WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 05:12 PM JST

PDB ID	:	6LON
Title	:	Crystal structure of HPSG
Authors	:	Liu, J.; Zhang, Y.; Yuchi, Z.
Deposited on	:	2020-01-06
Resolution	:	2.20 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.36
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)	:	2.36

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 2.20 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.
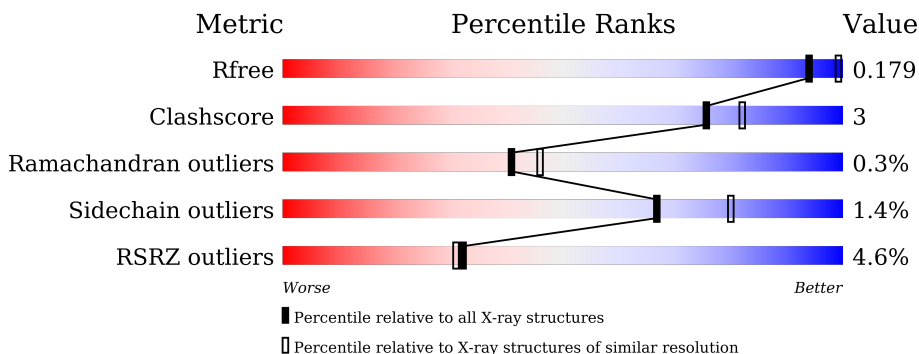
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	824	4% / 89% / 8% •
1	B	824	4% / 91% / 7% •
1	C	824	7% / 89% / 9% •
1	D	824	2% / 91% / 6% •

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LLQ	D	901	-	X	-	-
3	GOL	C	905	-	X	-	-
3	GOL	C	910	-	-	X	-
3	GOL	D	913	-	X	-	-

2   Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 52749 atoms, of which 24877 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 PFL2/glycerol dehydratase family glycyl radical enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	802	Total	C	H	N	O	S	0	4	0
			12444	4028	6100	1086	1194	36			
1	A	804	Total	C	H	N	O	S	0	4	0
			12463	4035	6104	1091	1197	36			
1	C	804	Total	C	H	N	O	S	0	6	0
			12427	4031	6073	1090	1196	37			
1	D	804	Total	C	H	N	O	S	0	6	0
			12578	4058	6184	1100	1199	37			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	129	ALA	THR	engineered mutation	UNP E5Y7I4
B	130	ALA	ASP	engineered mutation	UNP E5Y7I4
B	131	ALA	MET	engineered mutation	UNP E5Y7I4
B	132	ALA	GLN	engineered mutation	UNP E5Y7I4
A	129	ALA	THR	engineered mutation	UNP E5Y7I4
A	130	ALA	ASP	engineered mutation	UNP E5Y7I4
A	131	ALA	MET	engineered mutation	UNP E5Y7I4
A	132	ALA	GLN	engineered mutation	UNP E5Y7I4
C	129	ALA	THR	engineered mutation	UNP E5Y7I4
C	130	ALA	ASP	engineered mutation	UNP E5Y7I4
C	131	ALA	MET	engineered mutation	UNP E5Y7I4
C	132	ALA	GLN	engineered mutation	UNP E5Y7I4
D	129	ALA	THR	engineered mutation	UNP E5Y7I4
D	130	ALA	ASP	engineered mutation	UNP E5Y7I4
D	131	ALA	MET	engineered mutation	UNP E5Y7I4
D	132	ALA	GLN	engineered mutation	UNP E5Y7I4

- Molecule 2 is (2 {S})-2,3-bis(oxidanyl)propane-1-sulfonic acid (three-letter code: LLQ) (formula: $C_3H_8O_5S$) (labeled as "Ligand of Interest" by depositor).
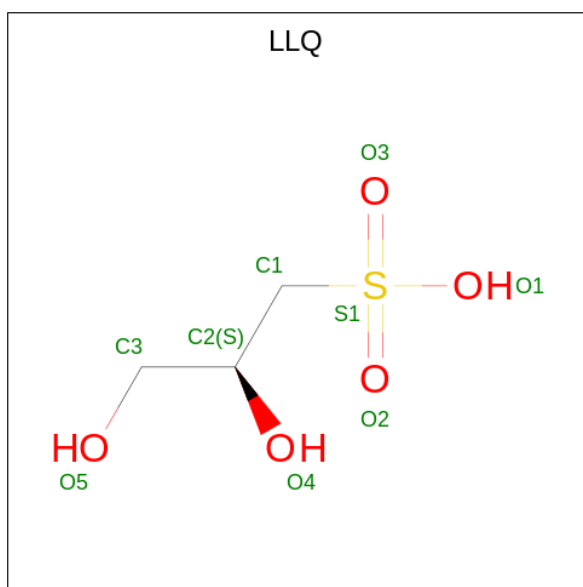
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	O	S	0	0
			16	3	7	5	1		
2	A	1	Total	C	H	O	S	0	0
			16	3	7	5	1		
2	C	1	Total	C	H	O	S	0	0
			16	3	7	5	1		
2	D	1	Total	C	H	O	S	0	0
			16	3	7	5	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
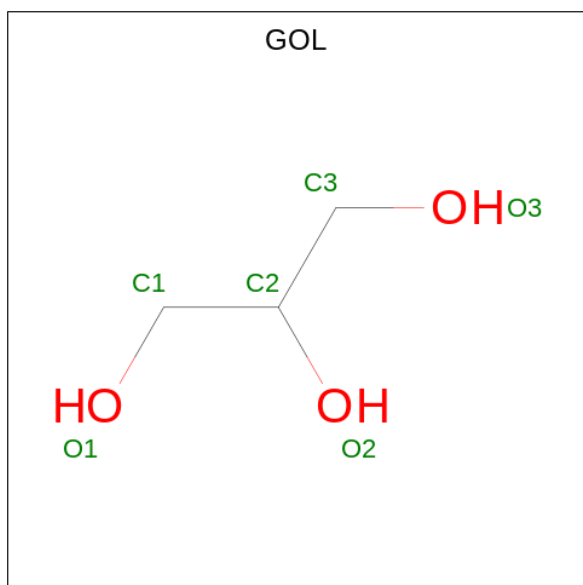
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 14	C 3	H 8	O 3	0	0
3	B	1	Total 13	C 3	H 7	O 3	0	0
3	B	1	Total 12	C 3	H 6	O 3	0	0
3	B	1	Total 11	C 3	H 5	O 3	0	0
3	B	1	Total 14	C 3	H 8	O 3	0	0
3	B	1	Total 13	C 3	H 7	O 3	0	0
3	B	1	Total 13	C 3	H 7	O 3	0	0
3	B	1	Total 13	C 3	H 7	O 3	0	0
3	B	1	Total 14	C 3	H 8	O 3	0	0
3	B	1	Total 13	C 3	H 7	O 3	0	0
3	B	1	Total 14	C 3	H 8	O 3	0	0
3	B	1	Total 13	C 3	H 7	O 3	0	0
3	B	1	Total 14	C 3	H 8	O 3	0	0
3	B	1	Total 13	C 3	H 7	O 3	0	0
3	B	1	Total 14	C 3	H 8	O 3	0	0
3	A	1	Total 14	C 3	H 8	O 3	0	0
3	A	1	Total 14	C 3	H 8	O 3	0	0
3	A	1	Total 14	C 3	H 8	O 3	0	0
3	A	1	Total 13	C 3	H 7	O 3	0	0
3	A	1	Total 13	C 3	H 7	O 3	0	0
3	A	1	Total 13	C 3	H 7	O 3	0	0
3	A	1	Total 11	C 3	H 5	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 3	H 8	O 3	0	0
3	A	1	Total 13	C 3	H 7	O 3	0	0
3	A	1	Total 13	C 3	H 7	O 3	0	0
3	A	1	Total 13	C 3	H 7	O 3	0	0
3	A	1	Total 13	C 3	H 7	O 3	0	0
3	A	1	Total 13	C 3	H 7	O 3	0	0
3	A	1	Total 14	C 3	H 8	O 3	0	0
3	A	1	Total 13	C 3	H 7	O 3	0	0
3	A	1	Total 14	C 3	H 8	O 3	0	0
3	A	1	Total 14	C 3	H 8	O 3	0	0
3	C	1	Total 14	C 3	H 8	O 3	0	0
3	C	1	Total 13	C 3	H 7	O 3	0	0
3	C	1	Total 13	C 3	H 7	O 3	0	0
3	C	1	Total 14	C 3	H 8	O 3	0	0
3	C	1	Total 13	C 3	H 7	O 3	0	0
3	C	1	Total 13	C 3	H 7	O 3	0	0
3	C	1	Total 14	C 3	H 8	O 3	0	0
3	C	1	Total 13	C 3	H 7	O 3	0	0
3	C	1	Total 14	C 3	H 8	O 3	0	0
3	C	1	Total 13	C 3	H 7	O 3	0	0
3	D	1	Total 12	C 3	H 6	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total 13	C 3	H 7	O 3	0	0
3	D	1	Total 12	C 3	H 6	O 3	0	0
3	D	1	Total 12	C 3	H 6	O 3	0	0
3	D	1	Total 11	C 3	H 5	O 3	0	0
3	D	1	Total 12	C 3	H 6	O 3	0	0
3	D	1	Total 13	C 3	H 7	O 3	0	0
3	D	1	Total 14	C 3	H 8	O 3	0	0
3	D	1	Total 13	C 3	H 7	O 3	0	0
3	D	1	Total 14	C 3	H 8	O 3	0	0
3	D	1	Total 14	C 3	H 8	O 3	0	0
3	D	1	Total 14	C 3	H 8	O 3	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	536	Total 536	O 536	0	0
5	A	544	Total 544	O 544	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	423	Total 423	O 423	0	0
5	D	554	Total 554	O 554	0	0

