



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2020 – 12:14 PM JST

PDB ID : 6LP1
Title : Crystal structure of acetate:succinate CoA transferase (ASCT) from Trypanosoma brucei.
Authors : Mochizuki, K.; Inaoka, D.K.; Shiba, T.; Fukuda, K.; Kurasawa, H.; Mazet, M.; Millerieux, Y.; Bringaud, F.; Boshart, M.; Balogun, E.O.; Harada, S.; Hirayama, K.; Kita, K.
Deposited on : 2020-01-08
Resolution : 2.01 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
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) : 2.14.6

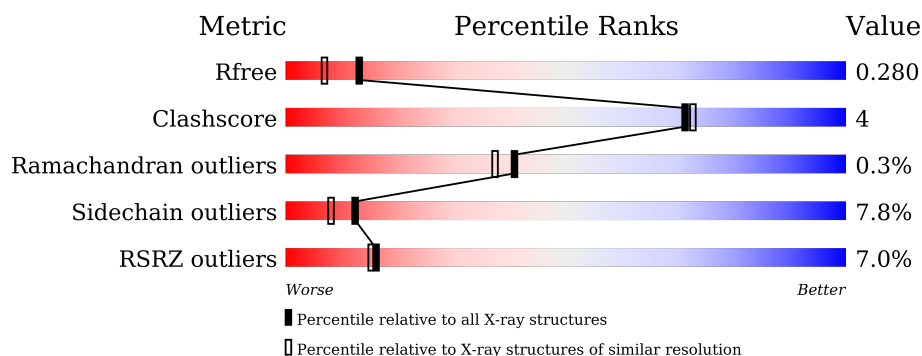
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	483	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>..</div> </div> </div>
1	B	483	<div> <div>11%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>.</div> </div> </div>
1	C	483	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>..</div> </div> </div>
1	D	483	<div> <div>9%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>..</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14484 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 Succinyl-CoA:3-ketoacid-coenzyme A transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3515	2209	615	668	23			
1	B	467	Total	C	N	O	S	0	0	0
			3520	2214	617	666	23			
1	C	469	Total	C	N	O	S	0	1	0
			3539	2225	619	672	23			
1	D	466	Total	C	N	O	S	0	2	0
			3524	2215	617	669	23			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by author).



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

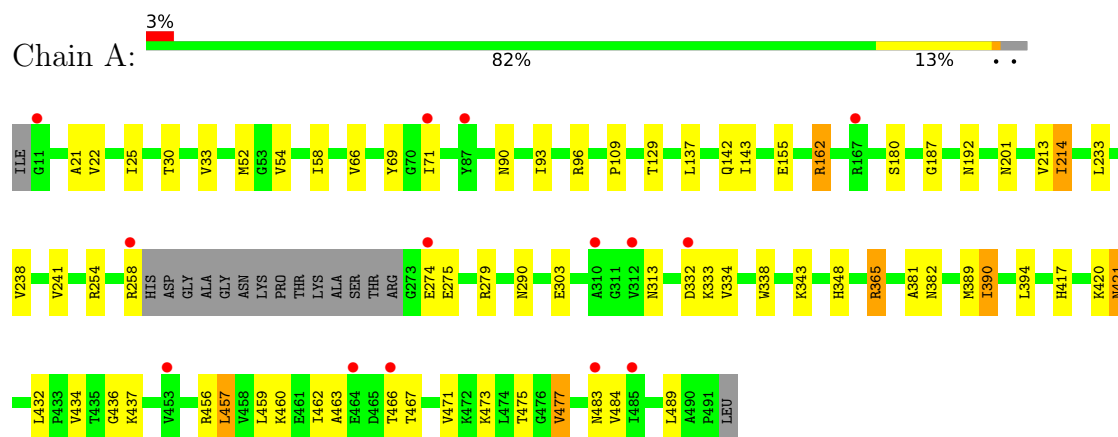
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total	O	0	0
			103	103		
4	B	88	Total	O	0	0
			88	88		
4	C	98	Total	O	0	0
			98	98		
4	D	81	Total	O	0	0
			81	81		

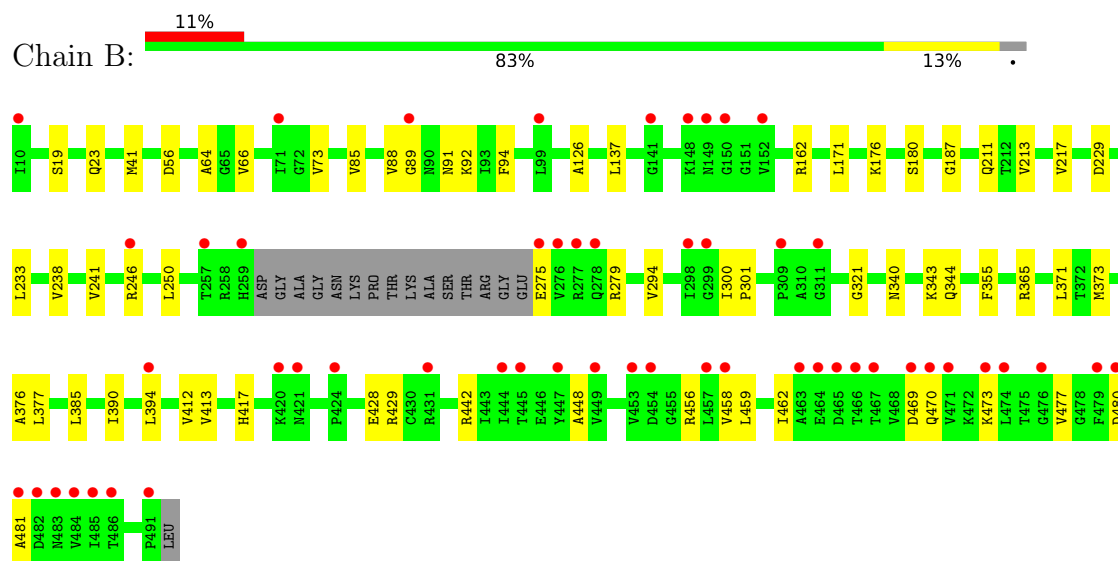
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

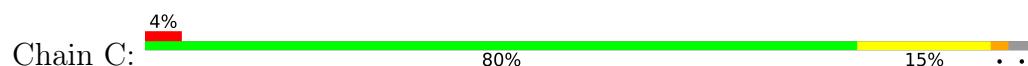
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase

