



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:11 AM UTC

PDB ID : 7TGM / pdb_00007tgm
Title : Crystal structure of HSC-AMS bound DesD, the desferrioxamine synthetase from the *Streptomyces griseoflavus* ferrimycin biosynthetic pathway
Authors : Patel, K.D.; Gulick, A.M.
Deposited on : 2022-01-07
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

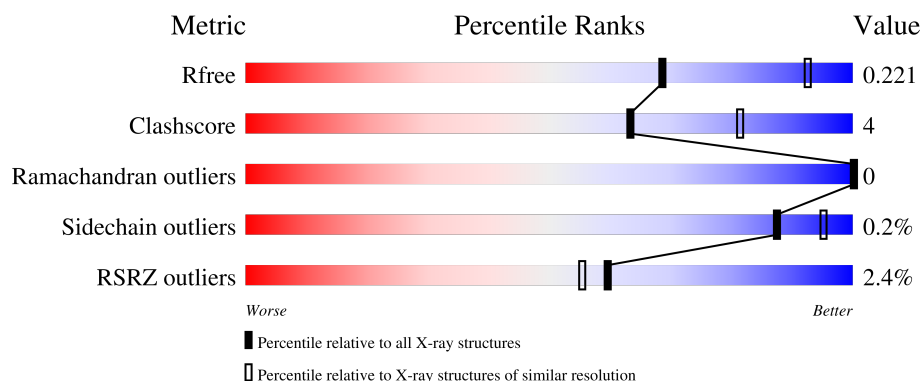
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

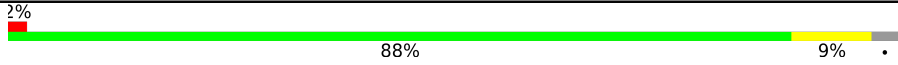
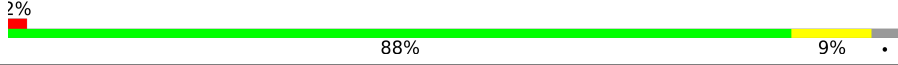
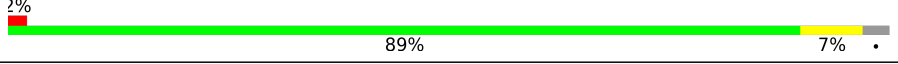
The reported resolution of this entry is 2.50 Å.

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	612	
1	B	612	
1	C	612	
1	D	612	
1	E	612	

2 Entry composition [i](#)

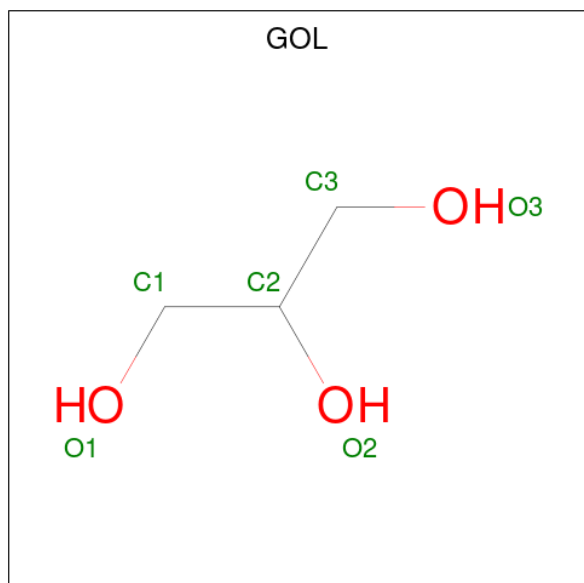
There are 8 unique types of molecules in this entry. The entry contains 24554 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Desferrioxamine synthetase DesD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	0	0
			4692	2984	817	875	16			
1	B	592	Total	C	N	O	S	0	0	0
			4674	2973	818	868	15			
1	C	592	Total	C	N	O	S	0	0	0
			4662	2967	810	870	15			
1	E	591	Total	C	N	O	S	0	0	0
			4658	2965	809	869	15			
1	D	592	Total	C	N	O	S	0	0	0
			4674	2975	816	868	15			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

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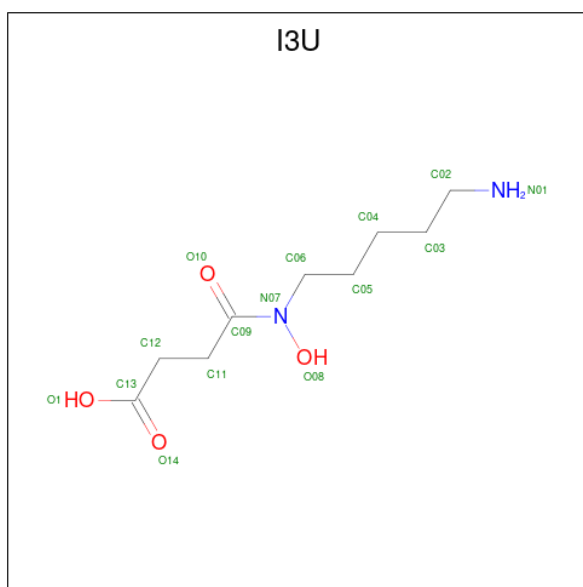
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		

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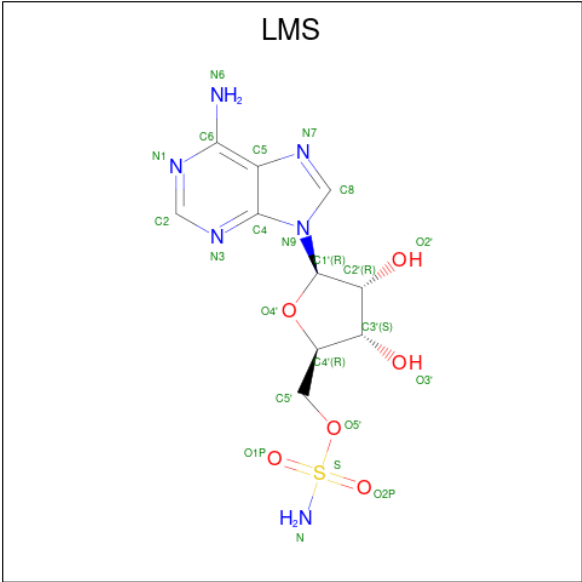
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 4-[(5-aminopentyl)(hydroxy)amino]-4-oxobutanoic acid (CCD ID: I3U) (formula: C₉H₁₈N₂O₄) (labeled as "Ligand of Interest" by depositor).



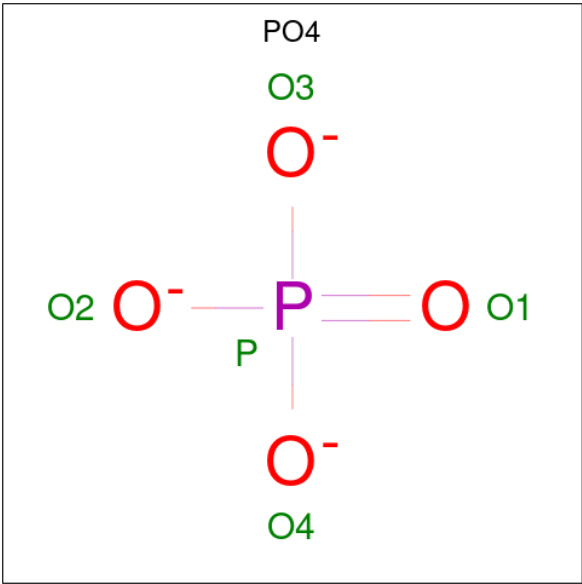
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	9	2	3		
3	B	1	Total	C	N	O	0	0
			14	9	2	3		
3	C	1	Total	C	N	O	0	0
			14	9	2	3		
3	E	1	Total	C	N	O	0	0
			14	9	2	3		
3	D	1	Total	C	N	O	0	0
			14	9	2	3		

- Molecule 4 is [(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3,4-DIHYDROXYTETRAHYDRO-2-FURANYL]METHYL SULFAMATE (CCD ID: LMS) (formula: C₁₀H₁₄N₆O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			23	10	6	6	1		
4	B	1	Total	C	N	O	S	0	0
			23	10	6	6	1		
4	C	1	Total	C	N	O	S	0	0
			23	10	6	6	1		
4	E	1	Total	C	N	O	S	0	0
			23	10	6	6	1		
4	D	1	Total	C	N	O	S	0	0
			23	10	6	6	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

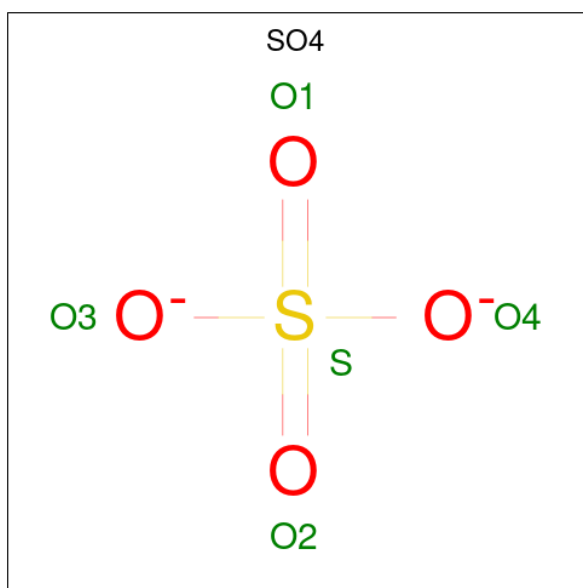


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	C	1	Total O P 5 4 1	0	0
5	E	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	B	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0
6	E	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		

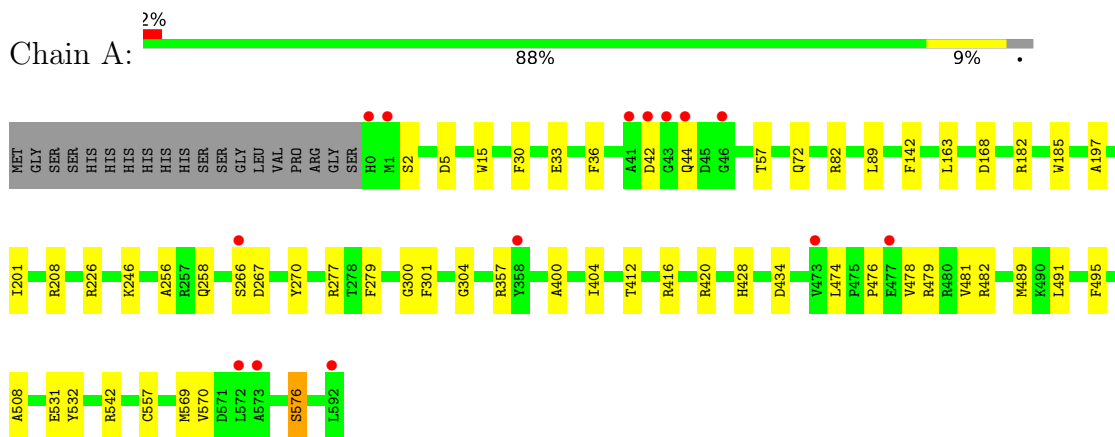
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	104	Total	O	0	0
			104	104		
8	B	110	Total	O	0	0
			110	110		
8	C	41	Total	O	0	0
			41	41		
8	E	43	Total	O	0	0
			43	43		
8	D	92	Total	O	0	0
			92	92		

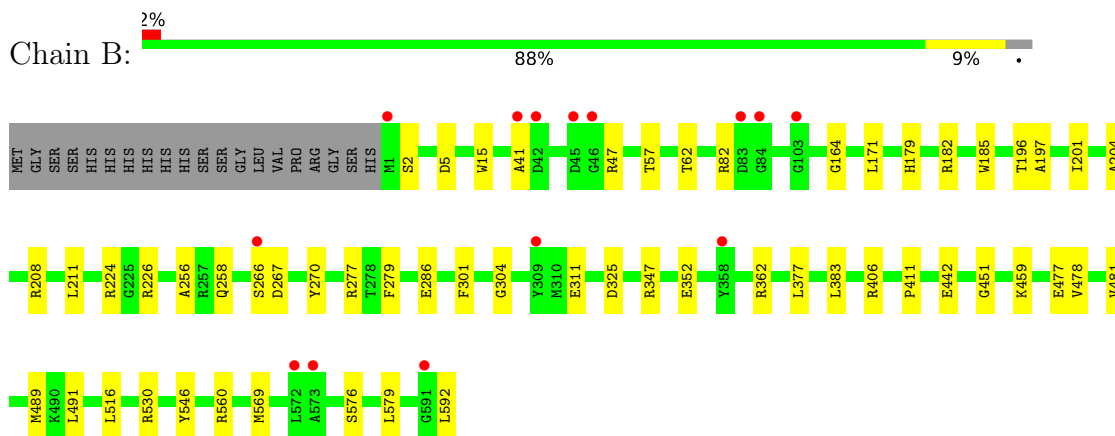
3 Residue-property plots [i](#)

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.

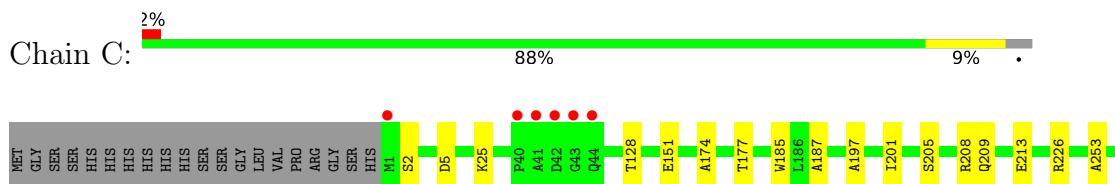
• Molecule 1: Desferrioxamine synthetase DesD

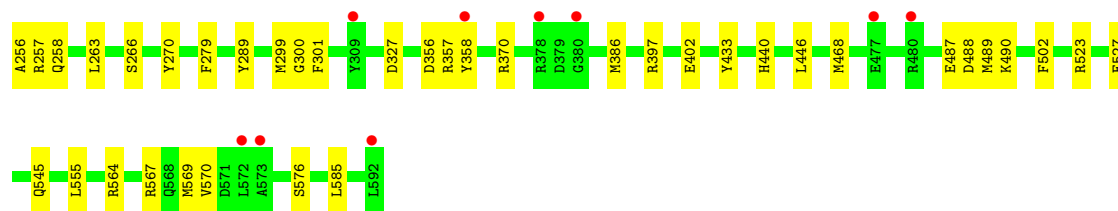


• Molecule 1: Desferrioxamine synthetase DesD

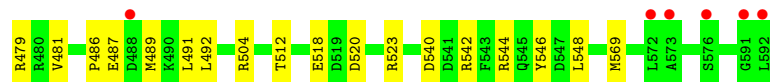
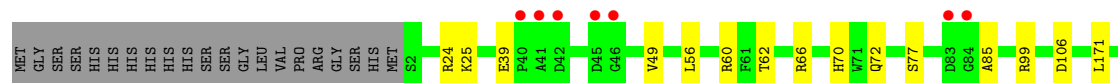
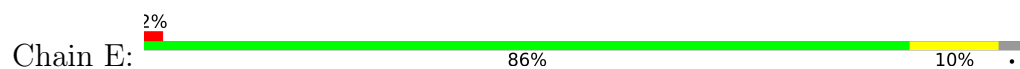


• Molecule 1: Desferrioxamine synthetase DesD

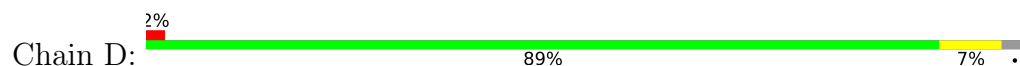




● Molecule 1: Desferrioxamine synthetase DesD



● Molecule 1: Desferrioxamine synthetase DesD



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	125.80Å 237.40Å 329.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.60 – 2.50 49.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.60-2.50) 93.3 (49.60-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.189 , 0.220 0.189 , 0.221	Depositor DCC
R_{free} test set	1862 reflections (1.10%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	24554	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: I3U, GOL, PO4, SO4, MG, LMS

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	0.35	0/4806	0.51	0/6542
1	B	0.36	0/4787	0.55	0/6516
1	C	0.30	0/4776	0.47	0/6505
1	D	0.34	0/4788	0.50	0/6519
1	E	0.33	0/4772	0.49	0/6499
All	All	0.34	0/23929	0.51	0/32581

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	4692	0	4573	38	0
1	B	4674	0	4560	44	0
1	C	4662	0	4527	34	0
1	D	4674	0	4556	33	0
1	E	4658	0	4524	42	0
2	A	78	0	103	3	0
2	B	84	0	112	9	0
2	C	54	0	72	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	90	0	119	5	0
2	E	48	0	64	2	0
3	A	14	0	0	0	0
3	B	14	0	0	0	0
3	C	14	0	0	0	0
3	D	14	0	0	0	0
3	E	14	0	0	0	0
4	A	23	0	12	0	0
4	B	23	0	12	0	0
4	C	23	0	12	0	0
4	D	23	0	13	0	0
4	E	23	0	12	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
7	A	40	0	0	0	0
7	B	60	0	0	0	0
7	C	50	0	0	0	0
7	D	50	0	0	1	0
7	E	35	0	0	0	0
8	A	104	0	0	1	0
8	B	110	0	0	2	0
8	C	41	0	0	2	0
8	D	92	0	0	3	0
8	E	43	0	0	0	0
All	All	24554	0	23271	188	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 4.