Full wwPDB X-ray Structure Validation Report

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.
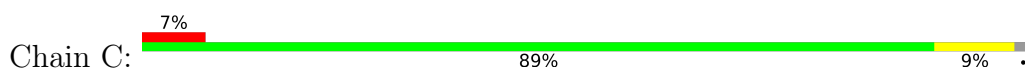
• Molecule 1: PFL2/glycerol dehydratase family glycyl radical enzyme
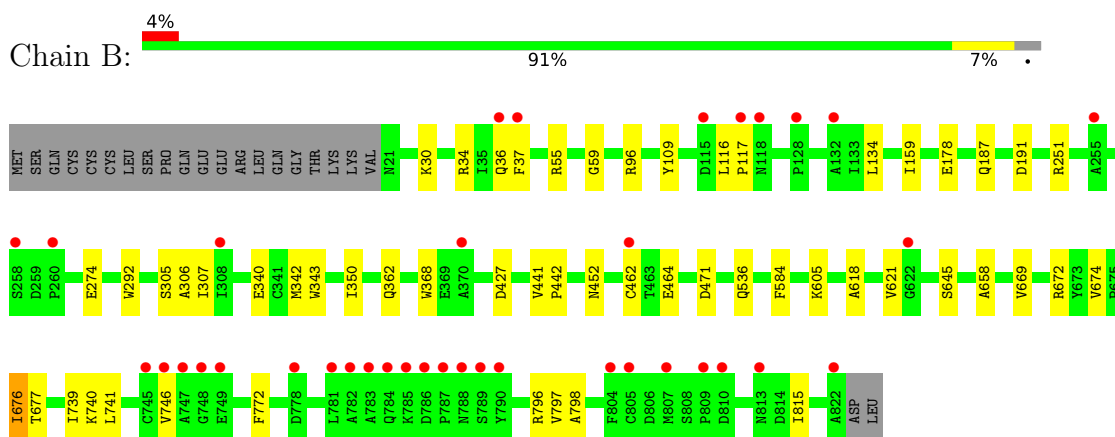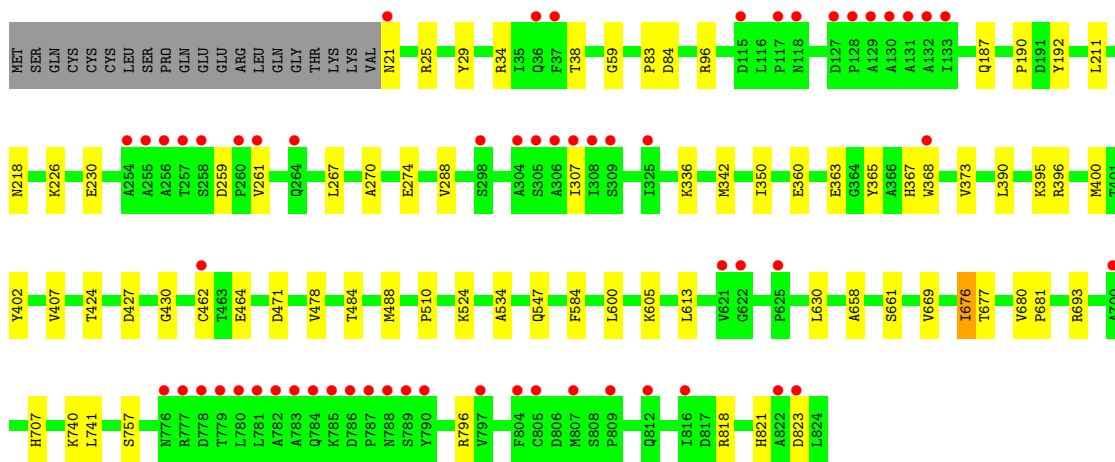

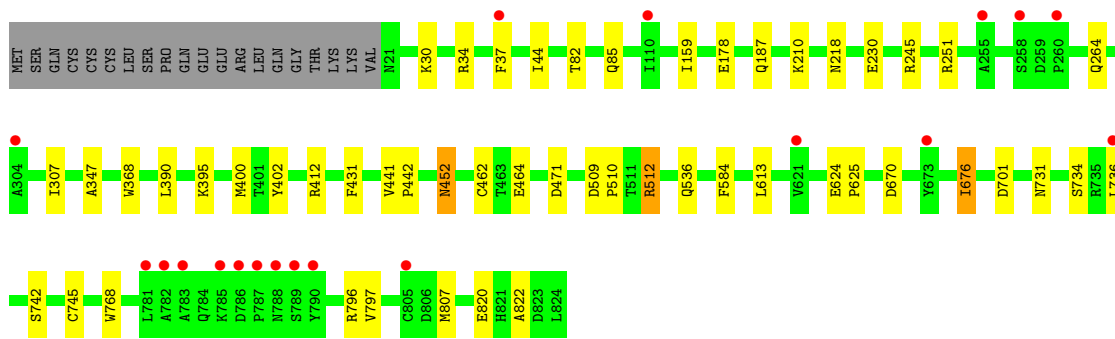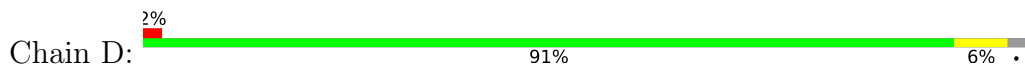• Molecule 1: PFL2/glycerol dehydratase family glycyl radical enzyme
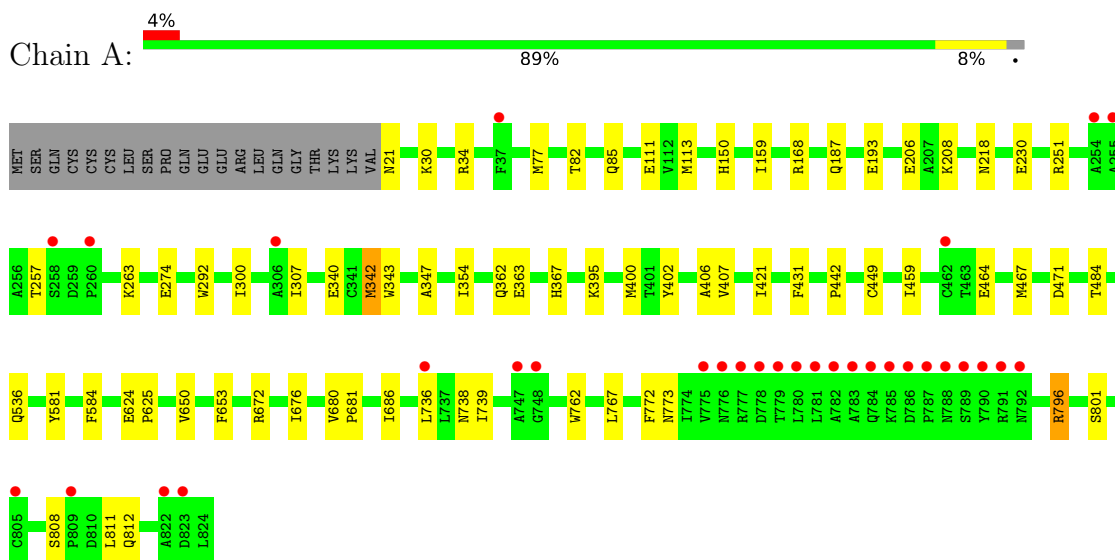
• Molecule 1: PFL2/glycerol dehydratase family glycyl radical enzyme

• Molecule 1: PFL2/glycerol dehydratase family glycyl radical enzyme

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	92.92Å 219.40Å 213.14Å 90.00° 98.04° 90.00°	Depositor
Resolution (Å)	36.25 – 2.20 36.25 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.25-2.20) 95.1 (36.25-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.143 , 0.179 0.143 , 0.179	Depositor DCC
R_{free} test set	1999 reflections (0.94%)	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 52.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	52749	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, NA, LLQ

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	0.54	0/6519	0.65	0/8852
1	B	0.54	1/6508 (0.0%)	0.66	1/8840 (0.0%)
1	C	0.53	0/6519	0.64	0/8855
1	D	0.57	0/6567	0.65	1/8914 (0.0%)
All	All	0.55	1/26113 (0.0%)	0.65	2/35461 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	797	VAL	C-O	-5.64	1.12	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	796	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	D	796	ARG	NE-CZ-NH1	5.06	122.83	120.30