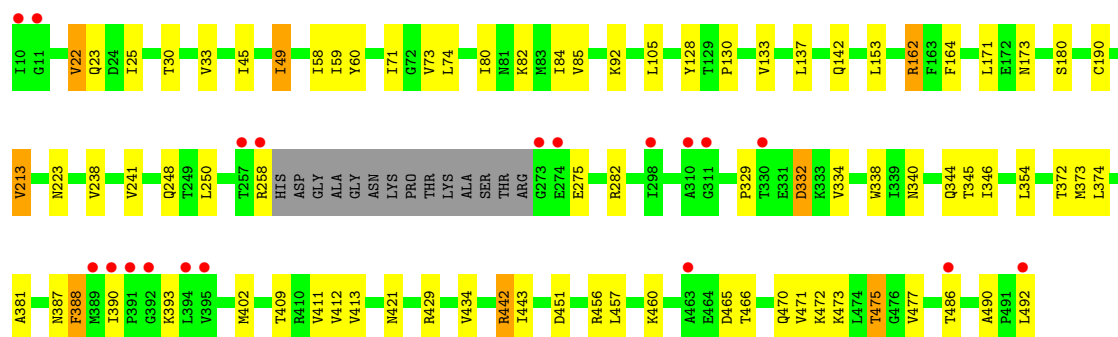


- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase

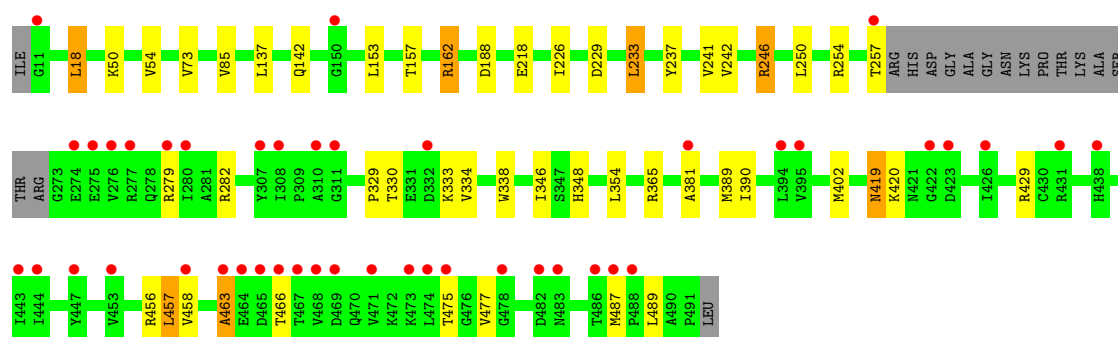
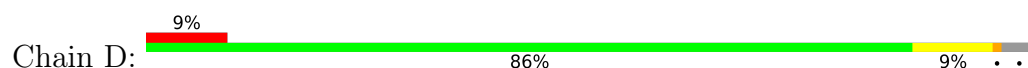


- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase





- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.89Å 164.63Å 187.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.01 19.97 – 2.01	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.97-2.01) 98.9 (19.97-2.01)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.225 , 0.279 0.231 , 0.280	Depositor DCC
R_{free} test set	6346 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14484	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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: GOL, CA

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	0.49	0/3572	0.81	5/4833 (0.1%)
1	B	0.48	0/3578	0.77	2/4842 (0.0%)
1	C	0.51	0/3596	0.79	2/4866 (0.0%)
1	D	0.50	0/3581	0.78	4/4844 (0.1%)
All	All	0.50	0/14327	0.79	13/19385 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
1	D	0	2
All	All	0	5

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	A	365	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	D	365	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	B	365	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	D	365	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	B	365	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	D	162	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	C	162	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	C	429	ARG	NE-CZ-NH1	6.31	123.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	D	162	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	162	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	477	VAL	CB-CA-C	-5.08	101.74	111.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	GLU	Peptide
1	A	463	ALA	Peptide
1	C	465	ASP	Peptide
1	D	420	LYS	Peptide
1	D	463	ALA	Peptide