All (188) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ARG:NH1	1:A:267:ASP:O	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:TRP:HE1	1:E:266:SER:HB3	1.50	0.76
1:A:476:PRO:HA	1:A:479:ARG:HD2	1.68	0.75
1:E:476:PRO:HA	1:E:479:ARG:HD2	1.71	0.72
1:C:185:TRP:HE1	1:C:266:SER:HB3	1.54	0.72
1:A:185:TRP:HE1	1:A:266:SER:HB3	1.57	0.70
1:D:530:ARG:HH11	1:D:530:ARG:HG2	1.57	0.69
1:B:406:ARG:HH11	2:B:603:GOL:H12	1.59	0.68
1:D:24:ARG:NH2	8:D:702:HOH:O	2.27	0.67
1:C:567:ARG:NH1	8:C:701:HOH:O	2.28	0.66
2:C:602:GOL:H12	1:D:246:LYS:NZ	2.12	0.65
1:E:310:MET:HE1	1:E:368:LEU:HD23	1.80	0.62
1:E:49:VAL:HG23	1:E:60:ARG:HG2	1.82	0.61
1:A:226:ARG:HH21	1:A:258:GLN:HE21	1.49	0.60
1:A:300:GLY:HA3	1:A:569:MET:HG3	1.83	0.60
1:C:300:GLY:HA3	1:C:569:MET:HG3	1.84	0.60
1:D:322:ARG:HD2	2:D:610:GOL:O2	2.02	0.60
1:E:487:GLU:OE2	1:E:546:TYR:OH	2.20	0.60
1:E:182:ARG:NH1	1:E:267:ASP:O	2.35	0.59
1:A:478:VAL:O	1:A:481:VAL:HG22	2.03	0.58
1:B:41:ALA:CB	1:B:47:ARG:HB3	2.33	0.58
1:B:442:GLU:O	1:B:459:LYS:HE3	2.03	0.57
1:B:224:ARG:NH1	8:B:701:HOH:O	2.31	0.56
1:C:205:SER:O	1:C:209:GLN:HG3	2.05	0.56
1:A:142:PHE:HB2	2:A:604:GOL:H2	1.88	0.55
1:A:197:ALA:HB1	1:A:201:ILE:HB	1.87	0.55
1:D:185:TRP:HE1	1:D:266:SER:HB3	1.71	0.55
1:B:41:ALA:HB2	1:B:47:ARG:C	2.31	0.55
1:E:277:ARG:NH1	1:E:304:GLY:O	2.39	0.55
1:E:300:GLY:HA3	1:E:569:MET:HG3	1.89	0.55
1:E:208:ARG:HE	1:E:216:VAL:HG11	1.71	0.55
1:B:377:LEU:HD11	1:B:383:LEU:CD2	2.36	0.54
1:D:72:GLN:OE1	1:D:512:THR:OG1	2.24	0.54
2:C:602:GOL:H12	1:D:246:LYS:HZ3	1.72	0.54
1:D:258:GLN:NE2	8:D:704:HOH:O	2.39	0.54
1:B:182:ARG:NH1	1:B:267:ASP:O	2.40	0.54
1:E:352:GLU:O	1:E:362:ARG:NH2	2.41	0.53
1:B:286:GLU:OE1	1:B:286:GLU:N	2.32	0.53
1:E:62:THR:HG23	1:E:77:SER:HB2	1.91	0.53
1:E:39:GLU:HG3	1:E:49:VAL:HG12	1.91	0.53
1:C:2:SER:HB3	1:C:5:ASP:HB2	1.91	0.53
1:B:377:LEU:HD11	1:B:383:LEU:HD22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ALA:HB2	1:C:263:LEU:HD11	1.92	0.52
1:B:226:ARG:HH21	1:B:258:GLN:HE21	1.58	0.52
1:B:477:GLU:H	1:B:477:GLU:CD	2.18	0.52
1:D:37:THR:H	2:D:612:GOL:H12	1.74	0.52
1:B:171:LEU:O	1:B:179:HIS:HD2	1.92	0.52
1:C:564:ARG:HB2	2:C:601:GOL:H12	1.92	0.52
1:C:386:MET:HE3	1:C:502:PHE:CE2	2.45	0.52
2:E:605:GOL:H32	2:E:607:GOL:H12	1.92	0.52
1:C:567:ARG:HH11	1:C:567:ARG:HG2	1.74	0.51
1:B:164:GLY:H	2:B:611:GOL:C1	2.23	0.51
1:B:57:THR:OG1	1:B:82:ARG:HD3	2.11	0.51
1:C:253:ALA:O	1:C:257:ARG:HG3	2.10	0.51
1:A:270:TYR:HB3	1:A:279:PHE:HB3	1.91	0.51
1:C:208:ARG:HG2	1:C:213:GLU:HG2	1.93	0.50
1:A:208:ARG:HH12	2:A:605:GOL:H31	1.74	0.50
1:A:434:ASP:OD1	1:A:542:ARG:NH2	2.44	0.50
1:D:286:GLU:O	2:D:609:GOL:O1	2.28	0.50
1:E:24:ARG:HG3	1:E:24:ARG:HH11	1.77	0.50
1:D:254:GLU:OE2	8:D:701:HOH:O	2.19	0.50
1:B:41:ALA:HB2	1:B:47:ARG:HB3	1.93	0.50
1:B:41:ALA:HB2	1:B:47:ARG:O	2.11	0.50
1:B:196:THR:HG21	1:B:311:GLU:O	2.12	0.49
1:C:226:ARG:HH21	1:C:258:GLN:HE21	1.59	0.49
1:C:270:TYR:HB3	1:C:279:PHE:HB3	1.94	0.49
1:B:226:ARG:NH2	8:B:703:HOH:O	2.44	0.49
1:D:60:ARG:NH2	7:D:621:SO4:S	2.85	0.49
1:B:47:ARG:HD2	1:B:62:THR:HG23	1.95	0.49
1:A:416:ARG:HG2	1:A:420:ARG:NE	2.28	0.49
1:C:356:ASP:OD1	1:C:358:TYR:N	2.42	0.49
1:E:491:LEU:HD21	1:E:548:LEU:HD12	1.95	0.49
1:A:72:GLN:HE21	1:A:508:ALA:HB1	1.78	0.49
1:B:204:ALA:O	1:B:208:ARG:HG2	2.12	0.49
1:B:347:ARG:HD2	1:B:352:GLU:OE2	2.13	0.49
1:C:397:ARG:NH1	1:C:402:GLU:OE2	2.45	0.49
1:E:291:LYS:NZ	5:E:611:PO4:O4	2.45	0.49
1:D:476:PRO:HA	1:D:479:ARG:HD2	1.94	0.49
1:A:256:ALA:HB1	1:B:15:TRP:HB2	1.95	0.48
1:A:357:ARG:HD2	1:E:85:ALA:HB2	1.95	0.48
1:E:478:VAL:O	1:E:481:VAL:HG22	2.12	0.48
1:B:489:MET:HE2	1:B:579:LEU:HD12	1.95	0.48
1:B:185:TRP:CZ2	1:B:211:LEU:HD21	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:GLY:H	2:B:603:GOL:C3	2.26	0.48
1:C:468:MET:O	1:C:490:LYS:NZ	2.33	0.48
1:D:153:HIS:CD2	1:D:299:MET:HE1	2.49	0.48
1:E:434:ASP:OD2	1:E:542:ARG:NH2	2.48	0.47
1:C:489:MET:HE1	1:C:576:SER:HB3	1.97	0.47
1:E:540:ASP:HB3	1:E:544:ARG:NH2	2.30	0.47
1:D:300:GLY:HA3	1:D:569:MET:HG3	1.96	0.47
1:B:491:LEU:HD22	1:B:546:TYR:HB3	1.96	0.47
1:D:24:ARG:HG3	1:D:25:LYS:N	2.29	0.47
1:E:431:TYR:OH	1:E:548:LEU:HD13	2.15	0.47
1:A:416:ARG:NH1	1:A:531:GLU:OE2	2.48	0.46
1:E:270:TYR:HB3	1:E:279:PHE:HB3	1.97	0.46
1:B:451:GLY:H	2:B:603:GOL:H31	1.80	0.46
1:C:488:ASP:OD2	1:C:488:ASP:N	2.35	0.46
1:B:47:ARG:HD2	1:B:62:THR:CG2	2.46	0.46
1:B:270:TYR:HB3	1:B:279:PHE:HB3	1.97	0.46
1:A:277:ARG:NH1	1:A:304:GLY:O	2.48	0.46
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.75	0.45
1:B:208:ARG:HG2	1:B:208:ARG:HH11	1.80	0.45
1:A:168:ASP:OD2	2:A:613:GOL:H11	2.15	0.45
1:E:357:ARG:HA	1:E:362:ARG:NH1	2.32	0.45
1:D:47:ARG:HH11	1:D:62:THR:HG23	1.81	0.45
2:C:602:GOL:H12	1:D:246:LYS:HZ2	1.81	0.45
1:A:300:GLY:CA	1:A:569:MET:HG3	2.46	0.45
1:C:301:PHE:CE2	1:C:569:MET:HE3	2.52	0.45
1:E:66:ARG:HG2	1:E:518:GLU:OE2	2.16	0.45
1:A:400:ALA:O	1:A:404:ILE:HG13	2.16	0.45
1:D:335:LEU:HD22	1:D:425:PRO:HB3	1.98	0.45
1:D:479:ARG:HB3	1:D:482:ARG:NH2	2.31	0.45
1:E:56:LEU:HD23	1:E:56:LEU:HA	1.77	0.44
1:A:489:MET:HE1	1:A:576:SER:CB	2.48	0.44
1:B:530:ARG:HH12	1:B:592:LEU:C	2.25	0.44
1:C:299:MET:O	1:C:569:MET:HE2	2.18	0.44
1:B:362:ARG:HH12	2:B:614:GOL:H2	1.82	0.44
1:D:476:PRO:HA	1:D:479:ARG:HG3	1.99	0.44
1:B:2:SER:HB3	1:B:5:ASP:HB2	1.99	0.44
1:E:171:LEU:HA	1:E:177:THR:HG21	1.99	0.44
1:B:185:TRP:HE1	1:B:266:SER:HB3	1.81	0.44
1:E:24:ARG:HG3	1:E:24:ARG:NH1	2.33	0.44
1:A:489:MET:HE1	1:A:576:SER:HB2	2.00	0.44
1:A:301:PHE:HZ	1:A:570:VAL:HG22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:GLU:H	1:B:286:GLU:CD	2.24	0.43
1:D:489:MET:CE	1:D:579:LEU:HD12	2.48	0.43
1:B:164:GLY:H	2:B:611:GOL:H11	1.83	0.43
1:B:301:PHE:CE2	1:B:569:MET:HE2	2.52	0.43
1:C:327:ASP:OD2	1:C:433:TYR:OH	2.33	0.43
1:D:488:ASP:OD2	1:D:488:ASP:N	2.47	0.43
1:C:289:TYR:HB2	1:C:370:ARG:HB3	1.99	0.43
1:A:2:SER:HB3	1:A:5:ASP:HB2	2.00	0.43
1:A:15:TRP:HB2	1:B:256:ALA:HB1	2.00	0.43
1:C:128:THR:OG1	2:C:607:GOL:H32	2.19	0.43
1:D:327:ASP:OD2	1:D:433:TYR:OH	2.27	0.43
1:B:197:ALA:HB1	1:B:201:ILE:HB	2.00	0.43
1:E:520:ASP:HA	1:E:523:ARG:NH1	2.34	0.43
1:E:486:PRO:HG2	1:E:489:MET:CE	2.48	0.43
1:D:220:ASP:OD2	2:D:608:GOL:H11	2.19	0.43
1:D:411:PRO:HB2	1:D:516:LEU:HD13	2.01	0.43
1:D:277:ARG:NH1	1:D:304:GLY:O	2.52	0.42
1:B:277:ARG:NH1	1:B:304:GLY:O	2.52	0.42
1:C:301:PHE:HZ	1:C:570:VAL:HG22	1.84	0.42
1:E:357:ARG:HA	1:E:362:ARG:HH11	1.84	0.42
1:A:226:ARG:NH2	1:A:258:GLN:HE21	2.14	0.42
1:E:386:MET:HE1	1:E:422:TYR:CZ	2.55	0.42
1:E:330:LEU:O	1:E:333:THR:OG1	2.33	0.42
1:A:491:LEU:HD23	1:A:495:PHE:CE2	2.55	0.42
1:E:339:ARG:NH2	1:E:371:GLU:OE2	2.39	0.42
1:D:257:ARG:O	1:D:258:GLN:HB2	2.19	0.42
1:C:487:GLU:OE1	1:C:545:GLN:NE2	2.52	0.42
1:E:249:VAL:HG11	2:E:602:GOL:H31	2.00	0.42
1:E:310:MET:HE3	1:E:367:ALA:O	2.20	0.42
1:B:560:ARG:HB3	2:B:602:GOL:H11	2.02	0.42
1:C:25:LYS:NZ	1:C:151:GLU:OE2	2.42	0.41
1:C:386:MET:HG3	1:C:446:LEU:HD11	2.02	0.41
1:E:70:HIS:HB2	1:E:504:ARG:HD2	2.02	0.41
1:E:72:GLN:OE1	1:E:512:THR:OG1	2.38	0.41
1:E:204:ALA:O	1:E:208:ARG:HD3	2.19	0.41
1:B:411:PRO:HB2	1:B:516:LEU:HD13	2.01	0.41
1:C:357:ARG:NH1	2:C:608:GOL:O2	2.54	0.41
1:C:523:ARG:HD2	1:C:527:GLU:OE2	2.19	0.41
1:A:33:GLU:OE1	1:A:557:CYS:HB3	2.19	0.41
1:E:204:ALA:O	1:E:208:ARG:CD	2.68	0.41
1:C:197:ALA:HB1	1:C:201:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:ARG:NH2	1:E:106:ASP:OD1	2.54	0.41
1:A:412:THR:HG23	8:A:780:HOH:O	2.21	0.41
1:C:440:HIS:HB2	8:C:729:HOH:O	2.21	0.41
1:B:286:GLU:O	2:B:612:GOL:O3	2.32	0.41
1:C:174:ALA:HB3	1:C:177:THR:HG23	2.03	0.41
1:A:428:HIS:HA	1:A:532:TYR:OH	2.21	0.41
1:A:482:ARG:HE	1:A:482:ARG:HB2	1.59	0.41
1:C:256:ALA:HB1	1:D:15:TRP:HB2	2.03	0.41
1:E:491:LEU:HD11	1:E:548:LEU:HD11	2.03	0.41
1:D:197:ALA:HB1	1:D:201:ILE:HB	2.02	0.41
1:A:30:PHE:HB2	1:A:36:PHE:CZ	2.56	0.40
1:A:246:LYS:NZ	2:B:611:GOL:O3	2.45	0.40
1:A:474:LEU:HD12	1:A:482:ARG:HD3	2.03	0.40
1:B:478:VAL:O	1:B:481:VAL:HG22	2.21	0.40
1:E:24:ARG:HG3	1:E:25:LYS:N	2.35	0.40
1:D:33:GLU:OE1	1:D:557:CYS:HB3	2.20	0.40
1:D:270:TYR:HB3	1:D:279:PHE:HB3	2.03	0.40
1:D:572:LEU:HD21	2:D:615:GOL:H31	2.03	0.40
1:A:42:ASP:HB3	1:A:44:GLN:OE1	2.21	0.40
1:A:89:LEU:HD23	1:A:89:LEU:HA	1.88	0.40
1:C:555:LEU:HD13	1:C:585:LEU:HD21	2.03	0.40
1:E:489:MET:HA	1:E:492:LEU:HG	2.02	0.40
1:A:57:THR:OG1	1:A:82:ARG:HD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	591/612 (97%)	575 (97%)	16 (3%)	0	100	100
1	B	590/612 (96%)	573 (97%)	17 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	590/612 (96%)	578 (98%)	12 (2%)	0	100	100
1	D	590/612 (96%)	575 (98%)	15 (2%)	0	100	100
1	E	589/612 (96%)	572 (97%)	17 (3%)	0	100	100
All	All	2950/3060 (96%)	2873 (97%)	77 (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	485/504 (96%)	484 (100%)	1 (0%)	87	95
1	B	481/504 (95%)	479 (100%)	2 (0%)	84	93
1	C	479/504 (95%)	479 (100%)	0	100	100
1	D	481/504 (95%)	480 (100%)	1 (0%)	87	95
1	E	479/504 (95%)	479 (100%)	0	100	100
All	All	2405/2520 (95%)	2401 (100%)	4 (0%)	87	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	576	SER
1	B	325	ASP
1	B	576	SER
1	D	576	SER

