Full wwPDB X-ray Structure Validation Report ⓘ

Jul 17, 2024 – 01:59 pm BST

PDB ID	:	8OPW
Title	:	Structure of Mycobacterium tuberculosis beta-oxidation trifunctional enzyme in complex with Caffeine (Fragment-B-51)
Authors	:	Dalwani, S.; Wierenga, R.K.; Venkatesan, R.
Deposited on	:	2023-04-10
Resolution	:	2.52 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:

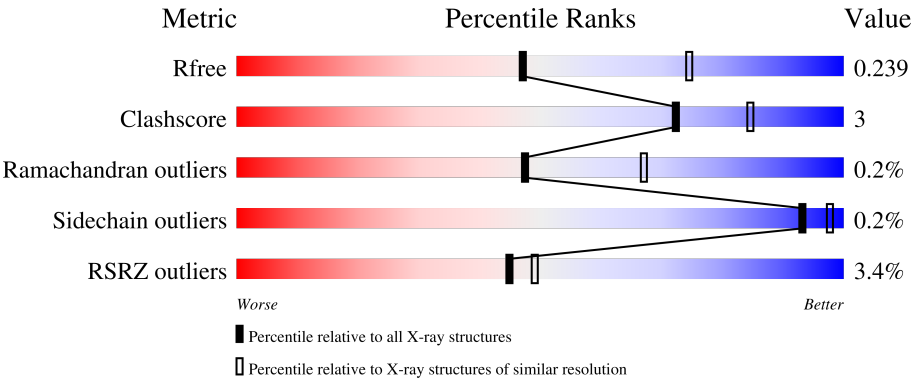
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 <=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	736	4% 90% 9%
1	B	736	2% 90% 8%
2	C	403	3% 88% 9%
2	D	403	4% 88% 10%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17040 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 3-hydroxyacyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	1	0
			5428	3435	934	1037	22			
1	B	727	Total	C	N	O	S	0	1	0
			5410	3423	929	1036	22			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP O53872
A	-14	GLY	-	expression tag	UNP O53872
A	-13	SER	-	expression tag	UNP O53872
A	-12	SER	-	expression tag	UNP O53872
A	-11	HIS	-	expression tag	UNP O53872
A	-10	HIS	-	expression tag	UNP O53872
A	-9	HIS	-	expression tag	UNP O53872
A	-8	HIS	-	expression tag	UNP O53872
A	-7	HIS	-	expression tag	UNP O53872
A	-6	HIS	-	expression tag	UNP O53872
A	-5	SER	-	expression tag	UNP O53872
A	-4	GLN	-	expression tag	UNP O53872
A	-3	ASP	-	expression tag	UNP O53872
A	-2	PRO	-	expression tag	UNP O53872
A	-1	ASN	-	expression tag	UNP O53872
A	0	SER	-	expression tag	UNP O53872
B	-15	MET	-	initiating methionine	UNP O53872
B	-14	GLY	-	expression tag	UNP O53872
B	-13	SER	-	expression tag	UNP O53872
B	-12	SER	-	expression tag	UNP O53872
B	-11	HIS	-	expression tag	UNP O53872
B	-10	HIS	-	expression tag	UNP O53872
B	-9	HIS	-	expression tag	UNP O53872
B	-8	HIS	-	expression tag	UNP O53872
B	-7	HIS	-	expression tag	UNP O53872

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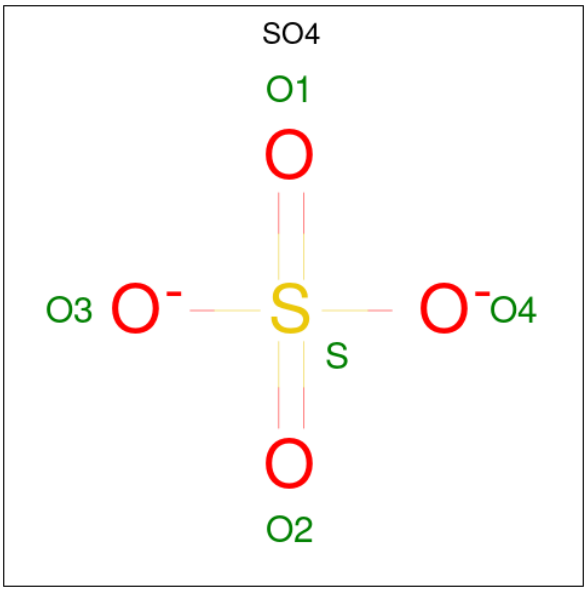
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP O53872
B	-5	SER	-	expression tag	UNP O53872
B	-4	GLN	-	expression tag	UNP O53872
B	-3	ASP	-	expression tag	UNP O53872
B	-2	PRO	-	expression tag	UNP O53872
B	-1	ASN	-	expression tag	UNP O53872
B	0	SER	-	expression tag	UNP O53872

- Molecule 2 is a protein called Putative acyltransferase Rv0859.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	394	Total	C	N	O	S	0	0	0
			2911	1816	517	563	15			
2	D	395	Total	C	N	O	S	0	0	0
			2917	1820	518	564	15			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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

