



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 11:23 AM BST

PDB ID : 6U4O
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

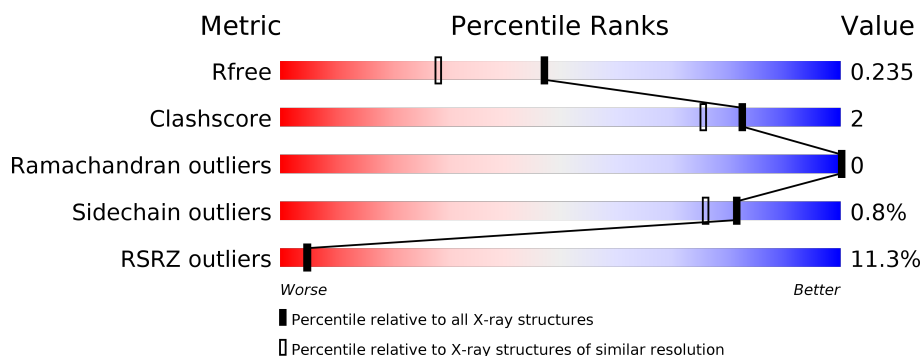
1 Overall quality at a glance

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}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (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 on 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	<div> <div>7%</div> <div>92%</div> <div>6%</div> </div>
1	B	488	<div> <div>11%</div> <div>90%</div> <div>8%</div> </div>
1	C	488	<div> <div>12%</div> <div>92%</div> <div>6%</div> </div>
1	D	488	<div> <div>15%</div> <div>91%</div> <div>7%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	C	502	-	-	-	X

2 Entry composition [i](#)

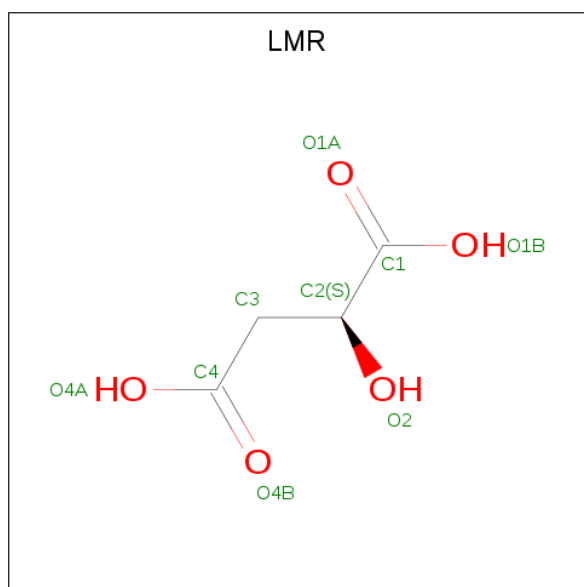
There are 5 unique types of molecules in this entry. The entry contains 29877 atoms, of which 14505 are hydrogens and 0 are deuteriums.

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 (three-letter code: LMR) (formula: C₄H₆O₅) (labeled as "Ligand of Interest" by author).



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 (three-letter code: 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 (three-letter code: 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		

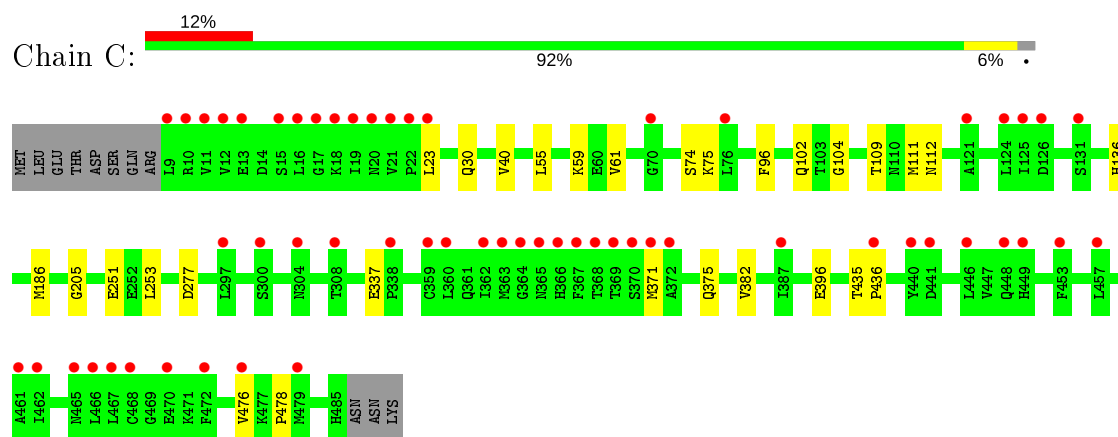
- Molecule 5 is water.

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		

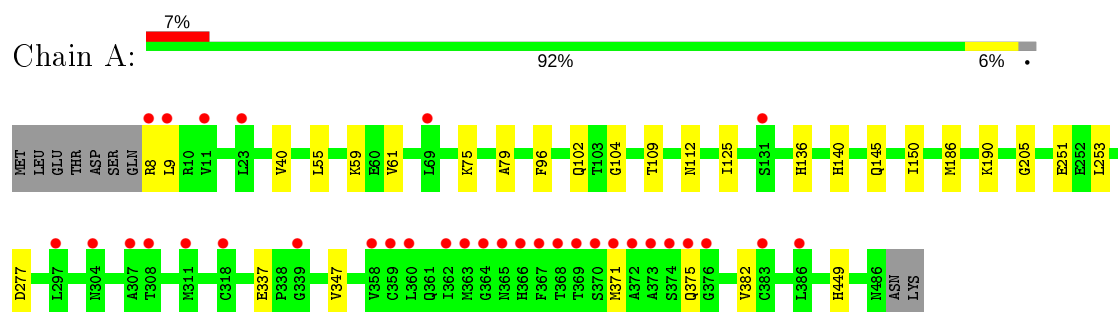
3 Residue-property plots [i](#)

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.

