



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 28, 2022 – 12:42 PM EDT

PDB ID : 7TGM
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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

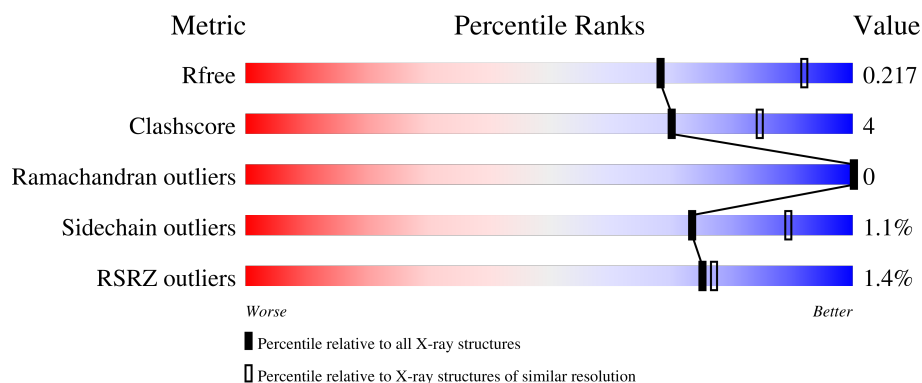
1 Overall quality at a glance

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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	<div> <div>0%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div></div> </div> <div>.</div> </div>
1	B	612	<div> <div>0%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div></div> </div> <div>.</div> </div>
1	C	612	<div> <div>0%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div></div> </div> <div>.</div> </div>
1	D	612	<div> <div>0%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div></div> </div> <div>.</div> </div>
1	E	612	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div></div> </div> <div>.</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	601	-	-	-	X
2	GOL	B	606	-	-	-	X
2	GOL	B	609	-	-	-	X
2	GOL	C	607	-	-	-	X
2	GOL	D	607	-	-	-	X
2	GOL	D	614	-	-	-	X
7	SO4	A	624	-	-	-	X
7	SO4	B	621	-	-	-	X
7	SO4	C	621	-	-	-	X
7	SO4	C	622	-	-	-	X
7	SO4	C	623	-	-	-	X
7	SO4	D	624	-	-	-	X
7	SO4	D	627	-	-	-	X
7	SO4	E	613	-	-	-	X
7	SO4	E	614	-	-	-	X
7	SO4	E	615	-	-	-	X

2 Entry composition [i](#)

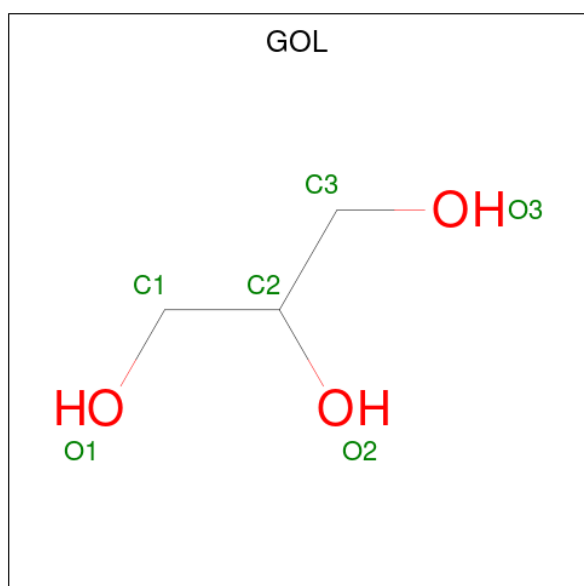
There are 8 unique types of molecules in this entry. The entry contains 24554 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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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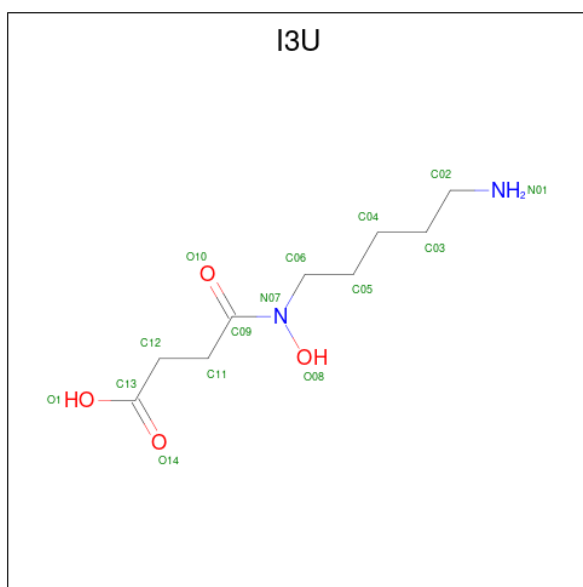
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	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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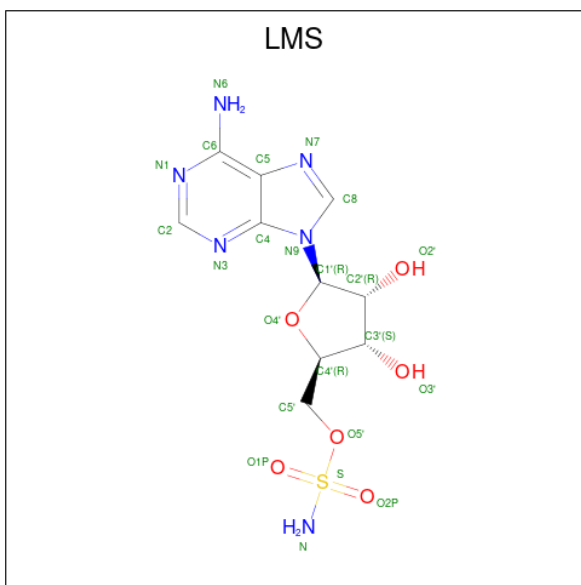
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	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 (three-letter code: I3U) (formula: C₉H₁₈N₂O₄) (labeled as "Ligand of Interest" by depositor).



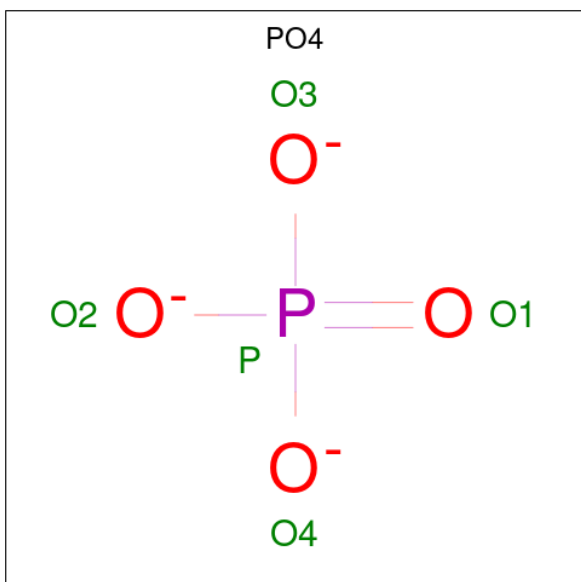
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	9	2	3		
3	B	1	Total	C	N	O	0	0
			14	9	2	3		
3	C	1	Total	C	N	O	0	0
			14	9	2	3		
3	E	1	Total	C	N	O	0	0
			14	9	2	3		
3	D	1	Total	C	N	O	0	0
			14	9	2	3		

- Molecule 4 is [(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3,4-DIHYDROXYTETRAHYDRO-2-FURANYL]METHYL SULFAMATE (three-letter code: 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 (three-letter code: PO4) (formula: O₄P).

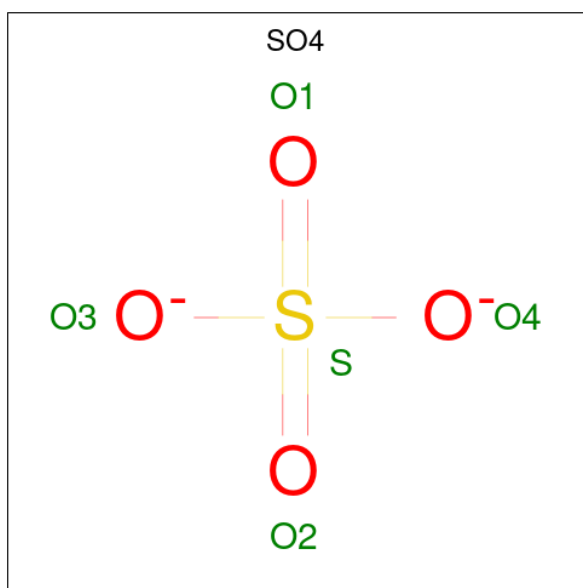


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	C	1	Total O P 5 4 1	0	0
5	E	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: 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 (three-letter code: 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		

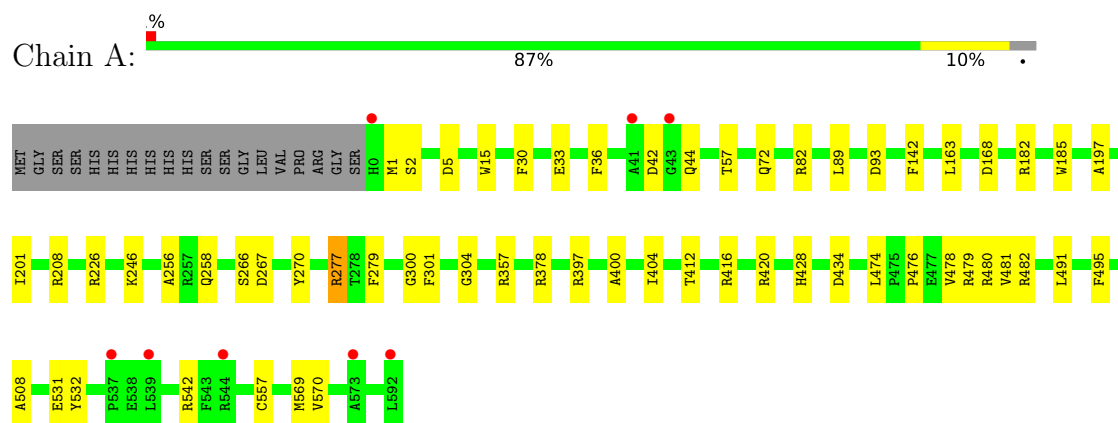
- Molecule 8 is water.

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		

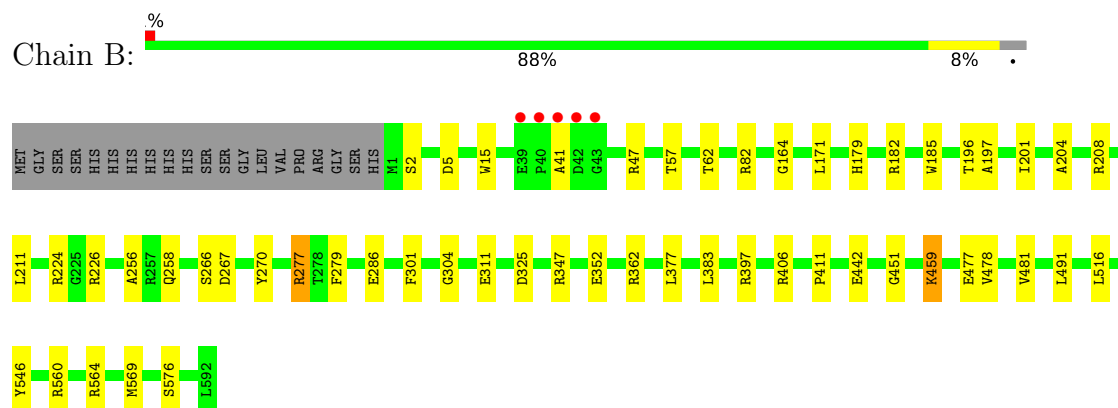
3 Residue-property plots

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.