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	3515	0	3527	30	0
1	B	3520	0	3536	17	0
1	C	3539	0	3554	35	0
1	D	3524	0	3538	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	C	6	0	8	1	0
3	D	6	0	8	0	0
4	A	103	0	0	1	0
4	B	88	0	0	0	0
4	C	98	0	0	1	0
4	D	81	0	0	0	0
All	All	14484	0	14171	100	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 (100) 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:C:340:ASN:HD21	1:C:344:GLN:HE21	1.30	0.80
1:B:340:ASN:HD21	1:B:344:GLN:HE21	1.34	0.76
1:C:22:VAL:HG21	1:C:49:ILE:HG22	1.67	0.76
1:A:459:LEU:HD11	1:A:462:ILE:HG23	1.69	0.74
1:C:22:VAL:HG22	1:C:25:ILE:HD12	1.73	0.71
1:A:471:VAL:O	1:A:475:THR:HG23	1.93	0.69
1:A:52:MET:SD	1:A:54:VAL:HG23	2.35	0.67
1:C:33:VAL:HG11	1:C:71:ILE:HD11	1.77	0.66
1:C:59:ILE:HD12	1:C:80:ILE:HD12	1.79	0.64
1:C:338:TRP:CH2	1:C:354:LEU:HD21	2.33	0.63
1:A:21:ALA:HB1	1:A:214:ILE:HD12	1.81	0.63
1:A:213:VAL:HG22	1:A:238:VAL:HA	1.82	0.61
1:C:190:CYS:H	1:C:223:ASN:HD21	1.49	0.60
1:C:471:VAL:O	1:C:475:THR:HG22	2.05	0.57
1:A:434:VAL:CG1	1:A:436:GLY:O	2.52	0.56
1:A:417:HIS:NE2	1:A:475:THR:HG22	2.20	0.56
1:A:279:ARG:HG2	1:A:489:LEU:HD21	1.88	0.55
1:A:30:THR:HG22	1:A:58:ILE:HB	1.89	0.55
1:B:428:GLU:O	1:B:429:ARG:NH1	2.41	0.53
1:B:126:ALA:HB1	1:B:171:LEU:HD11	1.89	0.53
1:C:213:VAL:HG22	1:C:238:VAL:HA	1.90	0.53
1:B:294:VAL:HG12	1:B:371:LEU:HB3	1.91	0.53
1:B:213:VAL:HG22	1:B:238:VAL:HA	1.91	0.51
1:C:329:PRO:HG2	1:C:334:VAL:HG22	1.92	0.51
1:A:290:ASN:HD22	1:A:313:ASN:H	1.59	0.51
1:A:109:PRO:HD3	1:A:137:LEU:HD23	1.94	0.50
1:D:381:ALA:HA	1:D:457:LEU:HD13	1.92	0.50
1:C:162:ARG:HG2	1:C:164:PHE:CE2	2.47	0.50
1:C:442:ARG:HD3	1:C:451:ASP:OD1	2.11	0.50
1:C:22:VAL:CG2	1:C:49:ILE:HG22	2.38	0.50
1:A:381:ALA:HA	1:A:457:LEU:HD13	1.93	0.49
1:D:463:ALA:CB	1:D:487:MET:HB3	2.42	0.49
1:C:381:ALA:HA	1:C:457:LEU:HD13	1.93	0.48
1:D:463:ALA:HB2	1:D:487:MET:HB3	1.96	0.47
1:D:18:LEU:HD13	1:D:242:VAL:HG11	1.97	0.47
1:D:254:ARG:NH2	1:D:334:VAL:HG21	2.30	0.47
1:A:187:GLY:HA2	1:A:192:ASN:O	2.14	0.47
1:C:137:LEU:HD13	1:C:402:MET:CE	2.43	0.47
1:A:33:VAL:HB	1:A:71:ILE:HD11	1.97	0.47
1:A:143:ILE:HD13	1:A:155:GLU:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ARG:NH1	1:C:490:ALA:O	2.48	0.46
1:D:18:LEU:HD22	1:D:242:VAL:CG1	2.46	0.46
1:A:66:VAL:HG12	1:A:69:TYR:HB3	1.97	0.46
1:C:49:ILE:HG13	1:C:74:LEU:HD21	1.98	0.46
1:D:246[B]:ARG:HD3	1:D:246[B]:ARG:HA	1.76	0.46
1:D:329:PRO:HG2	1:D:334:VAL:HG12	1.96	0.46
1:B:448:ALA:HB1	1:B:459:LEU:CD1	2.46	0.46
1:B:187:GLY:HA3	1:B:217:VAL:HG11	1.98	0.46
1:B:321:GLY:HA2	1:B:355:PHE:CE1	2.50	0.46
1:D:50:LYS:HD3	1:D:73:VAL:HG22	1.98	0.46
1:C:180:SER:HB2	1:C:213:VAL:HB	1.98	0.46
1:A:390:ILE:HB	1:A:432:LEU:HD22	1.98	0.45
1:D:218:GLU:O	1:D:246[B]:ARG:NE	2.50	0.45
1:A:390:ILE:HD13	1:A:432:LEU:CD2	2.46	0.45
1:B:480:ASP:OD1	1:B:481:ALA:N	2.50	0.45
1:C:60:TYR:CZ	1:C:84:ILE:HD13	2.52	0.45
1:C:137:LEU:HD11	1:C:388:PHE:CZ	2.52	0.45
1:C:413:VAL:CG1	1:C:443:ILE:HG12	2.46	0.45
1:B:64:ALA:O	1:B:91:ASN:ND2	2.51	0.44
1:A:25:ILE:O	1:A:54:VAL:HG21	2.17	0.44
1:B:180:SER:HB2	1:B:213:VAL:HB	1.99	0.44
1:C:471:VAL:O	1:C:475:THR:CG2	2.66	0.44
1:D:137:LEU:HD22	1:D:402:MET:CE	2.48	0.44
1:A:129:THR:OG1	1:A:365:ARG:HD2	2.17	0.44
1:C:486:THR:HG22	4:C:685:HOH:O	2.17	0.44
1:B:64:ALA:HB3	1:B:94:PHE:CD2	2.53	0.44
1:A:22:VAL:HG13	1:A:25:ILE:HD12	2.00	0.44
1:D:338:TRP:CZ3	1:D:348:HIS:HB3	2.53	0.44
1:B:412:VAL:HG13	1:B:442:ARG:HB3	1.99	0.44
1:C:60:TYR:CE2	1:C:84:ILE:HD13	2.52	0.44
1:D:18:LEU:HD22	1:D:242:VAL:HG11	2.00	0.44
1:C:30:THR:HG22	1:C:58:ILE:HB	2.00	0.43
1:A:180:SER:HB2	1:A:213:VAL:HB	2.01	0.43
1:A:390:ILE:HG23	1:A:394:LEU:HB3	2.00	0.43
1:A:254:ARG:NH1	1:A:334:VAL:HG21	2.34	0.43
1:A:466:THR:HG22	1:A:467:THR:H	1.82	0.43
1:D:330:THR:HG22	1:D:333:LYS:HD3	2.00	0.43
1:C:413:VAL:HG13	1:C:443:ILE:HA	2.01	0.43
1:C:173:ASN:HD22	3:C:502:GOL:C3	2.31	0.43
1:C:190:CYS:N	1:C:223:ASN:HD21	2.16	0.42
1:A:96:ARG:NH1	4:A:606:HOH:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ILE:N	1:B:301:PRO:CD	2.82	0.42
1:B:376:ALA:HB2	1:B:385:LEU:HD11	2.01	0.42
1:C:130:PRO:O	1:C:133:VAL:HG23	2.19	0.42
1:A:52:MET:SD	1:A:54:VAL:CG2	3.06	0.42
1:C:373:MET:HA	1:C:412:VAL:O	2.20	0.42
1:B:385:LEU:HD13	1:B:413:VAL:HG21	2.01	0.42
1:C:332:ASP:N	1:C:332:ASP:OD1	2.51	0.42
1:C:128:TYR:CZ	1:C:171:LEU:HD13	2.55	0.41
1:C:372:THR:OG1	1:C:411:VAL:HG22	2.20	0.41
1:D:188:ASP:HB3	1:D:226:ILE:HD12	2.02	0.41
1:A:338:TRP:CZ3	1:A:348:HIS:HB3	2.55	0.41
1:A:459:LEU:HD12	1:A:484:VAL:HG22	2.02	0.41
1:A:66:VAL:HG23	1:A:90:ASN:O	2.20	0.41
1:D:137:LEU:HD11	1:D:142:GLN:HE22	1.85	0.41
1:B:428:GLU:HA	1:B:477:VAL:HG11	2.03	0.40
1:D:233:LEU:HD22	1:D:237:TYR:CD2	2.56	0.40
1:D:257:THR:HG22	1:D:330:THR:HA	2.03	0.40
1:C:22:VAL:HG22	1:C:25:ILE:CD1	2.47	0.40
1:C:45:ILE:O	1:C:49:ILE:HG23	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	463/483 (96%)	446 (96%)	15 (3%)	2 (0%)	34	30
1	B	463/483 (96%)	445 (96%)	16 (4%)	2 (0%)	34	30
1	C	466/483 (96%)	448 (96%)	17 (4%)	1 (0%)	47	44
1	D	464/483 (96%)	446 (96%)	17 (4%)	1 (0%)	47	44
All	All	1856/1932 (96%)	1785 (96%)	65 (4%)	6 (0%)	41	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	388	PHE
1	B	89	GLY
1	A	421	ASN
1	D	419	ASN
1	A	201	ASN
1	B	458	VAL

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	375/387 (97%)	351 (94%)	24 (6%)	17	13
1	B	376/387 (97%)	345 (92%)	31 (8%)	11	7
1	C	378/387 (98%)	342 (90%)	36 (10%)	8	5
1	D	376/387 (97%)	349 (93%)	27 (7%)	14	9
All	All	1505/1548 (97%)	1387 (92%)	118 (8%)	12	8

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	ILE
1	A	142	GLN
1	A	162	ARG
1	A	214	ILE
1	A	233	LEU
1	A	241	VAL
1	A	258	ARG
1	A	274	GLU
1	A	303	GLU
1	A	332	ASP
1	A	333	LYS
1	A	343	LYS
1	A	382	ASN
1	A	389	MET