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	72	GLN
1	A	209	GLN
1	A	258	GLN

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Mol	Chain	Res	Type
1	B	160	ASN
1	B	179	HIS
1	B	258	GLN
1	B	274	GLN
1	B	391	HIS
1	B	536	HIS
1	C	143	GLN
1	C	209	GLN
1	C	258	GLN
1	C	273	GLN
1	C	454	GLN
1	C	536	HIS
1	C	568	GLN
1	E	391	HIS
1	E	454	GLN
1	D	143	GLN
1	D	273	GLN
1	D	454	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](#)

Of 126 ligands modelled in this entry, 5 are monoatomic - leaving 121 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	GOL	B	605	-	5,5,5	0.93	0	5,5,5	1.10	0
2	GOL	E	607	-	5,5,5	1.01	0	5,5,5	0.95	0
7	SO4	C	623	-	4,4,4	0.24	0	6,6,6	0.12	0
7	SO4	D	626	-	4,4,4	0.28	0	6,6,6	0.09	0
2	GOL	D	601	-	5,5,5	1.04	0	5,5,5	1.06	0
2	GOL	B	603	-	5,5,5	1.23	1 (20%)	5,5,5	0.75	0
2	GOL	B	610	-	5,5,5	1.36	1 (20%)	5,5,5	1.17	0
2	GOL	E	603	-	5,5,5	0.99	0	5,5,5	1.01	0
2	GOL	A	608	-	5,5,5	0.97	0	5,5,5	1.10	1 (20%)
7	SO4	E	616	-	4,4,4	0.24	0	6,6,6	0.19	0
5	PO4	D	618	6	4,4,4	0.97	0	6,6,6	0.66	0
2	GOL	B	613	-	5,5,5	1.14	0	5,5,5	0.79	0
2	GOL	D	610	-	5,5,5	1.18	1 (20%)	5,5,5	0.91	0
2	GOL	B	611	-	5,5,5	0.89	0	5,5,5	1.19	1 (20%)
4	LMS	C	611	6,3	25,25,25	3.66	12 (48%)	38,38,38	3.96	10 (26%)
7	SO4	B	619	-	4,4,4	0.26	0	6,6,6	0.09	0
3	I3U	D	616	4	12,13,14	2.89	2 (16%)	10,14,16	1.48	2 (20%)
5	PO4	C	612	6	4,4,4	0.70	0	6,6,6	0.80	0
2	GOL	C	601	-	5,5,5	1.10	0	5,5,5	1.04	0
7	SO4	E	619	-	4,4,4	0.29	0	6,6,6	0.14	0
7	SO4	D	624	-	4,4,4	0.26	0	6,6,6	0.10	0
2	GOL	E	606	-	5,5,5	0.96	0	5,5,5	0.99	0
7	SO4	C	614	-	4,4,4	0.27	0	6,6,6	0.17	0
7	SO4	A	618	-	4,4,4	0.29	0	6,6,6	0.17	0
2	GOL	C	604	-	5,5,5	0.83	0	5,5,5	1.07	0
2	GOL	D	607	-	5,5,5	0.89	0	5,5,5	1.22	0
7	SO4	D	629	-	4,4,4	0.26	0	6,6,6	0.07	0
7	SO4	B	627	-	4,4,4	0.25	0	6,6,6	0.14	0
7	SO4	D	622	-	4,4,4	0.27	0	6,6,6	0.31	0
2	GOL	C	605	-	5,5,5	0.89	0	5,5,5	1.12	0
2	GOL	D	611	-	5,5,5	1.41	1 (20%)	5,5,5	0.63	0
7	SO4	B	624	-	4,4,4	0.28	0	6,6,6	0.07	0
7	SO4	A	623	-	4,4,4	0.25	0	6,6,6	0.10	0
3	I3U	A	614	4	12,13,14	3.13	1 (8%)	10,14,16	1.56	2 (20%)
2	GOL	D	608	-	5,5,5	1.18	0	5,5,5	0.77	0
5	PO4	A	616	6	4,4,4	0.76	0	6,6,6	0.90	0
7	SO4	A	622	-	4,4,4	0.33	0	6,6,6	0.14	0
7	SO4	A	619	-	4,4,4	0.30	0	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	D	621	-	4,4,4	0.25	0	6,6,6	0.12	0
3	I3U	C	610	4	12,13,14	2.83	2 (16%)	10,14,16	1.75	2 (20%)
2	GOL	D	615	-	5,5,5	1.15	0	5,5,5	0.80	0
2	GOL	D	613	-	5,5,5	0.95	0	5,5,5	1.11	0
7	SO4	C	617	-	4,4,4	0.31	0	6,6,6	0.11	0
7	SO4	C	622	-	4,4,4	0.23	0	6,6,6	0.17	0
7	SO4	C	621	-	4,4,4	0.25	0	6,6,6	0.15	0
7	SO4	B	625	-	4,4,4	0.24	0	6,6,6	0.28	0
2	GOL	E	601	-	5,5,5	1.13	1 (20%)	5,5,5	1.03	0
5	PO4	E	611	6	4,4,4	0.95	0	6,6,6	0.89	0
2	GOL	B	614	-	5,5,5	1.22	0	5,5,5	0.79	0
2	GOL	B	606	-	5,5,5	1.19	0	5,5,5	0.60	0
7	SO4	E	614	-	4,4,4	0.23	0	6,6,6	0.10	0
7	SO4	B	622	-	4,4,4	0.25	0	6,6,6	0.17	0
7	SO4	B	621	-	4,4,4	0.29	0	6,6,6	0.18	0
7	SO4	C	618	-	4,4,4	0.27	0	6,6,6	0.13	0
2	GOL	A	605	-	5,5,5	0.95	0	5,5,5	0.98	0
2	GOL	E	602	-	5,5,5	1.01	0	5,5,5	1.14	0
7	SO4	D	627	-	4,4,4	0.28	0	6,6,6	0.15	0
2	GOL	D	612	-	5,5,5	0.85	0	5,5,5	1.05	0
2	GOL	C	603	-	5,5,5	0.67	0	5,5,5	1.22	1 (20%)
2	GOL	D	614	-	5,5,5	1.04	0	5,5,5	0.96	0
7	SO4	C	615	-	4,4,4	0.27	0	6,6,6	0.14	0
5	PO4	B	617	6	4,4,4	1.02	0	6,6,6	1.14	1 (16%)
7	SO4	D	625	-	4,4,4	0.24	0	6,6,6	0.12	0
2	GOL	A	607	-	5,5,5	1.28	1 (20%)	5,5,5	1.03	0
7	SO4	B	630	-	4,4,4	0.25	0	6,6,6	0.15	0
2	GOL	A	612	-	5,5,5	1.05	0	5,5,5	1.00	0
2	GOL	E	604	-	5,5,5	1.23	1 (20%)	5,5,5	1.22	0
7	SO4	C	619	-	4,4,4	0.28	0	6,6,6	0.16	0
7	SO4	A	625	-	4,4,4	0.26	0	6,6,6	0.20	0
2	GOL	E	605	-	5,5,5	0.94	0	5,5,5	0.87	0
2	GOL	A	613	-	5,5,5	1.35	0	5,5,5	0.81	0
2	GOL	D	609	-	5,5,5	1.07	0	5,5,5	1.15	0
7	SO4	E	613	-	4,4,4	0.25	0	6,6,6	0.16	0
2	GOL	A	611	-	5,5,5	0.94	0	5,5,5	1.20	1 (20%)
2	GOL	A	601	-	5,5,5	1.60	2 (40%)	5,5,5	0.79	0
4	LMS	B	616	6,3	25,25,25	3.81	11 (44%)	38,38,38	3.59	10 (26%)
2	GOL	A	602	-	5,5,5	1.18	1 (20%)	5,5,5	1.04	1 (20%)
2	GOL	A	604	-	5,5,5	1.20	1 (20%)	5,5,5	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	609	-	5,5,5	0.83	0	5,5,5	1.11	0
2	GOL	B	604	-	5,5,5	1.17	0	5,5,5	0.75	0
2	GOL	B	607	-	5,5,5	0.89	0	5,5,5	1.19	0
2	GOL	C	609	-	5,5,5	1.02	0	5,5,5	1.02	0
2	GOL	C	602	-	5,5,5	0.90	0	5,5,5	0.95	0
2	GOL	A	610	-	5,5,5	0.99	0	5,5,5	0.92	0
2	GOL	D	606	-	5,5,5	1.16	1 (20%)	5,5,5	1.05	0
3	I3U	B	615	4	12,13,14	3.03	2 (16%)	10,14,16	1.79	2 (20%)
7	SO4	E	618	-	4,4,4	0.21	0	6,6,6	0.35	0
7	SO4	B	623	-	4,4,4	0.27	0	6,6,6	0.05	0
2	GOL	B	601	-	5,5,5	1.06	0	5,5,5	1.38	0
7	SO4	B	628	-	4,4,4	0.24	0	6,6,6	0.20	0
2	GOL	B	608	-	5,5,5	1.06	0	5,5,5	0.84	0
2	GOL	B	609	-	5,5,5	0.88	0	5,5,5	1.04	0
2	GOL	B	612	-	5,5,5	1.01	0	5,5,5	0.92	0
7	SO4	A	621	-	4,4,4	0.28	0	6,6,6	0.24	0
2	GOL	B	602	-	5,5,5	0.77	0	5,5,5	1.14	0
2	GOL	E	608	-	5,5,5	0.93	0	5,5,5	1.02	0
7	SO4	E	615	-	4,4,4	0.28	0	6,6,6	0.10	0
7	SO4	D	620	-	4,4,4	0.29	0	6,6,6	0.11	0
7	SO4	B	629	-	4,4,4	0.28	0	6,6,6	0.12	0
2	GOL	A	606	-	5,5,5	0.76	0	5,5,5	1.36	1 (20%)
2	GOL	D	602	-	5,5,5	1.06	0	5,5,5	0.99	0
2	GOL	D	605	-	5,5,5	1.25	1 (20%)	5,5,5	1.12	0
7	SO4	A	620	-	4,4,4	0.27	0	6,6,6	0.14	0
7	SO4	C	616	-	4,4,4	0.25	0	6,6,6	0.12	0
7	SO4	A	624	-	4,4,4	0.25	0	6,6,6	0.21	0
7	SO4	B	626	-	4,4,4	0.28	0	6,6,6	0.14	0
3	I3U	E	609	4	12,13,14	3.07	2 (16%)	10,14,16	1.56	2 (20%)
7	SO4	C	620	-	4,4,4	0.25	0	6,6,6	0.10	0
7	SO4	D	623	-	4,4,4	0.26	0	6,6,6	0.07	0
7	SO4	D	628	-	4,4,4	0.25	0	6,6,6	0.10	0
2	GOL	D	603	-	5,5,5	1.28	1 (20%)	5,5,5	1.00	0
4	LMS	A	615	6,3	25,25,25	3.93	11 (44%)	38,38,38	3.33	12 (31%)
2	GOL	A	603	-	5,5,5	0.70	0	5,5,5	1.15	0
7	SO4	B	620	-	4,4,4	0.31	0	6,6,6	0.23	0
2	GOL	C	607	-	5,5,5	1.15	0	5,5,5	1.05	0
2	GOL	D	604	-	5,5,5	1.02	0	5,5,5	1.07	0
4	LMS	D	617	6,3	25,25,25	4.19	10 (40%)	38,38,38	3.18	11 (28%)
7	SO4	E	617	-	4,4,4	0.24	0	6,6,6	0.18	0
2	GOL	C	606	-	5,5,5	1.02	0	5,5,5	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	C	608	-	5,5,5	1.06	0	5,5,5	1.06	0
4	LMS	E	610	6,3	25,25,25	3.86	12 (48%)	38,38,38	3.21	11 (28%)