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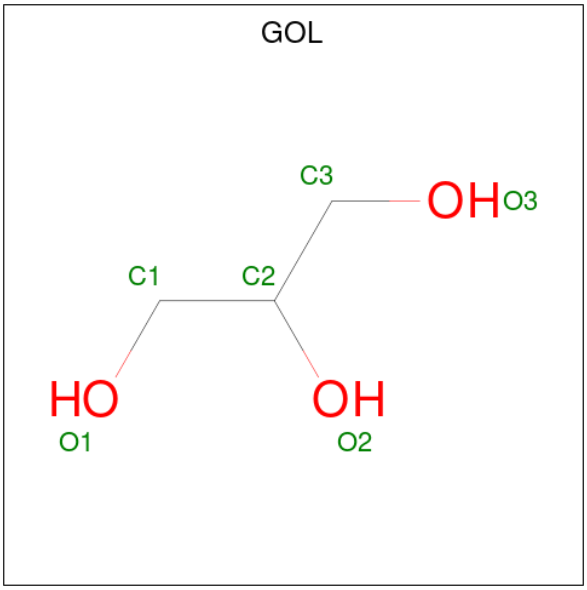
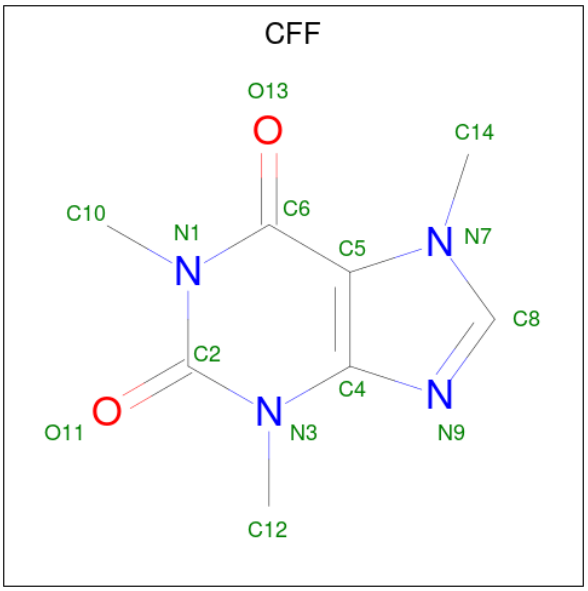
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 14 8 4 2	0	0
5	D	1	Total C N O 14 8 4 2	0	0

- Molecule 6 is water.

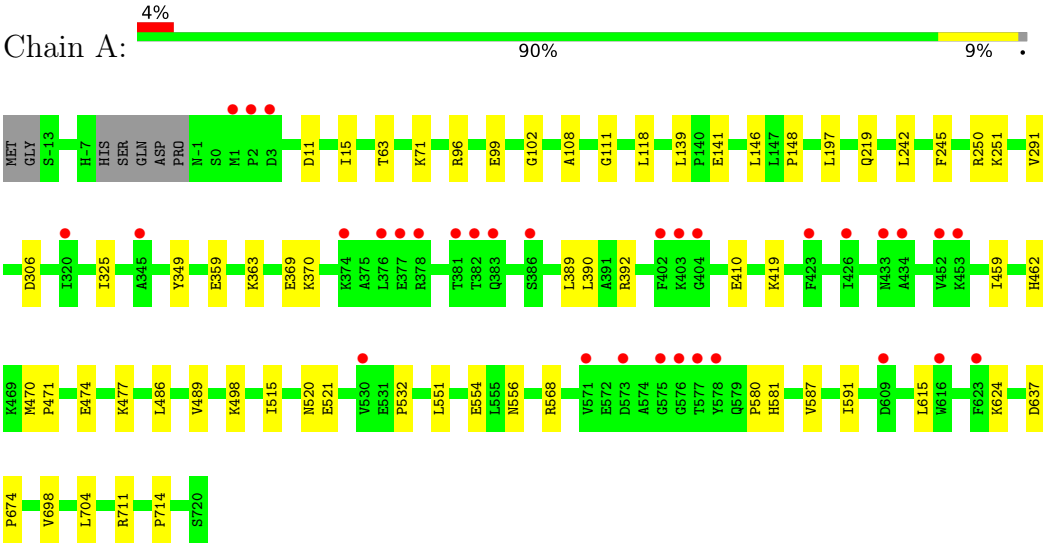
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	38	Total O 38 38	0	0
6	B	51	Total O 51 51	0	0
6	C	49	Total O 49 49	0	0
6	D	36	Total O 36 36	0	0

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.

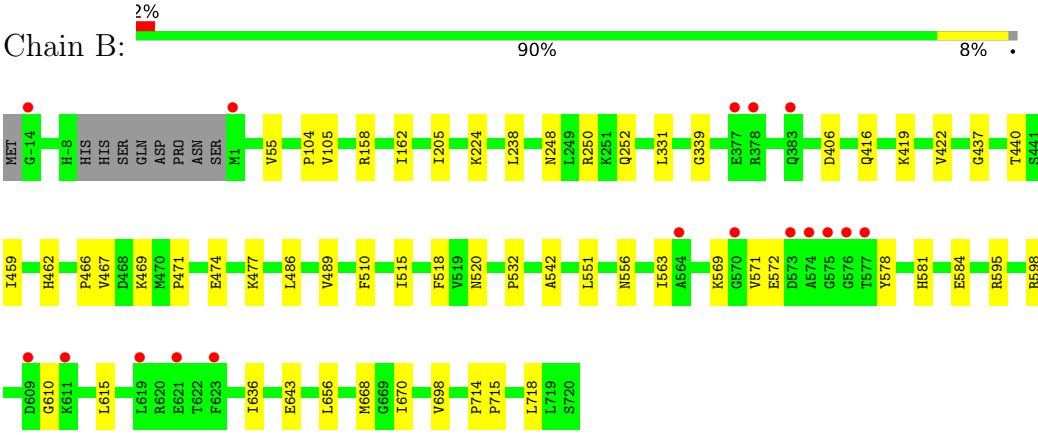
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