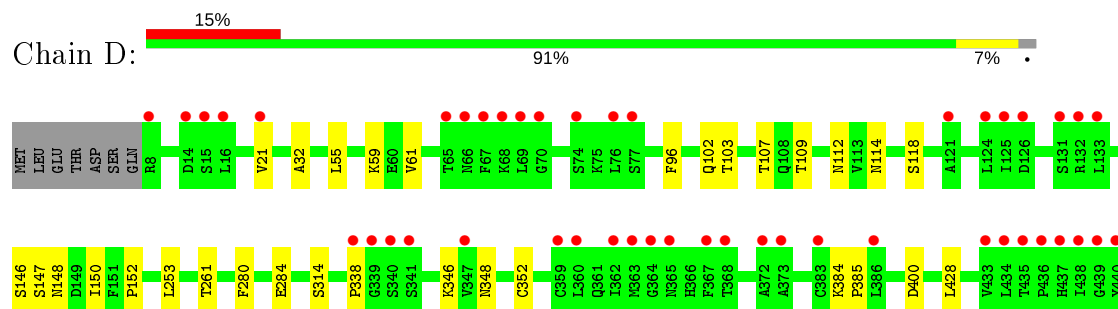
• Molecule 1: Fumarate hydratase

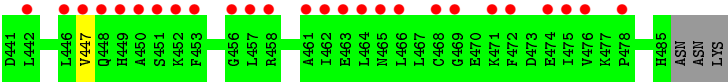


• Molecule 1: Fumarate hydratase

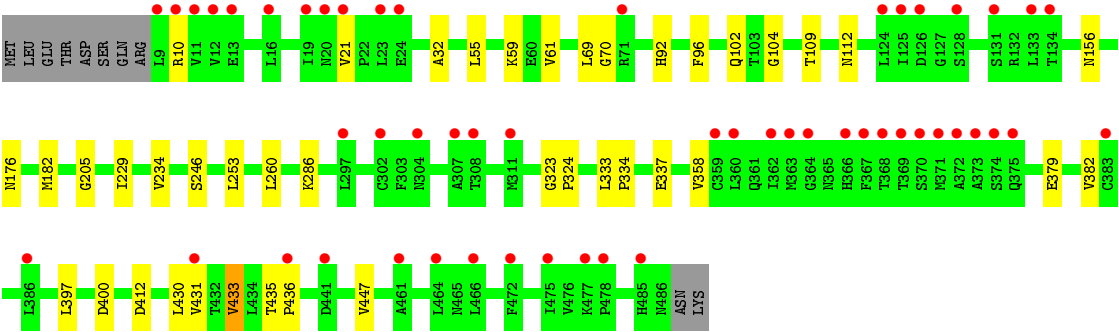
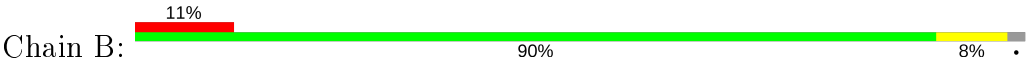


• Molecule 1: Fumarate hydratase





● 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 0.202 , 0.235	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 , 44.4	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, LMR, ACT

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	0.67	0/3714	0.74	0/5030
1	B	0.70	0/3662	0.74	0/4973
1	C	0.69	0/3642	0.73	0/4951
1	D	0.70	0/3622	0.74	0/4922
All	All	0.69	0/14640	0.74	0/19876

There are no bond length outliers.

There are no bond angle outliers.

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	16	0
1	B	3601	3626	3567	23	0
1	C	3580	3577	3495	16	0
1	D	3562	3531	3444	19	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	71	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 2.

All (71) 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:O	1:C:476:VAL:HG23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:334:PRO:HG3	1:B:412:ASP:HB2	1.93	0.50
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: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: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:A:40:VAL:HA	1:B:400:ASP:HB3	1.95	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:251:GLU:HG2	5:A:863:HOH:O	2.16	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:8:ARG:C	1:A:9:LEU:HD22	2.42	0.40
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
1:C:396:GLU:CD	5:C:694:HOH:O	2.59	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	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 [i](#)

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%)	409 (99%)	3 (1%)	84	79
1	B	399/428 (93%)	396 (99%)	3 (1%)	81	76
1	C	389/428 (91%)	383 (98%)	6 (2%)	65	53
1	D	384/428 (90%)	383 (100%)	1 (0%)	92	91
All	All	1584/1712 (92%)	1571 (99%)	13 (1%)	81	76

All (13) 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	337	GLU
1	C	478	PRO
1	A	190	LYS
1	A	277	ASP
1	A	337	GLU
1	D	284	GLU
1	B	337	GLU
1	B	379	GLU
1	B	433	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) 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
1	C	195	HIS
1	C	293	HIS
1	A	66	ASN
1	A	91	GLN
1	A	102	GLN
1	A	112	ASN
1	A	138	ASN
1	A	140	HIS

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Mol	Chain	Res	Type
1	A	195	HIS
1	A	293	HIS
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	231	HIS
1	D	348	ASN
1	D	375	GLN
1	B	91	GLN
1	B	92	HIS
1	B	94	ASN
1	B	102	GLN
1	B	112	ASN
1	B	195	HIS
1	B	375	GLN
1	B	377	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	GOL	A	502	-	5,5,5	0.07	0	5,5,5	0.24	0
3	GOL	C	502	-	5,5,5	0.12	0	5,5,5	0.34	0
2	LMR	B	501	-	2,8,8	0.49	0	3,10,10	2.80	2 (66%)
4	ACT	A	504	-	1,3,3	5.20	1 (100%)	0,3,3	0.00	-
3	GOL	B	502	-	5,5,5	0.05	0	5,5,5	0.35	0
4	ACT	C	503	-	1,3,3	5.28	1 (100%)	0,3,3	0.00	-
4	ACT	D	502	-	1,3,3	5.01	1 (100%)	0,3,3	0.00	-
3	GOL	A	503	-	5,5,5	0.12	0	5,5,5	0.31	0
2	LMR	A	501	-	2,8,8	0.23	0	3,10,10	2.30	1 (33%)
2	LMR	D	501	-	2,8,8	0.51	0	3,10,10	3.16	1 (33%)
2	LMR	C	501	-	2,8,8	0.32	0	3,10,10	2.37	1 (33%)
4	ACT	B	503	-	1,3,3	4.37	1 (100%)	0,3,3	0.00	-