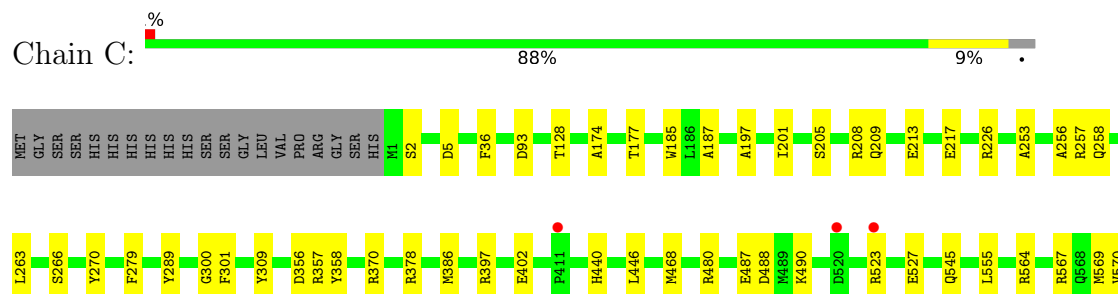
• Molecule 1: Desferrioxamine synthetase DesD

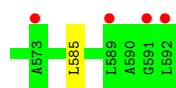


• Molecule 1: Desferrioxamine synthetase DesD

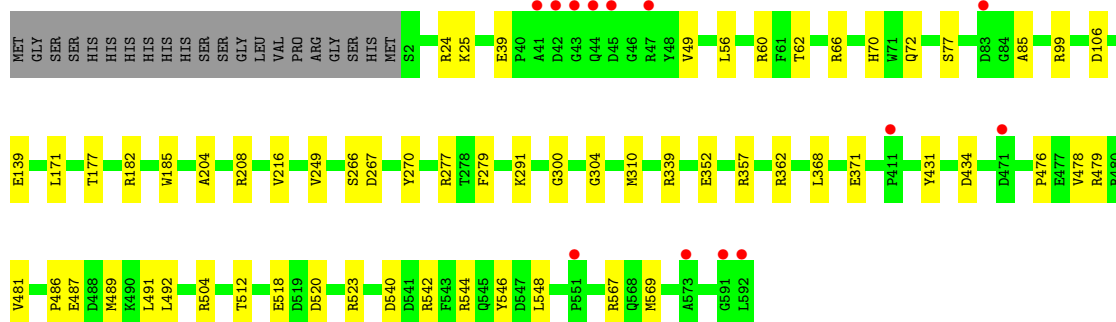
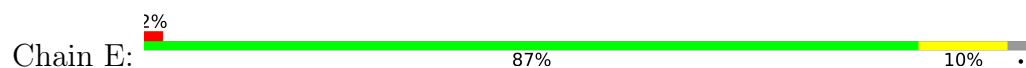


• Molecule 1: Desferrioxamine synthetase DesD

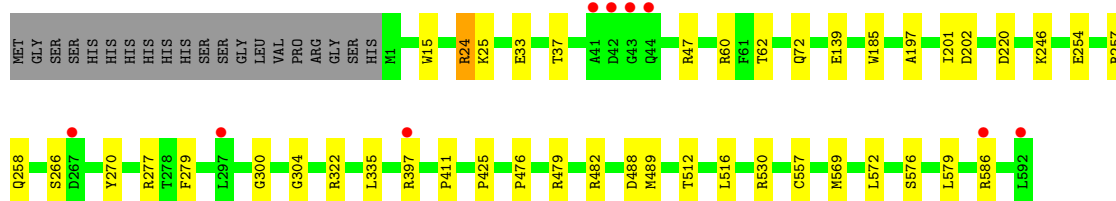
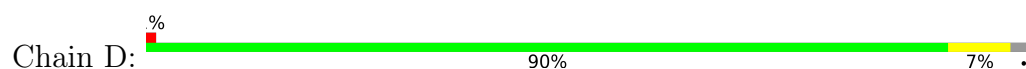




• Molecule 1: Desferrioxamine synthetase DesD



• 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 0.187 , 0.217	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)	0.34 , 38.7	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, MG, PO4, I3U, 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	0.43	0/4806	0.62	0/6542
1	B	0.43	0/4787	0.64	0/6516
1	C	0.38	0/4776	0.60	0/6505
1	D	0.41	0/4788	0.61	0/6519
1	E	0.39	0/4772	0.59	0/6499
All	All	0.41	0/23929	0.61	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

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	36	0
1	B	4674	0	4560	40	0
1	C	4662	0	4527	28	0
1	D	4674	0	4556	30	0
1	E	4658	0	4524	41	0
2	A	78	0	103	3	0
2	B	84	0	112	8	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	4	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	172	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 (172) 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: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: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
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
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:D:37:THR:H	2:D:612:GOL:H12	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:41:ALA:HB2	1:B:47:ARG:C	2.31	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: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
2:C:602:GOL:H12	1:D:246:LYS:HZ3	1.76	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
2:C:602:GOL:H12	1:D:246:LYS:HZ2	1.77	0.49
1:E:310:MET:HE3	1:E:368:LEU:HB3	1.95	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:185:TRP:CZ2	1:B:211:LEU:HD21	2.47	0.48
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:E:486:PRO:HG2	1:E:489:MET:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:GLU:H	1:B:477:GLU:CD	2.18	0.47
1:E:434:ASP:OD2	1:E:542:ARG:NH2	2.48	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
1:A:300:GLY:CA	1:A:569:MET:HG3	2.46	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:B:362:ARG:HH12	2:B:614:GOL:H2	1.82	0.44
1:E:310:MET:HE1	1:E:368:LEU:HD23	2.00	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:301:PHE:HZ	1:A:570:VAL:HG22	1.83	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: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:B:197:ALA:HB1	1:B:201:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:301:PHE:CE2	1:B:569:MET:HE2	2.53	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:B:560:ARG:HB3	2:B:602:GOL:H11	2.02	0.42
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [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	485/504 (96%)	479 (99%)	6 (1%)	71	88
1	B	481/504 (95%)	475 (99%)	6 (1%)	71	88
1	C	479/504 (95%)	473 (99%)	6 (1%)	69	87
1	D	481/504 (95%)	475 (99%)	6 (1%)	71	88
1	E	479/504 (95%)	477 (100%)	2 (0%)	91	97
All	All	2405/2520 (95%)	2379 (99%)	26 (1%)	73	89

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	93	ASP
1	A	277	ARG
1	A	378	ARG
1	A	397	ARG
1	A	480	ARG
1	B	277	ARG
1	B	325	ASP
1	B	397	ARG
1	B	459	LYS
1	B	564	ARG
1	B	576	SER
1	C	36	PHE
1	C	93	ASP
1	C	217	GLU
1	C	309	TYR
1	C	378	ARG
1	C	480	ARG
1	E	139	GLU
1	E	567	ARG
1	D	24	ARG
1	D	139	GLU
1	D	202	ASP
1	D	397	ARG
1	D	576	SER
1	D	586	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	209	GLN
1	A	258	GLN
1	B	179	HIS
1	B	258	GLN
1	C	209	GLN
1	C	258	GLN
1	D	143	GLN
1	D	273	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](#)