Chain A:



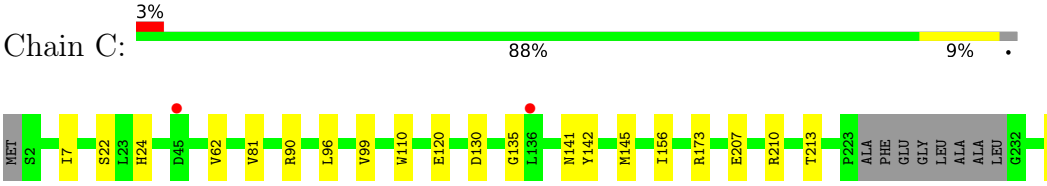
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

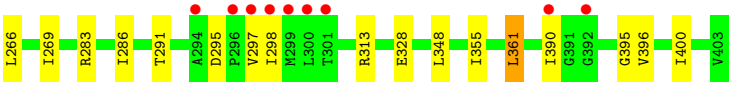
Chain B:



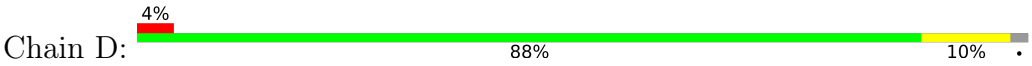
• Molecule 2: Putative acyltransferase Rv0859

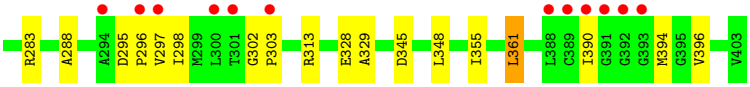
Chain C:





• Molecule 2: Putative acyltransferase Rv0859





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	249.51Å 134.50Å 118.98Å 90.00° 110.86° 90.00°	Depositor
Resolution (Å)	48.19 – 2.52 48.19 – 2.52	Depositor EDS
% Data completeness (in resolution range)	96.9 (48.19-2.52) 96.9 (48.19-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.205 , 0.240 0.204 , 0.239	Depositor DCC
R_{free} test set	2074 reflections (1.72%)	wwPDB-VP
Wilson B-factor (Å^2)	57.2	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17040	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: CFF, SO4, GOL

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	0.25	0/5533	0.46	0/7487
1	B	0.25	0/5510	0.46	0/7455
2	C	0.25	0/2954	0.50	0/3998
2	D	0.25	0/2960	0.49	0/4007
All	All	0.25	0/16957	0.47	0/22947