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	ACT	CH3-C	5.28	1.55	1.48
4	A	504	ACT	CH3-C	5.20	1.55	1.48
4	D	502	ACT	CH3-C	5.01	1.55	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	ACT	CH3-C	4.37	1.54	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	LMR	C3-C2-C1	-5.22	104.45	111.10
2	B	501	LMR	C3-C2-C1	-4.34	105.58	111.10
2	C	501	LMR	C3-C2-C1	-4.00	106.00	111.10
2	A	501	LMR	C3-C2-C1	-3.73	106.36	111.10
2	B	501	LMR	O2-C2-C3	2.14	113.20	108.50

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	502	GOL	O1-C1-C2-O2
3	C	502	GOL	O1-C1-C2-C3
3	C	502	GOL	C1-C2-C3-O3
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
3	B	502	GOL	O2-C2-C3-O3
3	A	502	GOL	C1-C2-C3-O3

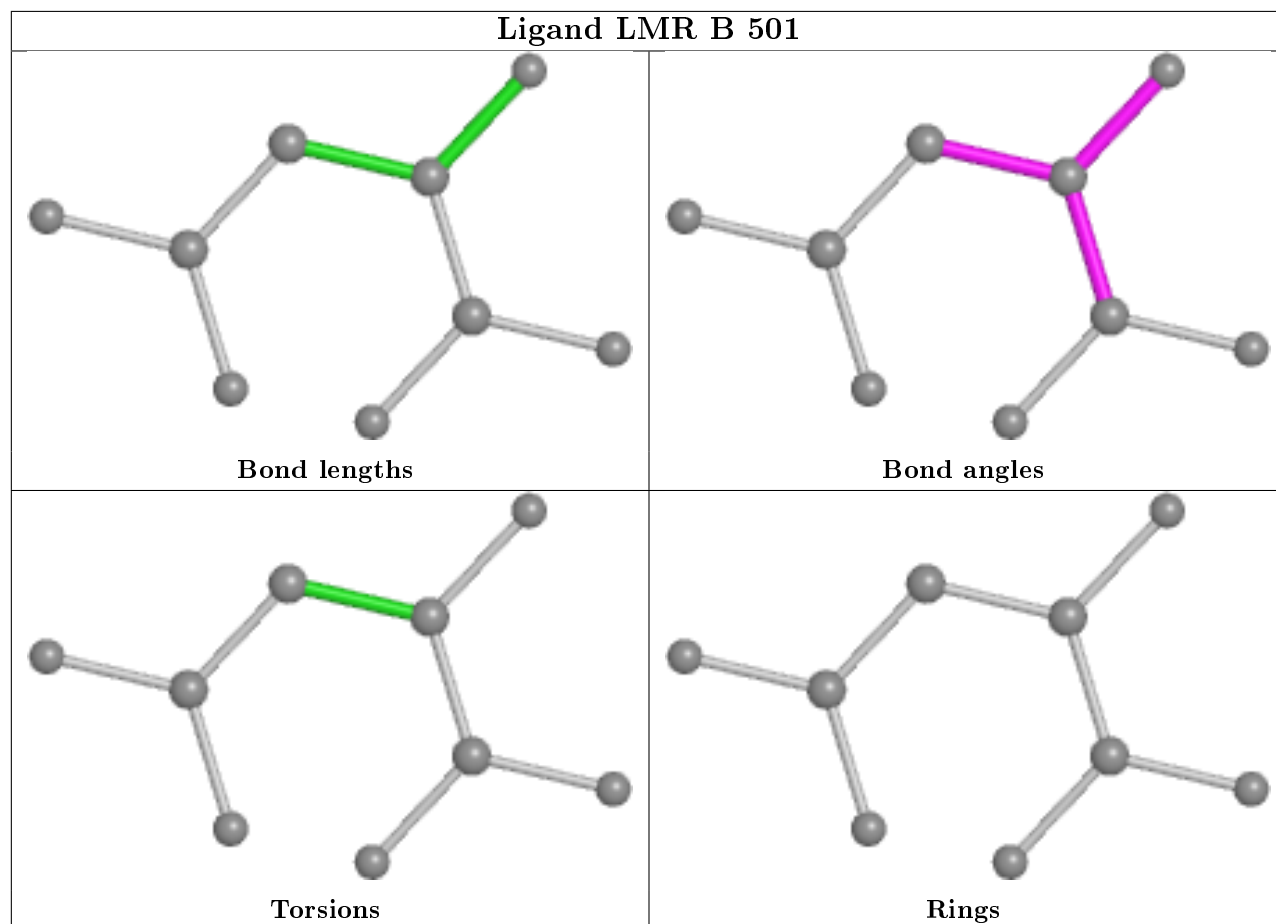
There are no ring outliers.