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	606	-	5,5,5	1.14	0	5,5,5	0.55	0
7	SO4	C	615	-	4,4,4	0.16	0	6,6,6	0.11	0
7	SO4	B	624	-	4,4,4	0.16	0	6,6,6	0.06	0
7	SO4	E	616	-	4,4,4	0.12	0	6,6,6	0.20	0
7	SO4	C	622	-	4,4,4	0.12	0	6,6,6	0.18	0
4	LMS	E	610	6,3	22,25,25	4.86	11 (50%)	25,38,38	3.28	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	609	-	5,5,5	0.80	0	5,5,5	1.03	0
7	SO4	D	629	-	4,4,4	0.14	0	6,6,6	0.07	0
2	GOL	A	603	-	5,5,5	0.68	0	5,5,5	1.07	0
2	GOL	C	604	-	5,5,5	0.80	0	5,5,5	1.00	0
2	GOL	A	601	-	5,5,5	1.51	1 (20%)	5,5,5	0.74	0
2	GOL	B	605	-	5,5,5	0.90	0	5,5,5	1.02	0
2	GOL	D	602	-	5,5,5	1.03	0	5,5,5	0.92	0
2	GOL	C	606	-	5,5,5	0.99	0	5,5,5	0.90	0
2	GOL	A	604	-	5,5,5	1.15	0	5,5,5	0.99	0
7	SO4	C	616	-	4,4,4	0.14	0	6,6,6	0.11	0
7	SO4	D	621	-	4,4,4	0.14	0	6,6,6	0.11	0
2	GOL	B	607	-	5,5,5	0.86	0	5,5,5	1.11	0
2	GOL	A	613	-	5,5,5	1.28	0	5,5,5	0.76	0
2	GOL	D	606	-	5,5,5	1.09	0	5,5,5	0.98	0
3	I3U	C	610	4	13,13,14	2.79	2 (15%)	10,14,16	1.82	2 (20%)
7	SO4	A	624	-	4,4,4	0.14	0	6,6,6	0.20	0
2	GOL	D	611	-	5,5,5	1.32	1 (20%)	5,5,5	0.59	0
2	GOL	D	601	-	5,5,5	1.01	0	5,5,5	0.98	0
7	SO4	A	621	-	4,4,4	0.17	0	6,6,6	0.31	0
2	GOL	B	602	-	5,5,5	0.74	0	5,5,5	1.06	0
2	GOL	D	615	-	5,5,5	1.11	0	5,5,5	0.74	0
7	SO4	C	619	-	4,4,4	0.16	0	6,6,6	0.15	0
2	GOL	D	614	-	5,5,5	0.99	0	5,5,5	0.89	0
2	GOL	E	603	-	5,5,5	0.94	0	5,5,5	0.94	0
7	SO4	B	625	-	4,4,4	0.13	0	6,6,6	0.28	0
7	SO4	D	624	-	4,4,4	0.15	0	6,6,6	0.09	0
3	I3U	D	616	4	13,13,14	2.84	1 (7%)	10,14,16	1.50	2 (20%)
2	GOL	B	612	-	5,5,5	0.96	0	5,5,5	0.85	0
7	SO4	C	620	-	4,4,4	0.14	0	6,6,6	0.10	0
2	GOL	A	610	-	5,5,5	0.97	0	5,5,5	0.85	0
2	GOL	C	603	-	5,5,5	0.64	0	5,5,5	1.14	1 (20%)
2	GOL	D	607	-	5,5,5	0.86	0	5,5,5	1.13	0
7	SO4	D	627	-	4,4,4	0.17	0	6,6,6	0.14	0
4	LMS	A	615	6,3	22,25,25	5.01	11 (50%)	25,38,38	3.58	7 (28%)
3	I3U	B	615	4	13,13,14	2.99	2 (15%)	10,14,16	1.93	2 (20%)
2	GOL	D	613	-	5,5,5	0.91	0	5,5,5	1.03	0
2	GOL	C	601	-	5,5,5	1.06	0	5,5,5	0.97	0
7	SO4	D	625	-	4,4,4	0.14	0	6,6,6	0.10	0
4	LMS	D	617	6,3	22,25,25	5.45	10 (45%)	25,38,38	3.26	5 (20%)
7	SO4	C	618	-	4,4,4	0.15	0	6,6,6	0.12	0
7	SO4	A	623	-	4,4,4	0.14	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	E	611	6	4,4,4	0.91	0	6,6,6	0.85	0
3	I3U	A	614	4	13,13,14	3.08	1 (7%)	10,14,16	1.68	2 (20%)
2	GOL	D	605	-	5,5,5	1.18	1 (20%)	5,5,5	1.04	0
2	GOL	A	611	-	5,5,5	0.93	0	5,5,5	1.12	1 (20%)
7	SO4	D	626	-	4,4,4	0.17	0	6,6,6	0.08	0
2	GOL	B	608	-	5,5,5	1.01	0	5,5,5	0.77	0
5	PO4	D	618	6	4,4,4	0.92	0	6,6,6	0.63	0
7	SO4	B	628	-	4,4,4	0.13	0	6,6,6	0.18	0
7	SO4	D	628	-	4,4,4	0.14	0	6,6,6	0.14	0
7	SO4	B	629	-	4,4,4	0.17	0	6,6,6	0.12	0
2	GOL	E	604	-	5,5,5	1.16	1 (20%)	5,5,5	1.14	0
2	GOL	C	607	-	5,5,5	1.09	0	5,5,5	0.98	0
2	GOL	A	606	-	5,5,5	0.73	0	5,5,5	1.27	1 (20%)
7	SO4	A	618	-	4,4,4	0.17	0	6,6,6	0.18	0
2	GOL	C	602	-	5,5,5	0.86	0	5,5,5	0.88	0
7	SO4	A	620	-	4,4,4	0.16	0	6,6,6	0.14	0
7	SO4	C	623	-	4,4,4	0.14	0	6,6,6	0.10	0
7	SO4	D	620	-	4,4,4	0.17	0	6,6,6	0.11	0
2	GOL	A	607	-	5,5,5	1.20	0	5,5,5	0.96	0
7	SO4	A	619	-	4,4,4	0.18	0	6,6,6	0.35	0
2	GOL	D	610	-	5,5,5	1.14	1 (20%)	5,5,5	0.84	0
7	SO4	B	627	-	4,4,4	0.13	0	6,6,6	0.14	0
2	GOL	B	613	-	5,5,5	1.10	0	5,5,5	0.73	0
2	GOL	B	601	-	5,5,5	1.02	0	5,5,5	1.29	0
2	GOL	E	602	-	5,5,5	0.98	0	5,5,5	1.06	0
7	SO4	D	622	-	4,4,4	0.16	0	6,6,6	0.32	0
7	SO4	C	621	-	4,4,4	0.14	0	6,6,6	0.13	0
7	SO4	B	626	-	4,4,4	0.17	0	6,6,6	0.12	0
7	SO4	C	614	-	4,4,4	0.16	0	6,6,6	0.14	0
2	GOL	A	608	-	5,5,5	0.92	0	5,5,5	1.03	1 (20%)
7	SO4	B	623	-	4,4,4	0.16	0	6,6,6	0.08	0
2	GOL	B	614	-	5,5,5	1.15	0	5,5,5	0.73	0
5	PO4	B	617	6	4,4,4	0.98	0	6,6,6	1.09	1 (16%)
7	SO4	D	623	-	4,4,4	0.15	0	6,6,6	0.10	0
7	SO4	E	618	-	4,4,4	0.12	0	6,6,6	0.36	0
2	GOL	C	608	-	5,5,5	1.01	0	5,5,5	0.98	0
2	GOL	B	603	-	5,5,5	1.18	0	5,5,5	0.70	0
2	GOL	D	609	-	5,5,5	1.04	0	5,5,5	1.07	0
2	GOL	E	607	-	5,5,5	0.97	0	5,5,5	0.88	0
7	SO4	A	625	-	4,4,4	0.15	0	6,6,6	0.19	0
3	I3U	E	609	4	13,13,14	3.02	2 (15%)	10,14,16	1.68	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	605	-	5,5,5	0.90	0	5,5,5	0.91	0
7	SO4	A	622	-	4,4,4	0.21	0	6,6,6	0.12	0
2	GOL	C	605	-	5,5,5	0.87	0	5,5,5	1.04	0
7	SO4	E	613	-	4,4,4	0.14	0	6,6,6	0.16	0
7	SO4	B	621	-	4,4,4	0.17	0	6,6,6	0.16	0
2	GOL	D	608	-	5,5,5	1.13	0	5,5,5	0.71	0
7	SO4	B	630	-	4,4,4	0.14	0	6,6,6	0.14	0
2	GOL	E	606	-	5,5,5	0.92	0	5,5,5	0.92	0
7	SO4	E	617	-	4,4,4	0.13	0	6,6,6	0.15	0
2	GOL	E	605	-	5,5,5	0.89	0	5,5,5	0.81	0
2	GOL	E	601	-	5,5,5	1.10	1 (20%)	5,5,5	0.95	0
2	GOL	C	609	-	5,5,5	0.97	0	5,5,5	0.95	0
7	SO4	E	619	-	4,4,4	0.18	0	6,6,6	0.19	0
2	GOL	A	612	-	5,5,5	0.99	0	5,5,5	0.93	0
2	GOL	B	610	-	5,5,5	1.27	1 (20%)	5,5,5	1.10	0
2	GOL	B	611	-	5,5,5	0.87	0	5,5,5	1.11	1 (20%)
2	GOL	D	604	-	5,5,5	0.98	0	5,5,5	0.99	0
2	GOL	D	603	-	5,5,5	1.23	1 (20%)	5,5,5	0.92	0
4	LMS	C	611	6,3	22,25,25	4.69	11 (50%)	25,38,38	4.40	4 (16%)
7	SO4	C	617	-	4,4,4	0.19	0	6,6,6	0.16	0
7	SO4	B	620	-	4,4,4	0.20	0	6,6,6	0.22	0
5	PO4	A	616	6	4,4,4	0.72	0	6,6,6	0.86	0
2	GOL	D	612	-	5,5,5	0.82	0	5,5,5	0.98	0
5	PO4	C	612	6	4,4,4	0.66	0	6,6,6	0.76	0
7	SO4	B	622	-	4,4,4	0.14	0	6,6,6	0.16	0
7	SO4	E	614	-	4,4,4	0.13	0	6,6,6	0.09	0
7	SO4	B	619	-	4,4,4	0.15	0	6,6,6	0.06	0
2	GOL	B	604	-	5,5,5	1.10	0	5,5,5	0.70	0
4	LMS	B	616	6,3	22,25,25	4.83	9 (40%)	25,38,38	3.99	4 (16%)
7	SO4	E	615	-	4,4,4	0.17	0	6,6,6	0.08	0
2	GOL	E	608	-	5,5,5	0.89	0	5,5,5	0.95	0
2	GOL	A	602	-	5,5,5	1.16	1 (20%)	5,5,5	0.96	0
2	GOL	B	609	-	5,5,5	0.84	0	5,5,5	0.97	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	606	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	I3U	D	616	4	-	1/13/14/15	-
2	GOL	B	612	-	-	2/4/4/4	-
2	GOL	A	607	-	-	4/4/4/4	-
2	GOL	E	606	-	-	0/4/4/4	-
2	GOL	D	610	-	-	4/4/4/4	-
2	GOL	E	605	-	-	0/4/4/4	-
4	LMS	E	610	6,3	-	1/6/26/26	0/3/3/3
2	GOL	A	609	-	-	0/4/4/4	-
2	GOL	B	613	-	-	2/4/4/4	-
2	GOL	C	609	-	-	1/4/4/4	-
2	GOL	A	610	-	-	2/4/4/4	-
2	GOL	A	603	-	-	0/4/4/4	-
2	GOL	E	601	-	-	0/4/4/4	-
2	GOL	C	604	-	-	0/4/4/4	-
2	GOL	B	601	-	-	0/4/4/4	-
2	GOL	C	603	-	-	2/4/4/4	-
2	GOL	D	607	-	-	0/4/4/4	-
2	GOL	A	601	-	-	0/4/4/4	-
2	GOL	E	602	-	-	2/4/4/4	-
2	GOL	A	612	-	-	2/4/4/4	-
2	GOL	B	610	-	-	4/4/4/4	-
4	LMS	A	615	6,3	-	3/6/26/26	0/3/3/3
3	I3U	B	615	4	-	2/13/14/15	-
2	GOL	B	611	-	-	0/4/4/4	-
2	GOL	B	605	-	-	1/4/4/4	-
2	GOL	D	604	-	-	0/4/4/4	-
2	GOL	D	603	-	-	2/4/4/4	-
2	GOL	A	608	-	-	4/4/4/4	-
2	GOL	D	613	-	-	2/4/4/4	-
2	GOL	C	601	-	-	1/4/4/4	-
2	GOL	B	614	-	-	0/4/4/4	-
2	GOL	C	606	-	-	2/4/4/4	-
2	GOL	A	604	-	-	2/4/4/4	-
2	GOL	D	602	-	-	0/4/4/4	-
4	LMS	C	611	6,3	-	2/6/26/26	0/3/3/3
2	GOL	B	607	-	-	2/4/4/4	-
2	GOL	A	613	-	-	1/4/4/4	-
2	GOL	D	606	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	I3U	C	610	4	-	2/13/14/15	-
4	LMS	D	617	6,3	-	2/6/26/26	0/3/3/3
2	GOL	D	611	-	-	4/4/4/4	-
2	GOL	D	612	-	-	0/4/4/4	-
2	GOL	D	601	-	-	2/4/4/4	-
3	I3U	A	614	4	-	1/13/14/15	-
2	GOL	C	608	-	-	2/4/4/4	-
2	GOL	A	611	-	-	2/4/4/4	-
2	GOL	B	603	-	-	2/4/4/4	-
2	GOL	B	608	-	-	1/4/4/4	-
2	GOL	D	605	-	-	0/4/4/4	-
2	GOL	D	609	-	-	0/4/4/4	-
2	GOL	E	607	-	-	4/4/4/4	-
2	GOL	B	604	-	-	2/4/4/4	-
2	GOL	E	604	-	-	2/4/4/4	-
2	GOL	A	605	-	-	2/4/4/4	-
2	GOL	C	607	-	-	0/4/4/4	-
2	GOL	B	602	-	-	0/4/4/4	-
2	GOL	A	606	-	-	0/4/4/4	-
2	GOL	C	605	-	-	2/4/4/4	-
2	GOL	D	615	-	-	2/4/4/4	-
3	I3U	E	609	4	-	1/13/14/15	-
4	LMS	B	616	6,3	-	0/6/26/26	0/3/3/3
2	GOL	C	602	-	-	2/4/4/4	-
2	GOL	D	614	-	-	1/4/4/4	-
2	GOL	E	603	-	-	1/4/4/4	-
2	GOL	E	608	-	-	2/4/4/4	-
2	GOL	D	608	-	-	2/4/4/4	-
2	GOL	A	602	-	-	2/4/4/4	-
2	GOL	B	609	-	-	1/4/4/4	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	617	LMS	O2P-S	14.36	1.54	1.42
4	D	617	LMS	O1P-S	13.37	1.53	1.42
4	A	615	LMS	O2P-S	12.77	1.52	1.42
4	A	615	LMS	O1P-S	12.31	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	610	LMS	O1P-S	12.03	1.52	1.42
4	B	616	LMS	O2P-S	11.48	1.51	1.42
4	B	616	LMS	O1P-S	11.43	1.51	1.42
4	C	611	LMS	O2P-S	11.27	1.51	1.42
4	E	610	LMS	O2P-S	10.94	1.51	1.42
4	C	611	LMS	O1P-S	10.89	1.51	1.42
3	A	614	I3U	C09-N07	10.73	1.49	1.34
4	E	610	LMS	S-N	10.63	1.70	1.58
3	E	609	I3U	C09-N07	10.31	1.48	1.34
3	B	615	I3U	C09-N07	10.30	1.48	1.34
4	B	616	LMS	S-N	10.16	1.69	1.58
4	D	617	LMS	S-N	9.95	1.69	1.58
3	D	616	I3U	C09-N07	9.58	1.47	1.34
3	C	610	I3U	C09-N07	9.47	1.47	1.34
4	C	611	LMS	S-N	9.30	1.68	1.58
4	A	615	LMS	S-N	9.09	1.68	1.58
4	D	617	LMS	O4'-C1'	8.42	1.52	1.41
4	C	611	LMS	O4'-C1'	7.75	1.51	1.41
4	A	615	LMS	O4'-C1'	7.66	1.51	1.41
4	E	610	LMS	O4'-C1'	7.41	1.51	1.41
4	B	616	LMS	O4'-C1'	7.41	1.51	1.41
4	D	617	LMS	O5'-S	6.01	1.66	1.57
4	A	615	LMS	O5'-S	5.47	1.65	1.57
4	B	616	LMS	O5'-S	4.62	1.64	1.57
4	C	611	LMS	O5'-S	4.56	1.64	1.57
4	E	610	LMS	O5'-S	4.54	1.64	1.57
4	E	610	LMS	C2'-C1'	-4.37	1.47	1.53
4	C	611	LMS	C2'-C1'	-4.34	1.47	1.53
4	B	616	LMS	C4-N3	-4.15	1.29	1.35
4	A	615	LMS	C2'-C1'	-4.14	1.47	1.53
4	B	616	LMS	C2'-C1'	-3.96	1.47	1.53
4	A	615	LMS	C4-N3	-3.94	1.30	1.35
4	D	617	LMS	C2'-C1'	-3.84	1.47	1.53
4	D	617	LMS	C4-N3	-3.81	1.30	1.35
4	C	611	LMS	C4-N3	-3.74	1.30	1.35
4	C	611	LMS	C2-N3	3.19	1.37	1.32
4	B	616	LMS	C2-N3	3.07	1.37	1.32
4	E	610	LMS	C4-N3	-2.99	1.31	1.35
4	B	616	LMS	C6-N6	2.81	1.44	1.34
4	A	615	LMS	C6-N6	2.75	1.44	1.34
4	E	610	LMS	C2-N3	2.74	1.36	1.32
4	E	610	LMS	C6-N6	2.74	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	617	LMS	C2-N3	2.59	1.36	1.32
4	D	617	LMS	C6-N6	2.54	1.43	1.34
4	C	611	LMS	C6-N6	2.50	1.43	1.34
2	B	610	GOL	C3-C2	2.40	1.61	1.51
2	A	602	GOL	O2-C2	-2.36	1.36	1.43
2	D	611	GOL	C1-C2	2.31	1.61	1.51
4	E	610	LMS	C5-N7	2.30	1.48	1.39
2	A	601	GOL	C1-C2	2.27	1.61	1.51
2	D	605	GOL	C3-C2	2.26	1.61	1.51
4	A	615	LMS	C5-N7	2.25	1.47	1.39
2	D	603	GOL	O2-C2	-2.25	1.36	1.43
4	E	610	LMS	C2'-C3'	-2.21	1.47	1.53
3	E	609	I3U	C11-C09	2.16	1.56	1.51
2	E	601	GOL	O2-C2	-2.15	1.37	1.43
4	C	611	LMS	C2'-C3'	-2.13	1.47	1.53
3	C	610	I3U	C11-C09	2.12	1.56	1.51
4	A	615	LMS	C2-N3	2.10	1.35	1.32
4	D	617	LMS	C5-N7	2.10	1.47	1.39
4	C	611	LMS	C5-N7	2.09	1.47	1.39
4	A	615	LMS	C2'-C3'	-2.04	1.47	1.53
2	D	610	GOL	O2-C2	-2.02	1.37	1.43
3	B	615	I3U	C11-C09	2.02	1.55	1.51
2	E	604	GOL	C1-C2	2.01	1.60	1.51