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	GOL	C	602	-	-	2/4/4/4	-
2	GOL	A	610	-	-	2/4/4/4	-
2	GOL	B	605	-	-	1/4/4/4	-
2	GOL	C	608	-	-	2/4/4/4	-
2	GOL	D	606	-	-	2/4/4/4	-
2	GOL	E	607	-	-	3/4/4/4	-
3	I3U	B	615	4	-	2/14/14/15	-
2	GOL	B	601	-	-	0/4/4/4	-
2	GOL	B	608	-	-	1/4/4/4	-
2	GOL	A	605	-	-	2/4/4/4	-
2	GOL	C	605	-	-	2/4/4/4	-
2	GOL	E	602	-	-	1/4/4/4	-
2	GOL	B	609	-	-	1/4/4/4	-
2	GOL	B	612	-	-	2/4/4/4	-
2	GOL	D	611	-	-	4/4/4/4	-
2	GOL	D	612	-	-	0/4/4/4	-
2	GOL	D	601	-	-	2/4/4/4	-
2	GOL	B	603	-	-	2/4/4/4	-
2	GOL	B	610	-	-	3/4/4/4	-
2	GOL	C	603	-	-	2/4/4/4	-
2	GOL	E	603	-	-	1/4/4/4	-
2	GOL	B	602	-	-	0/4/4/4	-
2	GOL	E	608	-	-	2/4/4/4	-
2	GOL	D	614	-	-	1/4/4/4	-
3	I3U	A	614	4	-	2/14/14/15	-
2	GOL	D	608	-	-	2/4/4/4	-
2	GOL	A	608	-	-	4/4/4/4	-
2	GOL	D	602	-	-	0/4/4/4	-
2	GOL	A	607	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	612	-	-	2/4/4/4	-
2	GOL	E	604	-	-	2/4/4/4	-
2	GOL	D	605	-	-	0/4/4/4	-
2	GOL	B	613	-	-	2/4/4/4	-
2	GOL	D	610	-	-	4/4/4/4	-
2	GOL	E	605	-	-	0/4/4/4	-
2	GOL	B	611	-	-	0/4/4/4	-
2	GOL	A	613	-	-	0/4/4/4	-
2	GOL	D	609	-	-	0/4/4/4	-
3	I3U	C	610	4	-	3/14/14/15	-
2	GOL	D	615	-	-	1/4/4/4	-
2	GOL	D	613	-	-	1/4/4/4	-
3	I3U	E	609	4	-	2/14/14/15	-
4	LMS	C	611	6,3	-	4/10/26/26	0/3/3/3
2	GOL	A	611	-	-	2/4/4/4	-
2	GOL	A	601	-	-	0/4/4/4	-
4	LMS	B	616	6,3	-	3/10/26/26	0/3/3/3
2	GOL	A	602	-	-	2/4/4/4	-
2	GOL	D	603	-	-	2/4/4/4	-
2	GOL	A	604	-	-	2/4/4/4	-
2	GOL	A	609	-	-	0/4/4/4	-
3	I3U	D	616	4	-	2/14/14/15	-
2	GOL	B	604	-	-	2/4/4/4	-
2	GOL	C	604	-	-	0/4/4/4	-
4	LMS	A	615	6,3	-	5/10/26/26	0/3/3/3
2	GOL	B	607	-	-	2/4/4/4	-
2	GOL	E	601	-	-	0/4/4/4	-
2	GOL	A	603	-	-	0/4/4/4	-
2	GOL	B	614	-	-	0/4/4/4	-
2	GOL	C	601	-	-	1/4/4/4	-
2	GOL	C	609	-	-	1/4/4/4	-
2	GOL	B	606	-	-	2/4/4/4	-
2	GOL	C	607	-	-	0/4/4/4	-
2	GOL	D	604	-	-	0/4/4/4	-
4	LMS	D	617	6,3	-	4/10/26/26	0/3/3/3
2	GOL	E	606	-	-	0/4/4/4	-
2	GOL	C	606	-	-	2/4/4/4	-
2	GOL	A	606	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LMS	E	610	6,3	-	2/10/26/26	0/3/3/3
2	GOL	D	607	-	-	0/4/4/4	-

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	617	LMS	O2P-S	10.93	1.54	1.42
3	A	614	I3U	C09-N07	10.44	1.49	1.35
4	D	617	LMS	O1P-S	10.18	1.53	1.42
3	E	609	I3U	C09-N07	10.02	1.48	1.35
3	B	615	I3U	C09-N07	10.01	1.48	1.35
4	E	610	LMS	S-N	9.86	1.70	1.58
4	A	615	LMS	O2P-S	9.72	1.52	1.42
4	B	616	LMS	S-N	9.42	1.69	1.58
4	A	615	LMS	O1P-S	9.37	1.52	1.42
3	D	616	I3U	C09-N07	9.30	1.47	1.35
4	D	617	LMS	S-N	9.23	1.69	1.58
3	C	610	I3U	C09-N07	9.20	1.47	1.35
4	E	610	LMS	O1P-S	9.16	1.52	1.42
4	B	616	LMS	O2P-S	8.75	1.51	1.42
4	B	616	LMS	O1P-S	8.71	1.51	1.42
4	C	611	LMS	S-N	8.64	1.68	1.58
4	C	611	LMS	O2P-S	8.59	1.51	1.42
4	A	615	LMS	S-N	8.44	1.68	1.58
4	E	610	LMS	O2P-S	8.34	1.51	1.42
4	C	611	LMS	O1P-S	8.30	1.51	1.42
4	D	617	LMS	O5'-S	6.08	1.66	1.57
4	A	615	LMS	O5'-S	5.54	1.65	1.57
4	E	610	LMS	C5-N7	4.92	1.48	1.39
4	A	615	LMS	C5-N7	4.82	1.47	1.39
4	D	617	LMS	O4'-C1'	4.69	1.52	1.42
4	B	616	LMS	O5'-S	4.68	1.64	1.57
4	C	611	LMS	O5'-S	4.63	1.64	1.57
4	E	610	LMS	O5'-S	4.60	1.64	1.57
4	D	617	LMS	C5-N7	4.52	1.47	1.39
4	C	611	LMS	C5-N7	4.50	1.47	1.39
4	C	611	LMS	O4'-C1'	4.28	1.51	1.42
4	A	615	LMS	O4'-C1'	4.23	1.51	1.42
4	B	616	LMS	C5-N7	4.22	1.46	1.39
4	E	610	LMS	O4'-C1'	4.08	1.51	1.42
4	B	616	LMS	O4'-C1'	4.07	1.51	1.42
4	B	616	LMS	C6-N6	3.94	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	615	LMS	C6-N6	3.86	1.44	1.34
4	E	610	LMS	C6-N6	3.84	1.44	1.34
4	D	617	LMS	C6-N6	3.55	1.43	1.34
4	C	611	LMS	C6-N6	3.50	1.43	1.34
4	A	615	LMS	C8-N7	3.00	1.37	1.31
4	A	615	LMS	C5-C4	2.98	1.44	1.39
4	B	616	LMS	C8-N7	2.81	1.37	1.31
4	C	611	LMS	C8-N7	2.79	1.37	1.31
4	E	610	LMS	C8-N7	2.71	1.36	1.31
4	E	610	LMS	C5-C4	2.68	1.43	1.39
2	B	610	GOL	C3-C2	2.58	1.61	1.51
4	D	617	LMS	C8-N7	2.54	1.36	1.31
4	B	616	LMS	C8-N9	-2.51	1.33	1.37
4	B	616	LMS	C5-C4	2.49	1.43	1.39
4	C	611	LMS	C5-C4	2.49	1.43	1.39
2	D	611	GOL	C1-C2	2.47	1.61	1.51
2	A	601	GOL	C1-C2	2.43	1.61	1.51
4	D	617	LMS	C5-C4	2.42	1.43	1.39
2	D	605	GOL	C3-C2	2.42	1.61	1.51
2	A	602	GOL	O2-C2	-2.42	1.36	1.43
4	B	616	LMS	C4-N3	-2.40	1.29	1.34
2	D	603	GOL	O2-C2	-2.30	1.36	1.43
4	A	615	LMS	C4-N3	-2.24	1.30	1.34
4	E	610	LMS	C2'-C3'	-2.24	1.47	1.53
3	E	609	I3U	C11-C09	2.23	1.56	1.51
2	E	601	GOL	O2-C2	-2.20	1.37	1.43
3	C	610	I3U	C11-C09	2.19	1.56	1.51
4	C	611	LMS	C2'-C3'	-2.16	1.47	1.53
2	E	604	GOL	C1-C2	2.16	1.60	1.51
4	D	617	LMS	C4-N3	-2.16	1.30	1.34
2	A	601	GOL	C3-C2	2.13	1.59	1.51
2	D	606	GOL	C3-C2	2.12	1.59	1.51
4	C	611	LMS	C4-N3	-2.10	1.30	1.34
2	A	607	GOL	C3-C2	2.09	1.59	1.51
3	B	615	I3U	C11-C09	2.09	1.55	1.51
4	A	615	LMS	C2'-C3'	-2.07	1.47	1.53
2	D	610	GOL	O2-C2	-2.06	1.37	1.43
3	D	616	I3U	C11-C09	2.04	1.55	1.51
4	E	610	LMS	C8-N9	-2.03	1.34	1.37
4	E	610	LMS	C2'-C1'	-2.02	1.47	1.53
2	B	603	GOL	O2-C2	-2.01	1.37	1.43
4	C	611	LMS	C2'-C1'	-2.01	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	604	GOL	O2-C2	-2.00	1.37	1.43

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	611	LMS	O2P-S-O1P	-19.29	100.31	119.94
4	B	616	LMS	O2P-S-O1P	-17.18	102.46	119.94
4	A	615	LMS	O2P-S-O1P	-14.83	104.85	119.94
4	E	610	LMS	O2P-S-O1P	-13.69	106.00	119.94
4	D	617	LMS	O2P-S-O1P	-13.56	106.14	119.94
4	C	611	LMS	C4-N9-C8	6.88	112.96	105.74
4	E	610	LMS	C4-N9-C8	6.88	112.96	105.74
4	D	617	LMS	C4-N9-C8	6.62	112.69	105.74
4	A	615	LMS	C4-N9-C8	6.56	112.63	105.74
4	C	611	LMS	C5-C4-N3	-6.27	118.09	126.72
4	B	616	LMS	C4-N9-C8	6.09	112.14	105.74
4	B	616	LMS	C5-C4-N3	-6.04	118.40	126.72
4	E	610	LMS	C5-C4-N3	-5.98	118.48	126.72
4	D	617	LMS	C5-C4-N3	-5.73	118.83	126.72
4	E	610	LMS	N3-C4-N9	5.64	136.76	127.17
4	A	615	LMS	C5-C4-N3	-5.62	118.98	126.72
4	C	611	LMS	N3-C4-N9	5.46	136.46	127.17
4	D	617	LMS	N3-C4-N9	5.14	135.92	127.17
4	B	616	LMS	N3-C4-N9	4.87	135.45	127.17
4	A	615	LMS	N3-C4-N9	4.85	135.41	127.17
4	C	611	LMS	N3-C2-N1	-4.75	121.39	128.58
4	E	610	LMS	N3-C2-N1	-4.60	121.62	128.58
4	D	617	LMS	N3-C2-N1	-4.55	121.70	128.58
4	B	616	LMS	N3-C2-N1	-4.42	121.89	128.58
3	C	610	I3U	O08-N07-C06	4.39	124.04	113.76
4	A	615	LMS	N3-C2-N1	-4.22	122.19	128.58
3	B	615	I3U	O08-N07-C06	4.10	123.37	113.76
4	B	616	LMS	C4-C5-N7	-4.01	105.99	110.58
3	D	616	I3U	O08-N07-C06	3.91	122.93	113.76
4	C	611	LMS	C2-N3-C4	3.82	121.16	111.83
4	A	615	LMS	C4-C5-N7	-3.77	106.28	110.58
4	C	611	LMS	C4-C5-N7	-3.68	106.38	110.58
3	E	609	I3U	O08-N07-C06	3.59	122.16	113.76
4	B	616	LMS	C2-N3-C4	3.55	120.51	111.83
3	B	615	I3U	C12-C11-C09	-3.54	105.22	111.95
3	A	614	I3U	O08-N07-C06	3.50	121.97	113.76
4	D	617	LMS	C2-N3-C4	3.50	120.38	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	610	LMS	C2-N3-C4	3.46	120.29	111.83
4	D	617	LMS	C4-C5-N7	-3.41	106.68	110.58
4	A	615	LMS	C2-N3-C4	3.38	120.08	111.83
4	C	611	LMS	N9-C8-N7	-3.24	109.33	113.94
4	A	615	LMS	O5'-C5'-C4'	3.18	113.23	107.57
3	E	609	I3U	C12-C11-C09	-3.17	105.92	111.95
3	A	614	I3U	C12-C11-C09	-3.15	105.97	111.95
4	E	610	LMS	C4-C5-N7	-2.97	107.19	110.58
4	C	611	LMS	C1'-N9-C8	-2.94	120.56	127.09
4	D	617	LMS	C1'-N9-C8	-2.93	120.58	127.09
4	D	617	LMS	N9-C8-N7	-2.92	109.80	113.94
3	C	610	I3U	C12-C11-C09	-2.89	106.45	111.95
4	E	610	LMS	C1'-N9-C8	-2.84	120.78	127.09
4	B	616	LMS	C1'-N9-C8	-2.81	120.87	127.09
4	A	615	LMS	N9-C8-N7	-2.71	110.09	113.94
4	A	615	LMS	C1'-N9-C8	-2.57	121.38	127.09
4	B	616	LMS	N9-C8-N7	-2.54	110.33	113.94
4	E	610	LMS	N9-C8-N7	-2.46	110.44	113.94
4	C	611	LMS	O1P-S-N	2.44	112.65	109.13
4	D	617	LMS	O1P-S-N	2.40	112.60	109.13
5	B	617	PO4	O4-P-O1	-2.39	102.50	110.95
2	A	606	GOL	C3-C2-C1	-2.38	103.08	111.80
2	A	611	GOL	C3-C2-C1	-2.37	103.09	111.80
2	C	603	GOL	C3-C2-C1	-2.37	103.12	111.80
4	A	615	LMS	O1P-S-N	2.32	112.48	109.13
2	A	608	GOL	C3-C2-C1	-2.30	103.35	111.80
4	E	610	LMS	O5'-S-N	2.24	112.73	105.54
4	D	617	LMS	C5'-O5'-S	2.17	120.06	117.29
2	B	611	GOL	C3-C2-C1	-2.16	103.87	111.80
4	B	616	LMS	C2'-C1'-N9	2.06	118.43	113.30
2	A	602	GOL	C3-C2-C1	-2.05	104.28	111.80
4	E	610	LMS	C5-C6-N6	-2.05	118.22	123.29
4	A	615	LMS	O5'-S-O1P	2.01	112.23	106.28
3	D	616	I3U	C12-C11-C09	-2.00	108.14	111.95

There are no chirality outliers.