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	6359	6104	6110	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6344	6100	6090	29	0
1	C	6354	6073	6078	49	0
1	D	6394	6184	6166	29	0
2	A	9	7	0	0	0
2	B	9	7	0	0	0
2	C	9	7	0	0	0
2	D	9	7	0	0	0
3	A	102	124	136	9	0
3	B	90	108	120	4	0
3	C	60	74	80	15	0
3	D	72	82	95	7	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	544	0	0	5	0
5	B	536	0	0	0	0
5	C	423	0	0	6	0
5	D	554	0	0	5	0
All	All	27872	24877	24875	156	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (156) 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)
3:A:907:GOL:HO3	3:A:907:GOL:HO1	1.15	0.86
1:C:661:SER:HA	3:C:903:GOL:H11	1.58	0.83
1:C:363:GLU:HB2	1:C:677:THR:HG21	1.71	0.72
1:B:645:SER:HA	3:B:913:GOL:H11	1.72	0.71
3:C:904:GOL:O2	3:D:914:GOL:H11	1.92	0.70
1:C:226:LYS:NZ	1:C:230:GLU:OE2	2.22	0.69
1:D:251[B]:ARG:NH2	5:D:1001:HOH:O	2.25	0.69
1:A:193:GLU:OE2	3:A:902:GOL:H31	1.94	0.68
1:D:509:ASP:O	1:D:512:ARG:HD3	1.95	0.67
3:C:903:GOL:H32	1:D:218:ASN:HA	1.77	0.66
1:C:21:ASN:N	5:C:1003:HOH:O	2.28	0.66
1:C:218:ASN:HA	3:D:913:GOL:H32	1.77	0.66
1:D:512:ARG:HH11	1:D:512:ARG:HG3	1.60	0.66
1:A:111:GLU:OE2	1:A:168:ARG:NH2	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:GLU:HA	3:A:910:GOL:H12	1.78	0.64
1:C:740:LYS:NZ	1:C:818:ARG:O	2.25	0.63
1:A:363:GLU:HG3	1:A:811:LEU:HD11	1.82	0.62
1:C:430:GLY:O	1:C:796:ARG:HD3	2.01	0.61
1:A:113:MET:CE	1:A:354:ILE:HD12	2.31	0.60
1:C:796:ARG:HD2	5:C:1086:HOH:O	2.00	0.60
1:C:96:ARG:HD2	1:C:350:ILE:HD11	1.84	0.59
1:B:159:ILE:HD11	1:B:536:GLN:OE1	2.03	0.59
1:C:707:HIS:CD2	3:C:910:GOL:H31	2.38	0.58
1:C:680:VAL:HB	1:C:681:PRO:HD3	1.84	0.58
1:A:801:SER:HB3	5:A:1059:HOH:O	2.02	0.58
1:A:251:ARG:NH2	1:A:274:GLU:OE2	2.32	0.58
1:C:818:ARG:CB	3:C:910:GOL:O3	2.52	0.58
1:A:113:MET:HE1	1:A:354:ILE:HD12	1.85	0.57
1:B:618:ALA:O	1:B:621:VAL:HG22	2.06	0.56
1:C:34:ARG:NH2	1:C:84:ASP:OD2	2.33	0.56
1:D:245:ARG:HE	3:D:910:GOL:H12	1.71	0.55
1:C:259:ASP:OD1	1:C:261:VAL:HG12	2.08	0.55
1:A:395:LYS:HE2	1:A:431:PHE:CD2	2.43	0.54
1:B:59:GLY:O	3:A:911:GOL:H32	2.07	0.54
1:B:191:ASP:OD2	3:B:902:GOL:H31	2.08	0.54
1:A:292:TRP:CZ3	1:A:342:MET:HG3	2.43	0.53
1:C:218:ASN:HA	3:D:913:GOL:C3	2.38	0.53
1:C:368:TRP:CE2	1:C:462[B]:CYS:SG	3.02	0.52
1:B:672:ARG:HG2	1:B:674:VAL:HG23	1.91	0.52
1:C:368:TRP:CH2	1:C:676:ILE:HG22	2.45	0.52
1:C:661:SER:CA	3:C:903:GOL:H11	2.35	0.51
1:C:270:ALA:O	1:C:274:GLU:HG2	2.10	0.51
3:C:909:GOL:H31	5:C:1045:HOH:O	2.09	0.51
1:B:251[B]:ARG:HH22	1:B:274:GLU:HG3	1.76	0.50
1:D:452:ASN:H	1:D:452:ASN:HD22	1.59	0.50
1:A:257:THR:O	1:A:263:LYS:NZ	2.44	0.50
1:A:406:ALA:HB1	1:A:459:ILE:HD13	1.93	0.50
1:D:512:ARG:HH11	1:D:512:ARG:CG	2.24	0.50
1:A:736:LEU:HD12	5:A:1116:HOH:O	2.11	0.49
1:B:368:TRP:CE2	1:B:462[B]:CYS:SG	3.05	0.49
1:C:600:LEU:HD12	1:C:630:LEU:HD23	1.95	0.49
1:C:360:GLU:O	1:C:677:THR:HG22	2.13	0.48
1:D:44:ILE:C	1:D:44:ILE:HD12	2.34	0.48
1:D:390:LEU:C	1:D:390:LEU:HD23	2.33	0.48
1:C:38:THR:HG22	1:C:96:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:823:ASP:OD1	1:C:823:ASP:N	2.47	0.47
3:C:910:GOL:H12	5:C:1184:HOH:O	2.14	0.47
1:A:159:ILE:HD11	1:A:536:GLN:OE1	2.13	0.47
1:C:373:VAL:CG2	1:C:407:VAL:HG22	2.45	0.47
1:A:581:TYR:CD1	1:A:672:ARG:HD3	2.49	0.47
1:C:336:LYS:HD2	1:C:390:LEU:HD11	1.97	0.47
1:C:395:LYS:NZ	1:C:400:MET:O	2.45	0.47
1:D:210:LYS:NZ	5:D:1015:HOH:O	2.47	0.47
1:D:510:PRO:HG2	1:D:613:LEU:HD11	1.97	0.47
1:C:350:ILE:HG23	1:C:365:TYR:HB3	1.95	0.47
1:B:739:ILE:HD11	1:B:772:PHE:CE1	2.51	0.46
1:C:367:HIS:CE1	1:C:402:TYR:CZ	3.04	0.46
1:A:367:HIS:CE1	1:A:402:TYR:CZ	3.03	0.46
1:B:96:ARG:HD2	1:B:350:ILE:HD11	1.98	0.46
3:A:906:GOL:H11	5:C:1142:HOH:O	2.14	0.46
1:B:368:TRP:CH2	1:B:676:ILE:HG22	2.50	0.46
1:C:336:LYS:HD2	1:C:390:LEU:CD1	2.46	0.46
1:A:773:ASN:HD21	1:A:796:ARG:H	1.63	0.46
1:D:395:LYS:HE3	1:D:431:PHE:CD2	2.51	0.46
1:B:251[B]:ARG:HH22	1:B:274:GLU:CG	2.28	0.45
1:A:484:THR:HG22	1:A:686:ILE:HD11	1.97	0.45
1:C:510:PRO:HG2	1:C:613:LEU:HD11	1.97	0.45
1:D:30:LYS:O	1:D:34:ARG:HG3	2.16	0.45
1:D:670:ASP:OD1	1:D:731:ASN:HA	2.16	0.45
1:C:190:PRO:HG2	1:C:192:TYR:CZ	2.52	0.45
1:D:368:TRP:CE2	1:D:462[B]:CYS:SG	3.09	0.45
3:D:905:GOL:H32	5:D:1112:HOH:O	2.16	0.45
1:C:547:GLN:HE22	3:C:906:GOL:C1	2.29	0.45
1:A:230[B]:GLU:OE2	5:A:1001:HOH:O	2.21	0.45
1:C:524:LYS:HZ1	3:C:909:GOL:H32	1.81	0.45
1:A:762:TRP:CD1	1:A:767:LEU:HB2	2.52	0.45
3:C:904:GOL:HO2	3:D:914:GOL:H11	1.81	0.45
1:D:159:ILE:HD11	1:D:536:GLN:OE1	2.17	0.45
1:A:736:LEU:CD1	1:A:738:ASN:OD1	2.64	0.44
1:C:677:THR:O	1:C:677:THR:CG2	2.65	0.44
1:B:340:GLU:HA	1:B:343:TRP:CD1	2.52	0.44
1:D:395:LYS:NZ	1:D:400:MET:O	2.47	0.44
1:D:807:MET:HG2	5:D:1034:HOH:O	2.17	0.44
1:C:83:PRO:O	1:C:84:ASP:HB2	2.17	0.44
1:C:707:HIS:CD2	3:C:910:GOL:C3	3.00	0.44
1:D:624:GLU:N	1:D:625:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASN:HA	3:A:905:GOL:H12	2.00	0.43
1:D:395:LYS:HE3	1:D:431:PHE:CE2	2.53	0.43
1:A:208:LYS:HZ1	3:A:919:GOL:C3	2.27	0.43
1:A:739:ILE:HD11	1:A:772:PHE:CE1	2.53	0.43
1:C:396:ARG:HD3	1:C:424:THR:HA	2.00	0.43
1:D:745:CYS:HB3	1:D:822:ALA:O	2.18	0.43
1:A:680:VAL:HB	1:A:681:PRO:CD	2.49	0.43
1:C:288:VAL:HG13	1:C:342:MET:CE	2.48	0.43
3:C:904:GOL:O3	1:D:230:GLU:OE1	2.37	0.43
1:D:368:TRP:CH2	1:D:676:ILE:HG22	2.54	0.43
1:B:441:VAL:HB	1:B:442:PRO:HD3	2.01	0.43
1:C:59:GLY:O	3:D:908:GOL:H32	2.18	0.43
1:D:347:ALA:HA	1:D:402:TYR:CZ	2.54	0.43
1:C:658:ALA:HB1	1:C:669:VAL:O	2.19	0.43
1:B:30:LYS:O	1:B:34:ARG:HG3	2.19	0.42
1:A:407:VAL:HG11	1:A:421:ILE:HD11	2.00	0.42
1:A:808:SER:O	1:A:812:GLN:HG3	2.19	0.42
1:B:621:VAL:HG23	1:B:621:VAL:O	2.18	0.42
1:B:740:LYS:NZ	1:B:815:ILE:O	2.50	0.42
1:D:82:THR:HB	1:D:85:GLN:CG	2.49	0.42
1:D:441:VAL:HB	1:D:442:PRO:HD3	2.02	0.42
1:B:305:SER:O	1:B:306:ALA:HB3	2.19	0.42
1:A:21:ASN:O	5:A:1002:HOH:O	2.22	0.42
1:A:193:GLU:OE2	3:A:902:GOL:C3	2.66	0.42
1:B:109:TYR:CE2	1:B:134:LEU:HD11	2.54	0.42
1:A:150:HIS:HE2	3:A:911:GOL:H32	1.84	0.42
1:C:478:VAL:HG11	1:C:534:ALA:HB1	2.02	0.42
1:C:484:THR:O	1:C:488:MET:HG3	2.20	0.42
1:C:741:LEU:HD23	1:C:821:HIS:HB2	2.01	0.42
1:C:547:GLN:HE22	3:C:906:GOL:H12	1.84	0.42
1:D:37:PHE:HB2	5:D:1072:HOH:O	2.18	0.42
1:A:347:ALA:HA	1:A:402:TYR:CZ	2.55	0.42
1:A:77:MET:CE	1:A:300:ILE:HD11	2.49	0.41
1:A:30:LYS:O	1:A:34:ARG:HG3	2.20	0.41
1:D:734:SER:HA	1:D:768:TRP:CD2	2.56	0.41
1:A:347:ALA:HB2	1:A:400:MET:HE2	2.03	0.41
1:A:363:GLU:CG	1:A:811:LEU:HD11	2.50	0.41
1:B:452:ASN:HD22	3:B:910:GOL:H12	1.85	0.41
1:A:77:MET:HE2	5:A:1120:HOH:O	2.21	0.41
1:B:658:ALA:HB1	1:B:669:VAL:O	2.19	0.41
1:D:742:SER:OG	1:D:820:GLU:OE1	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:TRP:CE3	1:B:342:MET:HG3	2.56	0.41
1:B:36:GLN:HG3	1:B:37:PHE:CD2	2.56	0.41
1:B:116:LEU:N	1:B:117:PRO:CD	2.84	0.41
1:B:741:LEU:HD23	1:B:746:VAL:HG11	2.03	0.41
3:C:910:GOL:H2	5:C:1307:HOH:O	2.21	0.41
1:A:449:CYS:SG	1:A:467:MET:HG2	2.61	0.41
1:A:624:GLU:N	1:A:625:PRO:CD	2.84	0.41
1:A:82:THR:HB	1:A:85:GLN:CG	2.51	0.40
1:A:340:GLU:HA	1:A:343:TRP:CD1	2.56	0.40
1:C:96:ARG:HB3	1:C:350:ILE:HD13	2.02	0.40
1:C:211:LEU:HD23	1:C:211:LEU:O	2.21	0.40
1:C:360:GLU:HB3	1:C:681:PRO:HG3	2.02	0.40
1:B:251[B]:ARG:NH2	1:B:274:GLU:HG3	2.36	0.40
1:B:292:TRP:CZ3	1:B:342:MET:HG3	2.57	0.40
1:B:452:ASN:HD22	3:B:910:GOL:C1	2.34	0.40
1:C:25:ARG:O	1:C:29:TYR:HD2	2.05	0.40
1:B:677:THR:HG22	1:B:798:ALA:CB	2.51	0.40
1:A:650:VAL:HA	1:A:653:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	806/824 (98%)	781 (97%)	23 (3%)	2 (0%)	47	55
1	B	804/824 (98%)	783 (97%)	19 (2%)	2 (0%)	47	55
1	C	808/824 (98%)	776 (96%)	29 (4%)	3 (0%)	34	37
1	D	808/824 (98%)	780 (96%)	26 (3%)	2 (0%)	47	55
All	All	3226/3296 (98%)	3120 (97%)	97 (3%)	9 (0%)	41	46