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	611	LMS	O2P-S-O1P	-20.79	100.31	119.97
4	B	616	LMS	O2P-S-O1P	-18.51	102.46	119.97
4	A	615	LMS	O2P-S-O1P	-15.98	104.85	119.97
4	E	610	LMS	O2P-S-O1P	-14.76	106.00	119.97
4	D	617	LMS	O2P-S-O1P	-14.63	106.13	119.97
4	C	611	LMS	N3-C2-N1	-4.66	121.39	128.68
4	E	610	LMS	N3-C2-N1	-4.51	121.62	128.68
4	D	617	LMS	N3-C2-N1	-4.47	121.70	128.68
4	B	616	LMS	N3-C2-N1	-4.34	121.90	128.68
3	B	615	I3U	C12-C11-C09	-4.22	105.22	111.77
3	C	610	I3U	O08-N07-C06	4.18	124.04	113.59
4	A	615	LMS	N3-C2-N1	-4.15	122.19	128.68
3	B	615	I3U	O08-N07-C06	3.91	123.37	113.59
3	E	609	I3U	C12-C11-C09	-3.77	105.92	111.77
3	A	614	I3U	C12-C11-C09	-3.74	105.97	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	616	I3U	O08-N07-C06	3.73	122.93	113.59
3	C	610	I3U	C12-C11-C09	-3.44	106.44	111.77
3	E	609	I3U	O08-N07-C06	3.43	122.16	113.59
3	A	614	I3U	O08-N07-C06	3.35	121.97	113.59
4	B	616	LMS	C4-C5-N7	-3.27	105.99	109.40
4	A	615	LMS	O5'-C5'-C4'	3.01	113.23	107.62
4	A	615	LMS	C4-C5-N7	-3.00	106.27	109.40
4	C	611	LMS	C4-C5-N7	-2.90	106.38	109.40
4	D	617	LMS	C4-C5-N7	-2.61	106.68	109.40
4	A	615	LMS	O4'-C1'-C2'	-2.42	103.39	106.93
4	B	616	LMS	O4'-C1'-C2'	-2.37	103.46	106.93
3	D	616	I3U	C12-C11-C09	-2.34	108.14	111.77
4	C	611	LMS	O1P-S-N	2.33	112.65	109.14
5	B	617	PO4	O4-P-O1	-2.29	102.51	110.89
4	D	617	LMS	O1P-S-N	2.29	112.60	109.14
4	E	610	LMS	O5'-S-N	2.28	112.73	105.31
4	D	617	LMS	C5'-O5'-S	2.27	120.06	117.21
2	A	606	GOL	C3-C2-C1	-2.22	103.08	111.70
2	A	611	GOL	C3-C2-C1	-2.22	103.09	111.70
4	A	615	LMS	O1P-S-N	2.21	112.48	109.14
2	C	603	GOL	C3-C2-C1	-2.21	103.12	111.70
2	A	608	GOL	C3-C2-C1	-2.15	103.35	111.70
4	E	610	LMS	C4-C5-N7	-2.12	107.19	109.40
4	A	615	LMS	C3'-C2'-C1'	2.07	104.09	100.98
2	B	611	GOL	C3-C2-C1	-2.01	103.87	111.70

There are no chirality outliers.

All (99) 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
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	602	GOL	C1-C2-C3-O3
2	C	603	GOL	C1-C2-C3-O3
2	C	603	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
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	B	615	I3U	C04-C05-C06-N07
3	C	610	I3U	C04-C05-C06-N07
3	E	609	I3U	C04-C05-C06-N07
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
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	A	607	GOL	O1-C1-C2-O2
2	A	607	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
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	607	GOL	C1-C2-C3-O3
2	D	610	GOL	O1-C1-C2-C3
2	D	610	GOL	C1-C2-C3-O3
2	B	610	GOL	O1-C1-C2-C3
2	B	613	GOL	C1-C2-C3-O3
2	A	608	GOL	O1-C1-C2-O2
2	D	614	GOL	O2-C2-C3-O3
3	C	610	I3U	C02-C03-C04-C05
2	B	608	GOL	O2-C2-C3-O3
2	B	610	GOL	O1-C1-C2-O2
2	E	603	GOL	O1-C1-C2-O2
2	B	605	GOL	C1-C2-C3-O3
2	E	602	GOL	O1-C1-C2-C3
2	E	607	GOL	C1-C2-C3-O3
2	E	608	GOL	O1-C1-C2-C3
2	D	611	GOL	C1-C2-C3-O3
2	D	615	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
2	D	611	GOL	O2-C2-C3-O3
2	C	609	GOL	O2-C2-C3-O3
4	D	617	LMS	C5'-O5'-S-N
2	A	613	GOL	O1-C1-C2-C3
2	B	610	GOL	C1-C2-C3-O3
2	C	608	GOL	O1-C1-C2-C3
2	D	613	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	615	I3U	C02-C03-C04-C05
2	B	609	GOL	O2-C2-C3-O3
2	E	608	GOL	O2-C2-C3-O3

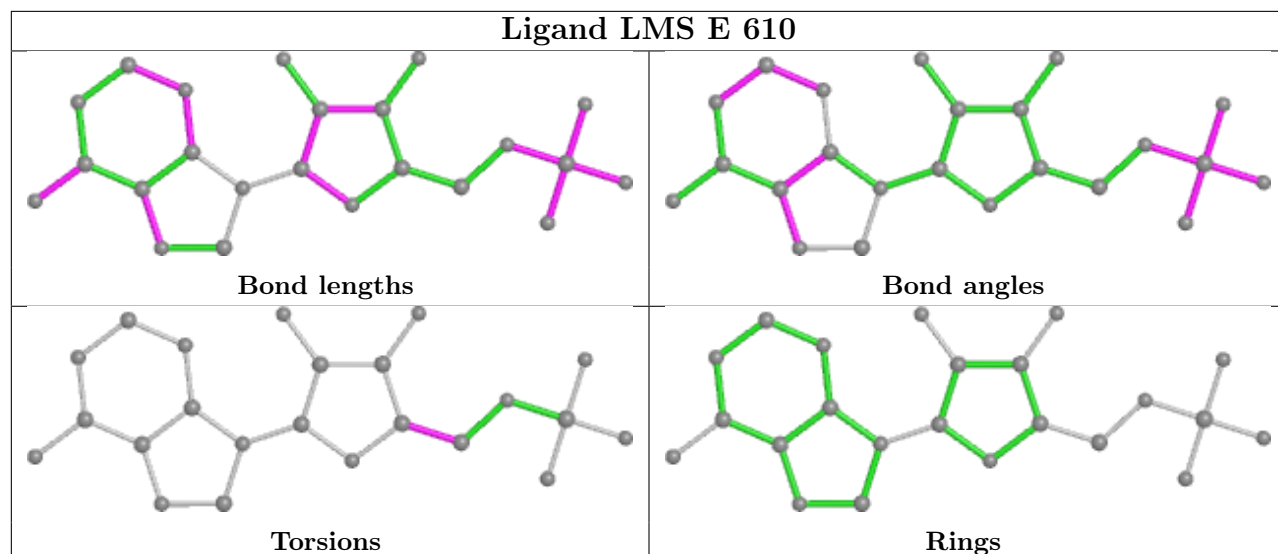
There are no ring outliers.

20 monomers are involved in 25 short contacts:

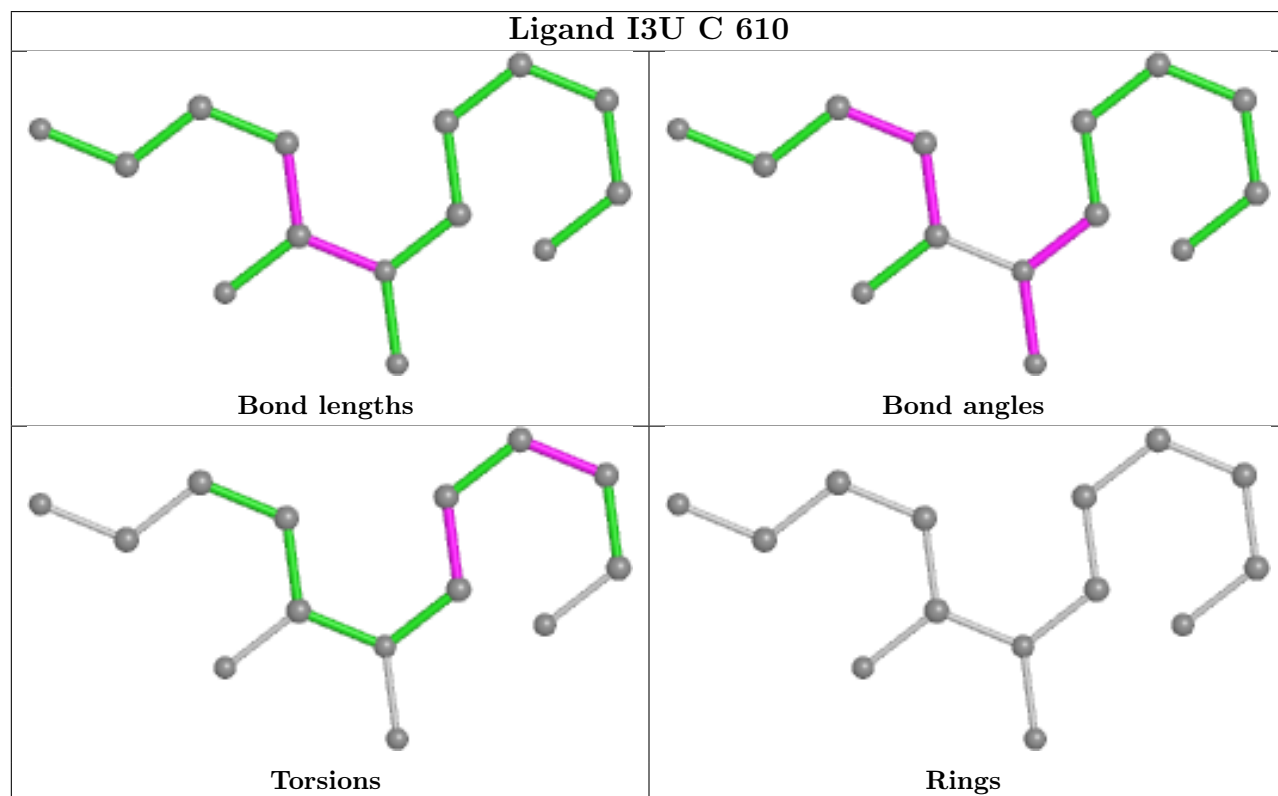
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	GOL	1	0
7	D	621	SO4	1	0
2	A	613	GOL	1	0
2	B	602	GOL	1	0
2	D	615	GOL	1	0
2	C	601	GOL	1	0
5	E	611	PO4	1	0
2	C	607	GOL	1	0
2	C	602	GOL	3	0
2	D	610	GOL	1	0
2	E	602	GOL	1	0
2	B	614	GOL	1	0
2	C	608	GOL	1	0
2	B	603	GOL	3	0
2	E	607	GOL	1	0
2	A	605	GOL	1	0
2	D	608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