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	GOL	O1-C1-C2-C3
2	A	604	GOL	C1-C2-C3-O3
2	A	608	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	610	GOL	C1-C2-C3-O3
2	A	612	GOL	O1-C1-C2-O2
2	A	612	GOL	O1-C1-C2-C3
2	B	604	GOL	O1-C1-C2-C3
2	B	607	GOL	O1-C1-C2-O2
2	B	612	GOL	C1-C2-C3-O3
2	C	603	GOL	C1-C2-C3-O3
2	C	603	GOL	O2-C2-C3-O3
2	C	606	GOL	O1-C1-C2-C3
2	E	604	GOL	O1-C1-C2-C3
2	D	603	GOL	O1-C1-C2-C3
2	D	608	GOL	C1-C2-C3-O3
3	A	614	I3U	C04-C05-C06-N07
3	A	614	I3U	C11-C12-C13-O14
3	B	615	I3U	C04-C05-C06-N07
3	C	610	I3U	C04-C05-C06-N07
3	C	610	I3U	C11-C12-C13-O14
3	E	609	I3U	C04-C05-C06-N07
3	E	609	I3U	C11-C12-C13-O14
3	D	616	I3U	C11-C12-C13-O14
4	A	615	LMS	C5'-O5'-S-N
4	A	615	LMS	C5'-O5'-S-O1P
4	A	615	LMS	C5'-O5'-S-O2P
4	C	611	LMS	C5'-O5'-S-N
4	C	611	LMS	C5'-O5'-S-O1P
4	E	610	LMS	C3'-C4'-C5'-O5'
4	D	617	LMS	C5'-O5'-S-O1P
2	A	605	GOL	O2-C2-C3-O3
2	B	612	GOL	O2-C2-C3-O3
2	A	605	GOL	C1-C2-C3-O3
2	A	607	GOL	O1-C1-C2-C3
2	A	608	GOL	O1-C1-C2-C3
2	A	611	GOL	O1-C1-C2-C3
2	B	603	GOL	O1-C1-C2-C3
2	B	606	GOL	O1-C1-C2-C3
2	B	607	GOL	O1-C1-C2-C3
2	C	605	GOL	O1-C1-C2-C3
2	E	607	GOL	O1-C1-C2-C3
2	D	601	GOL	O1-C1-C2-C3
2	D	606	GOL	O1-C1-C2-C3
2	D	611	GOL	O1-C1-C2-C3
2	A	602	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	604	GOL	O2-C2-C3-O3
2	A	608	GOL	O2-C2-C3-O3
2	E	604	GOL	O1-C1-C2-O2
2	D	601	GOL	O1-C1-C2-O2
2	D	603	GOL	O1-C1-C2-O2
2	D	606	GOL	O1-C1-C2-O2
3	D	616	I3U	C02-C03-C04-C05
2	A	610	GOL	O2-C2-C3-O3
2	A	611	GOL	O1-C1-C2-O2
2	D	608	GOL	O2-C2-C3-O3
2	C	602	GOL	C1-C2-C3-O3
2	A	607	GOL	O1-C1-C2-O2
2	A	607	GOL	O2-C2-C3-O3
2	B	604	GOL	O1-C1-C2-O2
2	B	610	GOL	O2-C2-C3-O3
2	C	606	GOL	O1-C1-C2-O2
2	C	608	GOL	O2-C2-C3-O3
2	D	611	GOL	O1-C1-C2-O2
2	D	615	GOL	O2-C2-C3-O3
2	B	613	GOL	O2-C2-C3-O3
2	C	601	GOL	O2-C2-C3-O3
2	C	602	GOL	O2-C2-C3-O3
2	E	602	GOL	O1-C1-C2-O2
2	E	607	GOL	O2-C2-C3-O3
2	D	610	GOL	O2-C2-C3-O3
2	D	613	GOL	O2-C2-C3-O3
2	A	608	GOL	O1-C1-C2-O2
2	D	614	GOL	O2-C2-C3-O3
2	B	610	GOL	O1-C1-C2-C3
2	B	608	GOL	O2-C2-C3-O3
2	B	610	GOL	O1-C1-C2-O2
2	E	603	GOL	O1-C1-C2-O2
3	C	610	I3U	C02-C03-C04-C05
2	E	608	GOL	O1-C1-C2-C3
2	D	610	GOL	O1-C1-C2-C3
2	D	610	GOL	C1-C2-C3-O3
2	D	611	GOL	C1-C2-C3-O3
2	B	603	GOL	O1-C1-C2-O2
2	B	606	GOL	O1-C1-C2-O2
2	C	605	GOL	O1-C1-C2-O2
2	E	607	GOL	O1-C1-C2-O2
2	D	610	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	D	611	GOL	O2-C2-C3-O3
2	C	609	GOL	O2-C2-C3-O3
4	D	617	LMS	O4'-C1'-N9-C8
2	A	607	GOL	C1-C2-C3-O3
2	C	608	GOL	O1-C1-C2-C3
2	E	608	GOL	O2-C2-C3-O3
4	B	616	LMS	O4'-C1'-N9-C8
4	A	615	LMS	O4'-C1'-N9-C8
4	C	611	LMS	O4'-C1'-N9-C8
2	B	609	GOL	O2-C2-C3-O3
4	B	616	LMS	C2'-C1'-N9-C8
4	D	617	LMS	C2'-C1'-N9-C8
2	B	613	GOL	C1-C2-C3-O3
3	B	615	I3U	C02-C03-C04-C05
4	A	615	LMS	O4'-C4'-C5'-O5'
4	B	616	LMS	O4'-C4'-C5'-O5'
4	C	611	LMS	O4'-C4'-C5'-O5'
4	E	610	LMS	O4'-C4'-C5'-O5'
4	D	617	LMS	O4'-C4'-C5'-O5'
2	B	605	GOL	O2-C2-C3-O3

There are no ring outliers.

22 monomers are involved in 27 short contacts:

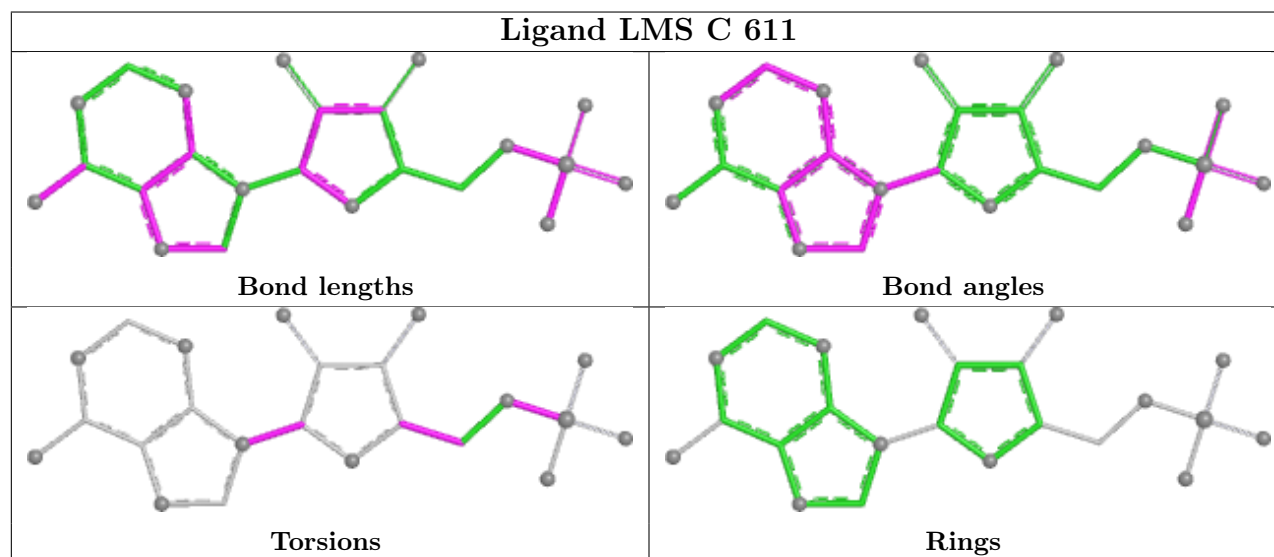
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	607	GOL	1	0
2	B	603	GOL	3	0
2	D	610	GOL	1	0
2	B	611	GOL	3	0
2	C	601	GOL	1	0
2	D	608	GOL	1	0
7	D	621	SO4	1	0
2	D	615	GOL	1	0
5	E	611	PO4	1	0
2	B	614	GOL	1	0
2	A	605	GOL	1	0
2	E	602	GOL	1	0
2	D	612	GOL	1	0
2	E	605	GOL	1	0
2	A	613	GOL	1	0
2	D	609	GOL	1	0
2	A	604	GOL	1	0

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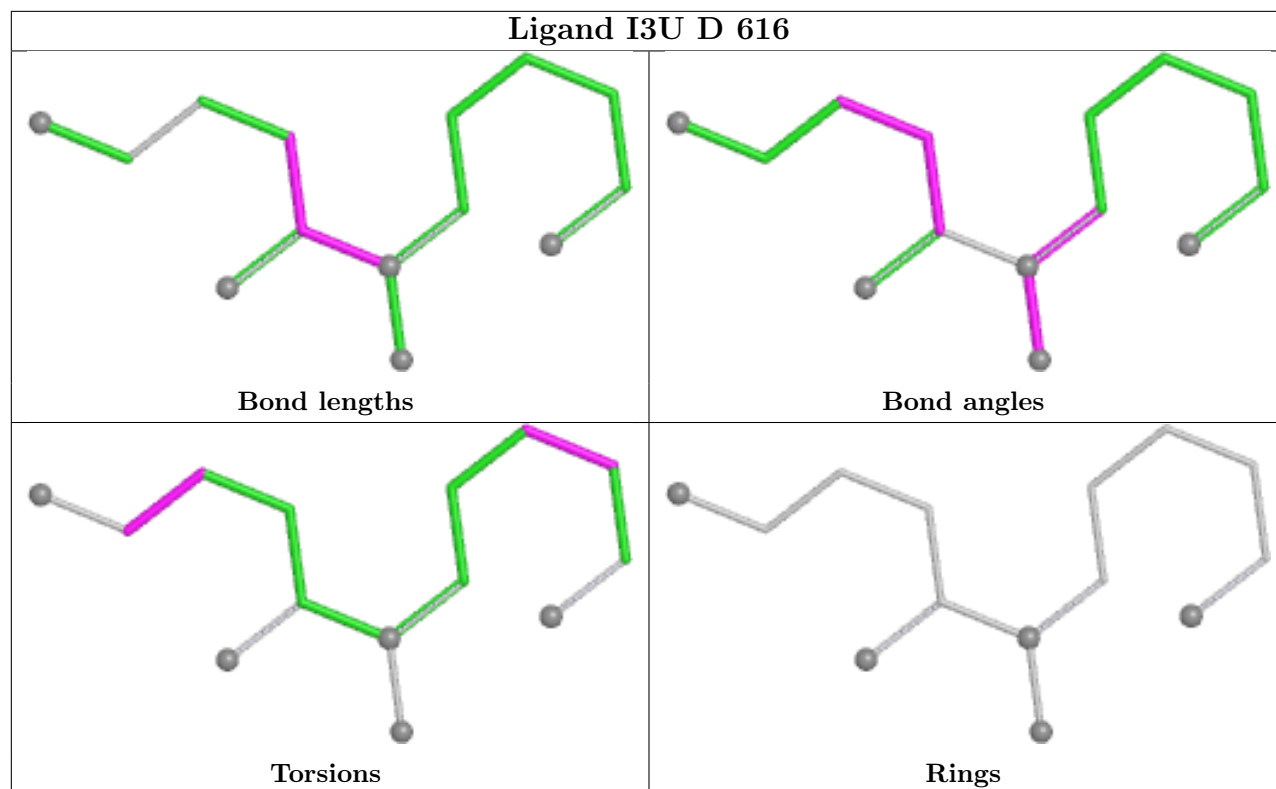
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	602	GOL	3	0
2	B	612	GOL	1	0
2	B	602	GOL	1	0
2	C	607	GOL	1	0
2	C	608	GOL	1	0

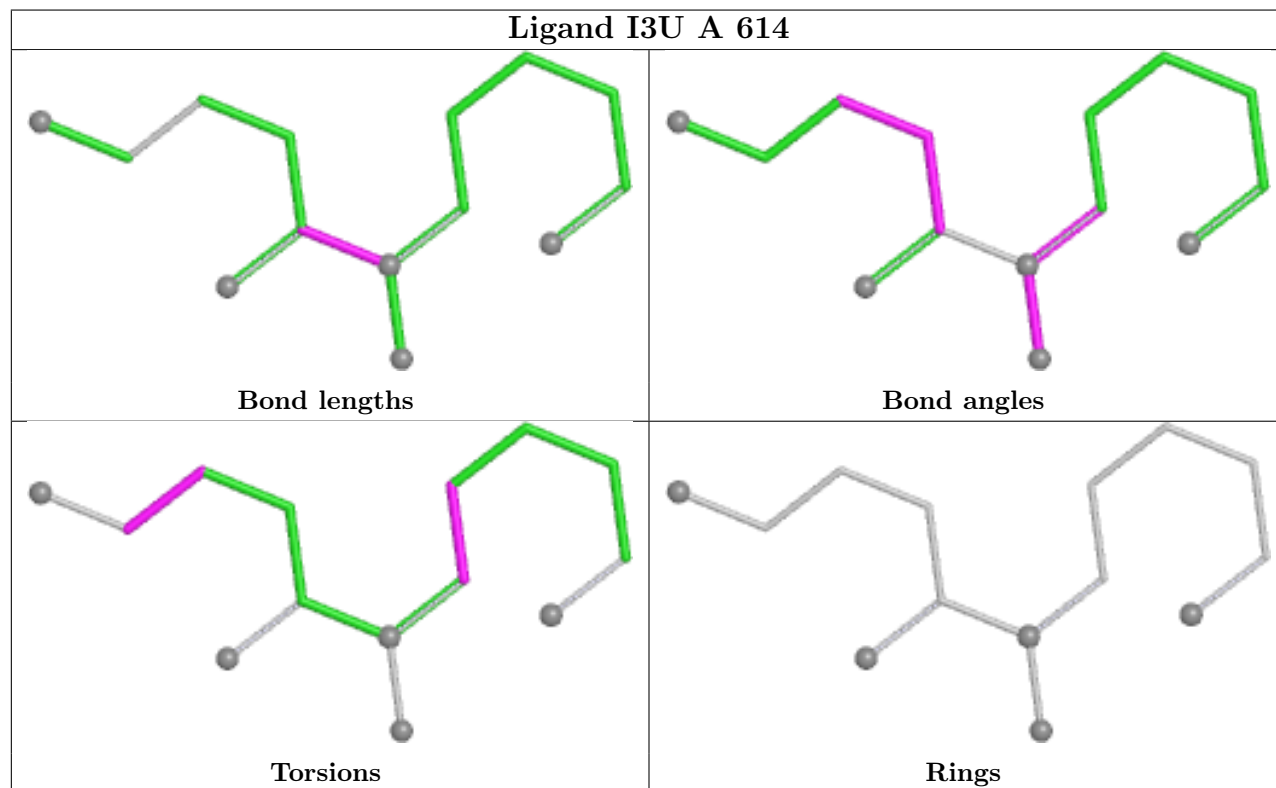
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