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	5428	0	5468	37	0
1	B	5410	0	5454	34	0
2	C	2911	0	2930	28	0
2	D	2917	0	2937	26	0
3	A	30	0	0	1	0
3	B	40	0	0	0	0
3	C	35	0	0	1	0
3	D	25	0	0	0	0
4	A	24	0	32	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	B	14	0	10	0	0
5	D	14	0	10	0	0
6	A	38	0	0	2	0
6	B	51	0	0	1	0
6	C	49	0	0	1	0
6	D	36	0	0	1	0
All	All	17040	0	16865	115	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 (115) 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:250:ARG:NH1	2:D:142:TYR:O	2.18	0.77
2:C:173:ARG:NH2	2:C:348:LEU:O	2.23	0.72
2:D:173:ARG:NH2	2:D:348:LEU:O	2.23	0.69
1:B:578:TYR:OH	1:B:584:GLU:OE2	2.11	0.68
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.75	0.68
1:A:251:LYS:HD2	2:D:233:GLY:HA2	1.79	0.63
2:C:81:VAL:HG11	2:D:296:PRO:HD3	1.81	0.62
1:B:698:VAL:HG13	1:B:714:PRO:HG3	1.82	0.61
1:B:520:ASN:HB3	1:B:581:HIS:CE1	2.37	0.60
1:A:462:HIS:HB3	1:A:474:GLU:HB3	1.85	0.58
1:B:532:PRO:HB2	1:B:615:LEU:HD13	1.85	0.58
1:A:297:LYS:NZ	6:A:901:HOH:O	2.33	0.57
1:A:520:ASN:HB3	1:A:581:HIS:CE1	2.39	0.57
2:D:99:VAL:HG13	2:D:269:ILE:HD11	1.87	0.56
2:C:249:ASN:ND2	3:C:501:SO4:O3	2.37	0.56
2:C:295:ASP:HB3	2:C:298:ILE:HG22	1.86	0.56
2:C:120:GLU:HG2	2:C:361:LEU:HB2	1.87	0.56
1:A:410:GLU:OE2	1:A:419:LYS:NZ	2.37	0.55
2:D:390:ILE:HB	2:D:394:MET:HB2	1.87	0.55
1:B:598:ARG:NH1	1:B:610:GLY:O	2.34	0.55
1:A:369:GLU:HG2	1:A:390:LEU:HD13	1.89	0.55
2:C:62:VAL:HG22	2:D:62:VAL:HG22	1.90	0.54
2:C:90:ARG:NH2	2:D:53:ASP:OD2	2.40	0.54
2:D:28:PRO:HG3	2:D:121:SER:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:173:ARG:NH1	6:D:603:HOH:O	2.41	0.53
1:B:104:PRO:HG2	1:B:205:ILE:HG23	1.91	0.53
1:B:477:LYS:HB2	1:B:486:LEU:HD11	1.91	0.52
2:D:62:VAL:HG21	2:D:130:ASP:HA	1.90	0.52
2:D:172:LEU:HD22	2:D:215:LYS:HG2	1.91	0.52
1:A:471:PRO:HG2	1:A:668:MET:HB3	1.91	0.52
1:A:470:MET:O	1:A:498:LYS:NZ	2.37	0.52
1:B:331:LEU:HD13	1:B:422:VAL:HG12	1.91	0.52
1:A:141:GLU:HG3	4:A:810:GOL:H32	1.92	0.51
1:B:419:LYS:HE2	1:B:440:THR:HB	1.93	0.51
2:C:96:LEU:HD23	2:C:396:VAL:HG13	1.91	0.51
2:C:110:TRP:CD1	2:D:313:ARG:HD3	2.46	0.51
3:A:803:SO4:O1	2:C:24:HIS:NE2	2.37	0.50
1:B:158:ARG:NH1	6:B:902:HOH:O	2.44	0.49
1:B:442:THR:HG21	1:B:563:ILE:HG12	1.94	0.49
2:C:241:LYS:HD2	2:C:297:VAL:HG21	1.94	0.49
1:B:55:VAL:HB	1:B:105:VAL:HG22	1.95	0.49
2:D:328:GLU:HB3	2:D:355:ILE:HG13	1.92	0.49
2:D:147:VAL:HG11	2:D:297:VAL:HG13	1.93	0.49
2:D:120:GLU:HG2	2:D:361:LEU:HB2	1.95	0.49
1:A:146:LEU:HD22	1:A:291:VAL:HG22	1.96	0.48
1:A:532:PRO:HB2	1:A:615:LEU:HD13	1.96	0.48
1:B:459:ILE:HD13	1:B:489:VAL:HG21	1.96	0.47
1:B:515:ILE:HD11	1:B:551:LEU:HD21	1.95	0.47
1:B:715:PRO:HD2	1:B:718:LEU:HD12	1.96	0.47
2:C:99:VAL:HG13	2:C:269:ILE:HD11	1.95	0.47
2:C:62:VAL:HG21	2:C:130:ASP:HA	1.96	0.47
1:B:250:ARG:NH1	2:C:145:MET:HG2	2.30	0.47
1:B:416:GLN:HG3	1:B:448:LEU:HD23	1.95	0.47
2:D:96:LEU:HD23	2:D:396:VAL:HG12	1.97	0.47
2:D:295:ASP:HB3	2:D:298:ILE:HG22	1.97	0.47
1:A:302:ALA:HA	1:A:306:ASP:HB2	1.96	0.46
1:B:515:ILE:HD12	1:B:670:ILE:HB	1.98	0.46
1:A:698:VAL:HG13	1:A:714:PRO:HG3	1.96	0.46
1:A:108:ALA:HB1	1:A:197:LEU:HB3	1.97	0.46
1:A:359:GLU:HG2	1:A:363:LYS:HE2	1.98	0.46
2:D:28:PRO:HD2	2:D:64:ASP:HB3	1.98	0.46
2:C:283:ARG:NH1	6:C:605:HOH:O	2.49	0.46
2:D:40:ARG:NH1	2:D:77:SER:O	2.41	0.46
2:C:156:ILE:HG12	2:C:298:ILE:HD11	1.97	0.45
1:A:63:THR:HA	1:A:111:GLY:HA3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLU:HG3	1:A:219:GLN:HE21	1.81	0.45
1:B:471:PRO:HG2	1:B:668:MET:HB3	1.99	0.45
1:A:568:ARG:HH12	1:A:580:PRO:HG3	1.82	0.45
2:C:7:ILE:HD11	2:C:286:ILE:HD11	1.98	0.44
1:B:248:ASN:O	1:B:252:GLN:HG2	2.17	0.44
1:B:466:PRO:HG2	1:B:469:LYS:HE3	1.98	0.44
2:D:54:VAL:HG22	2:D:115:LEU:HB2	2.00	0.44
1:A:515:ILE:HD11	1:A:551:LEU:HD21	2.00	0.43
2:C:291:THR:HG22	2:C:396:VAL:HG23	2.00	0.43
1:B:162:ILE:HD12	1:B:238:LEU:HD21	2.00	0.43
1:A:389:LEU:HA	1:A:392:ARG:NH1	2.34	0.43
1:B:518:PHE:HB2	1:B:643:GLU:CD	2.39	0.43
2:D:302:GLY:N	2:D:303:PRO:HD2	2.33	0.43
1:A:71:LYS:HE3	1:A:71:LYS:HB2	1.86	0.43
1:B:250:ARG:NH1	2:C:142:TYR:O	2.51	0.43
1:B:569:LYS:HA	1:B:572:GLU:HB3	2.01	0.43
1:A:587:VAL:O	1:A:591:ILE:HG12	2.19	0.43
1:B:339:GLY:HA3	1:B:467:VAL:HB	2.00	0.43
2:C:390:ILE:HD12	2:C:395:GLY:N	2.33	0.43
1:A:521:GLU:OE2	1:A:711:ARG:NE	2.31	0.42
2:C:22:SER:OG	2:C:207:GLU:OE2	2.28	0.42
1:B:510:PHE:CD1	1:B:656:LEU:HD11	2.54	0.42
1:A:242:LEU:HD12	1:A:245:PHE:CD2	2.54	0.42
2:C:313:ARG:HD3	2:D:110:TRP:CD1	2.54	0.42
1:B:224:LYS:HA	1:B:224:LYS:HD2	1.75	0.42
2:C:210:ARG:O	2:C:213:THR:OG1	2.29	0.42
1:A:102:GLY:N	6:A:903:HOH:O	2.52	0.42
1:A:477:LYS:HG3	1:A:486:LEU:HD21	2.01	0.42
2:C:110:TRP:CZ2	2:D:288:ALA:HA	2.55	0.42
1:A:118:LEU:HD23	1:A:139:LEU:HG	2.01	0.42
1:A:624:LYS:HE2	1:A:624:LYS:HB3	1.83	0.42
1:A:637:ASP:HB3	1:A:704:LEU:HD11	2.02	0.42
1:B:406:ASP:OD1	1:B:406:ASP:N	2.54	0.41
1:B:595:ARG:HG2	1:B:602:ALA:HB1	2.02	0.41
1:A:466:PRO:HB2	1:A:468:ASP:OD1	2.20	0.41
1:A:11:ASP:OD1	1:A:15:ILE:N	2.41	0.41
1:A:673:PRO:HA	1:A:674:PRO:HD3	1.96	0.41
2:D:38:GLU:HG3	2:D:42:ARG:HD2	2.01	0.41
1:A:96:ARG:NH1	1:A:99:GLU:OE1	2.50	0.41
1:A:370:LYS:HE3	1:A:370:LYS:HB2	1.91	0.41
2:C:135:GLY:HA2	2:C:141:ASN:HD22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:328:GLU:HB3	2:C:355:ILE:HG13	2.03	0.41
1:B:437:GLY:HA2	1:B:459:ILE:O	2.20	0.41
2:C:286:ILE:HD13	2:C:400:ILE:HG22	2.03	0.41
2:D:258:SER:HB3	2:D:329:ALA:HA	2.04	0.41
1:A:325:ILE:HB	1:A:349:TYR:CE1	2.56	0.40
1:A:459:ILE:HG21	1:A:489:VAL:HG21	2.03	0.40
1:B:542:ALA:HB2	1:B:636:ILE:HG23	2.03	0.40
1:B:595:ARG:HH22	1:B:606:GLU:HG2	1.86	0.40
2:C:266:LEU:HD23	2:C:266:LEU:HA	1.92	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	726/736 (99%)	705 (97%)	19 (3%)	2 (0%)	41	59
1	B	724/736 (98%)	694 (96%)	29 (4%)	1 (0%)	51	71
2	C	390/403 (97%)	382 (98%)	7 (2%)	1 (0%)	41	59
2	D	391/403 (97%)	378 (97%)	12 (3%)	1 (0%)	41	59
All	All	2231/2278 (98%)	2159 (97%)	67 (3%)	5 (0%)	47	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	361	LEU
2	D	361	LEU
1	B	556	ASN
1	A	556	ASN
1	A	148	PRO