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Mol	Chain	Res	Type
1	A	390	ILE
1	A	420	LYS
1	A	421	ASN
1	A	437	LYS
1	A	456	ARG
1	A	457	LEU
1	A	460	LYS
1	A	473	LYS
1	A	477	VAL
1	A	483	ASN
1	B	19	SER
1	B	23	GLN
1	B	41	MET
1	B	56	ASP
1	B	66	VAL
1	B	73	VAL
1	B	85	VAL
1	B	88	VAL
1	B	92	LYS
1	B	137	LEU
1	B	162	ARG
1	B	176	LYS
1	B	211	GLN
1	B	229	ASP
1	B	233	LEU
1	B	241	VAL
1	B	246	ARG
1	B	250	LEU
1	B	275	GLU
1	B	279	ARG
1	B	343	LYS
1	B	373	MET
1	B	377	LEU
1	B	390	ILE
1	B	394	LEU
1	B	417	HIS
1	B	456	ARG
1	B	462	ILE
1	B	469	ASP
1	B	470	GLN
1	B	473	LYS
1	C	22	VAL

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Mol	Chain	Res	Type
1	C	23	GLN
1	C	49	ILE
1	C	73	VAL
1	C	82	LYS
1	C	85	VAL
1	C	92	LYS
1	C	105	LEU
1	C	142	GLN
1	C	153	LEU
1	C	213	VAL
1	C	241	VAL
1	C	248	GLN
1	C	250	LEU
1	C	258	ARG
1	C	275	GLU
1	C	332	ASP
1	C	345	THR
1	C	346	ILE
1	C	374	LEU
1	C	387	ASN
1	C	390	ILE
1	C	393	LYS
1	C	409	THR
1	C	421	ASN
1	C	434	VAL
1	C	442	ARG
1	C	456	ARG
1	C	460	LYS
1	C	466	THR
1	C	470	GLN
1	C	472	LYS
1	C	473	LYS
1	C	475	THR
1	C	477	VAL
1	C	492	LEU
1	D	18	LEU
1	D	54	VAL
1	D	85	VAL
1	D	153	LEU
1	D	157	THR
1	D	162	ARG
1	D	229	ASP

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Mol	Chain	Res	Type
1	D	233	LEU
1	D	241	VAL
1	D	246[A]	ARG
1	D	246[B]	ARG
1	D	250	LEU
1	D	279	ARG
1	D	282	ARG
1	D	346	ILE
1	D	354	LEU
1	D	389	MET
1	D	390	ILE
1	D	419	ASN
1	D	429	ARG
1	D	456	ARG
1	D	457	LEU
1	D	458	VAL
1	D	466	THR
1	D	475	THR
1	D	477	VAL
1	D	489	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	97	GLN
1	A	208	GLN
1	A	290	ASN
1	A	421	ASN
1	A	470	GLN
1	B	47	GLN
1	B	77	ASN
1	B	97	GLN
1	B	208	GLN
1	B	290	ASN
1	B	306	ASN
1	B	344	GLN
1	B	438	HIS
1	B	470	GLN
1	C	110	GLN
1	C	142	GLN
1	C	173	ASN

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Mol	Chain	Res	Type
1	C	208	GLN
1	C	223	ASN
1	C	290	ASN
1	C	313	ASN
1	C	344	GLN
1	C	421	ASN
1	C	470	GLN
1	D	23	GLN
1	D	47	GLN
1	D	77	ASN
1	D	90	ASN
1	D	208	GLN
1	D	211	GLN
1	D	248	GLN
1	D	382	ASN
1	D	419	ASN

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	502	-	5,5,5	0.38	0	5,5,5	0.23	0
3	GOL	D	502	-	5,5,5	0.23	0	5,5,5	0.58	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	502	-	-	4/4/4/4	-
3	GOL	D	502	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

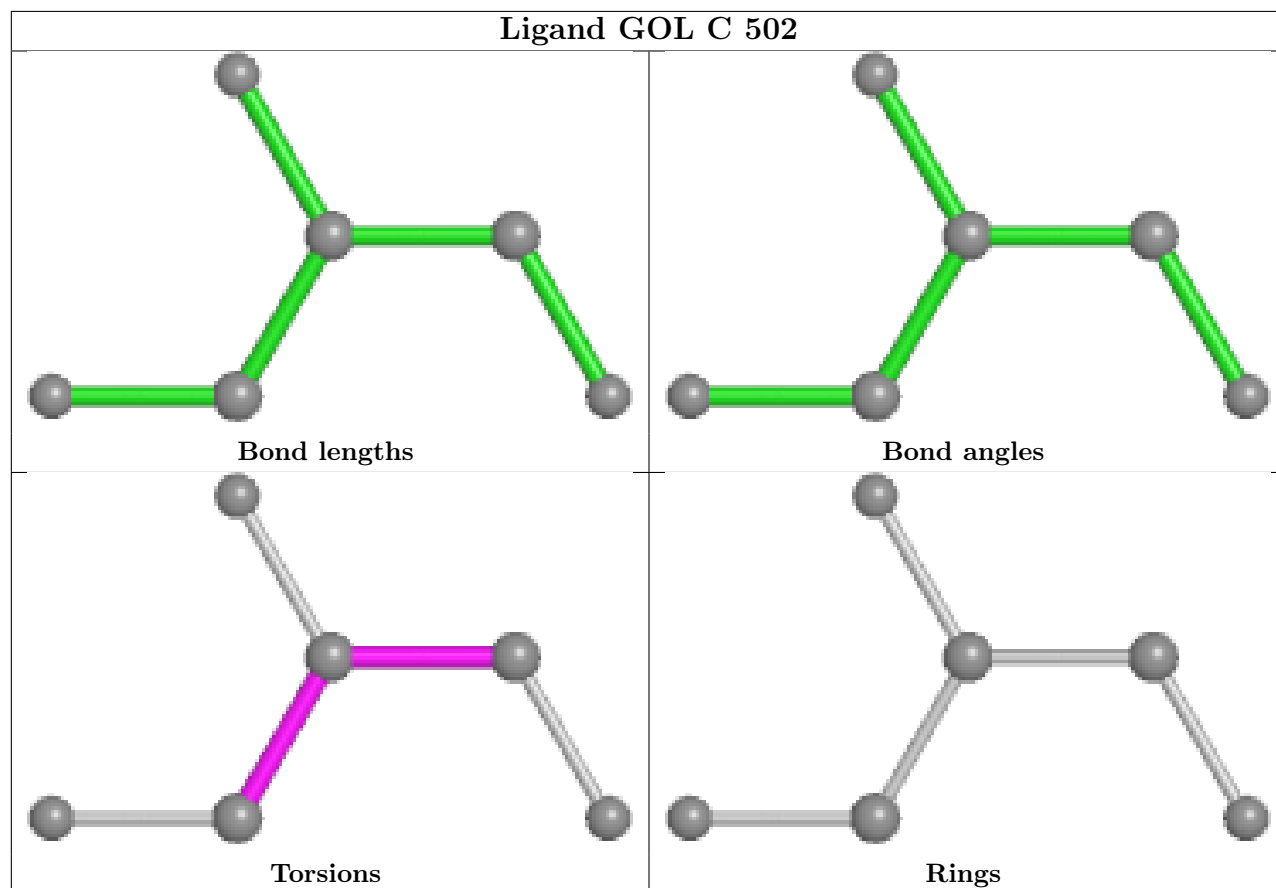
There are no ring outliers.