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	307	ILE
1	A	307	ILE
1	C	307	ILE
1	C	605	LYS
1	D	307	ILE
1	B	676	ILE
1	A	676	ILE
1	C	676	ILE
1	D	676	ILE

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	662/708 (94%)	654 (99%)	8 (1%)	71	83
1	B	662/708 (94%)	653 (99%)	9 (1%)	67	80
1	C	659/708 (93%)	652 (99%)	7 (1%)	73	85
1	D	672/708 (95%)	660 (98%)	12 (2%)	59	72
All	All	2655/2832 (94%)	2619 (99%)	36 (1%)	67	80

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	55	ARG
1	B	178	GLU
1	B	187	GLN
1	B	362	GLN
1	B	427	ASP
1	B	464	GLU
1	B	471	ASP
1	B	584	PHE
1	B	605	LYS
1	A	187	GLN
1	A	342	MET
1	A	362	GLN
1	A	442	PRO

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Mol	Chain	Res	Type
1	A	464	GLU
1	A	471	ASP
1	A	584	PHE
1	A	796	ARG
1	C	187	GLN
1	C	427	ASP
1	C	464	GLU
1	C	471	ASP
1	C	584	PHE
1	C	693	ARG
1	C	757	SER
1	D	178	GLU
1	D	187	GLN
1	D	264	GLN
1	D	412	ARG
1	D	452	ASN
1	D	464	GLU
1	D	471	ASP
1	D	512	ARG
1	D	584	PHE
1	D	701	ASP
1	D	736	LEU
1	D	797	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 62 ligands modelled in this entry, 4 are monoatomic - leaving 58 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
3	GOL	C	909	-	5,5,5	0.35	0	5,5,5	0.52	0
3	GOL	C	906	-	5,5,5	0.22	0	5,5,5	0.83	0
3	GOL	C	908	-	5,5,5	0.15	0	5,5,5	0.75	0
3	GOL	C	904	-	5,5,5	0.76	0	5,5,5	0.63	0
3	GOL	C	905	-	5,5,5	0.72	0	5,5,5	1.72	2 (40%)
3	GOL	D	911	-	5,5,5	0.35	0	5,5,5	0.63	0
2	LLQ	A	901	-	8,8,8	1.34	0	9,11,11	2.61	3 (33%)
2	LLQ	D	901	-	8,8,8	1.43	2 (25%)	9,11,11	2.57	4 (44%)
3	GOL	D	913	-	5,5,5	1.55	1 (20%)	5,5,5	2.90	3 (60%)
3	GOL	D	906	-	5,5,5	0.39	0	5,5,5	0.69	0
3	GOL	B	903	-	5,5,5	0.54	0	5,5,5	1.18	1 (20%)
3	GOL	B	913	-	5,5,5	0.29	0	5,5,5	1.32	0
3	GOL	A	917	-	5,5,5	0.41	0	5,5,5	0.63	0
3	GOL	D	903	-	5,5,5	0.31	0	5,5,5	0.60	0
3	GOL	A	907	-	5,5,5	0.54	0	5,5,5	1.20	0
3	GOL	A	913	-	5,5,5	0.35	0	5,5,5	0.53	0
3	GOL	D	910	-	5,5,5	0.48	0	5,5,5	0.56	0
3	GOL	A	903	-	5,5,5	0.15	0	5,5,5	0.78	0
3	GOL	A	902	-	5,5,5	0.23	0	5,5,5	0.68	0
3	GOL	B	907	-	5,5,5	0.46	0	5,5,5	0.50	0
3	GOL	C	910	-	5,5,5	0.15	0	5,5,5	1.25	1 (20%)
3	GOL	B	912	-	5,5,5	0.80	0	5,5,5	0.54	0
3	GOL	B	902	-	5,5,5	0.43	0	5,5,5	0.53	0
3	GOL	C	911	-	5,5,5	0.41	0	5,5,5	0.79	0
3	GOL	A	919	-	5,5,5	0.08	0	5,5,5	0.47	0
3	GOL	C	907	-	5,5,5	0.36	0	5,5,5	1.00	0
3	GOL	A	908	-	5,5,5	0.66	0	5,5,5	0.97	0
3	GOL	D	914	-	5,5,5	0.39	0	5,5,5	0.61	0
3	GOL	A	914	-	5,5,5	0.18	0	5,5,5	0.67	0
2	LLQ	C	901	-	8,8,8	1.42	1 (12%)	9,11,11	2.87	4 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	GOL	C	902	-	5,5,5	0.35	0	5,5,5	0.85	0
3	GOL	D	904	-	5,5,5	0.49	0	5,5,5	0.42	0
3	GOL	D	907	-	5,5,5	0.47	0	5,5,5	0.42	0
3	GOL	A	909	-	5,5,5	0.26	0	5,5,5	0.44	0
3	GOL	D	908	-	5,5,5	0.35	0	5,5,5	1.05	0
3	GOL	B	911	-	5,5,5	0.44	0	5,5,5	1.29	1 (20%)
3	GOL	A	906	-	5,5,5	0.31	0	5,5,5	1.00	0
3	GOL	D	902	-	5,5,5	0.33	0	5,5,5	0.79	0
3	GOL	D	909	-	5,5,5	0.50	0	5,5,5	0.89	0
3	GOL	C	903	-	5,5,5	0.78	0	5,5,5	1.91	2 (40%)
3	GOL	B	906	-	5,5,5	0.52	0	5,5,5	0.50	0
3	GOL	B	904	-	5,5,5	0.41	0	5,5,5	0.48	0
2	LLQ	B	901	-	8,8,8	1.54	2 (25%)	9,11,11	3.10	4 (44%)
3	GOL	A	915	-	5,5,5	0.26	0	5,5,5	0.55	0
3	GOL	A	918	-	5,5,5	0.28	0	5,5,5	1.22	0
3	GOL	A	911	-	5,5,5	0.53	0	5,5,5	0.82	0
3	GOL	D	905	-	5,5,5	0.57	0	5,5,5	0.86	0
3	GOL	A	904	-	5,5,5	0.13	0	5,5,5	0.43	0
3	GOL	B	914	-	5,5,5	0.21	0	5,5,5	0.28	0
3	GOL	B	915	-	5,5,5	0.30	0	5,5,5	1.12	0
3	GOL	A	910	-	5,5,5	0.39	0	5,5,5	0.70	0
3	GOL	B	917	-	5,5,5	0.31	0	5,5,5	0.87	0
3	GOL	A	912	-	5,5,5	0.41	0	5,5,5	0.90	0
3	GOL	B	909	-	5,5,5	0.55	0	5,5,5	0.96	0
3	GOL	B	910	-	5,5,5	0.38	0	5,5,5	0.64	0
3	GOL	A	905	-	5,5,5	0.34	0	5,5,5	0.66	0
3	GOL	B	908	-	5,5,5	0.38	0	5,5,5	0.39	0
3	GOL	B	905	-	5,5,5	0.24	0	5,5,5	1.18	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
3	GOL	C	909	-	-	0/4/4/4	-
3	GOL	C	906	-	-	2/4/4/4	-
3	GOL	C	908	-	-	0/4/4/4	-
3	GOL	C	904	-	-	3/4/4/4	-
3	GOL	C	905	-	-	4/4/4/4	-
3	GOL	D	911	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LLQ	A	901	-	-	2/7/7/7	-
2	LLQ	D	901	-	-	5/7/7/7	-
3	GOL	D	913	-	-	4/4/4/4	-
3	GOL	D	906	-	-	2/4/4/4	-
3	GOL	B	903	-	-	2/4/4/4	-
3	GOL	B	913	-	-	2/4/4/4	-
3	GOL	A	917	-	-	2/4/4/4	-
3	GOL	D	903	-	-	0/4/4/4	-
3	GOL	A	907	-	-	0/4/4/4	-
3	GOL	A	913	-	-	2/4/4/4	-
3	GOL	D	910	-	-	0/4/4/4	-
3	GOL	A	903	-	-	2/4/4/4	-
3	GOL	A	902	-	-	0/4/4/4	-
3	GOL	B	907	-	-	2/4/4/4	-
3	GOL	C	910	-	-	1/4/4/4	-
3	GOL	B	912	-	-	3/4/4/4	-
3	GOL	B	902	-	-	0/4/4/4	-
3	GOL	C	911	-	-	4/4/4/4	-
3	GOL	A	919	-	-	2/4/4/4	-
3	GOL	C	907	-	-	2/4/4/4	-
3	GOL	A	908	-	-	0/4/4/4	-
3	GOL	D	914	-	-	0/4/4/4	-
3	GOL	A	914	-	-	2/4/4/4	-
2	LLQ	C	901	-	-	0/7/7/7	-
3	GOL	C	902	-	-	0/4/4/4	-
3	GOL	D	904	-	-	0/4/4/4	-
3	GOL	D	907	-	-	2/4/4/4	-
3	GOL	A	909	-	-	0/4/4/4	-
3	GOL	D	908	-	-	2/4/4/4	-
3	GOL	B	911	-	-	0/4/4/4	-
3	GOL	A	906	-	-	2/4/4/4	-
3	GOL	D	902	-	-	0/4/4/4	-
3	GOL	D	909	-	-	2/4/4/4	-
3	GOL	C	903	-	-	1/4/4/4	-
3	GOL	B	906	-	-	4/4/4/4	-
3	GOL	B	904	-	-	0/4/4/4	-
2	LLQ	B	901	-	-	2/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	915	-	-	3/4/4/4	-
3	GOL	A	918	-	-	2/4/4/4	-
3	GOL	A	911	-	-	2/4/4/4	-
3	GOL	D	905	-	-	1/4/4/4	-
3	GOL	A	904	-	-	2/4/4/4	-
3	GOL	B	914	-	-	2/4/4/4	-
3	GOL	B	915	-	-	0/4/4/4	-
3	GOL	A	910	-	-	0/4/4/4	-
3	GOL	B	917	-	-	4/4/4/4	-
3	GOL	A	912	-	-	0/4/4/4	-
3	GOL	B	909	-	-	2/4/4/4	-
3	GOL	B	910	-	-	2/4/4/4	-
3	GOL	A	905	-	-	0/4/4/4	-
3	GOL	B	908	-	-	2/4/4/4	-
3	GOL	B	905	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	LLQ	O3-S1	3.08	1.54	1.45
2	C	901	LLQ	O2-S1	2.59	1.52	1.45
2	D	901	LLQ	O3-S1	2.26	1.51	1.45
2	D	901	LLQ	O2-S1	2.10	1.51	1.45
3	D	913	GOL	C3-C2	-2.08	1.43	1.51
2	B	901	LLQ	O2-S1	2.01	1.51	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	901	LLQ	O2-S1-C1	6.85	115.08	106.94
2	C	901	LLQ	O1-S1-C1	5.53	114.55	105.74
3	D	913	GOL	C3-C2-C1	-5.20	91.49	111.70
2	A	901	LLQ	O2-S1-C1	4.94	112.81	106.94
2	D	901	LLQ	O2-S1-C1	4.79	112.63	106.94
2	D	901	LLQ	O1-S1-C1	4.41	112.77	105.74
2	C	901	LLQ	O2-S1-C1	4.34	112.09	106.94
2	B	901	LLQ	O1-S1-C1	-4.24	98.98	105.74
2	A	901	LLQ	O1-S1-C1	4.19	112.41	105.74
2	C	901	LLQ	O3-S1-C1	-3.45	102.83	106.94
2	B	901	LLQ	O3-S1-C1	3.40	110.97	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	905	GOL	C3-C2-C1	-3.19	99.32	111.70
2	C	901	LLQ	O1-S1-O3	-2.91	104.17	111.27
3	C	903	GOL	O2-C2-C1	2.75	121.26	109.12
3	D	913	GOL	O2-C2-C1	2.67	120.86	109.12
3	C	903	GOL	O3-C3-C2	-2.61	97.68	110.20
2	A	901	LLQ	O4-C2-C3	-2.58	97.74	109.12
3	C	910	GOL	C3-C2-C1	-2.52	101.89	111.70
2	B	901	LLQ	C3-C2-C1	-2.52	102.70	111.65
2	D	901	LLQ	C3-C2-C1	-2.38	103.20	111.65
3	B	911	GOL	C3-C2-C1	-2.12	103.46	111.70
3	C	905	GOL	O2-C2-C3	2.11	118.44	109.12
3	D	913	GOL	O2-C2-C3	-2.07	100.00	109.12
2	D	901	LLQ	O3-S1-C1	-2.03	104.52	106.94
3	B	903	GOL	O3-C3-C2	2.03	119.93	110.20