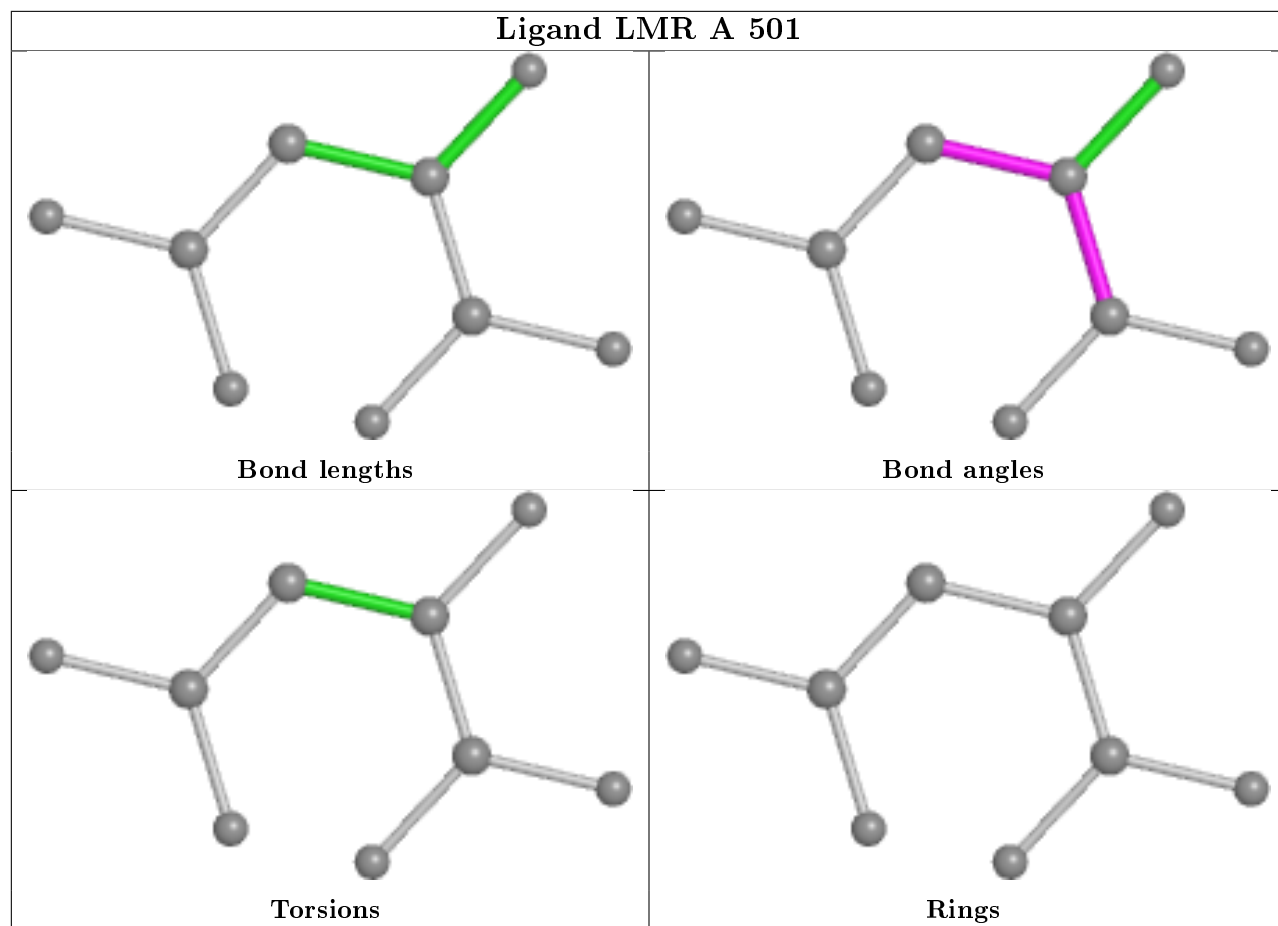
2 monomers are involved in 2 short contacts:

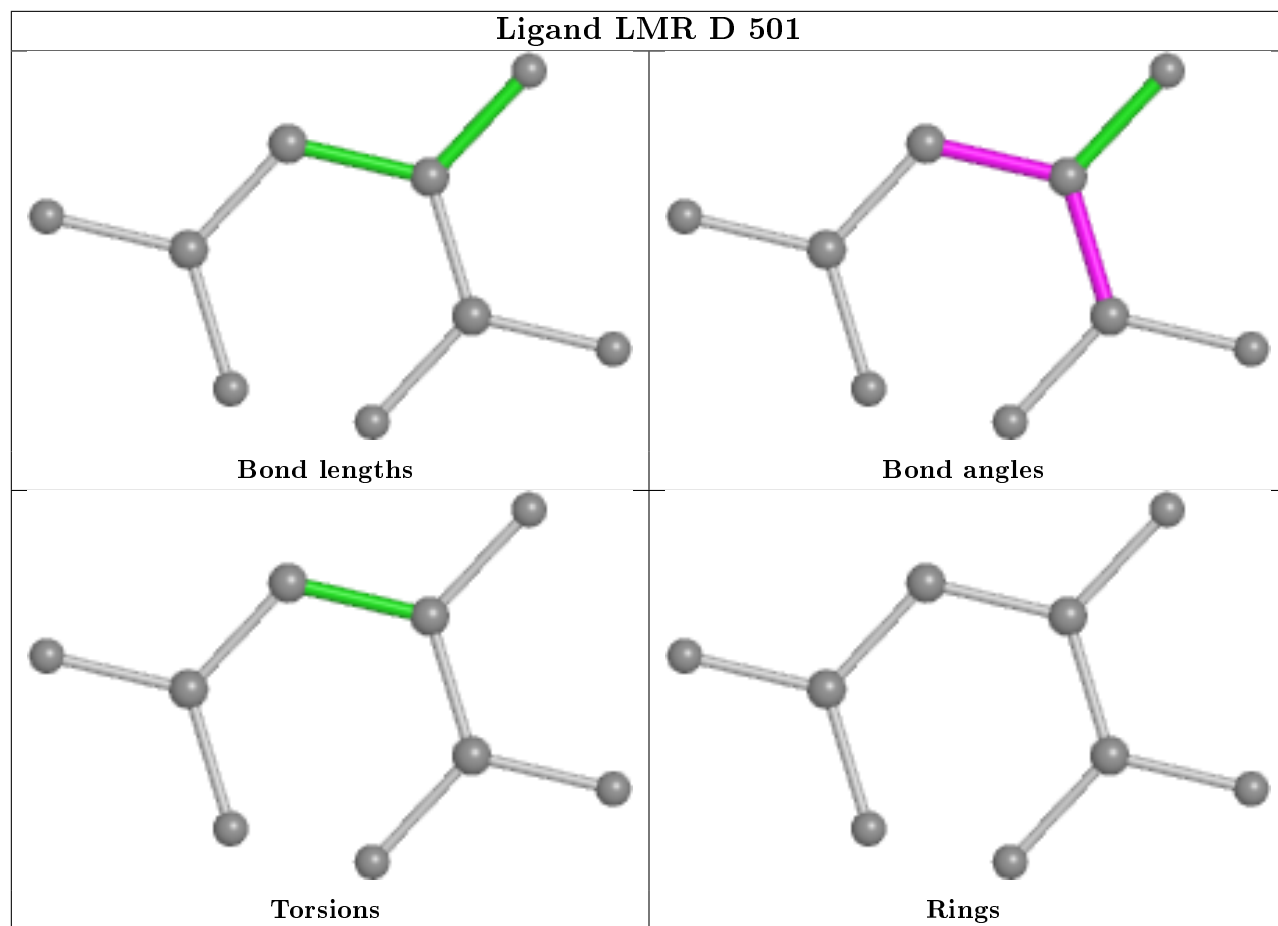
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	GOL	1	0
3	B	502	GOL	1	0