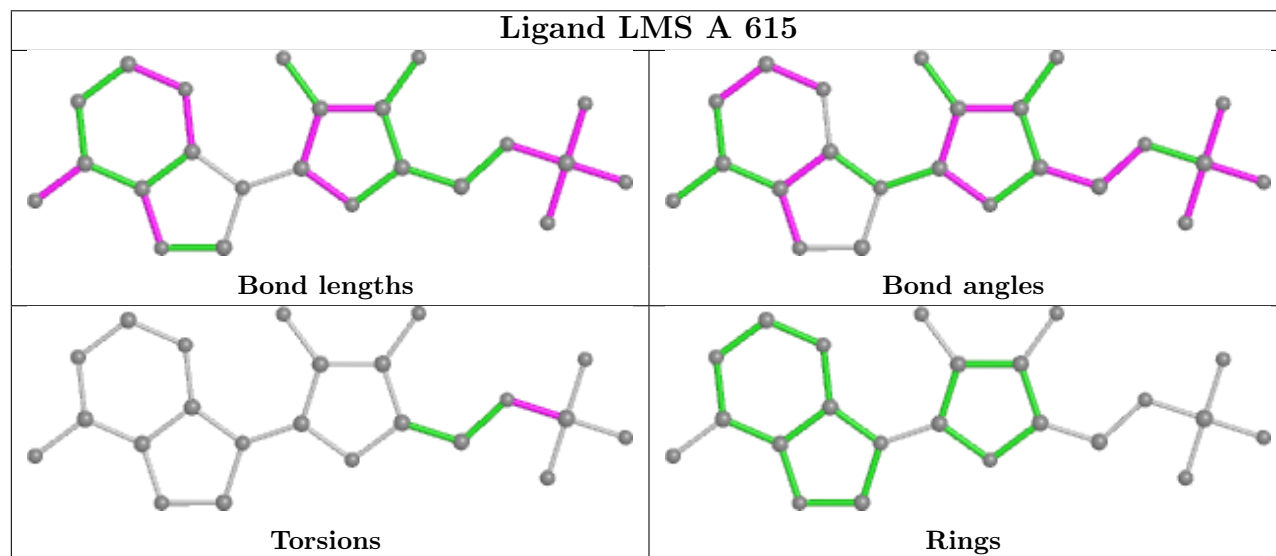
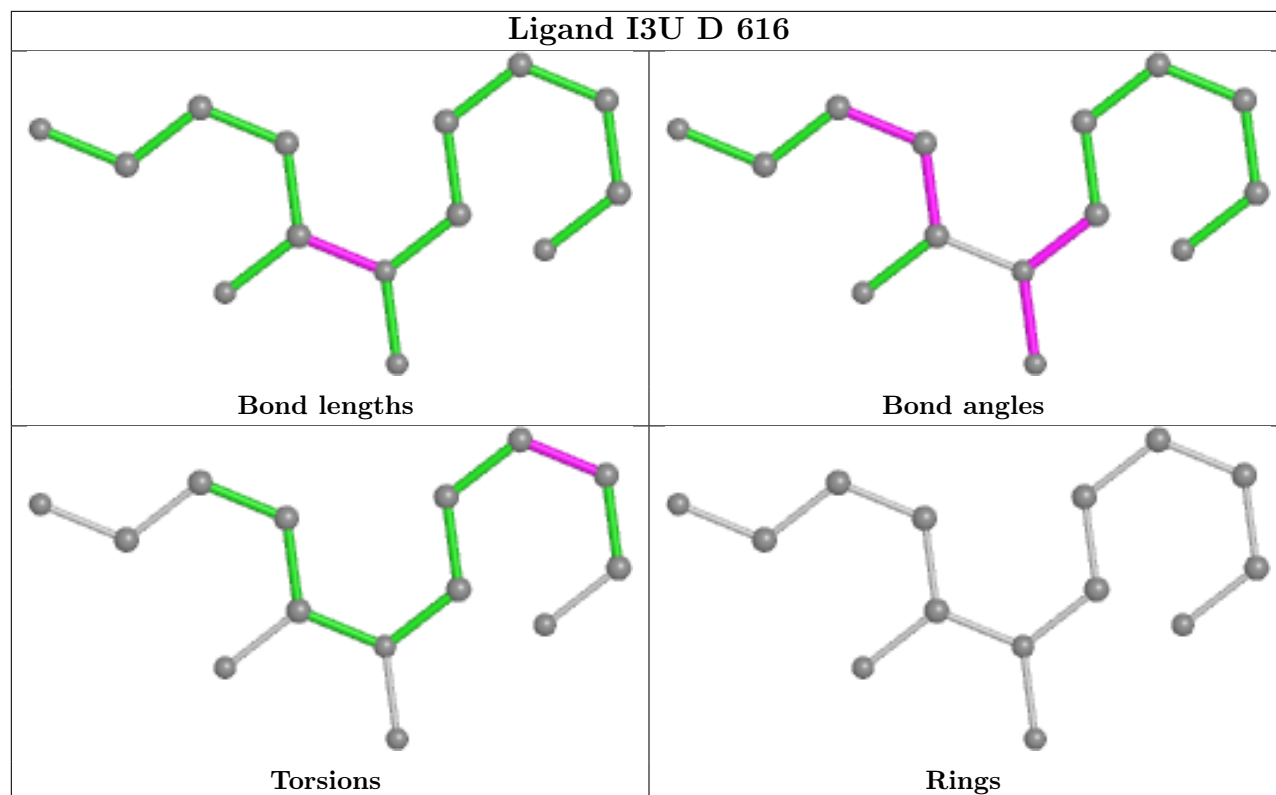
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

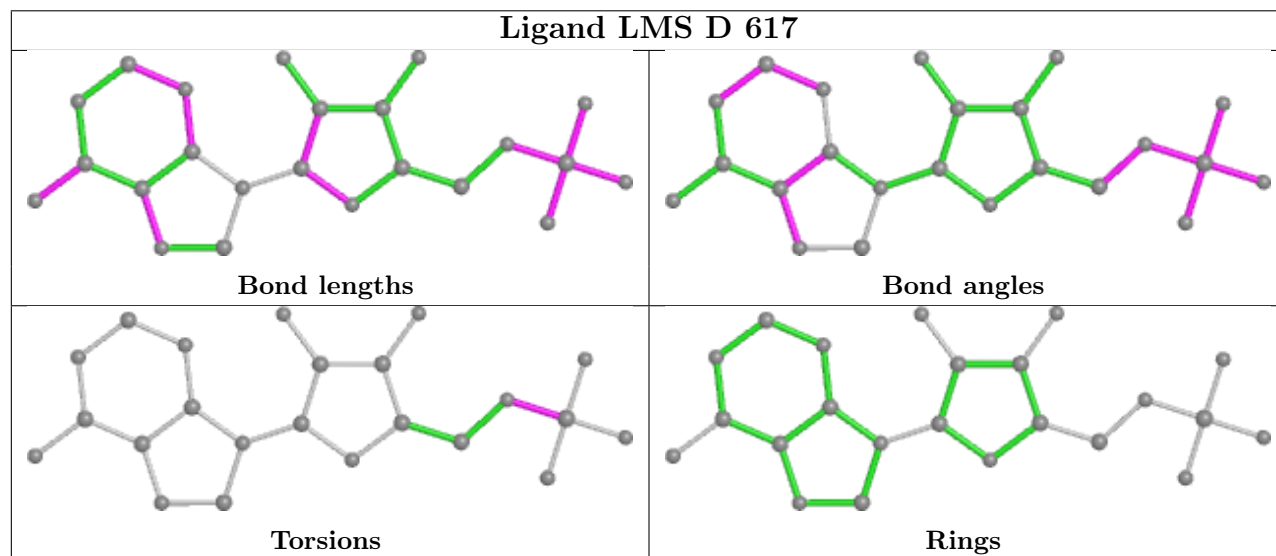
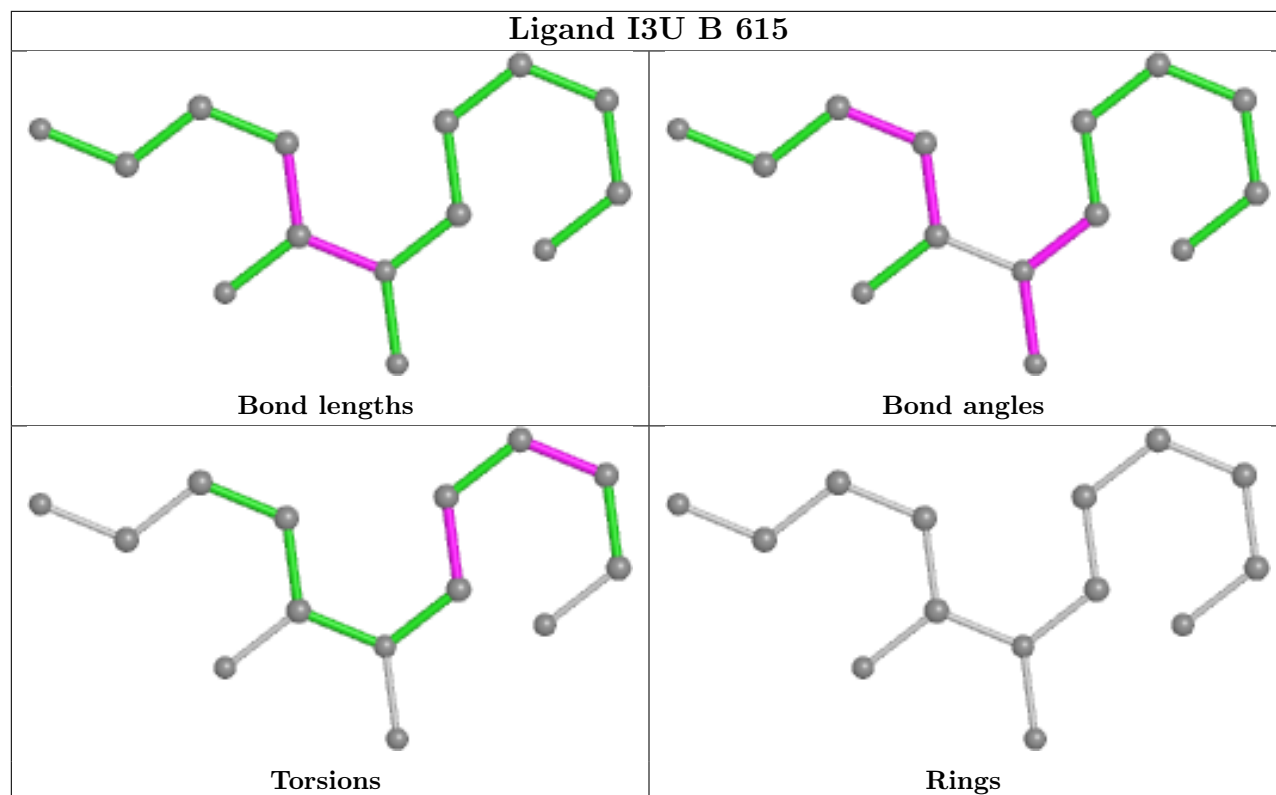
Ligand LMS E 610

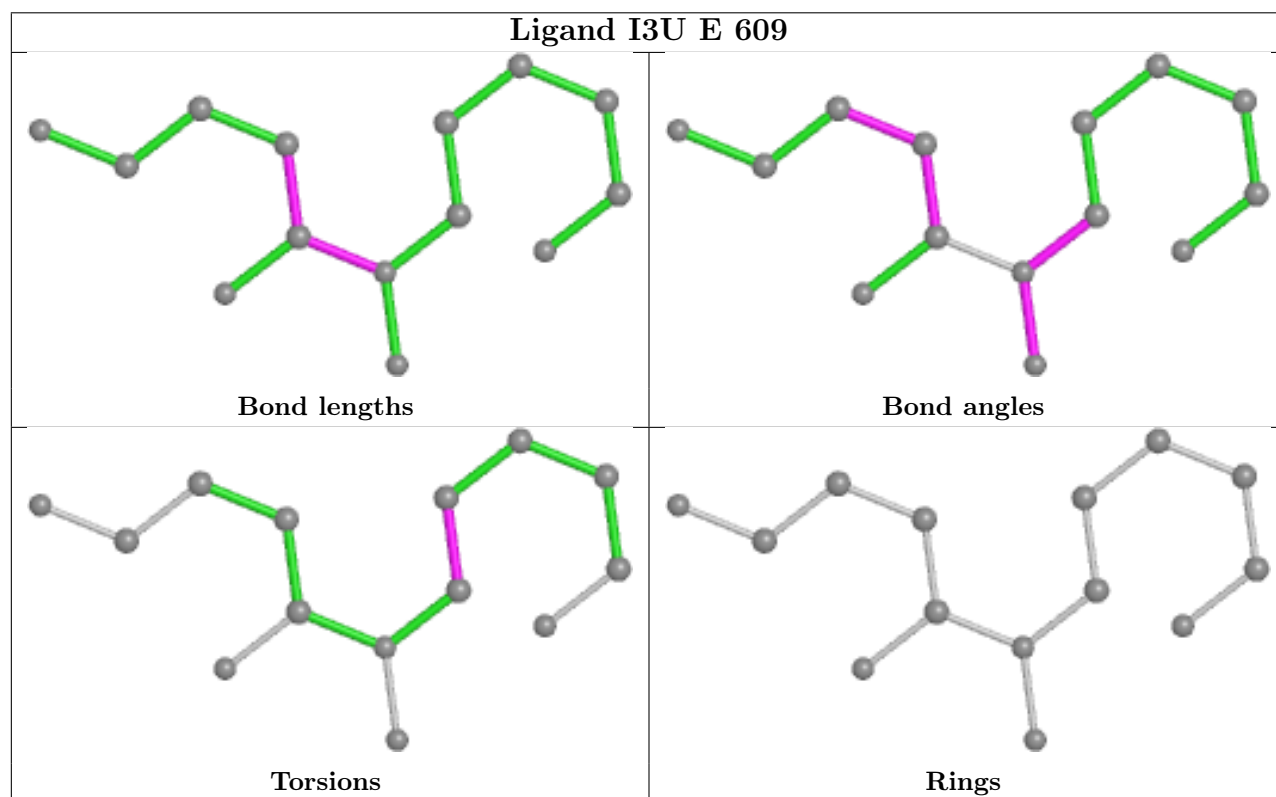
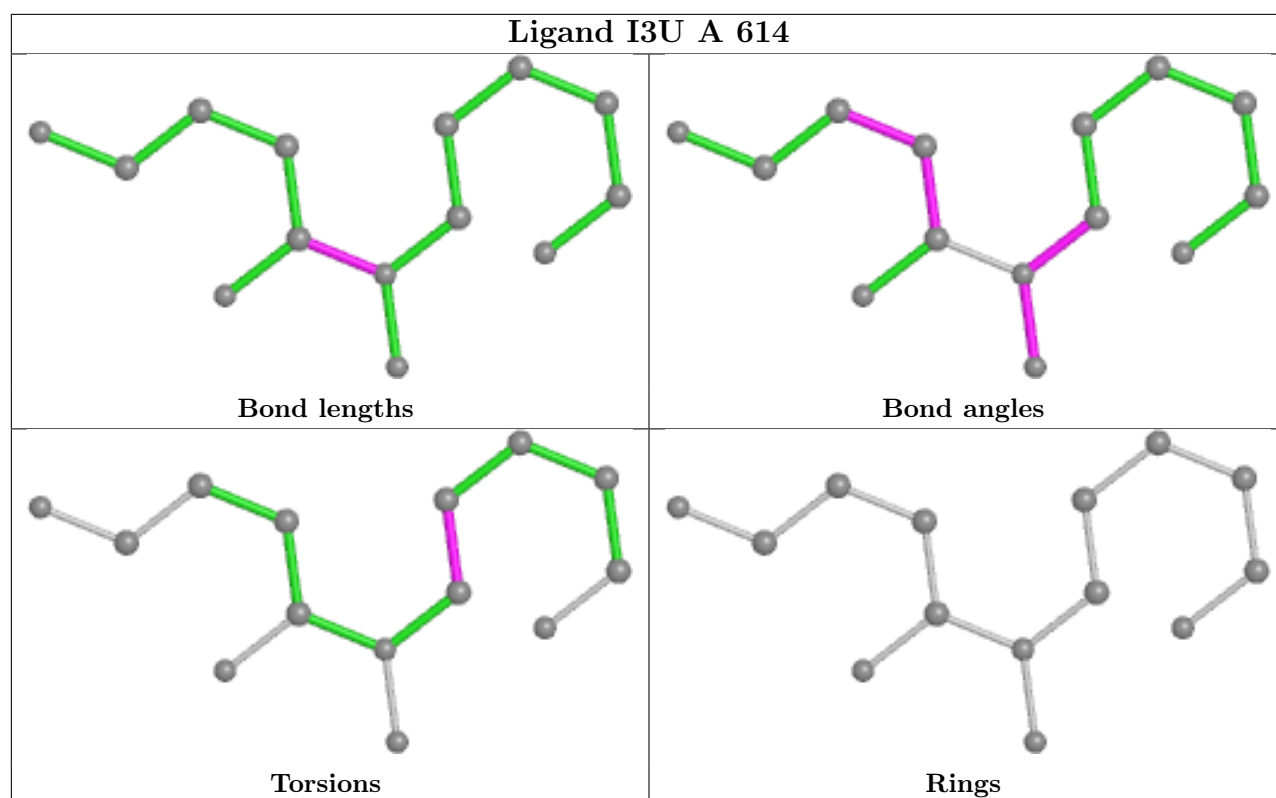