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	LLQ	C2-C1-S1-O1
2	D	901	LLQ	C2-C1-S1-O3
3	B	903	GOL	O1-C1-C2-C3
3	B	905	GOL	C1-C2-C3-O3
3	B	907	GOL	O1-C1-C2-C3
3	B	908	GOL	C1-C2-C3-O3
3	B	908	GOL	O2-C2-C3-O3
3	B	910	GOL	O1-C1-C2-O2
3	B	910	GOL	O1-C1-C2-C3
3	B	913	GOL	C1-C2-C3-O3
3	B	917	GOL	C1-C2-C3-O3
3	A	904	GOL	O1-C1-C2-C3
3	A	906	GOL	O1-C1-C2-C3
3	A	911	GOL	O1-C1-C2-C3
3	A	917	GOL	C1-C2-C3-O3
3	A	918	GOL	O1-C1-C2-C3
3	C	903	GOL	C1-C2-C3-O3
3	C	905	GOL	O1-C1-C2-C3
3	C	905	GOL	C1-C2-C3-O3
3	C	906	GOL	C1-C2-C3-O3
3	C	907	GOL	O1-C1-C2-C3
3	D	907	GOL	O1-C1-C2-C3
3	D	908	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	D	911	GOL	C1-C2-C3-O3
3	D	913	GOL	O1-C1-C2-C3
3	A	911	GOL	O1-C1-C2-O2
3	D	907	GOL	O1-C1-C2-O2
3	B	906	GOL	O1-C1-C2-C3
3	B	906	GOL	C1-C2-C3-O3
3	B	909	GOL	C1-C2-C3-O3
3	B	914	GOL	C1-C2-C3-O3
3	A	903	GOL	O1-C1-C2-C3
3	A	913	GOL	O1-C1-C2-C3
3	A	914	GOL	O1-C1-C2-C3
3	A	915	GOL	C1-C2-C3-O3
3	A	919	GOL	O1-C1-C2-C3
3	C	904	GOL	O1-C1-C2-C3
3	C	904	GOL	C1-C2-C3-O3
3	C	910	GOL	C1-C2-C3-O3
3	C	911	GOL	O1-C1-C2-C3
3	D	905	GOL	O1-C1-C2-C3
3	D	911	GOL	O1-C1-C2-C3
3	D	913	GOL	C1-C2-C3-O3
3	B	907	GOL	O1-C1-C2-O2
3	B	913	GOL	O2-C2-C3-O3
3	B	917	GOL	O2-C2-C3-O3
3	A	903	GOL	O1-C1-C2-O2
3	A	914	GOL	O1-C1-C2-O2
3	A	917	GOL	O2-C2-C3-O3
3	A	918	GOL	O1-C1-C2-O2
3	C	905	GOL	O1-C1-C2-O2
3	C	905	GOL	O2-C2-C3-O3
3	D	908	GOL	O1-C1-C2-O2
3	D	911	GOL	O2-C2-C3-O3
3	D	913	GOL	O1-C1-C2-O2
3	B	903	GOL	O1-C1-C2-O2
3	B	905	GOL	O2-C2-C3-O3
3	A	906	GOL	O1-C1-C2-O2
3	A	919	GOL	O1-C1-C2-O2
3	C	906	GOL	O2-C2-C3-O3
3	C	907	GOL	O1-C1-C2-O2
2	D	901	LLQ	C1-C2-C3-O5
3	B	909	GOL	O2-C2-C3-O3
3	B	914	GOL	O2-C2-C3-O3
3	B	917	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	904	GOL	O1-C1-C2-O2
3	A	915	GOL	O2-C2-C3-O3
3	C	911	GOL	O1-C1-C2-O2
3	D	913	GOL	O2-C2-C3-O3
3	B	906	GOL	O2-C2-C3-O3
3	B	912	GOL	O1-C1-C2-O2
3	B	912	GOL	O2-C2-C3-O3
3	A	913	GOL	O1-C1-C2-O2
3	C	911	GOL	O2-C2-C3-O3
2	D	901	LLQ	C2-C1-S1-O1
3	D	906	GOL	C1-C2-C3-O3
2	B	901	LLQ	C2-C1-S1-O3
2	A	901	LLQ	C2-C1-S1-O2
2	D	901	LLQ	C2-C1-S1-O2
3	B	906	GOL	O1-C1-C2-O2
3	D	909	GOL	O2-C2-C3-O3
3	B	917	GOL	O1-C1-C2-C3
3	C	911	GOL	C1-C2-C3-O3
3	C	904	GOL	O1-C1-C2-O2
3	D	906	GOL	O2-C2-C3-O3
2	D	901	LLQ	O4-C2-C3-O5
2	B	901	LLQ	C2-C1-S1-O1
3	B	912	GOL	O1-C1-C2-C3
3	D	909	GOL	O1-C1-C2-C3
3	A	915	GOL	O1-C1-C2-O2

There are no ring outliers.

20 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	909	GOL	2	0
3	C	906	GOL	2	0
3	C	904	GOL	3	0
3	D	913	GOL	2	0
3	B	913	GOL	1	0
3	A	907	GOL	1	0
3	D	910	GOL	1	0
3	A	902	GOL	2	0
3	C	910	GOL	5	0
3	B	902	GOL	1	0
3	A	919	GOL	1	0
3	D	914	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	908	GOL	1	0
3	A	906	GOL	1	0
3	C	903	GOL	3	0
3	A	911	GOL	2	0
3	D	905	GOL	1	0
3	A	910	GOL	1	0
3	B	910	GOL	2	0
3	A	905	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 then 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 LLQ A 901