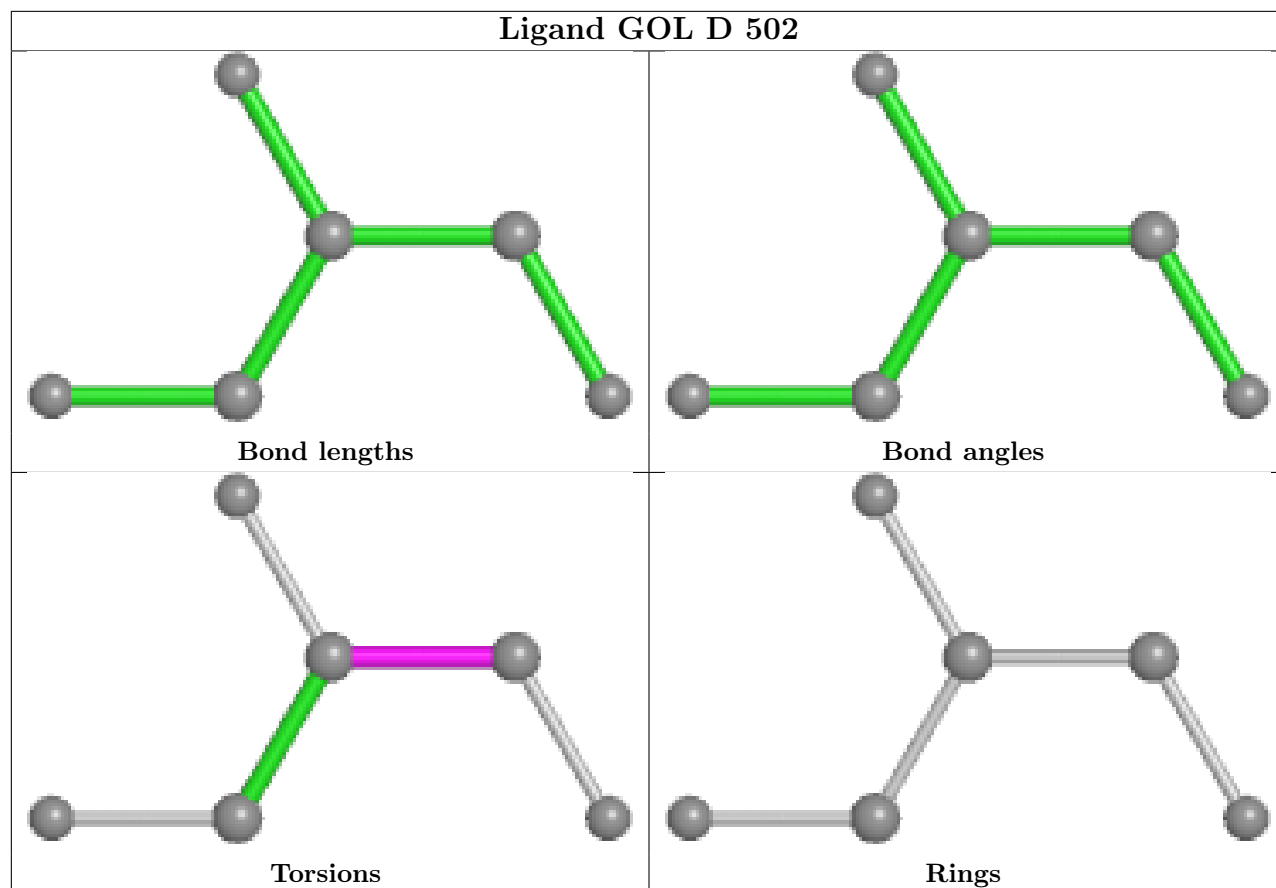
1 monomer is involved in 1 short contact:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	467/483 (96%)	0.05	14 (2%) 50 49	15, 27, 46, 62	1 (0%)
1	B	467/483 (96%)	0.52	53 (11%) 5 4	15, 33, 68, 82	1 (0%)
1	C	469/483 (97%)	0.11	19 (4%) 37 36	16, 28, 45, 82	1 (0%)
1	D	466/483 (96%)	0.37	44 (9%) 8 8	16, 30, 66, 85	1 (0%)
All	All	1869/1932 (96%)	0.26	130 (6%) 16 15	15, 28, 60, 85	4 (0%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	391	PRO	6.1
1	D	469	ASP	5.8
1	C	10	ILE	5.5
1	D	308	ILE	5.3
1	B	276	VAL	4.7
1	C	273	GLY	4.6
1	A	310	ALA	4.5
1	D	11	GLY	4.5
1	D	310	ALA	4.5
1	C	492	LEU	4.3
1	B	463	ALA	4.3
1	C	394	LEU	4.3
1	B	466	THR	4.3
1	D	422	GLY	4.2
1	B	465	ASP	4.2
1	B	149	ASN	4.1
1	A	258	ARG	4.1
1	B	277	ARG	4.1
1	B	457	LEU	4.1
1	B	474	LEU	4.0
1	B	259	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	467	THR	4.0
1	B	444	ILE	4.0
1	D	447	TYR	3.9
1	B	486	THR	3.8
1	B	483	ASN	3.7
1	B	458	VAL	3.7
1	B	421	ASN	3.7
1	B	10	ILE	3.6
1	D	466	THR	3.6
1	A	11	GLY	3.5
1	D	463	ALA	3.5
1	D	257	THR	3.5
1	C	311	GLY	3.5
1	B	447	TYR	3.5
1	B	141	GLY	3.4
1	D	483	ASN	3.4
1	D	475	THR	3.4
1	D	277	ARG	3.4
1	D	464	GLU	3.3
1	B	299	GLY	3.3
1	C	310	ALA	3.3
1	D	458	VAL	3.3
1	B	298	ILE	3.3
1	D	279	ARG	3.2
1	B	482	ASP	3.2
1	B	449	VAL	3.2
1	B	480	ASP	3.1
1	D	276	VAL	3.1
1	D	465	ASP	3.1
1	D	453	VAL	3.1
1	D	332	ASP	3.1
1	D	431	ARG	3.1
1	B	431	ARG	3.1
1	A	332	ASP	3.0
1	D	473	LYS	3.0
1	C	258	ARG	3.0
1	D	486	THR	3.0
1	A	274	GLU	3.0
1	B	311	GLY	3.0
1	B	420	LYS	3.0
1	B	257	THR	2.9
1	D	482	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	467	THR	2.9
1	B	71	ILE	2.9
1	B	473	LYS	2.9
1	C	11	GLY	2.8
1	B	394	LEU	2.8
1	B	454	ASP	2.7
1	C	257	THR	2.7
1	D	423	ASP	2.7
1	D	274	GLU	2.7
1	B	469	ASP	2.7
1	B	484	VAL	2.6
1	B	275	GLU	2.6
1	D	394	LEU	2.6
1	B	424	PRO	2.6
1	C	330	THR	2.6
1	D	311	GLY	2.6
1	C	395	VAL	2.5
1	C	392	GLY	2.5
1	B	309	PRO	2.5
1	B	453	VAL	2.5
1	B	148	LYS	2.5
1	C	486	THR	2.5
1	D	478	GLY	2.5
1	B	152	VAL	2.5
1	B	150	GLY	2.5
1	C	390	ILE	2.5
1	D	150	GLY	2.5
1	D	426	ILE	2.5
1	D	444	ILE	2.5
1	D	487	MET	2.4
1	A	464	GLU	2.4
1	B	464	GLU	2.4
1	D	468	VAL	2.4
1	D	280	ILE	2.4
1	B	99	LEU	2.4
1	B	278	GLN	2.4
1	B	481	ALA	2.4
1	A	167	ARG	2.4
1	A	485	ILE	2.3
1	B	470	GLN	2.3
1	B	485	ILE	2.3
1	D	443	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	87	TYR	2.3
1	D	275	GLU	2.3
1	D	488	PRO	2.3
1	C	298	ILE	2.3
1	B	445	THR	2.2
1	B	491	PRO	2.2
1	D	307	TYR	2.2
1	D	474	LEU	2.2
1	D	395	VAL	2.2
1	A	312	VAL	2.2
1	B	479	PHE	2.2
1	A	466	THR	2.1
1	A	453	VAL	2.1
1	C	274	GLU	2.1
1	C	463	ALA	2.1
1	B	471	VAL	2.1
1	A	71	ILE	2.1
1	D	438	HIS	2.1
1	C	389	MET	2.1
1	B	89	GLY	2.0
1	A	483	ASN	2.0
1	D	381	ALA	2.0
1	B	246	ARG	2.0
1	B	476	GLY	2.0
1	D	471	VAL	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 ⓘ