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	559/566 (99%)	558 (100%)	1 (0%)	93 98
1	B	557/566 (98%)	556 (100%)	1 (0%)	93 98
2	C	305/310 (98%)	305 (100%)	0	100 100
2	D	305/310 (98%)	303 (99%)	2 (1%)	84 93
All	All	1726/1752 (98%)	1722 (100%)	4 (0%)	93 98

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

Mol	Chain	Res	Type
1	A	554	GLU
1	B	571	VAL
2	D	283	ARG
2	D	345	ASP

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

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)

35 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	B	806	-	4,4,4	0.14	0	6,6,6	0.05	0
5	CFF	D	501	-	8,15,15	1.22	1 (12%)	8,23,23	2.67	3 (37%)
3	SO4	A	803	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	A	802	-	4,4,4	0.15	0	6,6,6	0.06	0
4	GOL	D	507	-	5,5,5	0.90	0	5,5,5	1.00	0
3	SO4	B	803	-	4,4,4	0.15	0	6,6,6	0.07	0
3	SO4	D	503	-	4,4,4	0.13	0	6,6,6	0.06	0
3	SO4	C	505	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	802	-	4,4,4	0.13	0	6,6,6	0.07	0
4	GOL	A	810	-	5,5,5	0.89	0	5,5,5	1.00	0
3	SO4	C	503	-	4,4,4	0.15	0	6,6,6	0.05	0
4	GOL	A	809	-	5,5,5	0.94	0	5,5,5	0.95	0
3	SO4	D	505	-	4,4,4	0.13	0	6,6,6	0.07	0
3	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	D	506	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	C	504	-	4,4,4	0.13	0	6,6,6	0.08	0
3	SO4	D	504	-	4,4,4	0.13	0	6,6,6	0.08	0
3	SO4	D	502	-	4,4,4	0.13	0	6,6,6	0.07	0
3	SO4	A	801	-	4,4,4	0.14	0	6,6,6	0.07	0
4	GOL	B	810	-	5,5,5	0.89	0	5,5,5	1.02	0
3	SO4	A	805	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	C	507	-	4,4,4	0.14	0	6,6,6	0.10	0
4	GOL	C	508	-	5,5,5	0.90	0	5,5,5	1.02	0
4	GOL	A	807	-	5,5,5	0.88	0	5,5,5	1.04	0
5	CFF	B	801	-	8,15,15	1.23	1 (12%)	8,23,23	2.68	3 (37%)
4	GOL	A	808	-	5,5,5	0.92	0	5,5,5	0.99	0
3	SO4	B	808	-	4,4,4	0.15	0	6,6,6	0.03	0
3	SO4	B	805	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	A	804	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	807	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	A	806	-	4,4,4	0.14	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	B	804	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	C	506	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	B	809	-	4,4,4	0.14	0	6,6,6	0.04	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
4	GOL	A	808	-	-	0/4/4/4	-
4	GOL	A	809	-	-	0/4/4/4	-
4	GOL	B	810	-	-	0/4/4/4	-
5	CFF	D	501	-	-	-	0/2/2/2
5	CFF	B	801	-	-	-	0/2/2/2
4	GOL	D	507	-	-	0/4/4/4	-
4	GOL	C	508	-	-	0/4/4/4	-
4	GOL	A	807	-	-	0/4/4/4	-
4	GOL	A	810	-	-	1/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	801	CFF	C5-C4	-2.18	1.36	1.39
5	D	501	CFF	C5-C4	-2.15	1.36	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	801	CFF	C5-C6-N1	-5.44	112.40	118.20
5	D	501	CFF	C5-C6-N1	-5.42	112.42	118.20
5	B	801	CFF	C4-C5-C6	4.56	122.89	119.96
5	D	501	CFF	C4-C5-C6	4.55	122.89	119.96
5	D	501	CFF	C12-N3-C4	2.32	121.54	118.25
5	B	801	CFF	C12-N3-C4	2.29	121.50	118.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	810	GOL	O2-C2-C3-O3