Ligand LLQ D 901

Bond lengths

Bond angles

Torsions

Rings

Ligand LLQ C 901

Bond lengths

Bond angles

Torsions

Rings

Ligand LLQ B 901

Bond lengths

Bond angles

Torsions

Rings
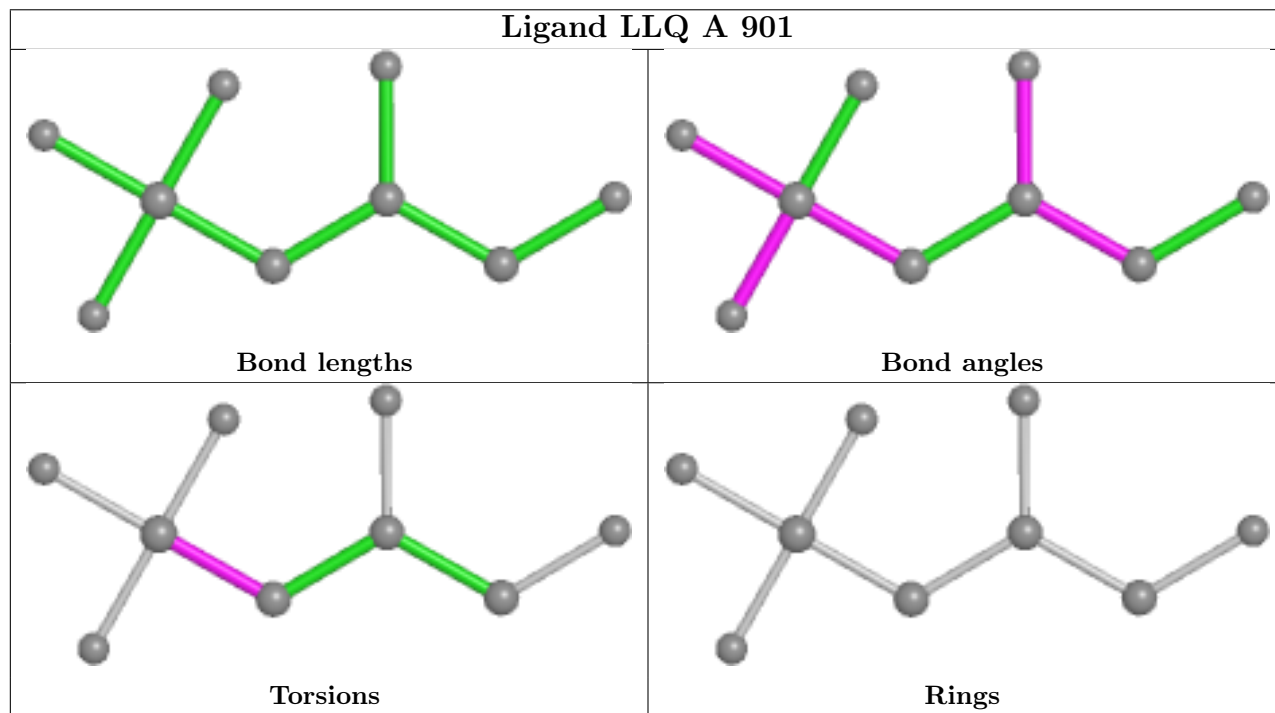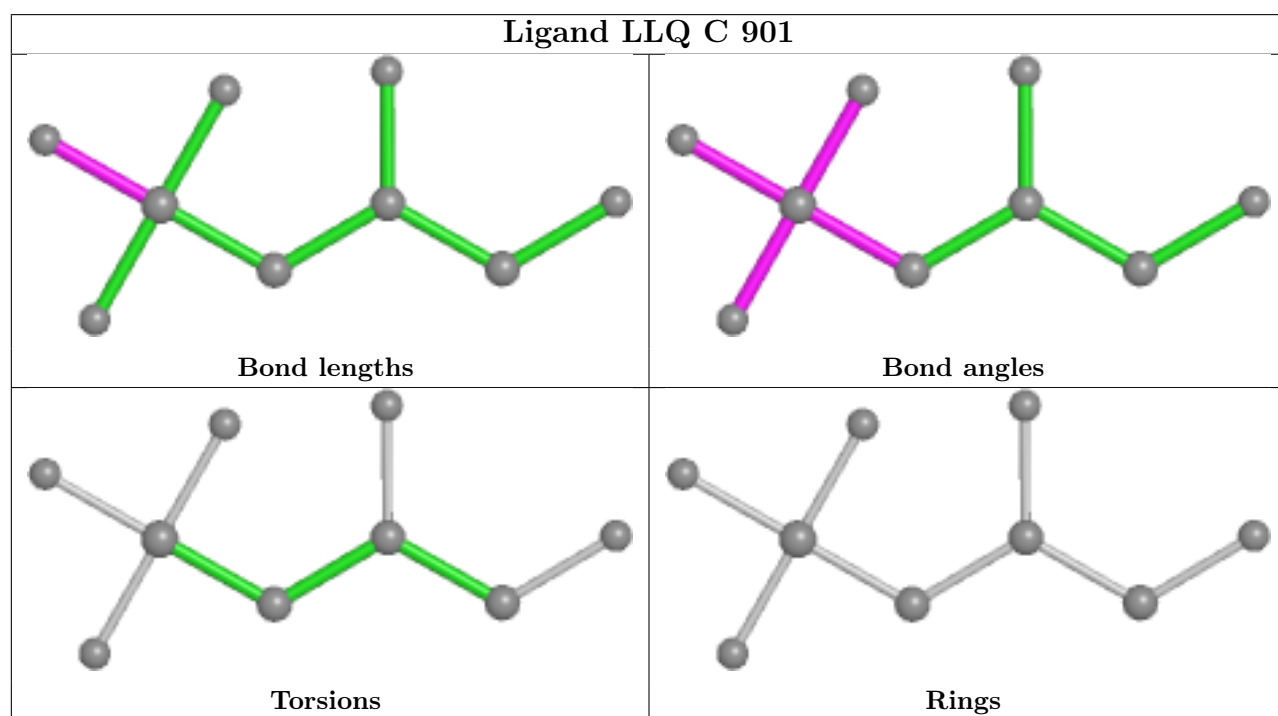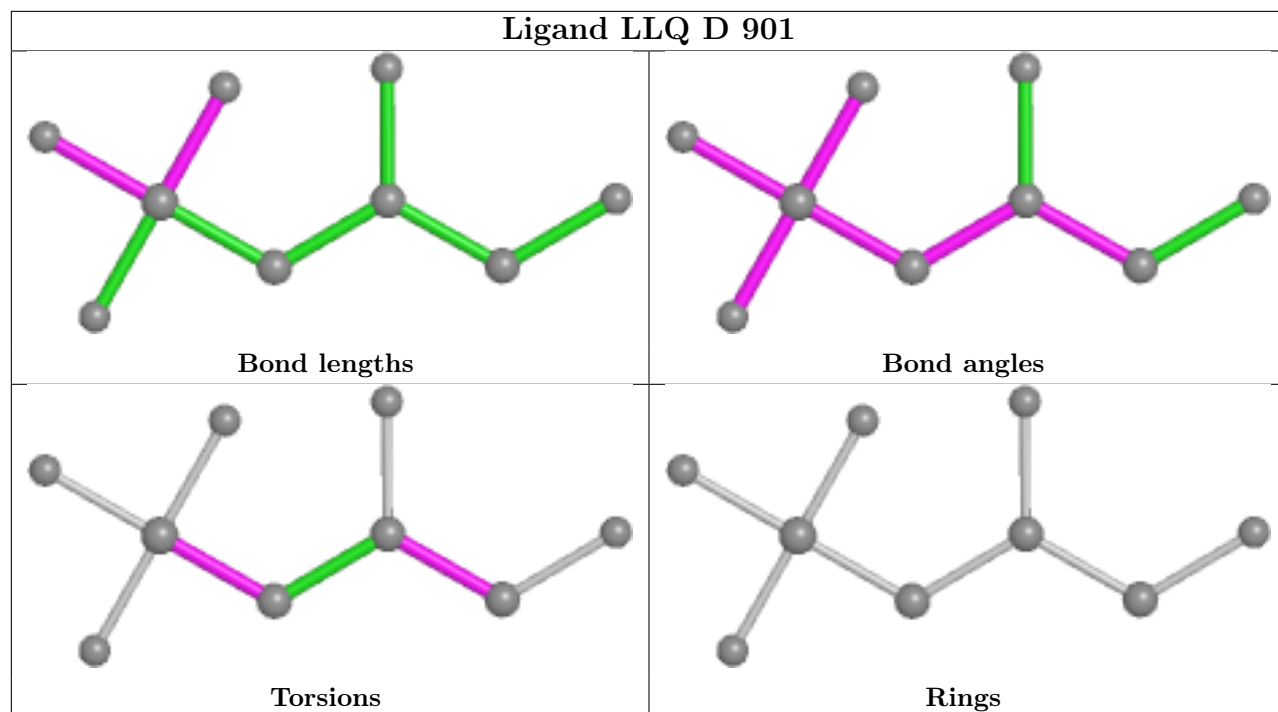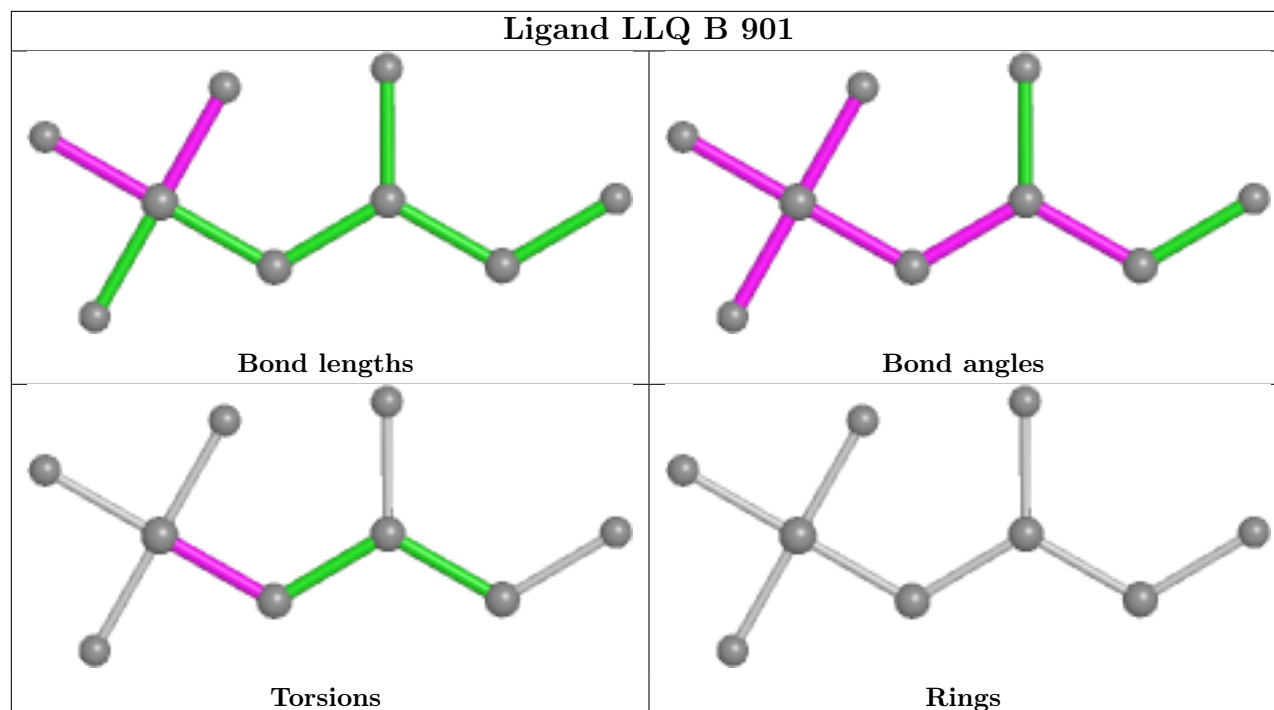
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	804/824 (97%)	-0.17	32 (3%)	38	36	16, 26, 49, 80	0
1	B	802/824 (97%)	-0.14	37 (4%)	32	31	16, 27, 50, 75	0
1	C	804/824 (97%)	0.09	59 (7%)	15	14	18, 34, 61, 83	0
1	D	804/824 (97%)	-0.27	19 (2%)	59	56	16, 25, 44, 68	0
All	All	3214/3296 (97%)	-0.12	147 (4%)	32	31	16, 27, 54, 83	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	790	TYR	6.5
1	B	790	TYR	6.2
1	C	790	TYR	5.8
1	A	789	SER	5.7
1	C	783	ALA	5.3
1	A	787	PRO	5.3
1	A	823	ASP	5.2
1	C	781	LEU	5.0
1	C	621	VAL	4.9
1	C	822	ALA	4.7
1	A	788	ASN	4.6
1	C	786	ASP	4.6
1	B	783	ALA	4.6
1	A	778	ASP	4.6
1	A	805	CYS	4.5
1	C	37	PHE	4.4
1	B	805	CYS	4.3
1	C	780	LEU	4.3
1	D	789	SER	4.2
1	B	787	PRO	4.1
1	D	790	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	789	SER	4.1
1	A	786	ASP	4.0
1	C	258	SER	4.0
1	D	786	ASP	4.0
1	A	781	LEU	3.9
1	A	782	ALA	3.9
1	A	37	PHE	3.8
1	C	779	THR	3.8
1	C	128	PRO	3.7
1	A	791	ARG	3.7
1	B	37	PHE	3.7
1	D	782	ALA	3.7
1	C	782	ALA	3.6
1	B	809	PRO	3.6
1	B	781	LEU	3.6
1	B	462[A]	CYS	3.6
1	C	785	LYS	3.6
1	C	784	GLN	3.6
1	B	747	ALA	3.6
1	A	783	ALA	3.5
1	D	787	PRO	3.5
1	C	257	THR	3.4
1	B	782	ALA	3.4
1	D	788	ASN	3.4
1	B	804	PHE	3.4
1	A	785	LYS	3.4
1	C	255	ALA	3.4
1	B	785	LYS	3.4
1	D	110	ILE	3.3
1	C	805	CYS	3.3
1	A	780	LEU	3.3
1	B	789	SER	3.3
1	B	748	GLY	3.3
1	A	822	ALA	3.2
1	C	807	MET	3.2
1	B	128	PRO	3.2
1	D	781	LEU	3.2
1	C	308	ILE	3.2
1	B	370	ALA	3.2
1	A	784	GLN	3.2
1	A	779	THR	3.1
1	C	787	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	306	ALA	3.1
1	C	823	ASP	3.0
1	C	132	ALA	3.0
1	C	804	PHE	3.0
1	B	746	VAL	3.0
1	D	37	PHE	2.9
1	B	778	ASP	2.9
1	B	788	ASN	2.9
1	B	786	ASP	2.9
1	A	777	ARG	2.9
1	C	809	PRO	2.9
1	D	736	LEU	2.8
1	D	805	CYS	2.8
1	C	462[A]	CYS	2.8
1	C	307	ILE	2.7
1	C	260	PRO	2.7
1	C	788	ASN	2.7
1	B	255	ALA	2.7
1	C	118	ASN	2.7
1	C	127	ASP	2.7
1	D	783	ALA	2.6
1	A	747	ALA	2.6
1	A	462[A]	CYS	2.6
1	D	304	ALA	2.6