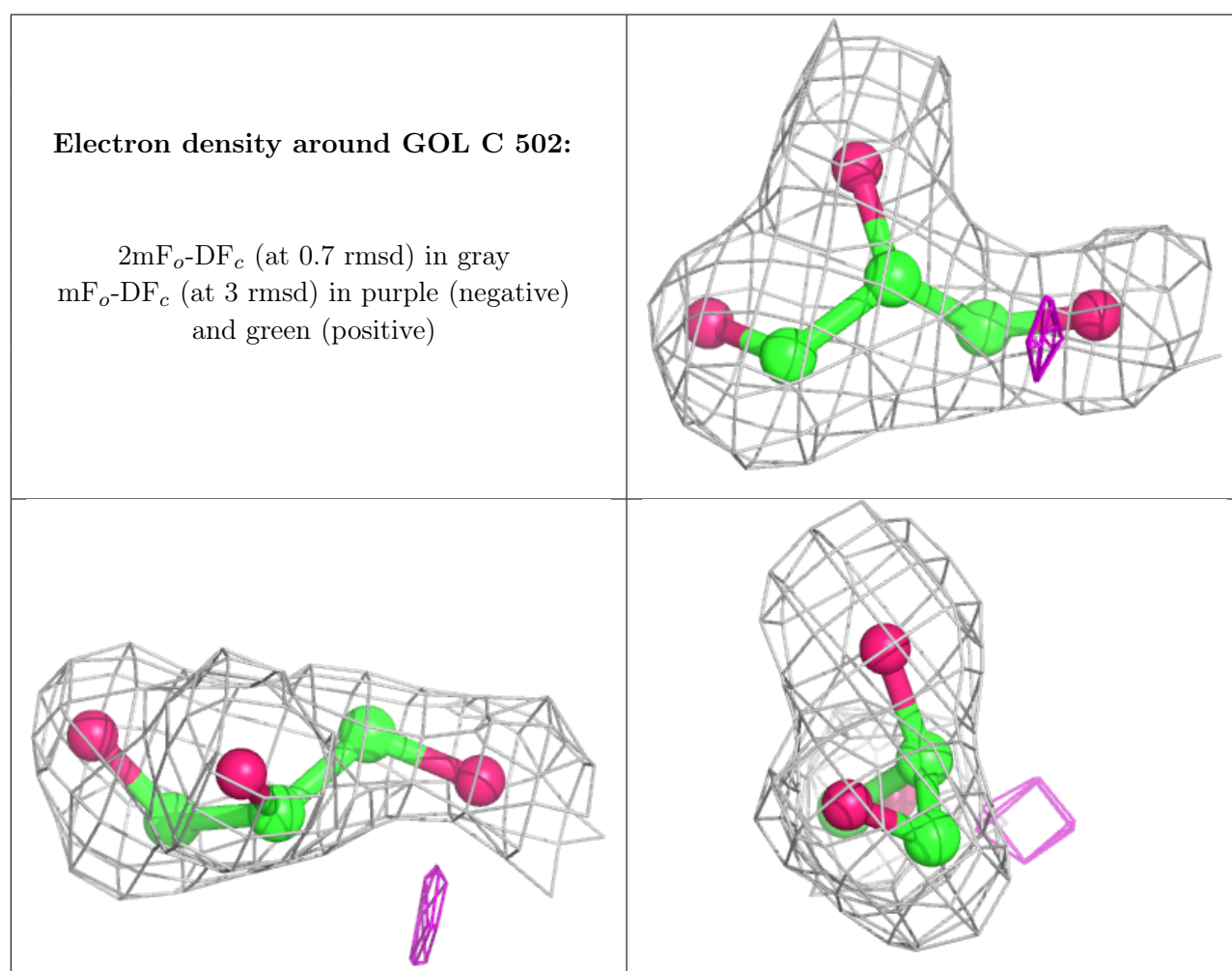
There are no monosaccharides in this entry.

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.

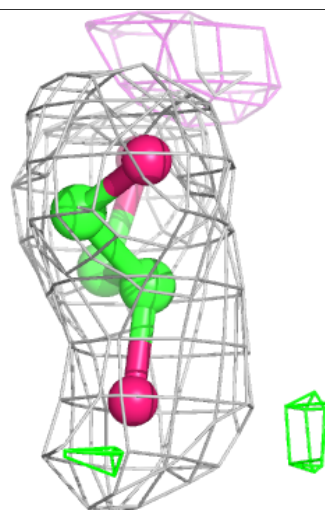
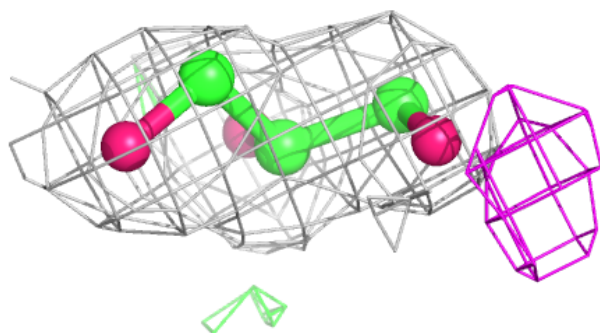
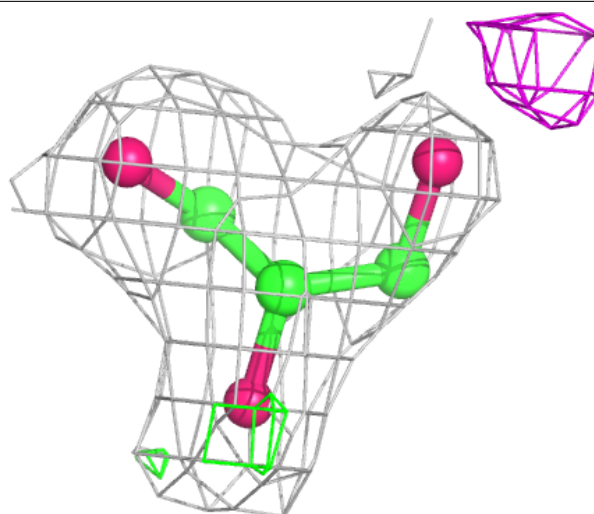
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	C	502	6/6	0.74	0.17	40,41,42,43	0
3	GOL	D	502	6/6	0.79	0.19	30,36,37,41	0
2	CA	B	501	1/1	0.91	0.09	64,64,64,64	0
2	CA	D	501	1/1	0.92	0.05	39,39,39,39	0
2	CA	A	501	1/1	0.94	0.06	40,40,40,40	0
2	CA	C	501	1/1	0.99	0.04	47,47,47,47	0

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.