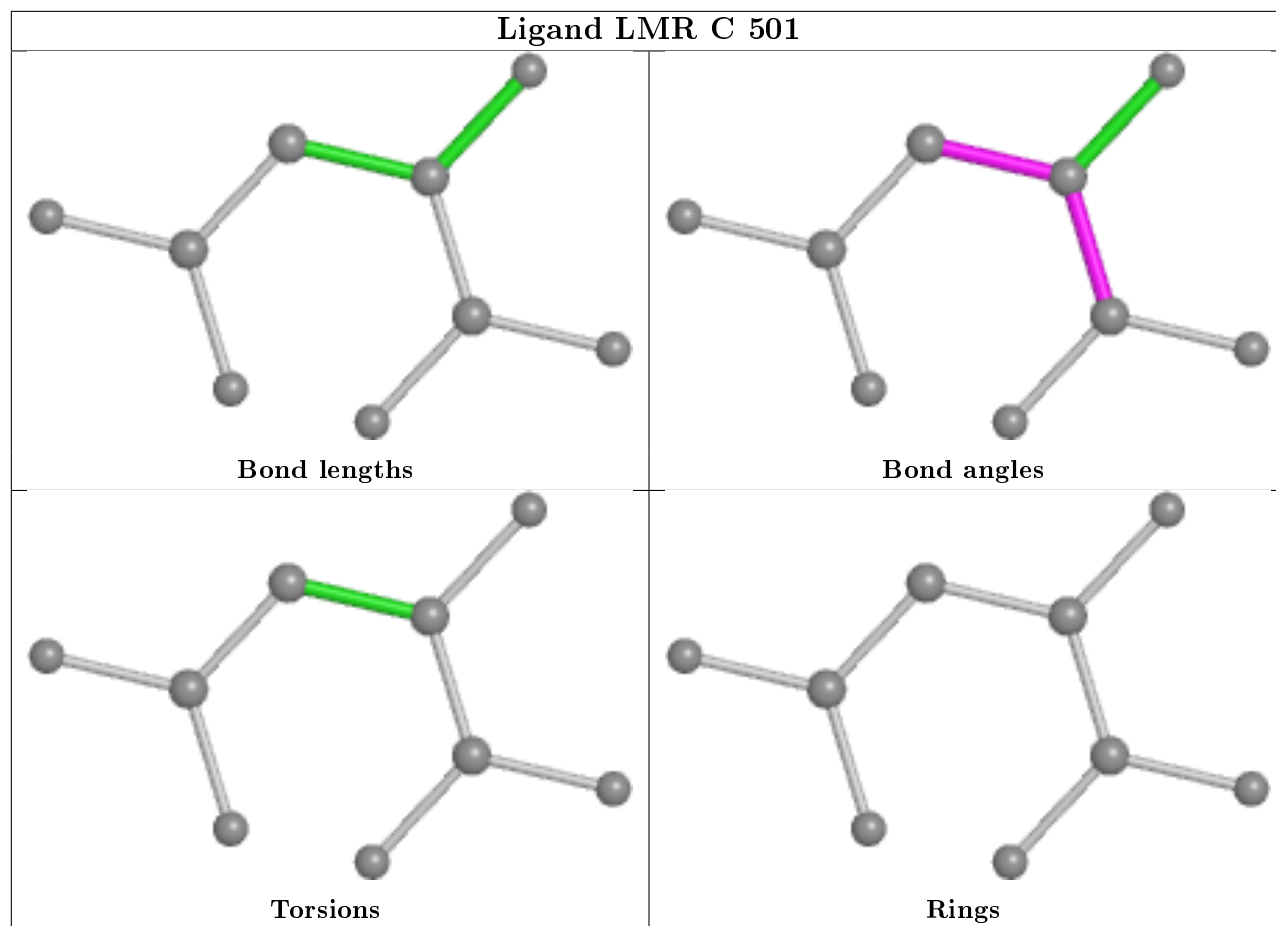
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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%)	0.28	33 (6%) 16 16	15, 25, 45, 68	0
1	B	478/488 (97%)	0.49	53 (11%) 5 5	16, 26, 58, 69	0
1	C	477/488 (97%)	0.63	58 (12%) 4 4	19, 30, 69, 86	1 (0%)
1	D	478/488 (97%)	0.63	72 (15%) 2 2	19, 30, 74, 90	0
All	All	1912/1952 (97%)	0.51	216 (11%) 5 5	15, 28, 64, 90	1 (0%)