1	C	625	PRO	2.6
1	C	261	VAL	2.6
1	C	622	GLY	2.6
1	A	792	ASN	2.5
1	B	745	CYS	2.5
1	A	775	VAL	2.5
1	B	784	GLN	2.5
1	B	822	ALA	2.5
1	C	36	GLN	2.5
1	C	254	ALA	2.5
1	A	809	PRO	2.5
1	C	256	ALA	2.5
1	C	117	PRO	2.5
1	B	813	ASN	2.4
1	C	812	GLN	2.4
1	C	21	ASN	2.4
1	C	777	ARG	2.4
1	C	133	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	816	ILE	2.4
1	B	118	ASN	2.3
1	A	258	SER	2.3
1	B	308	ILE	2.3
1	D	258	SER	2.3
1	B	117	PRO	2.3
1	C	264	GLN	2.3
1	B	749	GLU	2.3
1	B	807	MET	2.3
1	A	748	GLY	2.3
1	B	36	GLN	2.3
1	C	129	ALA	2.3
1	C	700	ALA	2.3
1	C	304	ALA	2.2
1	D	255	ALA	2.2
1	C	309	SER	2.2
1	D	785	LYS	2.2
1	C	776	ASN	2.2
1	A	254	ALA	2.2
1	C	797	VAL	2.1
1	C	778	ASP	2.1
1	C	305	SER	2.1
1	B	258	SER	2.1
1	B	622	GLY	2.1
1	C	368	TRP	2.1
1	B	132	ALA	2.1
1	A	736	LEU	2.1
1	D	260	PRO	2.1
1	C	130	ALA	2.1
1	D	621	VAL	2.1
1	B	810	ASP	2.1
1	A	776	ASN	2.1
1	B	260	PRO	2.1
1	A	260	PRO	2.1
1	C	131	ALA	2.0
1	C	115	ASP	2.0
1	D	673	TYR	2.0
1	C	325	ILE	2.0
1	A	255	ALA	2.0
1	B	115	ASP	2.0
1	C	298	SER	2.0
1	A	306	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	902	6/6	0.68	0.29	32,42,57,59	0
3	GOL	B	912	6/6	0.79	0.33	34,45,55,56	0
3	GOL	C	903	6/6	0.79	0.24	30,41,45,53	0
3	GOL	D	910	6/6	0.81	0.30	32,42,50,57	0
3	GOL	B	907	6/6	0.82	0.34	34,44,53,61	0
3	GOL	B	917	6/6	0.83	0.24	32,43,58,61	0
3	GOL	A	913	6/6	0.84	0.34	41,50,58,60	0
3	GOL	B	913	6/6	0.84	0.44	32,44,51,59	0
3	GOL	C	911	6/6	0.84	0.27	34,47,58,61	0
3	GOL	A	910	6/6	0.84	0.40	38,48,59,60	0
3	GOL	B	909	6/6	0.85	0.30	37,46,55,56	0
3	GOL	A	915	6/6	0.85	0.32	36,48,59,60	0
3	GOL	C	902	6/6	0.85	0.30	29,47,54,61	0
3	GOL	A	918	6/6	0.86	0.23	34,42,62,62	0
3	GOL	C	906	6/6	0.87	0.20	35,43,59,59	0
3	GOL	B	914	6/6	0.87	0.41	38,49,61,62	0
3	GOL	A	919	6/6	0.87	0.43	30,46,58,63	0
3	GOL	A	902	6/6	0.88	0.24	35,46,59,67	0
3	GOL	B	911	6/6	0.88	0.25	26,38,50,50	0
3	GOL	A	912	6/6	0.88	0.19	29,40,51,51	0
3	GOL	C	905	6/6	0.89	0.19	33,40,48,56	0
3	GOL	D	903	6/6	0.89	0.16	31,39,49,50	0
3	GOL	D	905	6/6	0.89	0.18	19,39,46,46	0
3	GOL	C	909	6/6	0.89	0.27	36,44,48,51	0
3	GOL	D	913	6/6	0.89	0.33	28,38,59,60	0
3	GOL	D	914	6/6	0.89	0.23	33,44,57,65	0
3	GOL	A	905	6/6	0.90	0.15	22,37,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	D	904	6/6	0.90	0.25	33,40,48,52	0
3	GOL	A	906	6/6	0.90	0.17	31,40,49,59	0