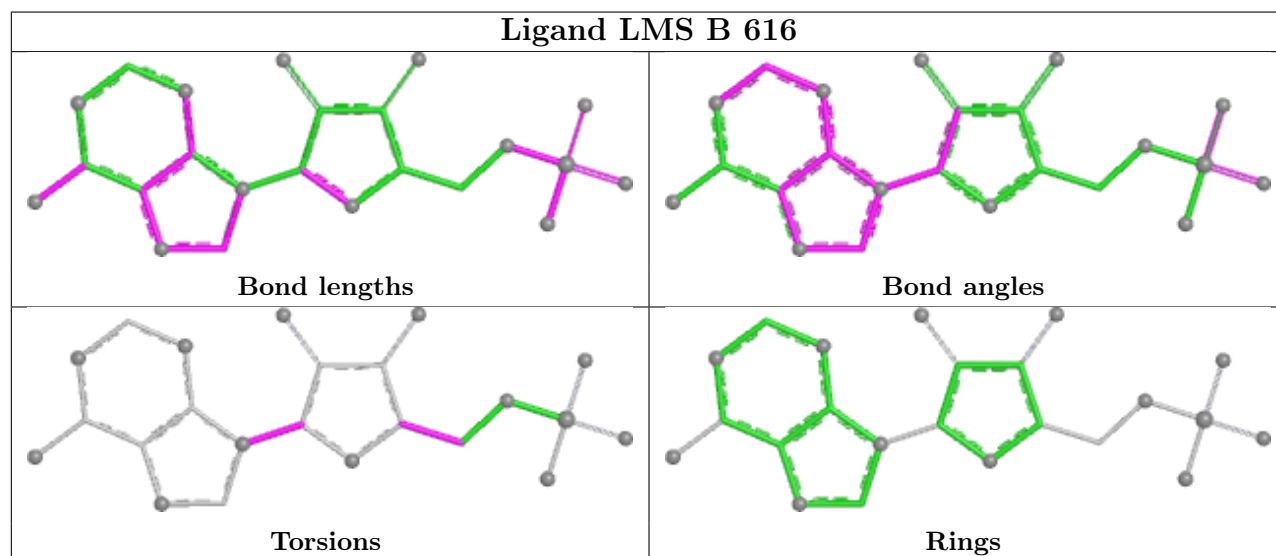
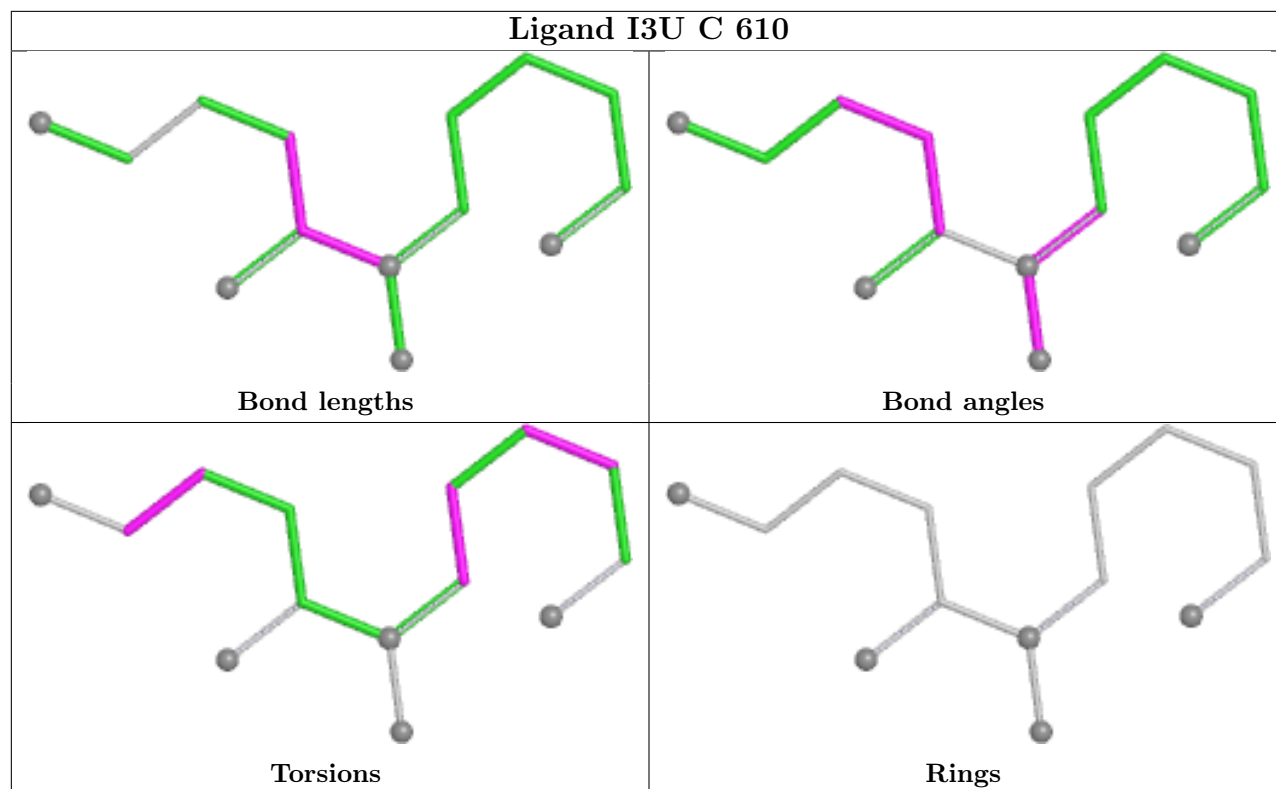