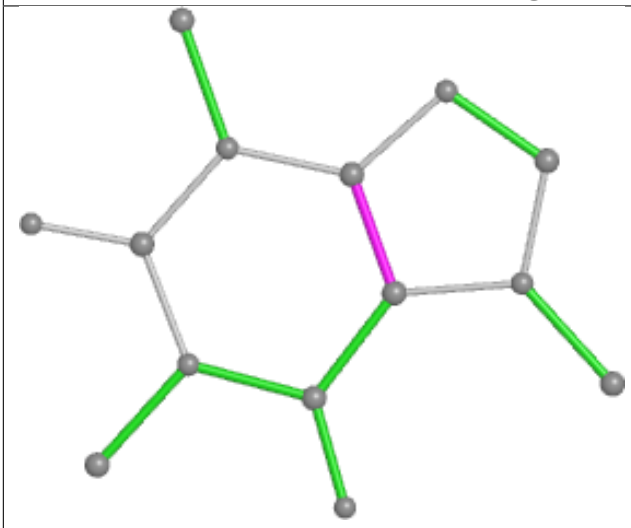
There are no ring outliers.

3 monomers are involved in 3 short contacts:

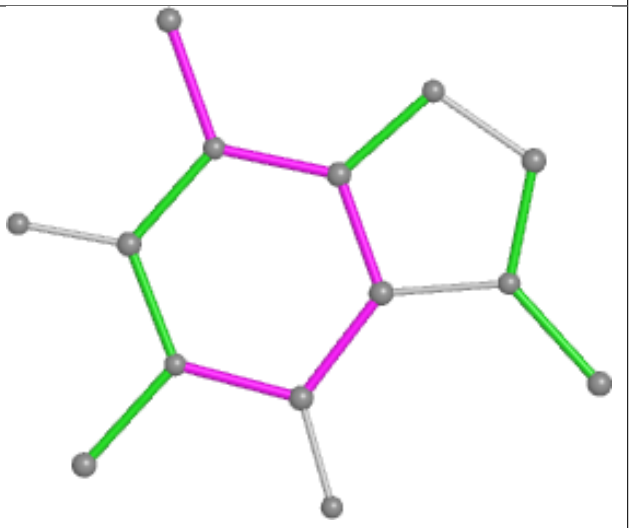
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	SO4	1	0
4	A	810	GOL	1	0
3	C	501	SO4	1	0

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.