3	GOL	D	909	6/6	0.90	0.18	25,39,54,58	0
3	GOL	B	906	6/6	0.90	0.16	21,42,51,51	0
3	GOL	D	911	6/6	0.90	0.29	38,46,55,60	0
3	GOL	A	911	6/6	0.90	0.16	31,40,48,48	0
3	GOL	B	910	6/6	0.90	0.22	29,36,51,61	0
3	GOL	A	908	6/6	0.91	0.23	30,38,45,45	0
3	GOL	A	904	6/6	0.91	0.29	34,41,56,58	0
3	GOL	D	908	6/6	0.92	0.14	30,38,47,47	0
3	GOL	A	914	6/6	0.92	0.24	37,44,54,57	0
3	GOL	B	904	6/6	0.92	0.12	32,41,48,48	0
3	GOL	A	909	6/6	0.92	0.26	32,39,46,46	0
3	GOL	B	903	6/6	0.92	0.12	25,37,50,60	0
3	GOL	C	907	6/6	0.92	0.14	35,45,52,63	0
3	GOL	A	907	6/6	0.93	0.15	34,40,46,47	0
3	GOL	C	910	6/6	0.93	0.18	36,48,58,58	0
3	GOL	B	915	6/6	0.93	0.31	39,46,53,55	0
3	GOL	C	908	6/6	0.93	0.19	34,41,50,60	0
3	GOL	A	903	6/6	0.95	0.14	30,38,49,59	0
3	GOL	A	917	6/6	0.95	0.17	32,41,58,60	0
3	GOL	B	908	6/6	0.95	0.10	31,40,52,56	0
3	GOL	B	905	6/6	0.95	0.19	29,34,46,46	0
3	GOL	D	906	6/6	0.95	0.15	30,36,42,44	0
3	GOL	D	907	6/6	0.95	0.24	35,43,51,57	0
3	GOL	D	902	6/6	0.96	0.17	26,33,38,47	0
3	GOL	C	904	6/6	0.97	0.13	30,41,54,55	0
2	LLQ	C	901	9/9	0.98	0.19	25,38,49,49	0
4	NA	C	912	1/1	0.98	0.11	24,24,24,24	0
2	LLQ	B	901	9/9	0.99	0.14	22,35,49,49	0
2	LLQ	D	901	9/9	0.99	0.21	14,26,43,52	0
4	NA	B	916	1/1	0.99	0.09	20,20,20,20	0
4	NA	A	916	1/1	0.99	0.16	21,21,21,21	0
2	LLQ	A	901	9/9	0.99	0.21	18,26,45,47	0
4	NA	D	912	1/1	1.00	0.16	20,20,20,20	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.
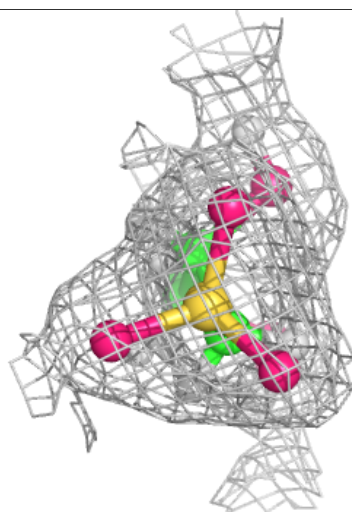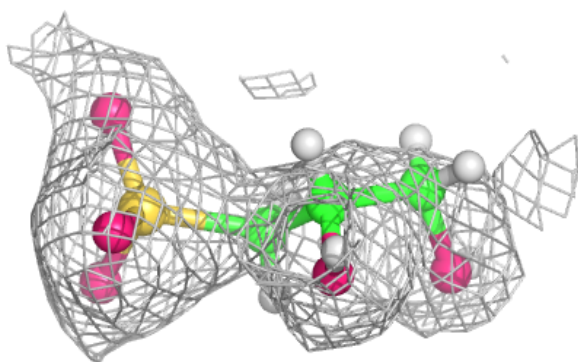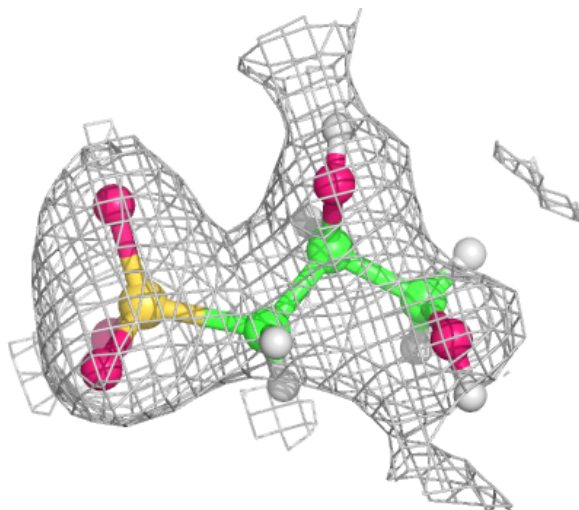
Electron density around LLQ C 901:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
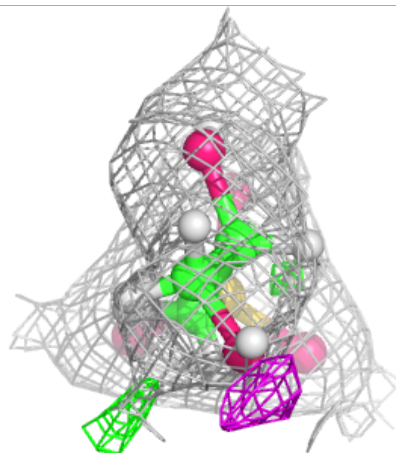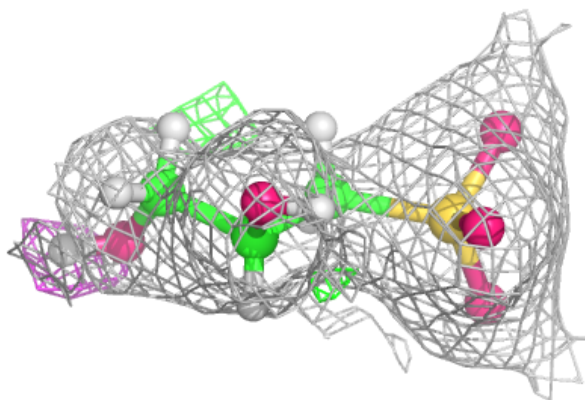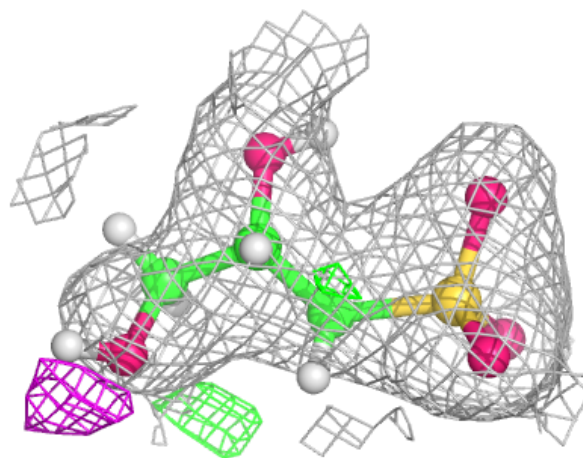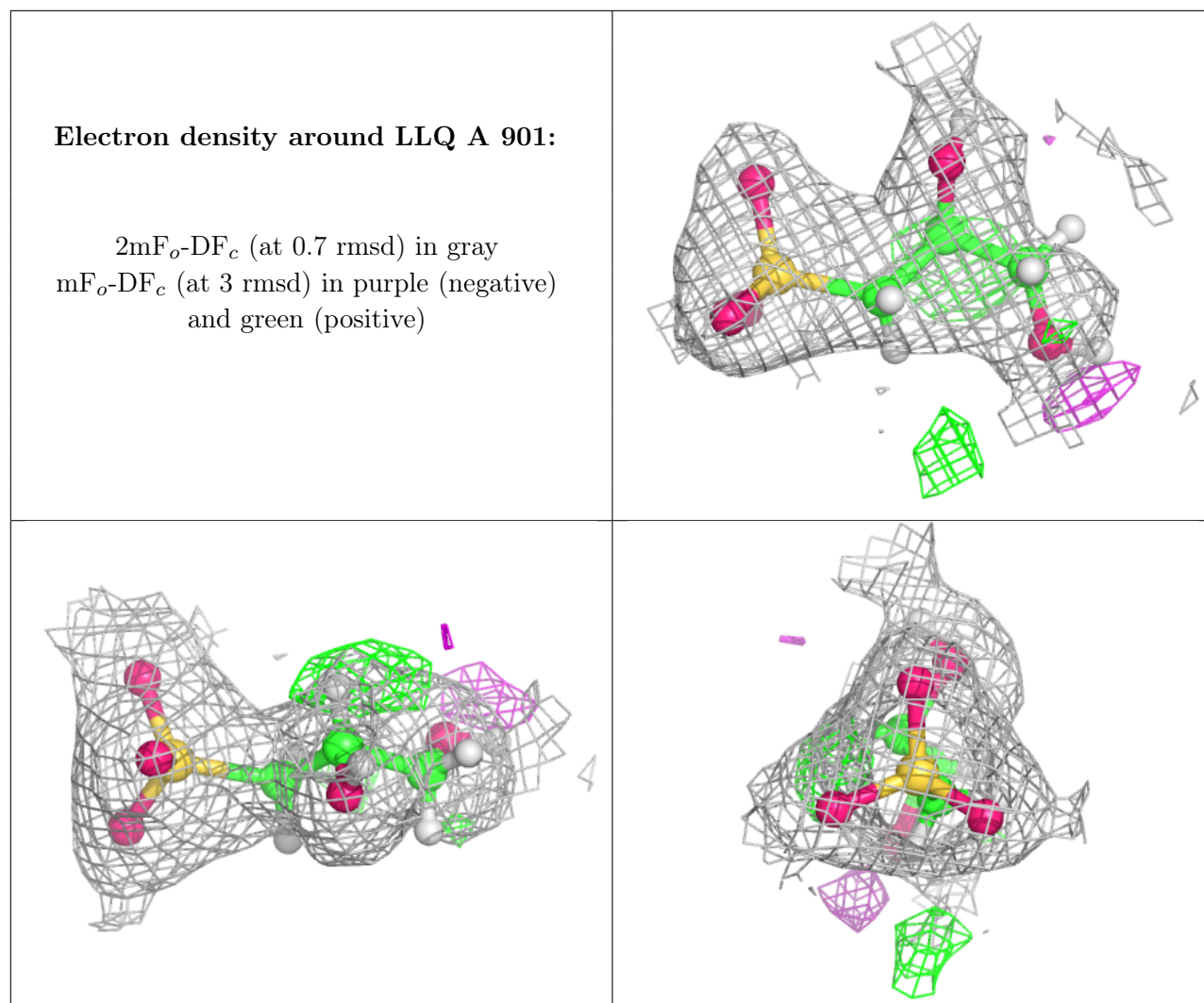and green (positive)
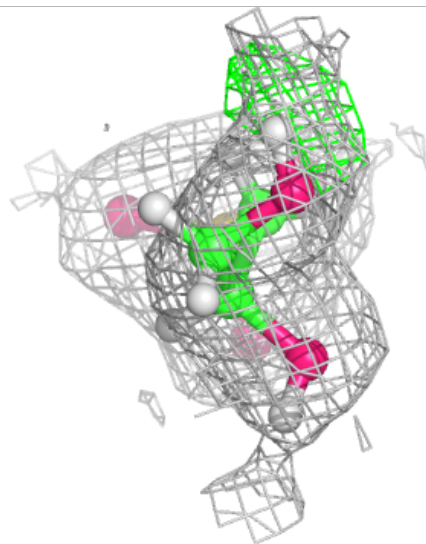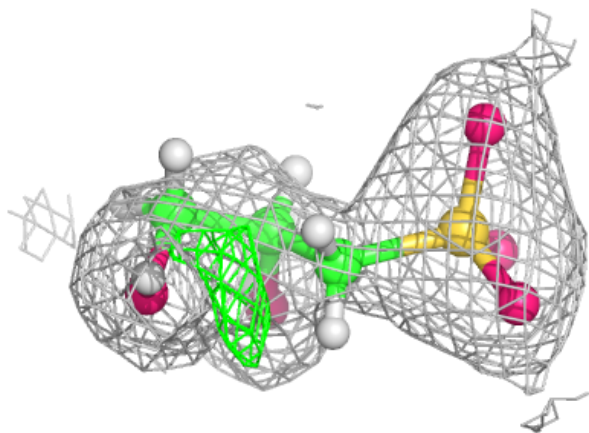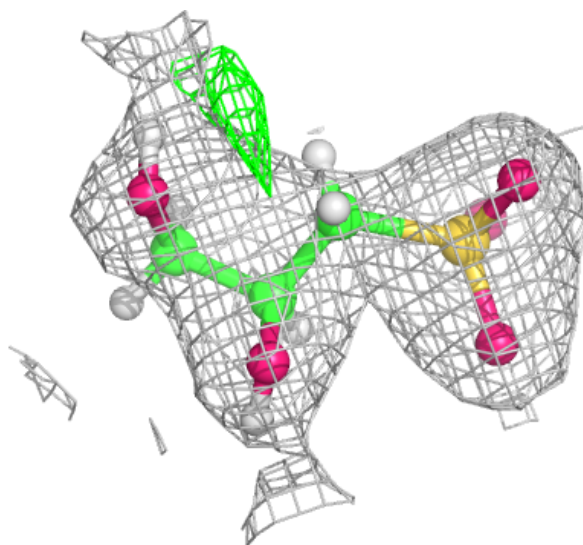
Electron density around LLQ B 901:

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

Electron density around LLQ D 901:

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

Electron density around LLQ A 901:

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 ⓘ

There are no such residues in this entry.