Ligand I3U D 616

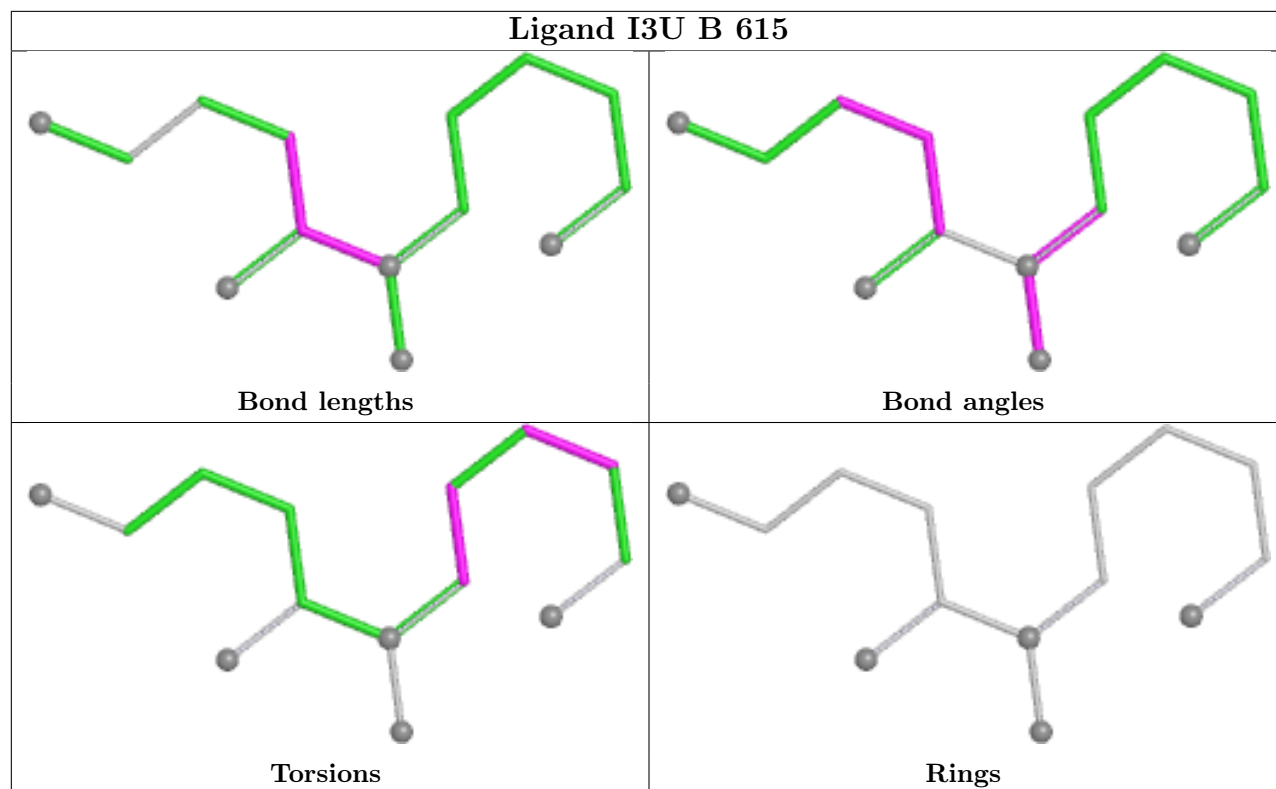


Ligand I3U A 614

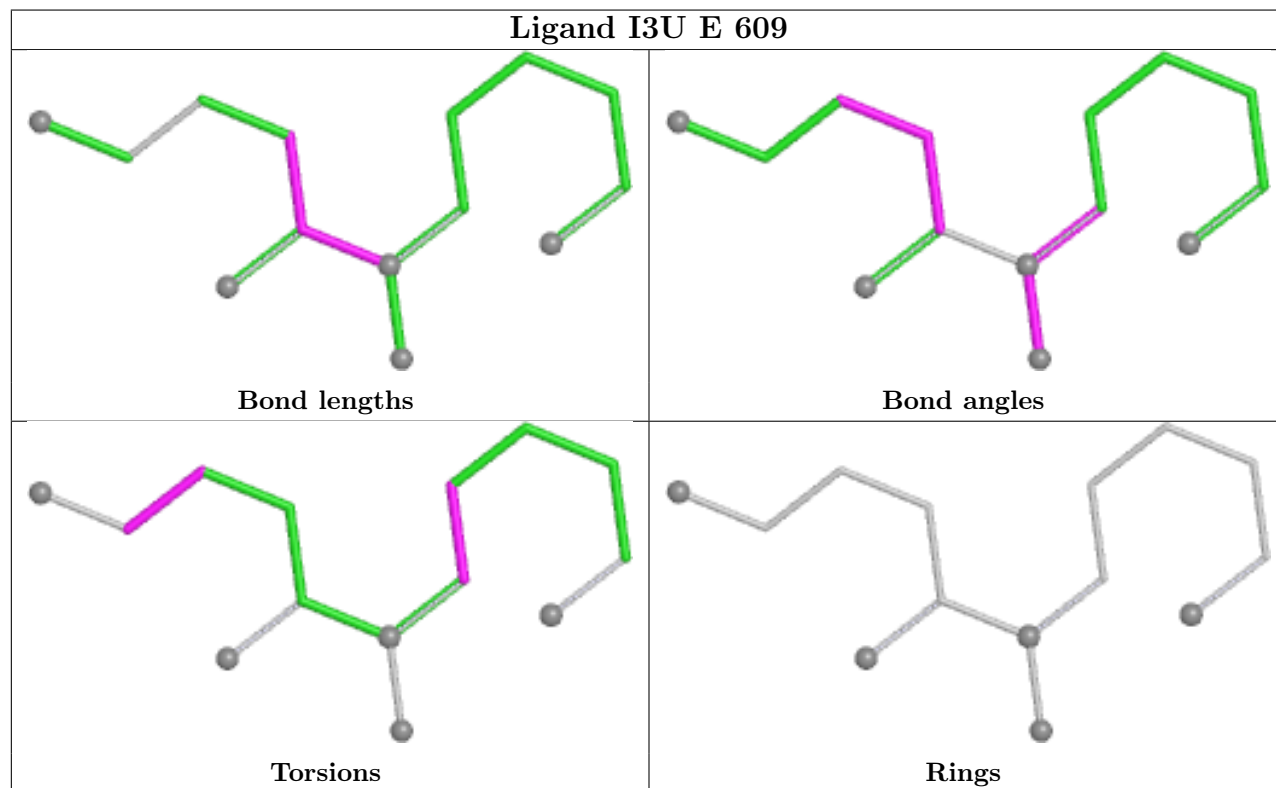




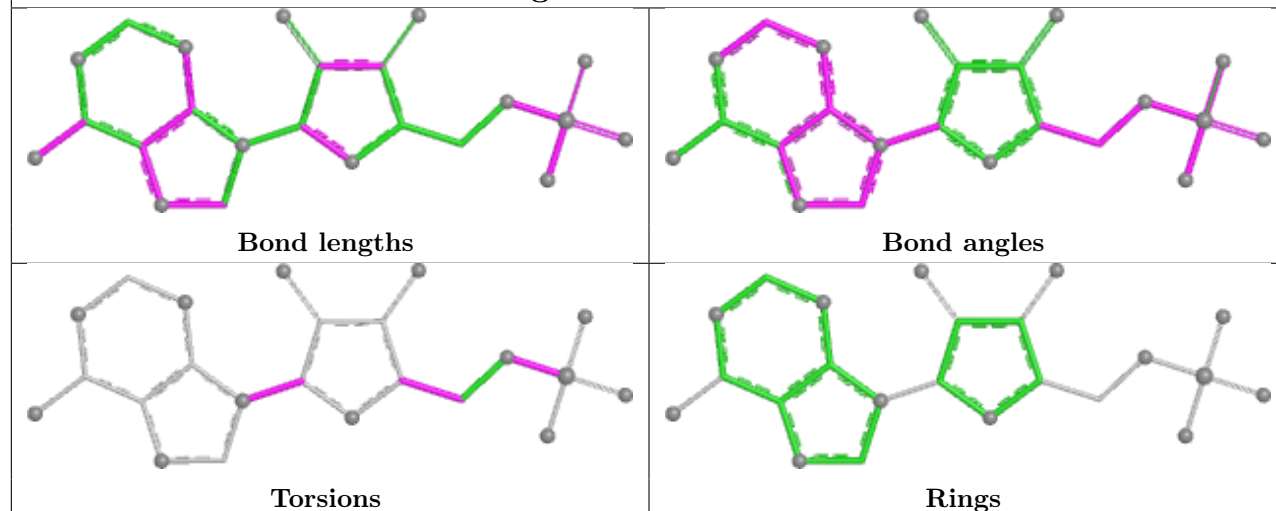
Ligand I3U B 615



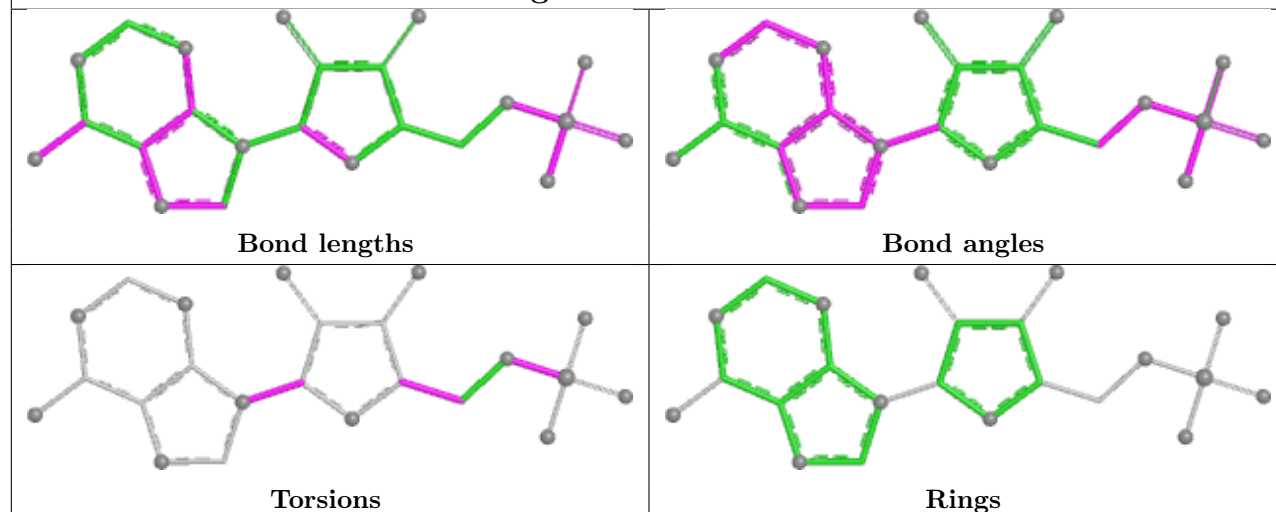
Ligand I3U E 609



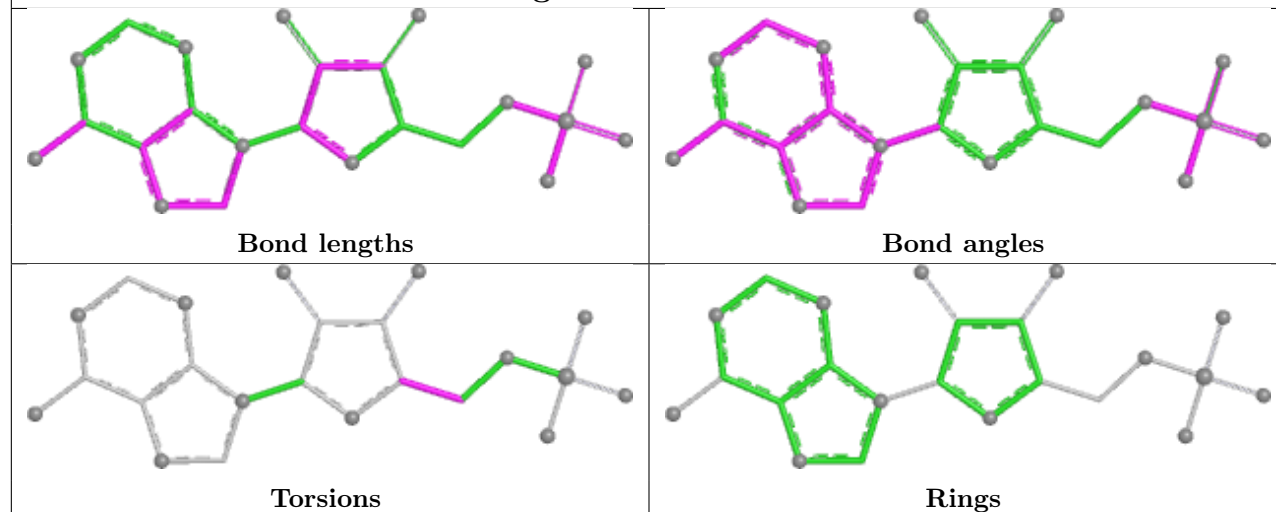
Ligand LMS A 615



Ligand LMS D 617



Ligand LMS E 610



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	593/612 (96%)	-0.12	14 (2%) 59 55	39, 56, 88, 157	0
1	B	592/612 (96%)	-0.17	14 (2%) 59 55	39, 54, 78, 145	0
1	C	592/612 (96%)	0.15	15 (2%) 58 54	47, 67, 96, 148	0
1	D	592/612 (96%)	-0.14	12 (2%) 65 61	46, 56, 79, 130	0
1	E	591/612 (96%)	0.20	15 (2%) 58 54	47, 67, 96, 157	0
All	All	2960/3060 (96%)	-0.02	70 (2%) 59 55	39, 59, 91, 157	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	42	ASP	6.0
1	D	1	MET	5.8
1	C	42	ASP	5.7
1	C	1	MET	5.7
1	E	83	ASP	5.2
1	A	572	LEU	4.9
1	D	573	ALA	4.7
1	E	573	ALA	4.6
1	E	42	ASP	4.5
1	A	0	HIS	4.3
1	C	573	ALA	4.3
1	B	1	MET	4.3
1	B	45	ASP	4.2
1	C	43	GLY	4.1
1	D	591	GLY	3.7
1	A	358	TYR	3.7
1	E	592	LEU	3.6
1	D	572	LEU	3.6
1	C	572	LEU	3.5
1	E	572	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	44	GLN	3.5
1	C	41	ALA	3.4
1	A	1	MET	3.3
1	A	477	GLU	3.3
1	E	41	ALA	3.3
1	A	573	ALA	3.3
1	D	358	TYR	3.2
1	A	43	GLY	3.2
1	E	358	TYR	3.2
1	C	309	TYR	3.1
1	C	592	LEU	3.1
1	D	309	TYR	3.1
1	C	44	GLN	3.0
1	A	42	ASP	3.0
1	B	572	LEU	3.0
1	D	267	ASP	2.9
1	E	84	GLY	2.9
1	B	358	TYR	2.9
1	A	46	GLY	2.9
1	D	45	ASP	2.8
1	A	266	SER	2.7
1	A	41	ALA	2.7
1	B	573	ALA	2.7
1	B	84	GLY	2.6
1	E	576	SER	2.6
1	B	83	ASP	2.5
1	E	591	GLY	2.5
1	B	591	GLY	2.5
1	B	41	ALA	2.5
1	C	378	ARG	2.5
1	D	592	LEU	2.4
1	D	43	GLY	2.4
1	E	488	ASP	2.4
1	B	309	TYR	2.4
1	E	45	ASP	2.3
1	E	477	GLU	2.3
1	B	103	GLY	2.3
1	D	83	ASP	2.3
1	C	40	PRO	2.3
1	E	46	GLY	2.3
1	C	358	TYR	2.3
1	C	480	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	592	LEU	2.2
1	D	266	SER	2.2
1	B	46	GLY	2.1
1	C	380	GLY	2.1
1	C	477	GLU	2.1
1	A	473	VAL	2.0
1	E	40	PRO	2.0
1	B	266	SER	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
2	GOL	C	609	6/6	0.59	0.24	80,84,91,102	0
7	SO4	C	617	5/5	0.59	0.14	110,111,115,122	0
7	SO4	A	622	5/5	0.63	0.16	110,110,111,116	0
7	SO4	A	619	5/5	0.63	0.17	103,103,114,118	0
7	SO4	B	621	5/5	0.64	0.17	107,108,117,118	0
7	SO4	D	624	5/5	0.64	0.12	95,96,98,102	5
7	SO4	A	621	5/5	0.65	0.23	119,119,120,120	0
7	SO4	E	619	5/5	0.67	0.22	124,125,125,126	0
7	SO4	B	619	5/5	0.67	0.09	115,115,126,129	0
2	GOL	E	606	6/6	0.68	0.18	77,82,83,85	0
2	GOL	D	614	6/6	0.68	0.22	73,74,74,77	6
7	SO4	B	624	5/5	0.69	0.12	123,124,127,132	0
2	GOL	E	607	6/6	0.69	0.24	92,93,97,98	0
2	GOL	D	608	6/6	0.70	0.21	72,77,80,81	0
2	GOL	D	607	6/6	0.71	0.21	90,91,101,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	D	629	5/5	0.71	0.13	130,130,131,131	0
7	SO4	D	627	5/5	0.72	0.20	132,132,133,133	0
7	SO4	A	623	5/5	0.72	0.13	123,123,125,126	0
7	SO4	A	625	5/5	0.73	0.27	80,81,81,89	5
7	SO4	C	622	5/5	0.73	0.25	91,91,92,92	5
7	SO4	D	621	5/5	0.74	0.11	105,106,107,107	0
7	SO4	B	628	5/5	0.74	0.19	102,102,102,102	5
7	SO4	C	615	5/5	0.75	0.16	111,112,124,129	0
7	SO4	E	613	5/5	0.75	0.18	127,127,128,132	0
7	SO4	E	615	5/5	0.75	0.16	94,94,99,107	5
7	SO4	A	618	5/5	0.75	0.20	122,123,125,128	0
7	SO4	A	620	5/5	0.76	0.17	108,108,109,113	0
7	SO4	E	616	5/5	0.76	0.27	96,97,98,104	5
2	GOL	D	602	6/6	0.76	0.21	82,83,84,85	0
7	SO4	D	620	5/5	0.76	0.17	127,127,130,132	0
2	GOL	C	608	6/6	0.76	0.17	80,81,85,86	0
7	SO4	D	622	5/5	0.76	0.18	111,111,112,112	0
7	SO4	D	623	5/5	0.76	0.19	133,133,134,134	5
7	SO4	C	621	5/5	0.76	0.20	105,106,112,115	5
2	GOL	A	601	6/6	0.76	0.24	74,75,77,78	0
7	SO4	B	627	5/5	0.76	0.19	94,94,96,98	5
2	GOL	D	611	6/6	0.77	0.25	73,75,76,77	0
7	SO4	B	629	5/5	0.77	0.15	95,96,98,100	5
2	GOL	C	606	6/6	0.77	0.19	79,81,85,86	0
7	SO4	A	624	5/5	0.77	0.30	81,82,86,88	5
7	SO4	C	620	5/5	0.77	0.17	89,89,93,96	5
2	GOL	B	609	6/6	0.77	0.22	86,87,88,92	0
7	SO4	C	616	5/5	0.78	0.13	128,128,128,129	0
2	GOL	B	613	6/6	0.78	0.29	95,96,96,97	0
7	SO4	C	623	5/5	0.79	0.23	131,132,133,133	0
2	GOL	B	612	6/6	0.79	0.17	58,62,67,69	0
7	SO4	B	620	5/5	0.79	0.17	103,103,103,105	0
2	GOL	A	613	6/6	0.79	0.20	83,83,84,84	0
7	SO4	C	614	5/5	0.79	0.15	122,123,123,123	0
2	GOL	B	614	6/6	0.79	0.17	69,73,78,85	0
2	GOL	B	607	6/6	0.80	0.19	74,75,77,81	0
2	GOL	B	608	6/6	0.80	0.19	76,77,78,78	0
2	GOL	A	607	6/6	0.80	0.25	88,90,92,98	0
2	GOL	B	610	6/6	0.80	0.26	70,71,72,73	0
2	GOL	B	606	6/6	0.80	0.22	78,81,82,82	0
2	GOL	E	604	6/6	0.80	0.17	79,80,80,81	0
2	GOL	D	613	6/6	0.80	0.19	78,79,80,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	B	625	5/5	0.81	0.18	100,100,100,102	5
2	GOL	D	605	6/6	0.81	0.21	67,71,74,74	0
2	GOL	C	607	6/6	0.81	0.18	76,77,78,84	0
7	SO4	E	618	5/5	0.81	0.27	90,91,92,92	5
7	SO4	D	628	5/5	0.82	0.13	94,94,95,95	5
7	SO4	D	625	5/5	0.82	0.10	90,91,98,101	5
2	GOL	A	609	6/6	0.83	0.17	65,67,68,69	0
2	GOL	B	603	6/6	0.83	0.20	63,65,68,74	0
7	SO4	E	614	5/5	0.83	0.17	100,100,102,106	5
7	SO4	C	618	5/5	0.83	0.20	81,81,83,88	5
7	SO4	D	626	5/5	0.84	0.14	95,96,102,108	5
2	GOL	D	610	6/6	0.84	0.17	82,83,84,85	0
2	GOL	D	606	6/6	0.85	0.25	78,80,80,80	0
2	GOL	E	608	6/6	0.85	0.17	75,76,76,82	0
2	GOL	C	604	6/6	0.85	0.22	87,89,89,90	0
2	GOL	A	604	6/6	0.85	0.15	65,66,67,68	0
2	GOL	A	606	6/6	0.86	0.14	63,65,69,72	0
2	GOL	A	605	6/6	0.86	0.16	76,77,77,81	0
2	GOL	B	611	6/6	0.86	0.20	75,76,77,78	0
2	GOL	E	605	6/6	0.86	0.19	85,86,87,87	0
2	GOL	D	609	6/6	0.86	0.14	69,70,73,84	0
2	GOL	A	612	6/6	0.87	0.18	80,81,82,84	0
7	SO4	B	626	5/5	0.87	0.16	83,83,89,91	5
2	GOL	E	603	6/6	0.87	0.15	78,84,87,90	0
7	SO4	C	619	5/5	0.87	0.18	83,83,91,92	5
2	GOL	D	615	6/6	0.87	0.17	80,81,81,82	0
2	GOL	C	601	6/6	0.87	0.18	71,72,75,75	0
7	SO4	B	623	5/5	0.87	0.17	111,112,115,121	5
2	GOL	D	612	6/6	0.87	0.19	91,91,91,91	0
2	GOL	B	605	6/6	0.88	0.15	86,87,87,87	0
2	GOL	B	602	6/6	0.88	0.15	61,62,68,68	0
2	GOL	B	601	6/6	0.88	0.14	54,56,58,62	0
7	SO4	B	630	5/5	0.89	0.14	111,112,112,119	5
2	GOL	C	605	6/6	0.89	0.16	78,79,79,79	0
2	GOL	E	602	6/6	0.89	0.15	72,73,73,75	0
2	GOL	C	602	6/6	0.90	0.14	62,64,65,66	0
2	GOL	C	603	6/6	0.90	0.15	57,59,60,70	0
2	GOL	A	610	6/6	0.90	0.16	82,82,83,86	0
7	SO4	E	617	5/5	0.90	0.19	78,78,81,82	5
2	GOL	A	608	6/6	0.91	0.17	60,62,62,63	0
2	GOL	D	601	6/6	0.91	0.16	67,69,71,75	0
2	GOL	A	603	6/6	0.92	0.15	68,69,69,70	0

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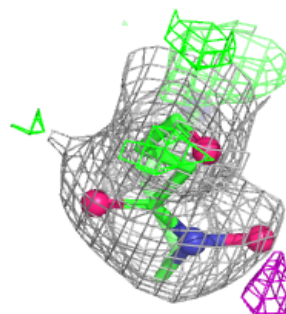
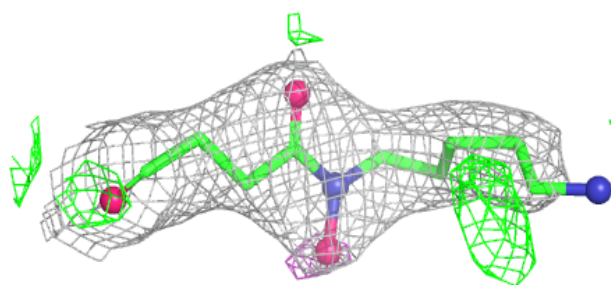
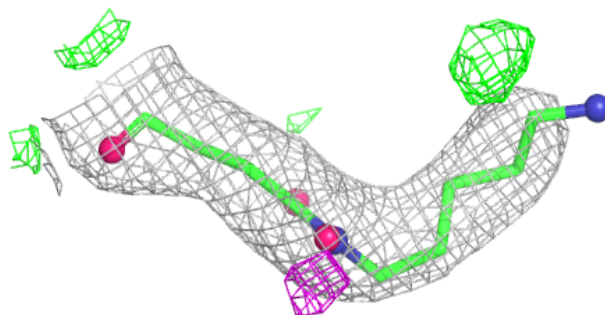
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	604	6/6	0.92	0.15	61,64,64,66	0
2	GOL	A	602	6/6	0.92	0.12	50,58,59,60	0
7	SO4	B	622	5/5	0.93	0.14	104,105,105,105	5
6	MG	A	617	1/1	0.93	0.06	58,58,58,58	0
2	GOL	A	611	6/6	0.93	0.13	51,52,53,54	6
3	I3U	D	616	14/15	0.93	0.14	50,58,66,73	0
3	I3U	E	609	14/15	0.94	0.14	59,68,81,84	0
2	GOL	E	601	6/6	0.94	0.13	58,60,64,66	0
2	GOL	D	603	6/6	0.95	0.10	50,51,57,57	0
3	I3U	A	614	14/15	0.95	0.11	50,59,68,74	0
6	MG	E	612	1/1	0.95	0.11	62,62,62,62	0
3	I3U	C	610	14/15	0.95	0.11	55,60,70,75	0
2	GOL	D	604	6/6	0.95	0.11	55,57,60,62	0
4	LMS	C	611	23/23	0.96	0.07	52,56,58,63	0
5	PO4	C	612	5/5	0.96	0.08	61,62,65,66	0
3	I3U	B	615	14/15	0.96	0.10	52,56,62,73	0
4	LMS	E	610	23/23	0.97	0.07	53,56,59,65	0
5	PO4	E	611	5/5	0.97	0.07	58,61,62,67	0
4	LMS	D	617	23/23	0.97	0.07	43,49,52,57	0
6	MG	C	613	1/1	0.97	0.05	61,61,61,61	0
4	LMS	B	616	23/23	0.98	0.06	44,47,49,51	0
4	LMS	A	615	23/23	0.98	0.06	44,49,54,56	0
6	MG	D	619	1/1	0.98	0.07	57,57,57,57	0
5	PO4	D	618	5/5	0.98	0.05	51,53,57,58	0
5	PO4	A	616	5/5	0.98	0.05	52,54,57,60	0
5	PO4	B	617	5/5	0.99	0.04	51,52,53,58	0
6	MG	B	618	1/1	0.99	0.05	58,58,58,58	0