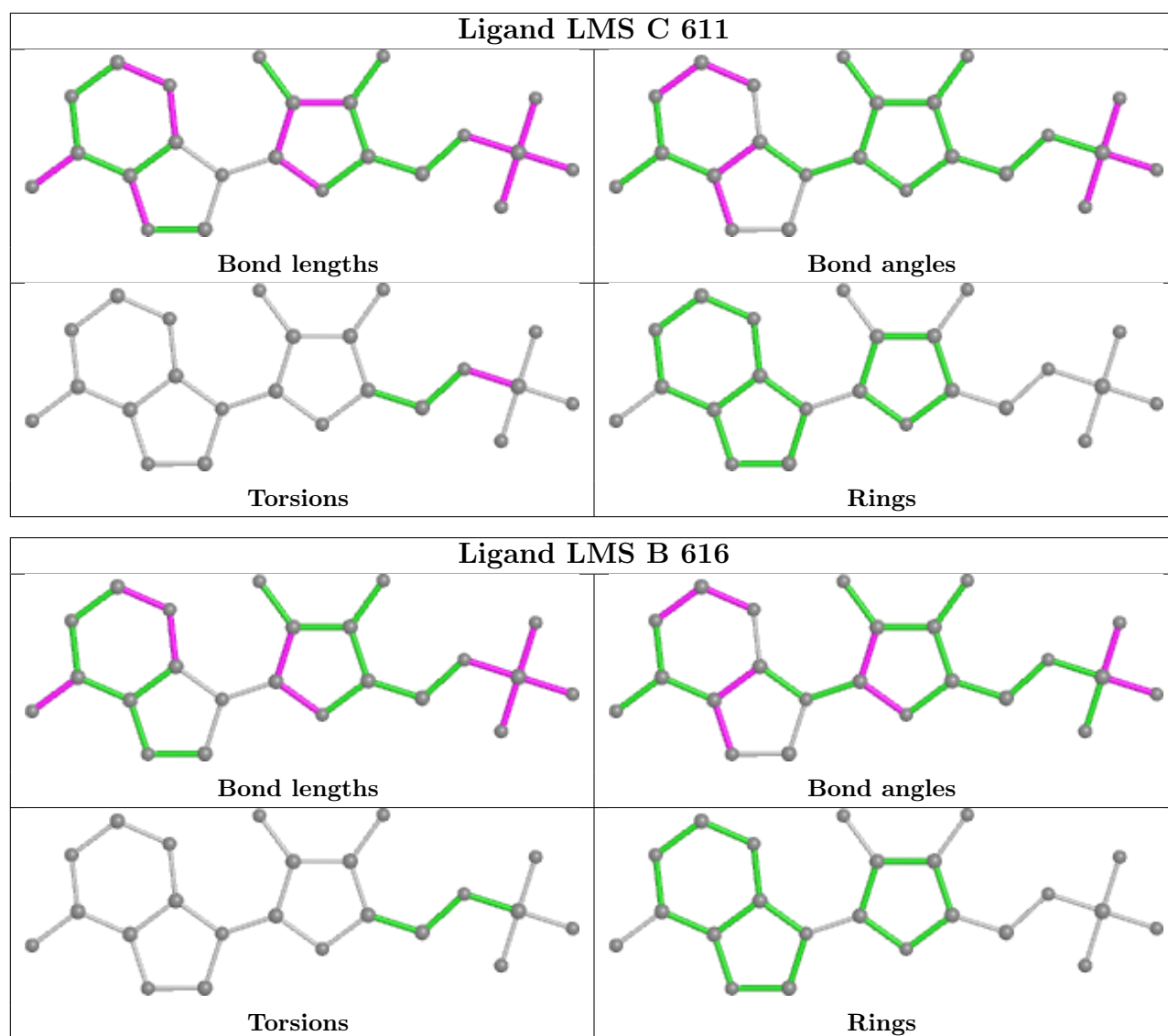
Ligand I3U C 610











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%)	-0.20	8 (1%) 77 79	39, 56, 88, 157	0
1	B	592/612 (96%)	-0.15	5 (0%) 86 87	39, 54, 78, 145	0
1	C	592/612 (96%)	-0.06	7 (1%) 79 80	47, 67, 96, 148	0
1	D	592/612 (96%)	-0.23	9 (1%) 73 75	46, 56, 79, 130	0
1	E	591/612 (96%)	-0.15	13 (2%) 62 65	47, 67, 96, 157	0
All	All	2960/3060 (96%)	-0.16	42 (1%) 75 77	39, 59, 91, 157	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	42	ASP	6.4
1	B	41	ALA	5.5
1	E	41	ALA	4.8
1	D	42	ASP	4.7
1	A	592	LEU	4.1
1	E	42	ASP	4.1
1	D	41	ALA	3.5
1	E	573	ALA	3.4
1	E	591	GLY	3.3
1	C	591	GLY	3.2
1	C	592	LEU	3.2
1	D	267	ASP	3.2
1	E	592	LEU	3.1
1	E	471	ASP	2.9
1	E	551	PRO	2.8
1	E	44	GLN	2.8
1	E	43	GLY	2.7
1	D	43	GLY	2.7
1	A	41	ALA	2.6
1	C	520	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	573	ALA	2.6
1	D	397	ARG	2.5
1	A	539	LEU	2.4
1	E	45	ASP	2.4
1	C	411	PRO	2.4
1	D	592	LEU	2.4
1	A	0	HIS	2.3
1	E	411	PRO	2.3
1	E	83	ASP	2.3
1	A	537	PRO	2.2
1	B	43	GLY	2.2
1	B	39	GLU	2.2
1	B	40	PRO	2.2
1	C	523	ARG	2.2
1	A	43	GLY	2.2
1	E	47	ARG	2.2
1	A	544	ARG	2.2
1	D	44	GLN	2.2
1	C	573	ALA	2.1
1	C	589	LEU	2.1
1	D	586	ARG	2.1
1	D	297	LEU	2.1

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
2	GOL	D	614	6/6	0.61	0.54	73,74,74,77	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	D	608	6/6	0.62	0.34	72,77,80,81	0
2	GOL	A	607	6/6	0.64	0.35	88,90,92,98	0
2	GOL	E	607	6/6	0.68	0.27	92,93,97,98	0
7	SO4	E	619	5/5	0.68	0.26	124,125,125,126	0
7	SO4	A	624	5/5	0.70	0.60	81,82,86,88	5
7	SO4	E	614	5/5	0.70	0.48	100,100,102,106	5
2	GOL	A	601	6/6	0.70	0.45	74,75,77,78	0
7	SO4	C	622	5/5	0.71	0.43	91,91,92,92	5
2	GOL	A	605	6/6	0.71	0.31	76,77,77,81	0
2	GOL	C	609	6/6	0.71	0.39	80,84,91,102	0
2	GOL	B	609	6/6	0.72	0.52	86,87,88,92	0
7	SO4	E	616	5/5	0.72	0.33	96,97,98,104	5
2	GOL	D	607	6/6	0.72	0.46	90,91,101,109	0
2	GOL	B	613	6/6	0.73	0.39	95,96,96,97	0
7	SO4	E	615	5/5	0.73	0.50	94,94,99,107	5
2	GOL	B	610	6/6	0.73	0.35	70,71,72,73	0
7	SO4	E	613	5/5	0.73	0.46	127,127,128,132	0
2	GOL	B	606	6/6	0.75	0.53	78,81,82,82	0
7	SO4	A	618	5/5	0.76	0.30	122,123,125,128	0
7	SO4	B	630	5/5	0.76	0.34	111,112,112,119	5
7	SO4	D	620	5/5	0.76	0.34	127,127,130,132	0
7	SO4	D	627	5/5	0.76	0.45	132,132,133,133	0
7	SO4	C	621	5/5	0.77	0.43	105,106,112,115	5
2	GOL	C	608	6/6	0.77	0.20	80,81,85,86	0
7	SO4	A	619	5/5	0.77	0.31	103,103,114,118	0
7	SO4	D	624	5/5	0.78	0.42	95,96,98,102	5
7	SO4	A	625	5/5	0.78	0.31	80,81,81,89	5
2	GOL	A	612	6/6	0.79	0.23	80,81,82,84	0
2	GOL	D	611	6/6	0.79	0.36	73,75,76,77	0
2	GOL	D	612	6/6	0.79	0.35	91,91,91,91	0
7	SO4	C	623	5/5	0.79	0.48	131,132,133,133	0
2	GOL	C	607	6/6	0.79	0.41	76,77,78,84	0
7	SO4	B	621	5/5	0.79	0.43	107,108,117,118	0
7	SO4	C	618	5/5	0.80	0.49	81,81,83,88	5
7	SO4	D	626	5/5	0.80	0.36	95,96,102,108	5
2	GOL	D	610	6/6	0.80	0.27	82,83,84,85	0
7	SO4	B	625	5/5	0.81	0.40	100,100,100,102	5
7	SO4	B	626	5/5	0.81	0.41	83,83,89,91	5
7	SO4	A	621	5/5	0.81	0.51	119,119,120,120	0
7	SO4	C	614	5/5	0.81	0.46	122,123,123,123	0
2	GOL	B	614	6/6	0.81	0.24	69,73,78,85	0
7	SO4	C	620	5/5	0.81	0.42	89,89,93,96	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	A	613	6/6	0.81	0.28	83,83,84,84	0
2	GOL	E	605	6/6	0.81	0.34	85,86,87,87	0
7	SO4	B	624	5/5	0.81	0.63	123,124,127,132	0
2	GOL	D	605	6/6	0.82	0.23	67,71,74,74	0
7	SO4	C	616	5/5	0.82	0.47	128,128,128,129	0
7	SO4	B	627	5/5	0.82	0.30	94,94,96,98	5
7	SO4	B	623	5/5	0.82	0.37	111,112,115,121	5
7	SO4	D	629	5/5	0.82	0.36	130,130,131,131	0
2	GOL	A	609	6/6	0.83	0.25	65,67,68,69	0
7	SO4	B	628	5/5	0.83	0.70	102,102,102,102	5
7	SO4	E	618	5/5	0.83	0.26	90,91,92,92	5
2	GOL	E	608	6/6	0.84	0.40	75,76,76,82	0
2	GOL	C	601	6/6	0.84	0.29	71,72,75,75	0
2	GOL	B	603	6/6	0.84	0.26	63,65,68,74	0
7	SO4	A	622	5/5	0.84	0.37	110,110,111,116	0
7	SO4	C	617	5/5	0.84	0.22	110,111,115,122	0
2	GOL	D	613	6/6	0.84	0.29	78,79,80,83	0
7	SO4	D	628	5/5	0.84	0.40	94,94,95,95	5
2	GOL	B	607	6/6	0.84	0.21	74,75,77,81	0
7	SO4	D	622	5/5	0.85	0.33	111,111,112,112	0
2	GOL	D	606	6/6	0.85	0.34	78,80,80,80	0
2	GOL	B	602	6/6	0.85	0.25	61,62,68,68	0
2	GOL	D	602	6/6	0.85	0.23	82,83,84,85	0
2	GOL	E	603	6/6	0.85	0.21	78,84,87,90	0
7	SO4	A	623	5/5	0.85	0.39	123,123,125,126	0
2	GOL	C	606	6/6	0.86	0.40	79,81,85,86	0
2	GOL	B	608	6/6	0.86	0.39	76,77,78,78	0
7	SO4	B	629	5/5	0.86	0.30	95,96,98,100	5
2	GOL	E	604	6/6	0.86	0.35	79,80,80,81	0
2	GOL	C	605	6/6	0.86	0.28	78,79,79,79	0
7	SO4	B	620	5/5	0.87	0.40	103,103,103,105	0
7	SO4	A	620	5/5	0.87	0.48	108,108,109,113	0
7	SO4	E	617	5/5	0.87	0.29	78,78,81,82	5
7	SO4	C	619	5/5	0.87	0.29	83,83,91,92	5
6	MG	E	612	1/1	0.88	0.08	62,62,62,62	0
2	GOL	A	608	6/6	0.88	0.25	60,62,62,63	0
2	GOL	B	612	6/6	0.88	0.16	58,62,67,69	0
2	GOL	C	604	6/6	0.88	0.25	87,89,89,90	0
2	GOL	A	610	6/6	0.88	0.31	82,82,83,86	0
2	GOL	E	602	6/6	0.88	0.24	72,73,73,75	0
7	SO4	D	623	5/5	0.89	0.24	133,133,134,134	5
7	SO4	B	622	5/5	0.89	0.22	104,105,105,105	5