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	16	LEU	6.6
1	C	466	LEU	5.7
1	C	23	LEU	5.5
1	C	131	SER	5.2
1	B	131	SER	5.1
1	B	11	VAL	4.9
1	D	475	ILE	4.8
1	D	461	ALA	4.8
1	C	9	LEU	4.7
1	B	133	LEU	4.7
1	D	367	PHE	4.6
1	B	19	ILE	4.6
1	B	461	ALA	4.5
1	A	367	PHE	4.5
1	D	69	LEU	4.5
1	C	21	VAL	4.5
1	C	11	VAL	4.5
1	A	9	LEU	4.4
1	C	367	PHE	4.4
1	D	457	LEU	4.4
1	D	453	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	367	PHE	4.4
1	D	447	VAL	4.4
1	D	466	LEU	4.3
1	B	9	LEU	4.3
1	B	23	LEU	4.3
1	D	472	PHE	4.2
1	C	19	ILE	4.2
1	D	446	LEU	4.2
1	D	439	GLY	4.1
1	B	12	VAL	4.1
1	D	442	LEU	4.0
1	D	341	SER	4.0
1	C	15	SER	3.9
1	A	8	ARG	3.8
1	B	360	LEU	3.8
1	A	360	LEU	3.8
1	D	464	LEU	3.8
1	B	16	LEU	3.8
1	D	469	GLY	3.8
1	D	440	TYR	3.8
1	C	125	ILE	3.7
1	C	465	ASN	3.7
1	D	338	PRO	3.7
1	D	16	LEU	3.7
1	C	17	GLY	3.5
1	D	364	GLY	3.5
1	D	433	VAL	3.5
1	D	465	ASN	3.5
1	D	478	PRO	3.5
1	B	368	THR	3.5
1	A	339	GLY	3.4
1	D	462	ILE	3.4
1	D	458	ARG	3.4
1	D	368	THR	3.4
1	C	461	ALA	3.4
1	D	468	CYS	3.4
1	A	371	MET	3.4
1	C	10	ARG	3.3
1	C	472	PHE	3.3
1	C	468	CYS	3.3
1	B	21	VAL	3.3
1	A	372	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	131	SER	3.2
1	A	11	VAL	3.2
1	C	12	VAL	3.2
1	B	359	CYS	3.1
1	B	372	ALA	3.1
1	C	368	THR	3.1
1	A	368	THR	3.1
1	D	436	PRO	3.0
1	D	67	PHE	3.0
1	B	475	ILE	3.0
1	B	134	THR	3.0
1	C	372	ALA	3.0
1	D	131	SER	3.0
1	C	20	ASN	3.0
1	C	436	PRO	3.0
1	B	472	PHE	3.0
1	D	448	GLN	3.0
1	A	364	GLY	3.0
1	C	467	LEU	3.0
1	D	471	LYS	3.0
1	B	125	ILE	3.0
1	B	364	GLY	2.9
1	C	18	LYS	2.9
1	B	297	LEU	2.9
1	D	15	SER	2.9
1	A	69	LEU	2.9
1	D	124	LEU	2.9
1	B	126	ASP	2.9
1	A	362	ILE	2.9
1	B	304	ASN	2.9
1	B	24	GLU	2.9
1	D	340	SER	2.8
1	C	366	HIS	2.8
1	C	360	LEU	2.8
1	C	441	ASP	2.8
1	D	14	ASP	2.8
1	D	456	GLY	2.7
1	D	133	LEU	2.7
1	B	478	PRO	2.7
1	D	451	SER	2.7
1	A	373	ALA	2.7
1	C	363	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	125	ILE	2.7
1	D	362	ILE	2.7
1	D	74	SER	2.7
1	C	371	MET	2.7
1	C	457	LEU	2.7
1	A	297	LEU	2.7
1	C	479	MET	2.6
1	D	68	LYS	2.6
1	A	369	THR	2.6
1	D	450	ALA	2.6
1	A	363	MET	2.6
1	C	369	THR	2.6
1	D	360	LEU	2.6
1	A	359	CYS	2.6
1	C	449	HIS	2.6
1	A	308	THR	2.6
1	D	65	THR	2.6
1	C	124	LEU	2.6
1	D	434	LEU	2.6
1	B	373	ALA	2.6
1	C	448	GLN	2.6
1	D	363	MET	2.6
1	C	453	PHE	2.6
1	D	435	THR	2.6
1	D	372	ALA	2.6
1	D	449	HIS	2.6
1	C	338	PRO	2.6
1	C	364	GLY	2.6
1	B	431	VAL	2.6
1	B	369	THR	2.5
1	A	383	CYS	2.5
1	C	440	TYR	2.5
1	C	387	ILE	2.5
1	D	21	VAL	2.5
1	D	474	GLU	2.5
1	B	441	ASP	2.5
1	D	132	ARG	2.5
1	D	359	CYS	2.5
1	B	466	LEU	2.5
1	A	366	HIS	2.5
1	B	366	HIS	2.4
1	D	76	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	66	ASN	2.4
1	B	375	GLN	2.4
1	D	438	ILE	2.4
1	B	362	ILE	2.4
1	A	358	VAL	2.4
1	B	485	HIS	2.4
1	D	77	SER	2.4
1	B	374	SER	2.4
1	B	308	THR	2.4
1	C	362	ILE	2.4
1	C	22	PRO	2.4
1	C	70	GLY	2.4
1	D	476	VAL	2.4
1	A	307	ALA	2.4
1	C	365	ASN	2.4
1	A	376	GLY	2.3
1	B	370	SER	2.3
1	B	13	GLU	2.3
1	A	318	CYS	2.3
1	C	462	ILE	2.3
1	B	383	CYS	2.3
1	C	300	SER	2.3
1	B	464	LEU	2.3
1	D	383	CYS	2.3
1	B	71	ARG	2.3
1	A	23	LEU	2.2
1	A	375	GLN	2.2
1	C	304	ASN	2.2
1	A	311	MET	2.2
1	C	370	SER	2.2
1	C	76	LEU	2.2
1	B	10	ARG	2.2
1	B	311	MET	2.2
1	B	371	MET	2.2
1	C	121	ALA	2.2
1	D	365	ASN	2.2
1	C	297	LEU	2.2
1	D	437	HIS	2.2
1	A	370	SER	2.1
1	A	386	LEU	2.1
1	D	463	GLU	2.1
1	A	365	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	20	ASN	2.1
1	B	477	LYS	2.1
1	B	128	SER	2.1
1	B	363	MET	2.1
1	C	359	CYS	2.1
1	B	124	LEU	2.1
1	B	386	LEU	2.1
1	D	8	ARG	2.1
1	C	470	GLU	2.1
1	C	476	VAL	2.1
1	B	302	CYS	2.1
1	B	307	ALA	2.1
1	D	386	LEU	2.1
1	D	70	GLY	2.1
1	C	308	THR	2.1
1	D	347	VAL	2.1
1	C	13	GLU	2.1
1	D	373	ALA	2.1
1	C	446	LEU	2.1
1	D	339	GLY	2.1
1	C	126	ASP	2.0
1	A	374	SER	2.0
1	B	436	PRO	2.0
1	D	126	ASP	2.0
1	A	304	ASN	2.0
1	D	452	LYS	2.0
1	D	121	ALA	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 monosaccharides 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,