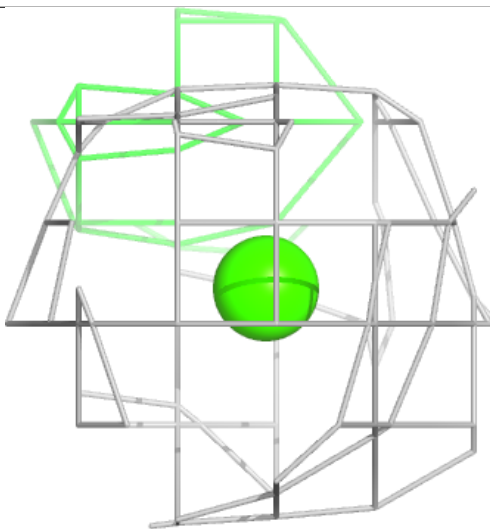
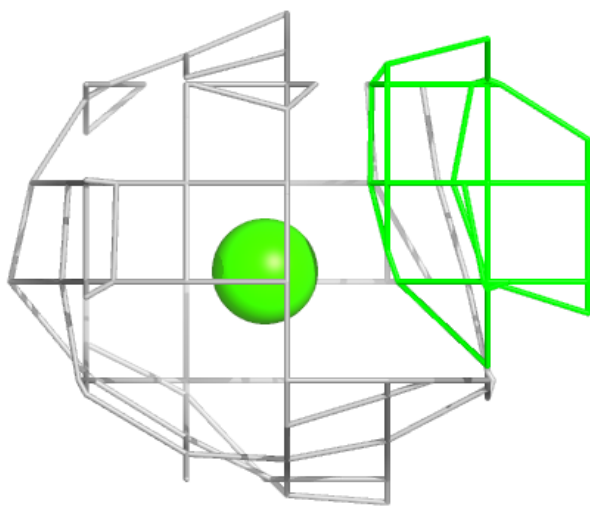
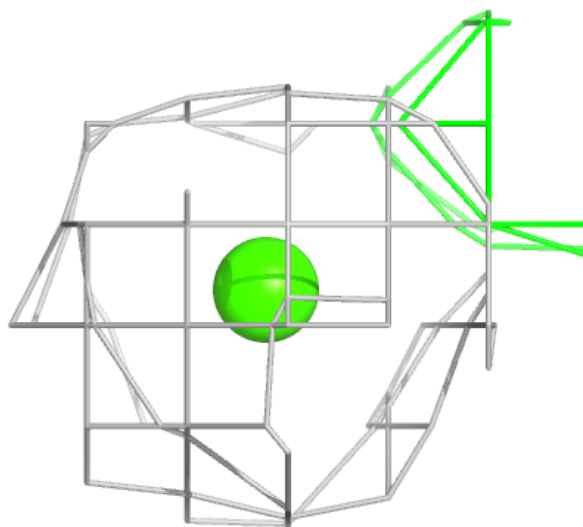
Electron density around GOL D 502:

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



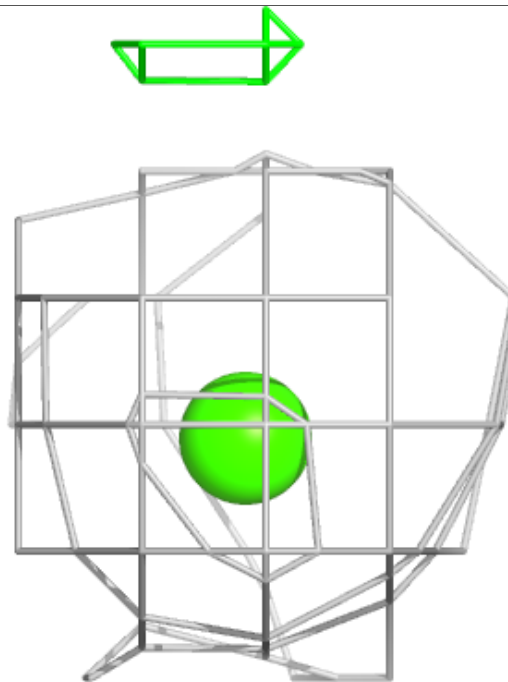
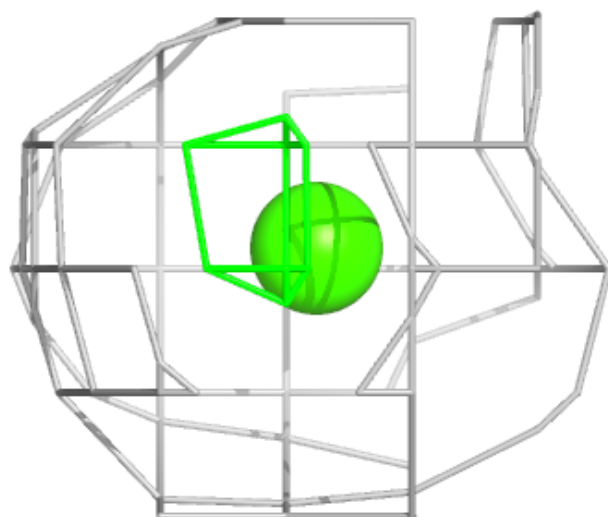
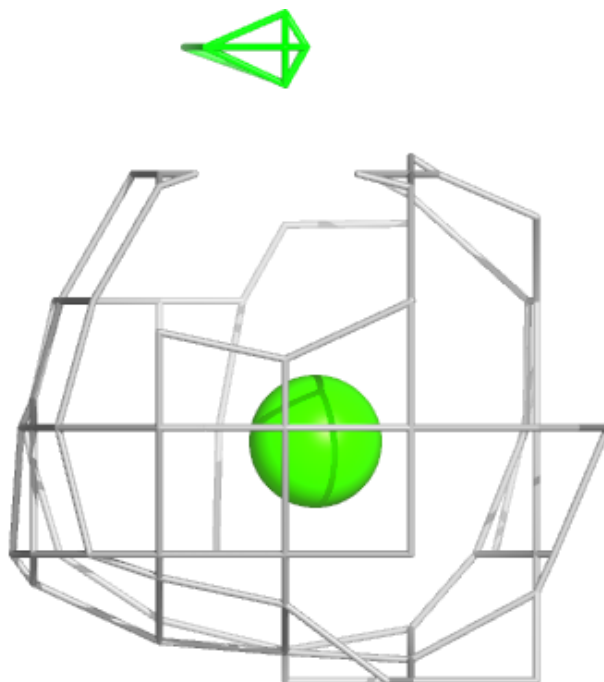
Electron density around CA B 501:

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



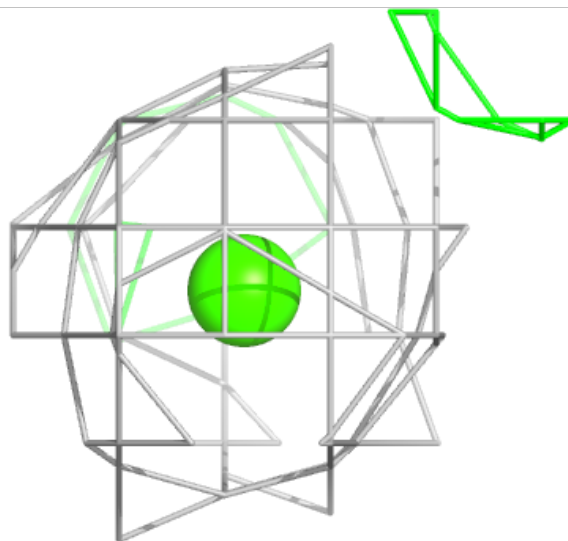
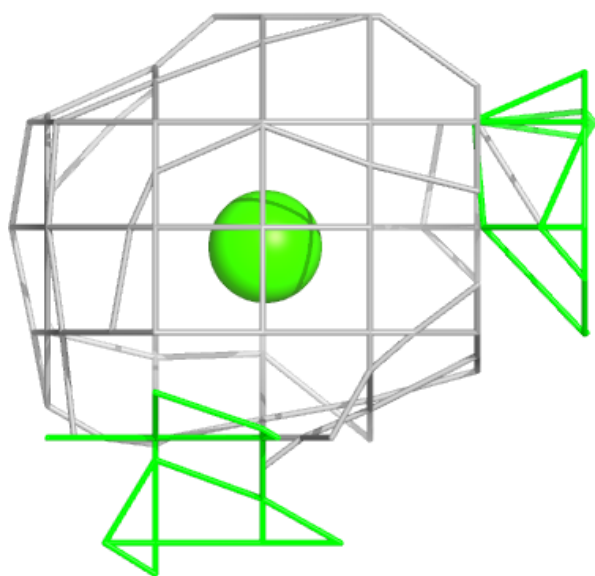
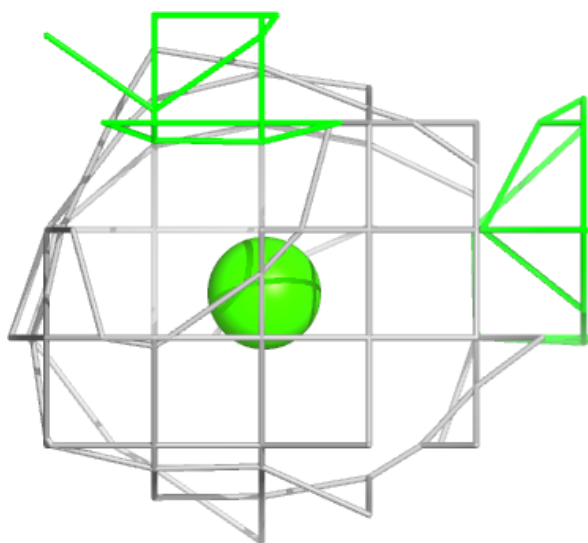
Electron density around CA D 501:

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



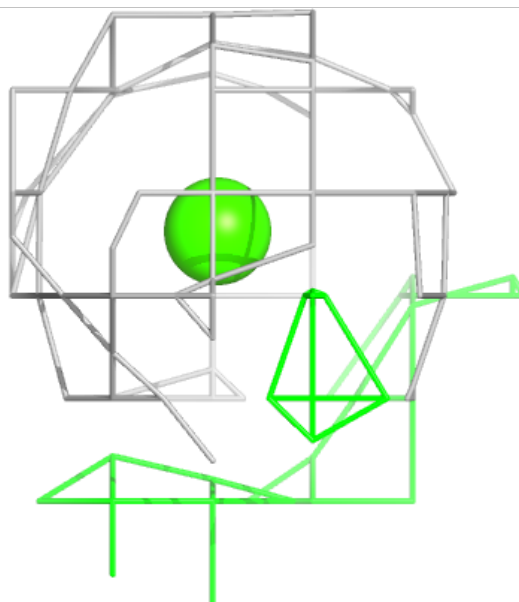
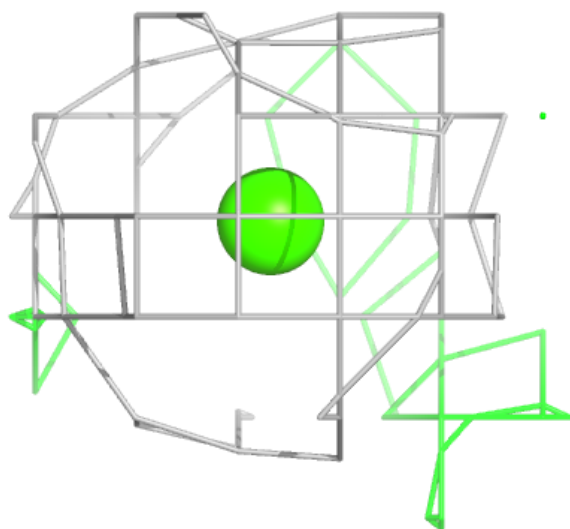
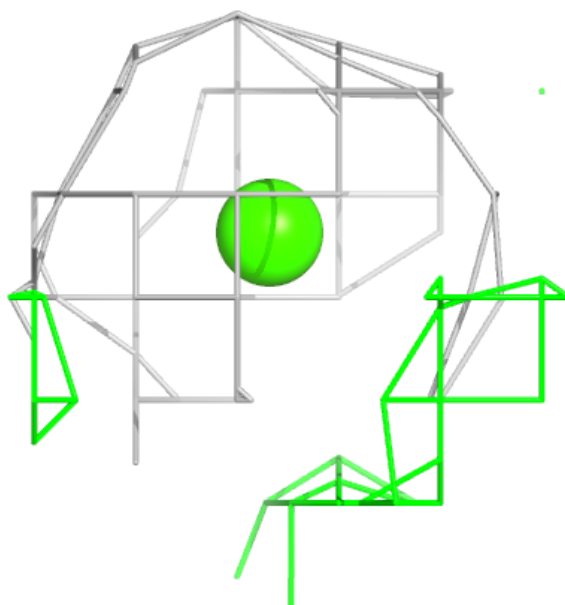
Electron density around CA A 501:

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



Electron density around CA C 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.