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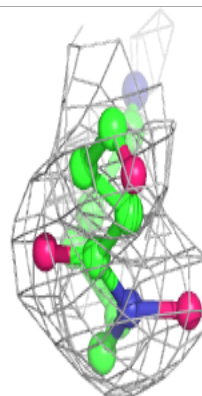
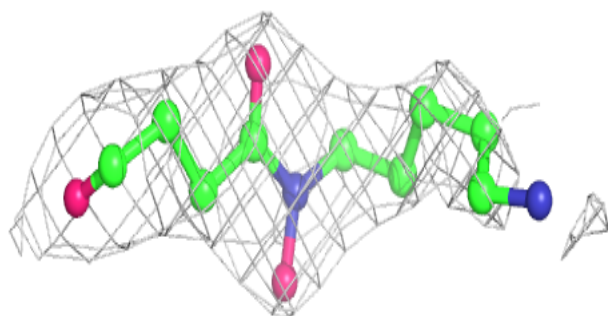
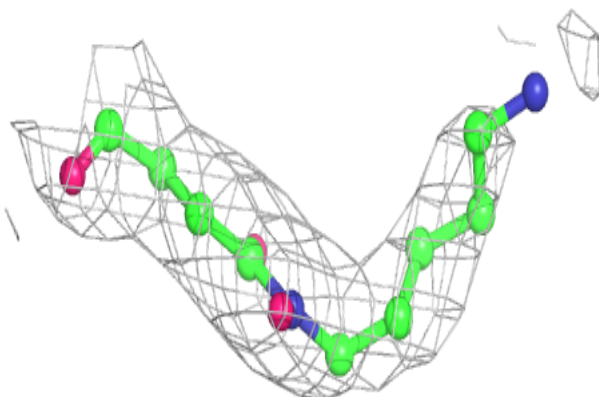
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	E	606	6/6	0.89	0.30	77,82,83,85	0
7	SO4	C	615	5/5	0.89	0.19	111,112,124,129	0
2	GOL	B	604	6/6	0.89	0.22	61,64,64,66	0
2	GOL	B	611	6/6	0.89	0.26	75,76,77,78	0
2	GOL	A	604	6/6	0.90	0.23	65,66,67,68	0
7	SO4	D	625	5/5	0.90	0.33	90,91,98,101	5
2	GOL	A	606	6/6	0.90	0.22	63,65,69,72	0
7	SO4	D	621	5/5	0.91	0.42	105,106,107,107	0
2	GOL	B	605	6/6	0.91	0.30	86,87,87,87	0
2	GOL	D	615	6/6	0.91	0.23	80,81,81,82	0
6	MG	A	617	1/1	0.92	0.20	58,58,58,58	0
7	SO4	B	619	5/5	0.92	0.32	115,115,126,129	0
2	GOL	E	601	6/6	0.92	0.17	58,60,64,66	0
2	GOL	D	609	6/6	0.92	0.19	69,70,73,84	0
2	GOL	A	603	6/6	0.93	0.22	68,69,69,70	0
2	GOL	C	602	6/6	0.93	0.19	62,64,65,66	0
2	GOL	D	601	6/6	0.93	0.22	67,69,71,75	0
3	I3U	C	610	14/15	0.93	0.21	55,60,70,75	0
3	I3U	D	616	14/15	0.93	0.23	50,58,66,73	0
2	GOL	C	603	6/6	0.93	0.25	57,59,60,70	0
2	GOL	A	611	6/6	0.94	0.28	51,52,53,54	6
3	I3U	A	614	14/15	0.94	0.20	50,59,68,74	0
2	GOL	D	604	6/6	0.94	0.23	55,57,60,62	0
3	I3U	E	609	14/15	0.94	0.16	59,68,81,84	0
2	GOL	B	601	6/6	0.94	0.24	54,56,58,62	0
2	GOL	A	602	6/6	0.94	0.20	50,58,59,60	0
2	GOL	D	603	6/6	0.95	0.19	50,51,57,57	0
6	MG	C	613	1/1	0.95	0.17	61,61,61,61	0
6	MG	D	619	1/1	0.96	0.07	57,57,57,57	0
3	I3U	B	615	14/15	0.96	0.23	52,56,62,73	0
6	MG	B	618	1/1	0.96	0.11	58,58,58,58	0
4	LMS	D	617	23/23	0.98	0.17	43,49,52,57	0
5	PO4	C	612	5/5	0.98	0.19	61,62,65,66	0
5	PO4	E	611	5/5	0.98	0.12	58,61,62,67	0
5	PO4	D	618	5/5	0.98	0.15	51,53,57,58	0
4	LMS	A	615	23/23	0.98	0.20	44,49,54,56	0
4	LMS	B	616	23/23	0.98	0.21	44,47,49,51	0
4	LMS	C	611	23/23	0.98	0.18	52,56,58,63	0
4	LMS	E	610	23/23	0.98	0.14	53,56,59,65	0
5	PO4	B	617	5/5	0.99	0.19	51,52,53,58	0
5	PO4	A	616	5/5	0.99	0.19	52,54,57,60	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.

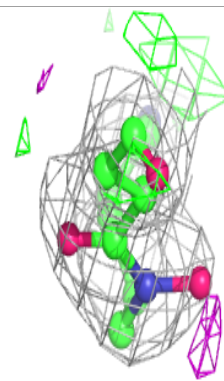
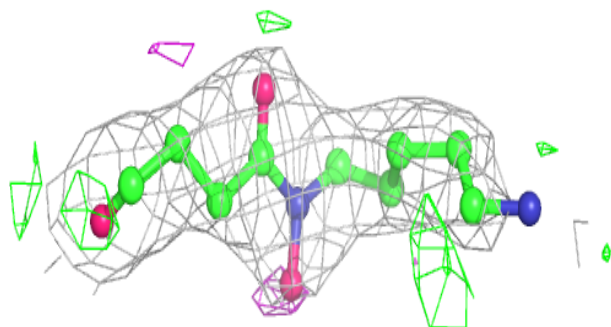
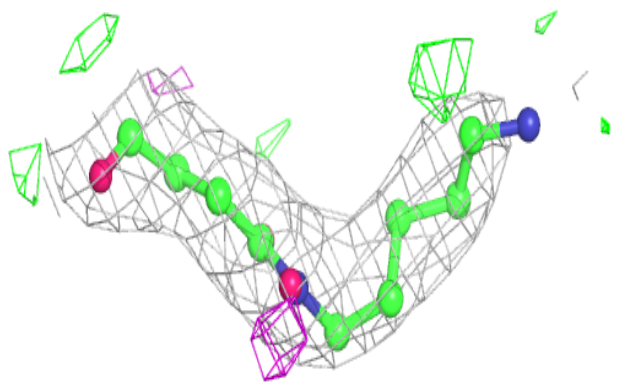
Electron density around I3U C 610:

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

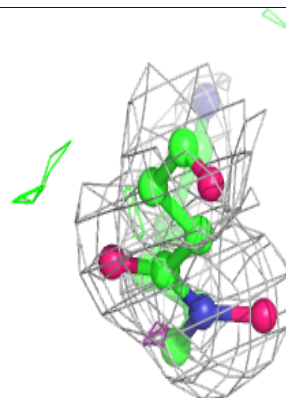
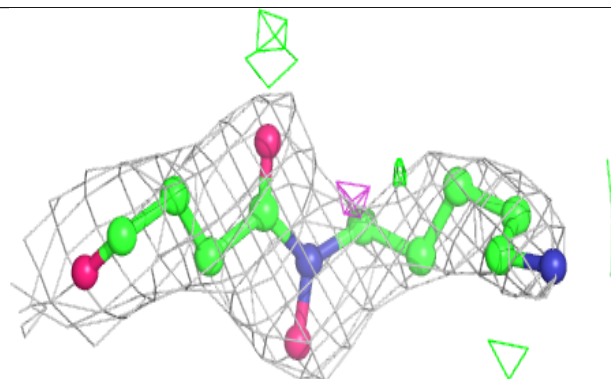
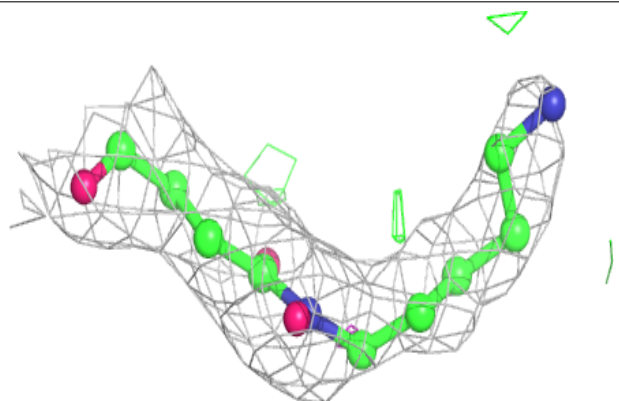


Electron density around I3U D 616:

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

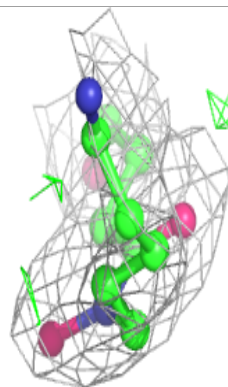
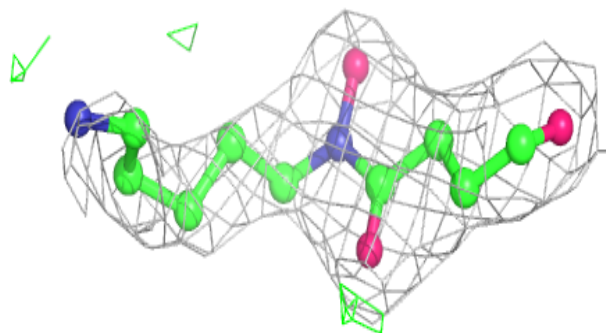
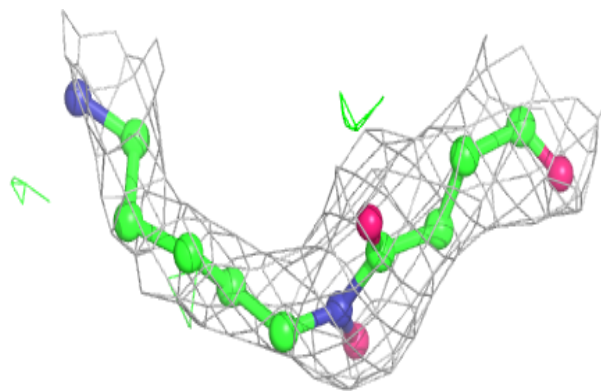
**Electron density around I3U A 614:**

