449	HIS	2.9
1	D	76	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	469	GLY	2.9
1	B	456	GLY	2.9
1	B	478	PRO	2.9
1	B	455	LYS	2.9
1	D	439	GLY	2.9
1	C	67	PHE	2.8
1	C	470	GLU	2.8
1	D	80	ILE	2.8
1	C	476	VAL	2.8
1	B	472	PHE	2.8
1	B	466	LEU	2.8
1	B	476	VAL	2.8
1	D	9	LEU	2.7
1	C	11	VAL	2.7
1	C	74	SER	2.7
1	C	131	SER	2.7
1	B	12	VAL	2.7
1	C	77	SER	2.7
1	B	133	LEU	2.7
1	C	448	GLN	2.6
1	C	442	LEU	2.6
1	C	130	SER	2.6
1	B	125	ILE	2.5
1	B	475	ILE	2.5
1	D	433	VAL	2.5
1	C	132	ARG	2.5
1	A	9	LEU	2.5
1	D	442	LEU	2.5
1	B	461	ALA	2.5
1	D	141	VAL	2.5
1	C	478	PRO	2.5
1	D	77	SER	2.5
1	D	125	ILE	2.5
1	C	121	ALA	2.5
1	D	29	ALA	2.5
1	D	477	LYS	2.5
1	D	465	ASN	2.4
1	C	453	PHE	2.4
1	D	463	GLU	2.4
1	D	451	SER	2.4
1	C	339	GLY	2.4
1	C	479	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	69	LEU	2.4
1	D	132	ARG	2.4
1	D	470	GLU	2.4
1	D	460	SER	2.4
1	D	79	ALA	2.4
1	C	338	PRO	2.4
1	C	135	VAL	2.4
1	B	16	LEU	2.3
1	D	67	PHE	2.3
1	C	462	ILE	2.3
1	C	17	GLY	2.3
1	A	127	GLY	2.3
1	D	128	SER	2.3
1	C	133	LEU	2.3
1	D	449	HIS	2.3
1	C	19	ILE	2.3
1	C	459	GLU	2.3
1	C	124	LEU	2.3
1	B	485	HIS	2.3
1	D	455	LYS	2.3
1	D	340	SER	2.3
1	D	83	ALA	2.2
1	B	470	GLU	2.2
1	C	475	ILE	2.2
1	D	452	LYS	2.2
1	C	13	GLU	2.2
1	C	341	SER	2.2
1	D	446	LEU	2.2
1	B	473	ASP	2.2
1	D	20	ASN	2.2
1	D	66	ASN	2.2
1	D	122	SER	2.2
1	D	436	PRO	2.2
1	B	479	MET	2.1
1	B	431	VAL	2.1
1	D	456	GLY	2.1
1	D	63	ALA	2.1
1	D	130	SER	2.1
1	C	438	ILE	2.1
1	B	446	LEU	2.1
1	C	72	ILE	2.0
1	D	445	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	19	ILE	2.0
1	D	26	TYR	2.0
1	C	70	GLY	2.0
1	D	17	GLY	2.0
1	B	471	LYS	2.0
1	A	340	SER	2.0
1	C	127	GLY	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](#)