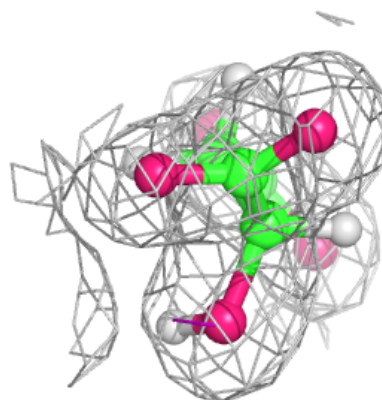
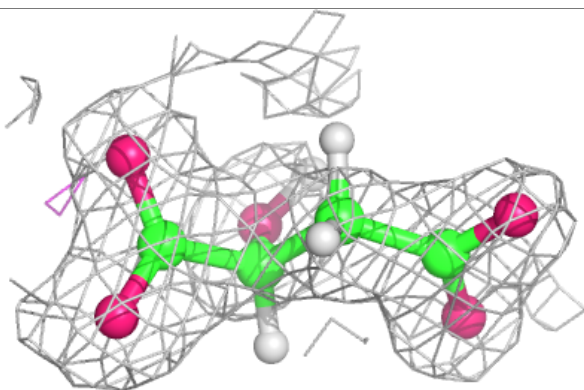
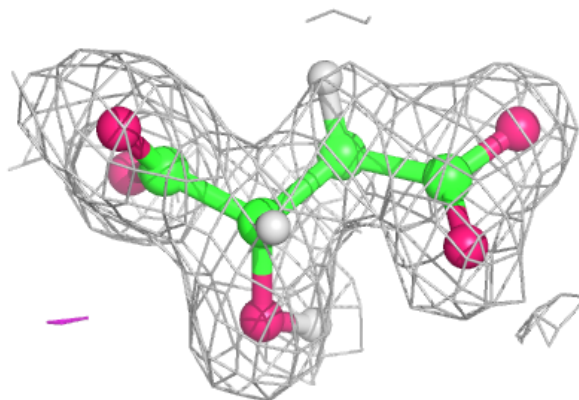
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	C	502	6/6	0.77	0.44	45,47,51,51	2
3	GOL	A	503	6/6	0.81	0.35	43,45,50,50	2
3	GOL	A	502	6/6	0.83	0.19	31,38,41,41	2
4	ACT	B	503	4/4	0.84	0.36	25,28,28,32	0
3	GOL	B	502	6/6	0.86	0.19	39,43,44,44	2
4	ACT	C	503	4/4	0.87	0.33	25,29,29,32	0
2	LMR	B	501	9/9	0.89	0.12	27,28,31,32	1
2	LMR	D	501	9/9	0.90	0.12	34,35,37,37	1
4	ACT	D	502	4/4	0.90	0.31	23,30,31,36	0
4	ACT	A	504	4/4	0.91	0.27	19,24,25,26	0
2	LMR	C	501	9/9	0.94	0.09	30,33,35,36	1
2	LMR	A	501	9/9	0.96	0.10	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.

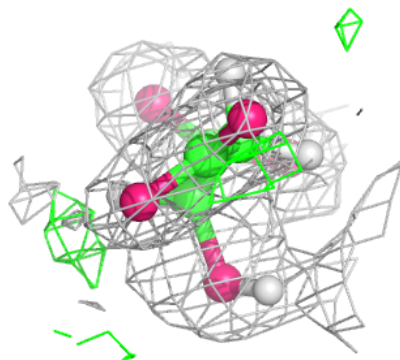
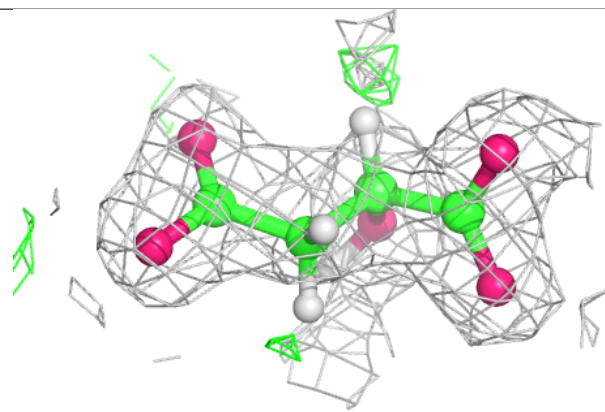
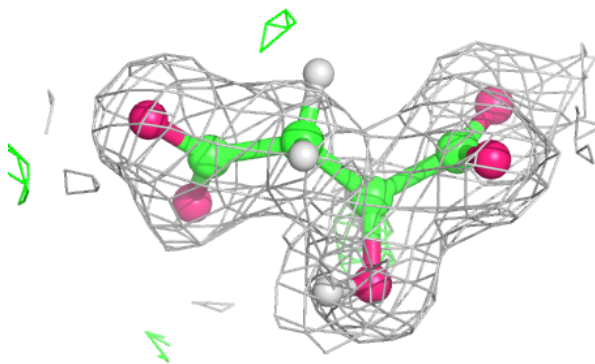
Electron density around LMR B 501:

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



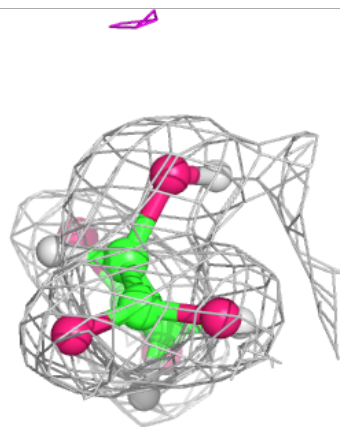
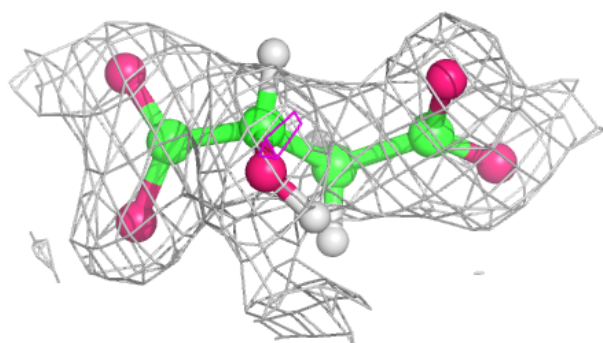
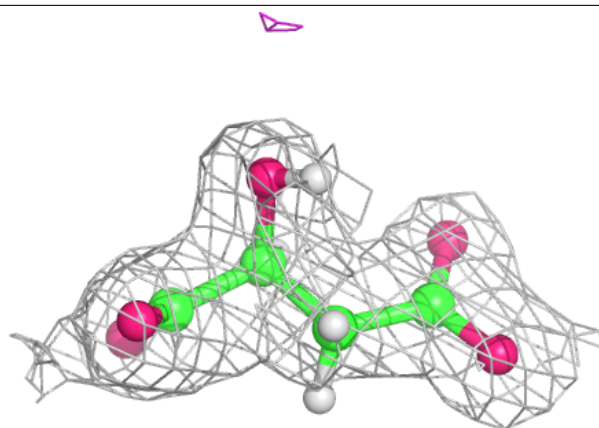
Electron density around LMR D 501:

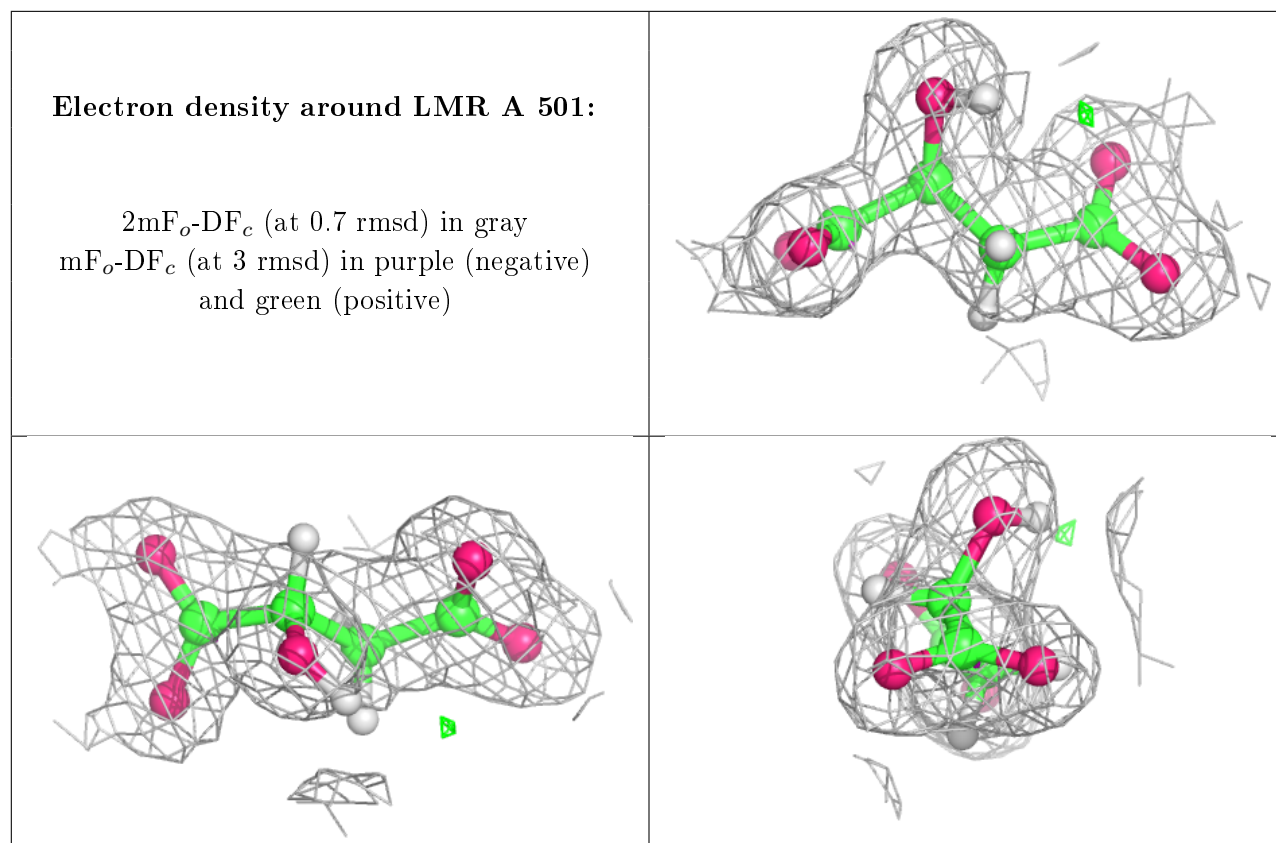
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMR C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 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.