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

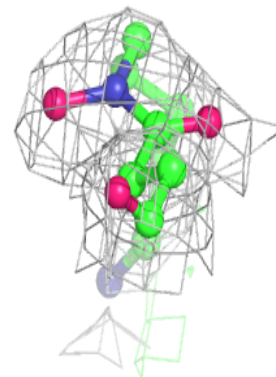
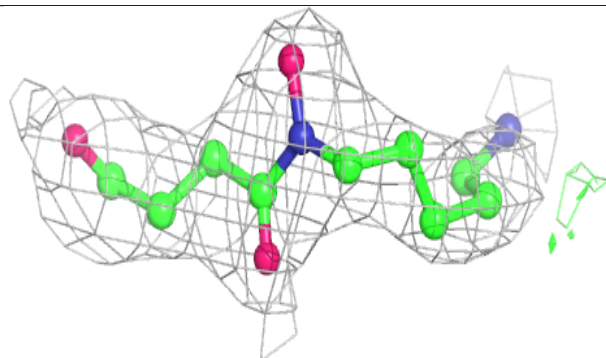
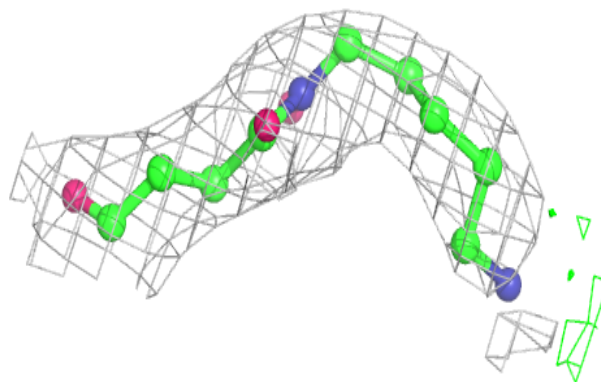


Electron density around I3U E 609:

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

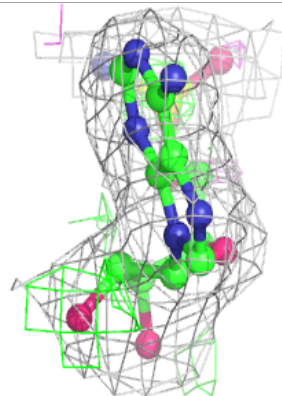
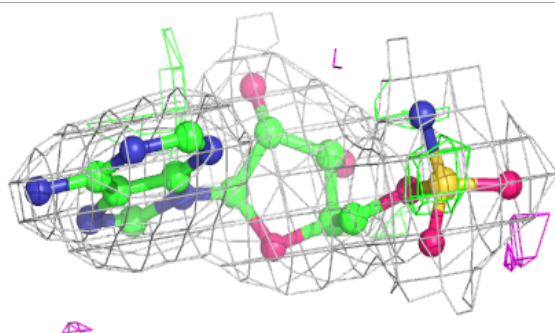
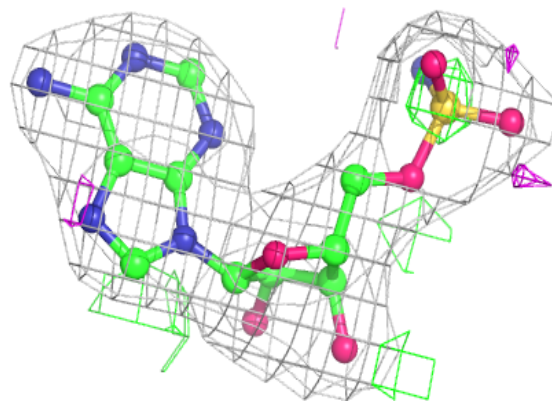
**Electron density around I3U B 615:**

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

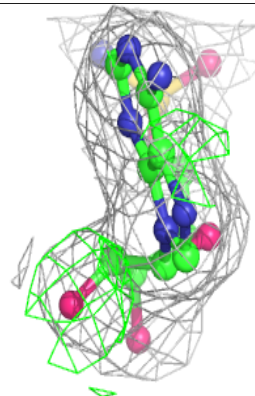
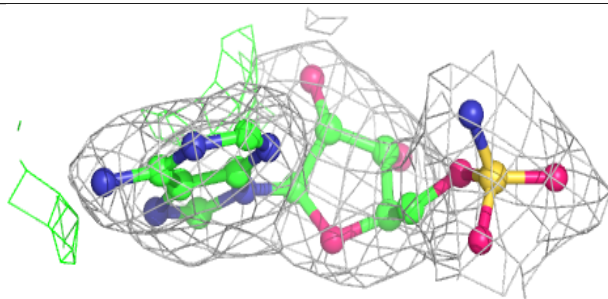
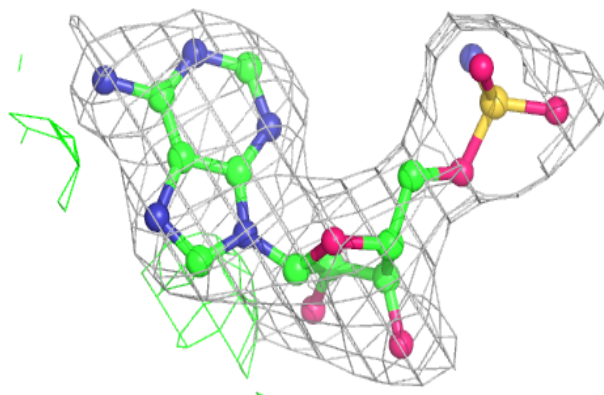


Electron density around LMS D 617:

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

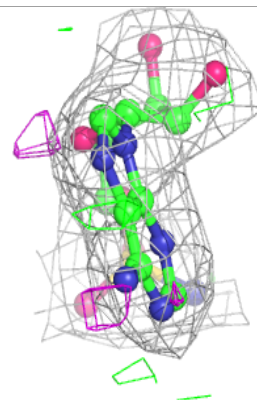
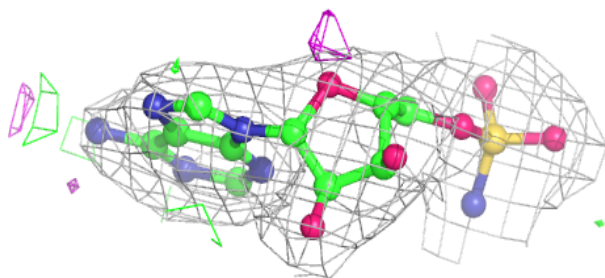
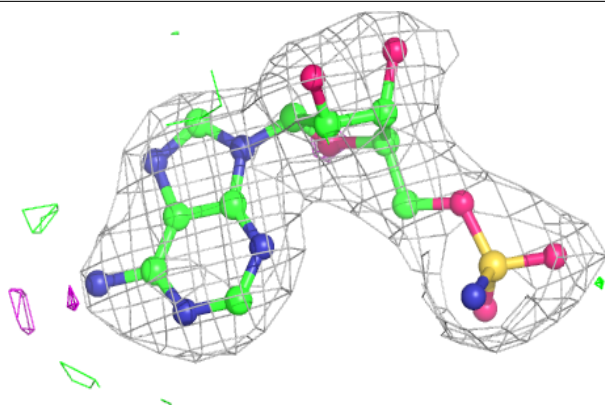
**Electron density around LMS A 615:**

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

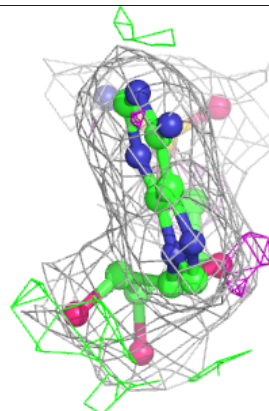
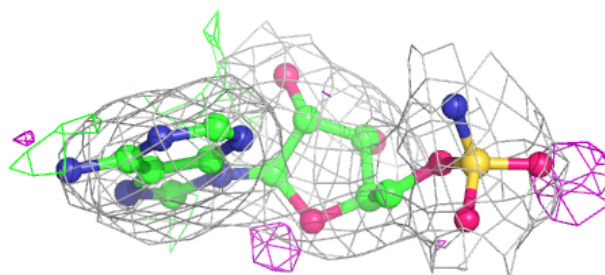
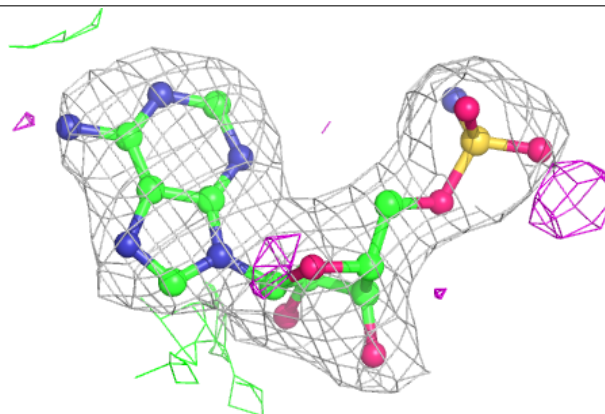


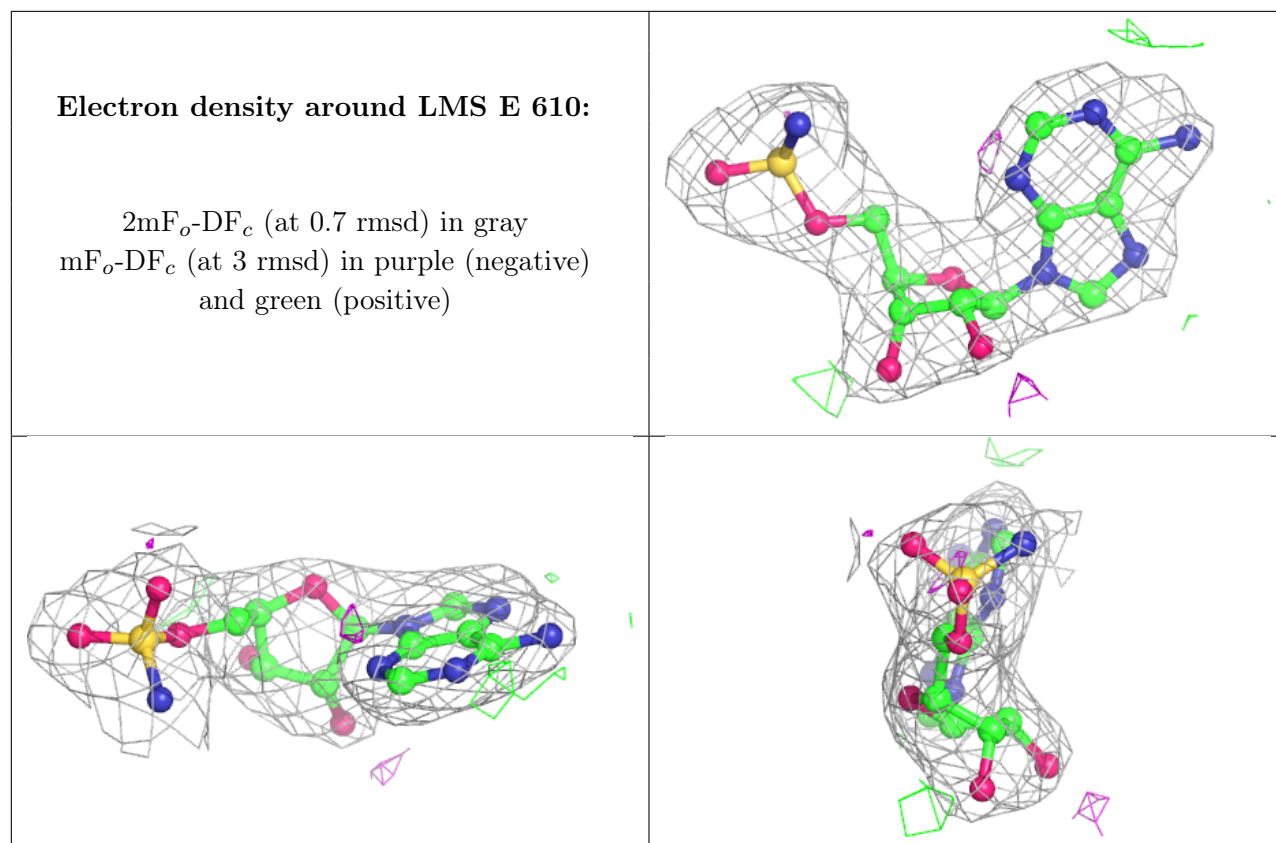
Electron density around LMS B 616:

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

**Electron density around LMS 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.