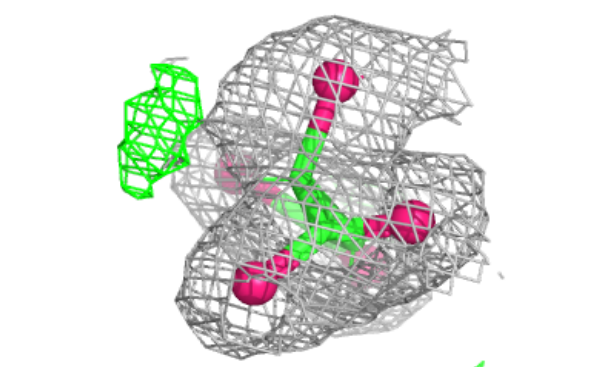
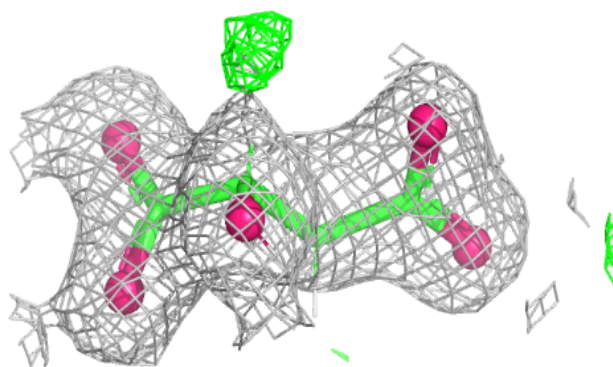
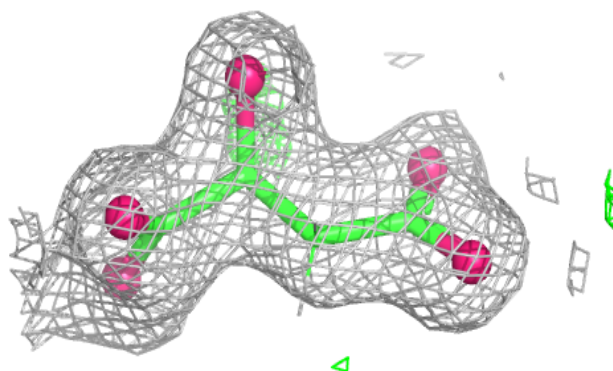
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACT	C	503	4/4	0.82	0.17	25,29,29,32	0
3	GOL	C	502	6/6	0.85	0.15	45,47,51,51	2
4	ACT	B	503	4/4	0.86	0.16	25,28,28,32	0
3	GOL	A	503	6/6	0.87	0.15	43,45,50,50	2
4	ACT	A	504	4/4	0.88	0.17	19,24,25,26	0
3	GOL	B	502	6/6	0.89	0.13	39,43,44,44	2
4	ACT	D	502	4/4	0.91	0.13	23,30,31,36	0
2	LMR	D	501	9/9	0.92	0.09	34,35,37,37	1
3	GOL	A	502	6/6	0.92	0.11	31,38,41,41	2
2	LMR	C	501	9/9	0.93	0.08	30,33,35,36	1
2	LMR	B	501	9/9	0.93	0.08	27,28,31,32	1
2	LMR	A	501	9/9	0.96	0.06	21,22,24,25	1

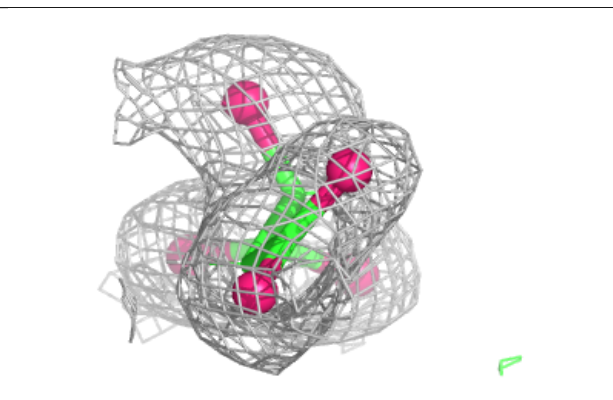
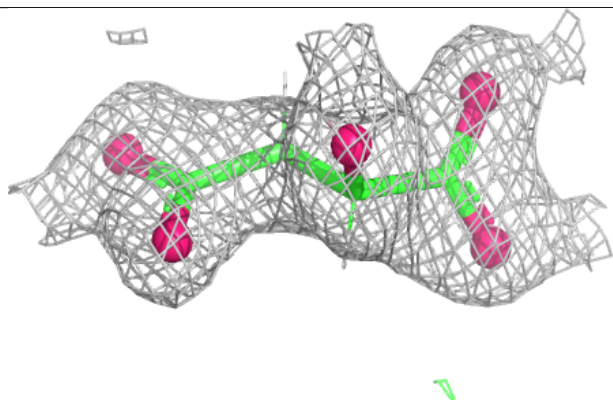
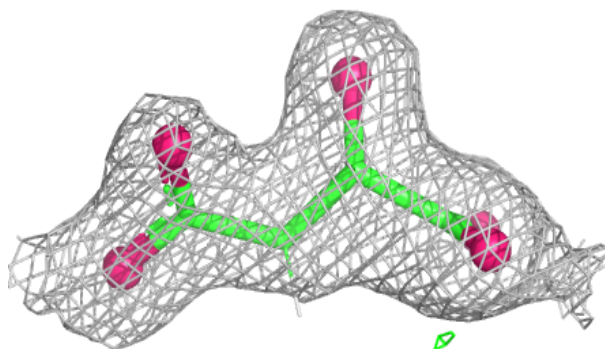
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMR D 501:

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

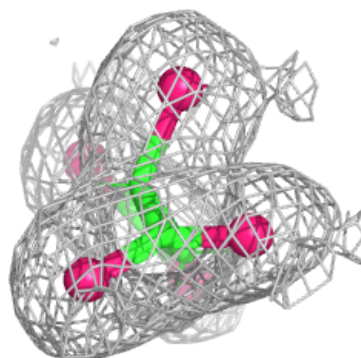
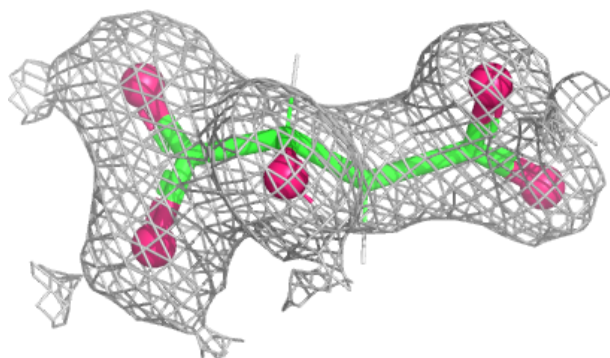
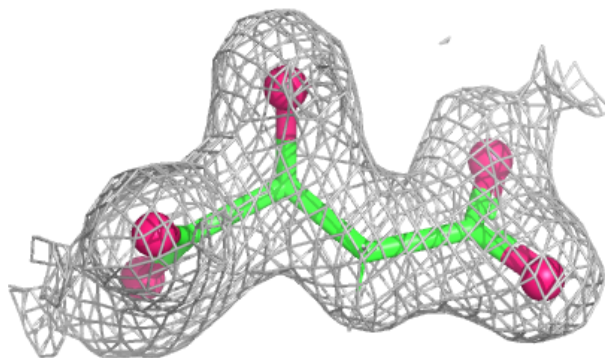
**Electron density around LMR C 501:**

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

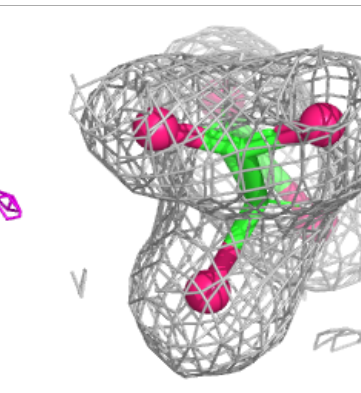
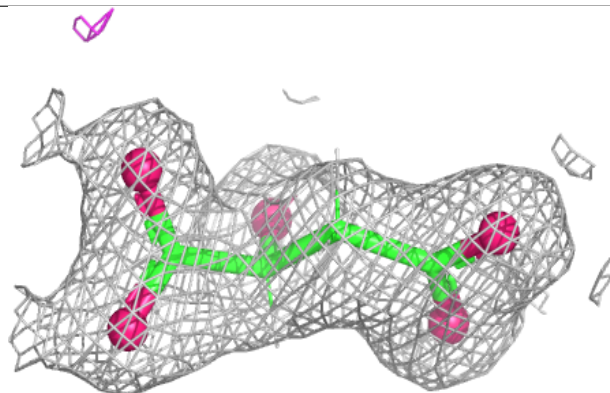
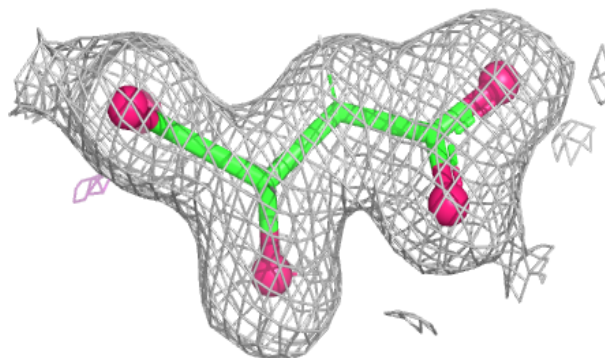


Electron density around LMR B 501:

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

**Electron density around LMR A 501:**

$2mF_o-DF_c$ (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.