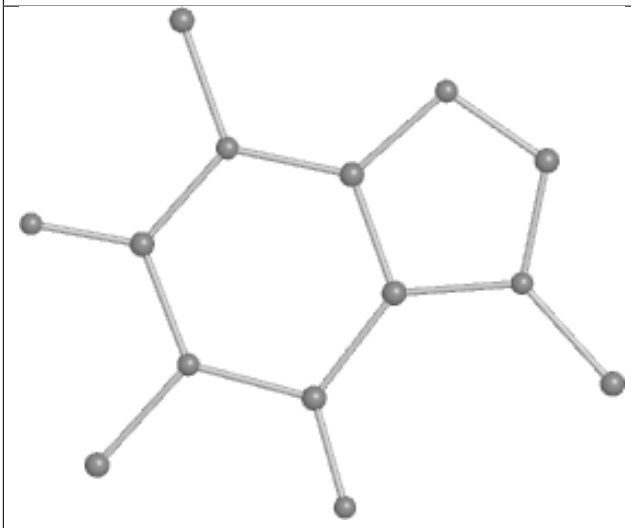
Ligand CFF D 501



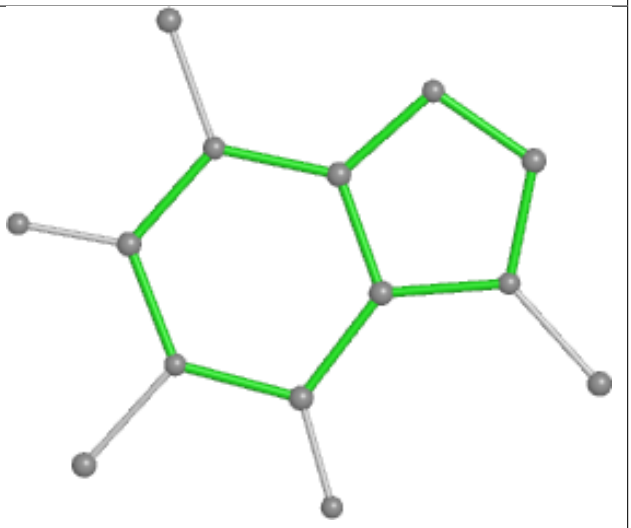
Bond lengths



Bond angles

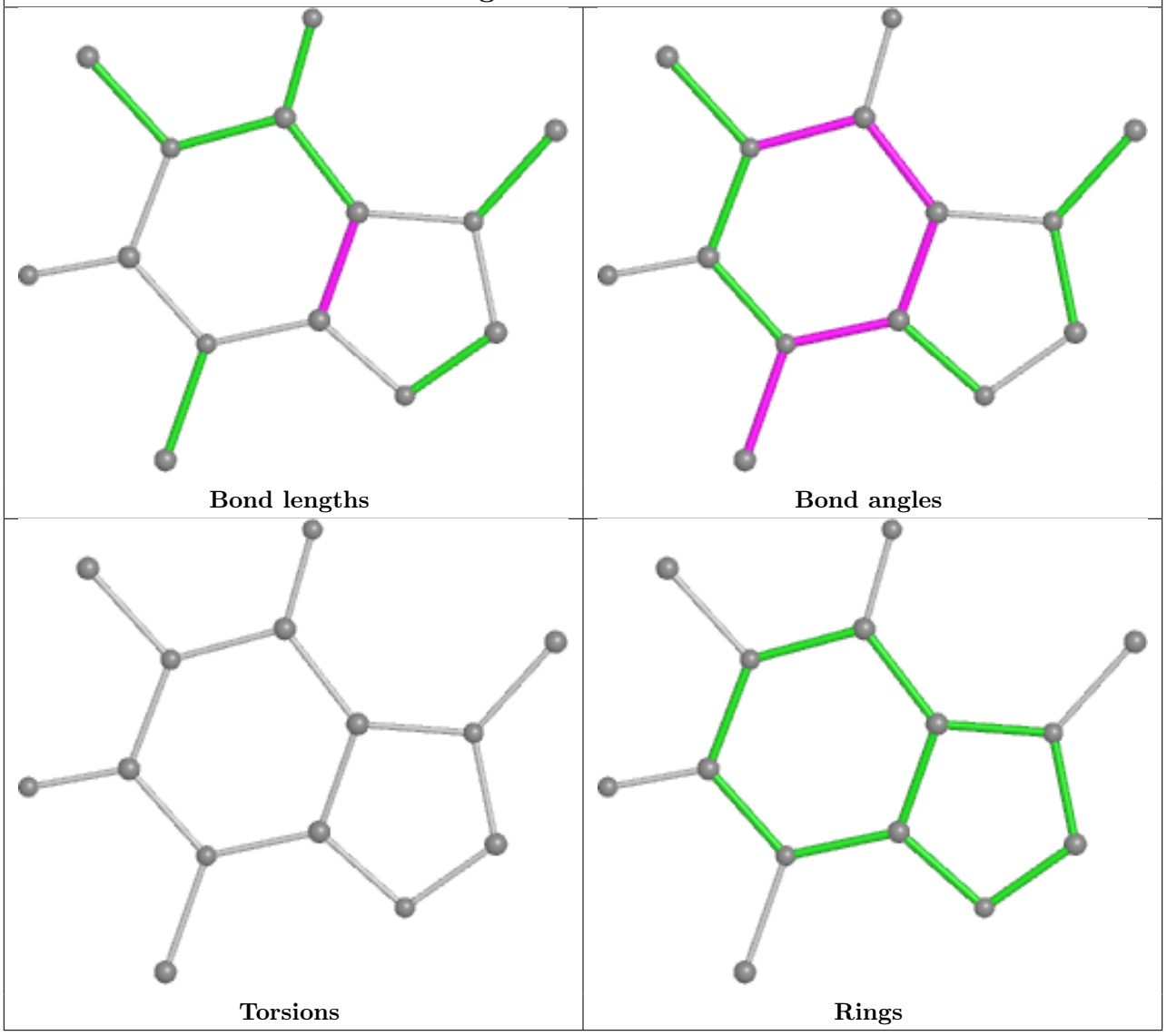


Torsions



Rings

Ligand CFF B 801



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, 95^{th} 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	729/736 (99%)	0.11	32 (4%)	34	37	39, 69, 105, 144	0
1	B	727/736 (98%)	-0.01	17 (2%)	60	64	41, 62, 99, 162	0
2	C	394/403 (97%)	0.13	11 (2%)	53	57	39, 52, 93, 139	0
2	D	395/403 (98%)	0.19	16 (4%)	37	41	40, 56, 95, 165	0
All	All	2245/2278 (98%)	0.09	76 (3%)	45	49	39, 61, 100, 165	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	575	GLY	10.9
1	B	574	ALA	6.2
1	B	576	GLY	5.8
2	D	301	THR	5.7
2	C	300	LEU	5.5
1	A	2	PRO	5.3
2	D	390	ILE	4.4
1	A	382	THR	4.2
1	A	377	GLU	3.9
1	A	575	GLY	3.9
1	A	3	ASP	3.9
2	D	391	GLY	3.8
1	B	564	ALA	3.8
1	B	570	GLY	3.8
1	B	577	THR	3.8
2	D	296	PRO	3.8
2	C	297	VAL	3.7
1	A	378	ARG	3.7
2	D	389	CYS	3.7
1	A	404	GLY	3.6
1	B	573	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	390	ILE	3.3
2	C	301	THR	3.3
1	A	376	LEU	3.2
1	B	1	MET	3.2
1	A	573	ASP	3.1
1	A	383	GLN	3.1
2	C	296	PRO	3.0
1	A	623	PHE	3.0
1	A	434	ALA	2.9
1	B	377	GLU	2.8
1	B	378	ARG	2.8
2	D	300	LEU	2.8
2	C	45	ASP	2.8
2	C	136	LEU	2.7
1	B	611	LYS	2.7
1	A	578	TYR	2.7
1	B	621	GLU	2.6
2	D	1	MET	2.6
1	A	374	LYS	2.6
1	A	403	LYS	2.6
1	A	1	MET	2.5
1	A	433	ASN	2.5
1	A	345	ALA	2.5
2	D	294	ALA	2.5
1	A	571	VAL	2.4
1	A	402	PHE	2.4
1	A	577	THR	2.4
1	A	453	LYS	2.3
1	A	452	VAL	2.3
1	A	320	ILE	2.3
1	B	-14	GLY	2.3
1	A	616	TRP	2.3
2	C	299	MET	2.3
2	D	392	GLY	2.3
2	D	303	PRO	2.3
1	A	386	SER	2.3
1	A	576	GLY	2.3
1	B	383	GLN	2.2