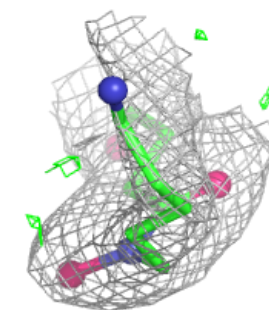
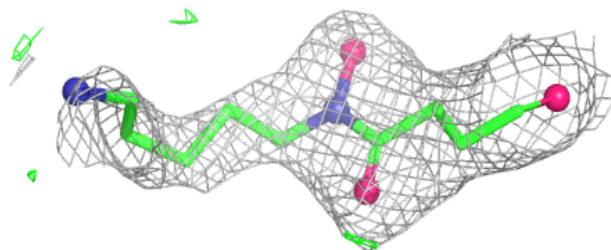
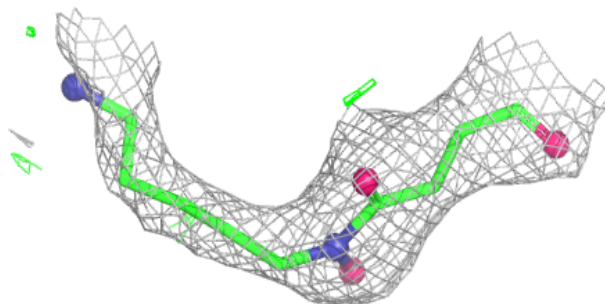
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around I3U D 616:

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

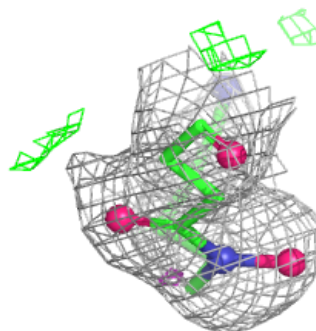
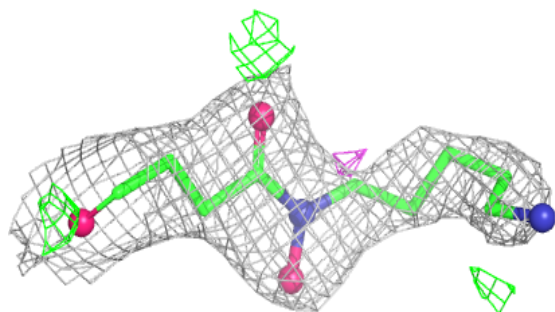
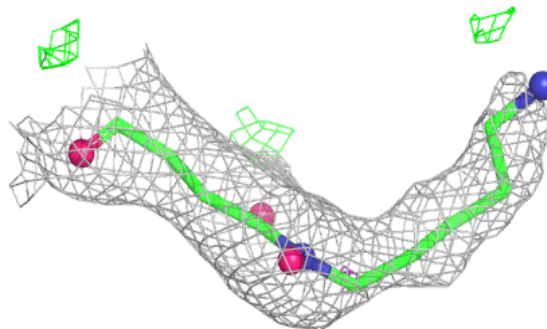
**Electron density around I3U E 609:**

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

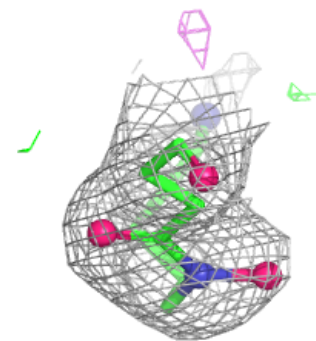
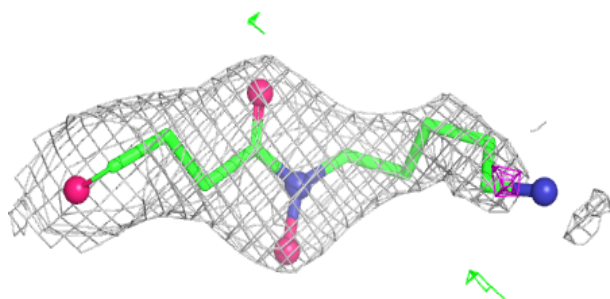
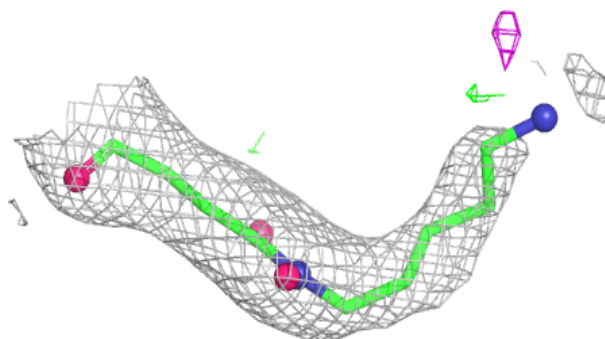


Electron density around I3U A 614:

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

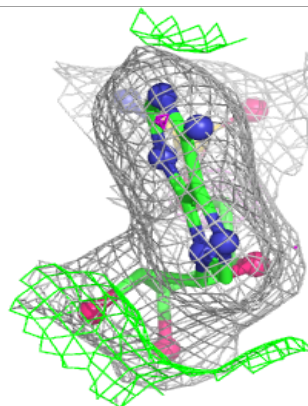
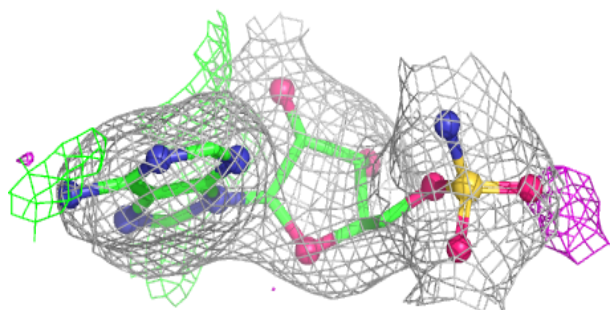
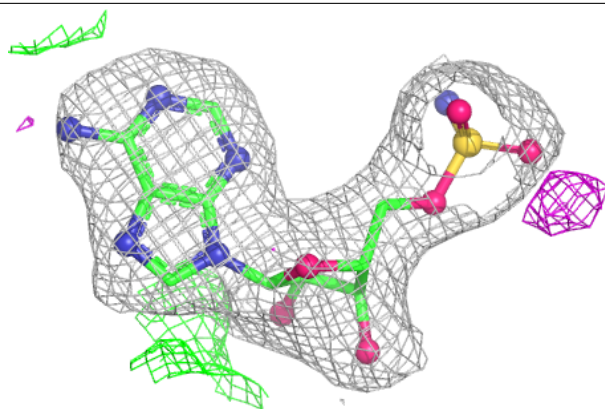
**Electron density around I3U C 610:**

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

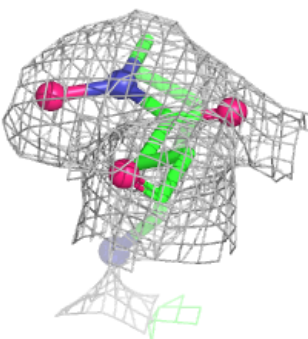
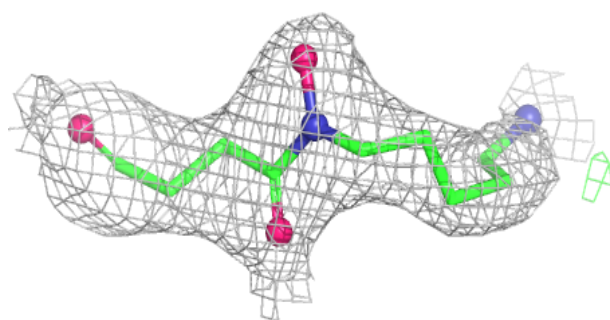
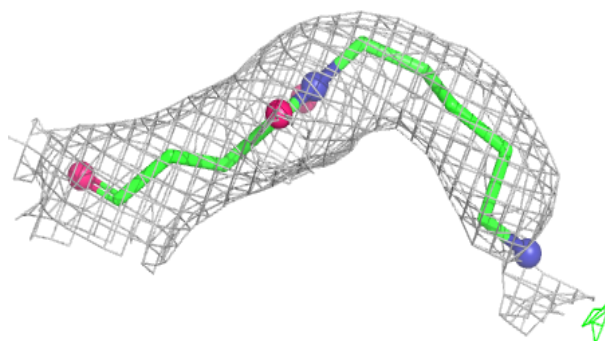


Electron density around LMS C 611:

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

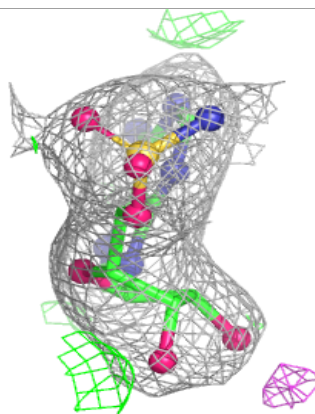
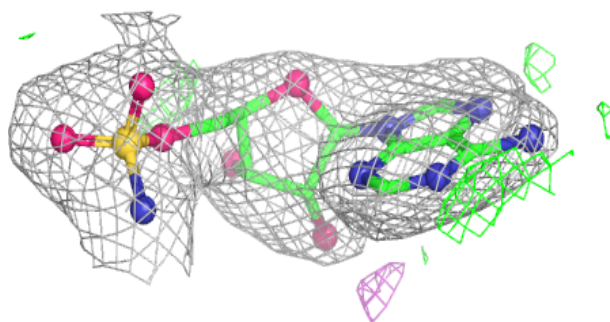
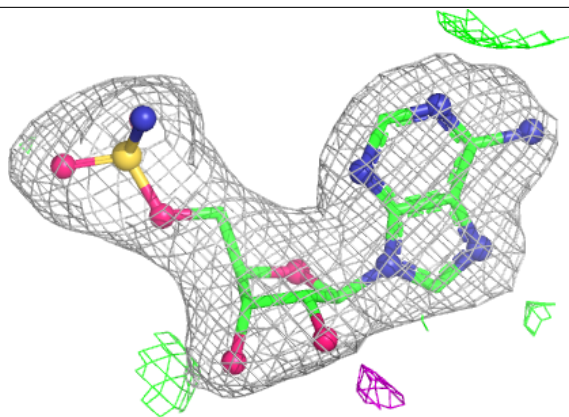
**Electron density around I3U B 615:**

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

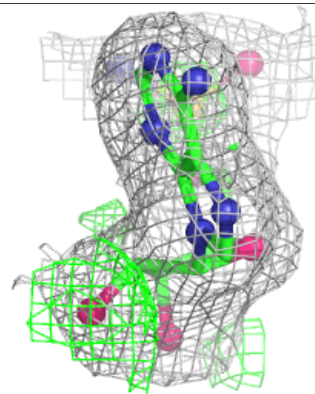
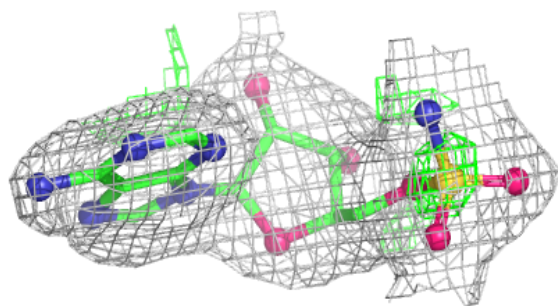
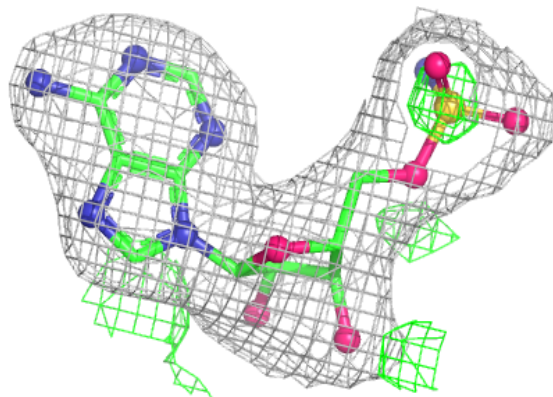


Electron density around LMS E 610:

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

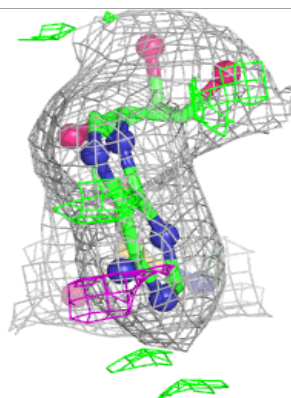
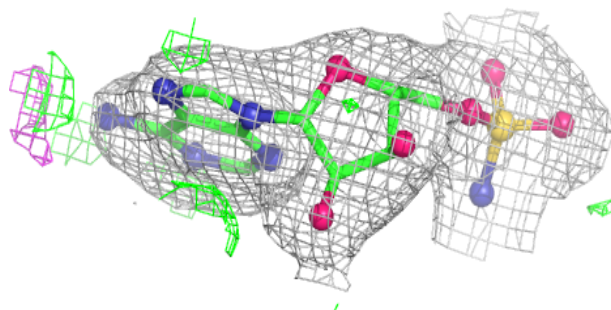
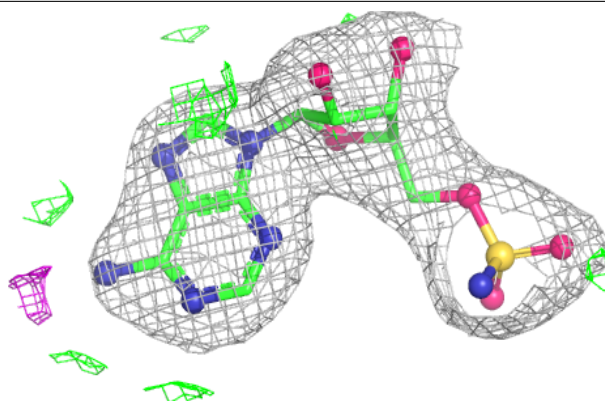
**Electron density around LMS D 617:**

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

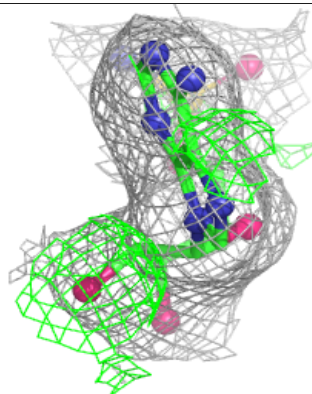
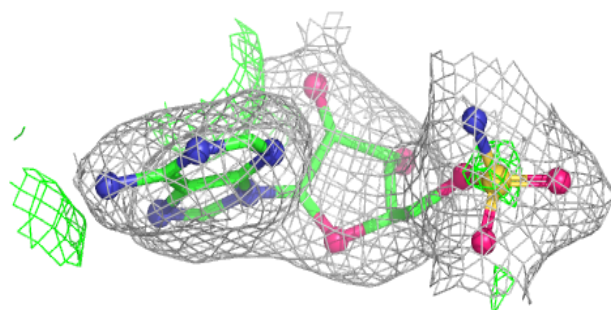
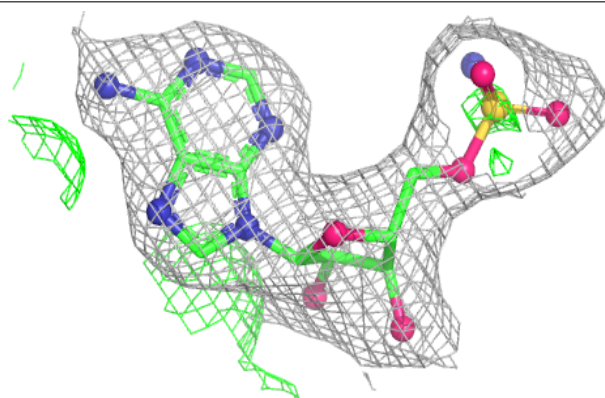


Electron density around LMS B 616:

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

**Electron density around LMS A 615:**

$2mF_o-DF_c$ (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.