2	D	134	MET	2.2
1	B	609	ASP	2.2
1	A	381	THR	2.2
2	C	294	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	426	ILE	2.1
2	C	298	ILE	2.1
2	D	393	GLY	2.1
2	D	2	SER	2.1
2	D	297	VAL	2.1
1	A	530	VAL	2.1
2	D	93	ALA	2.0
2	C	392	GLY	2.0
1	B	619	LEU	2.0
1	A	423	PHE	2.0
2	D	388	LEU	2.0
1	B	623	PHE	2.0
1	A	609	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
4	GOL	A	810	6/6	0.81	0.33	89,93,106,109	0
3	SO4	B	806	5/5	0.82	0.30	131,143,150,162	0
4	GOL	A	807	6/6	0.87	0.33	59,82,86,96	0
3	SO4	B	807	5/5	0.88	0.17	146,148,160,166	0
4	GOL	D	507	6/6	0.88	0.40	54,72,81,83	0
3	SO4	B	809	5/5	0.89	0.34	119,119,149,158	0
4	GOL	B	810	6/6	0.90	0.19	45,66,72,78	0
3	SO4	B	805	5/5	0.90	0.41	108,117,131,152	0
3	SO4	C	503	5/5	0.91	0.14	88,98,107,111	0
3	SO4	A	806	5/5	0.91	0.33	124,134,142,153	0

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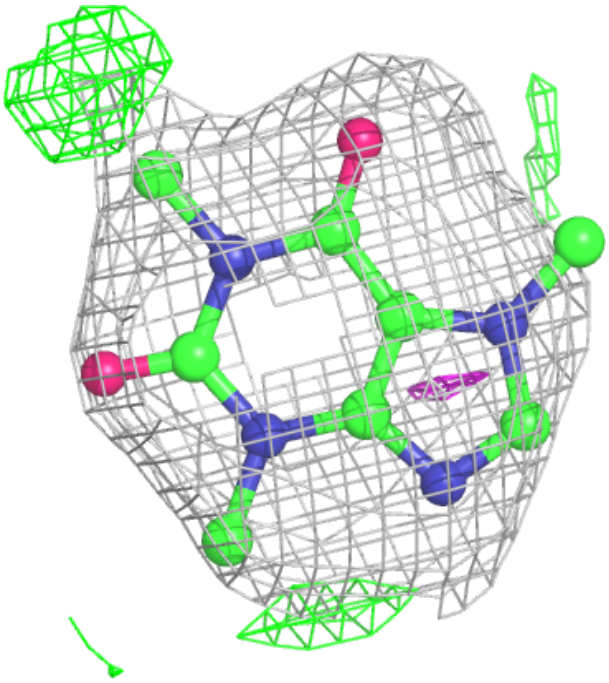
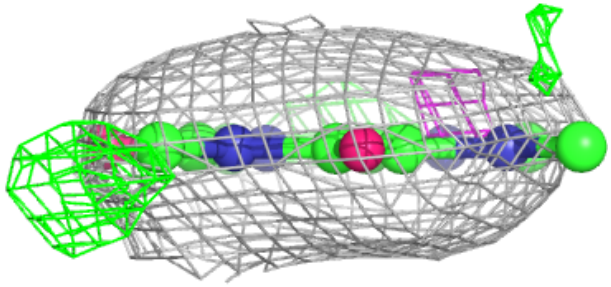
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	809	6/6	0.91	0.23	59,62,77,78	0
3	SO4	A	802	5/5	0.92	0.14	91,94,95,104	0
3	SO4	A	804	5/5	0.92	0.18	108,115,144,149	0
3	SO4	C	506	5/5	0.92	0.39	114,123,146,157	0
4	GOL	C	508	6/6	0.92	0.37	60,65,76,86	0
3	SO4	B	808	5/5	0.92	0.21	104,106,142,150	0
3	SO4	B	804	5/5	0.93	0.21	88,97,112,133	0
5	CFF	B	801	14/14	0.93	0.18	71,79,93,96	0
5	CFF	D	501	14/14	0.93	0.21	66,77,86,93	0
4	GOL	A	808	6/6	0.94	0.14	80,85,90,97	0
3	SO4	C	504	5/5	0.94	0.12	81,89,102,112	0
3	SO4	C	501	5/5	0.95	0.17	90,90,99,100	0
3	SO4	C	507	5/5	0.95	0.14	83,101,108,119	0
3	SO4	D	504	5/5	0.95	0.11	69,91,102,104	0
3	SO4	A	805	5/5	0.95	0.08	118,123,129,151	0
3	SO4	A	803	5/5	0.95	0.22	97,101,123,126	0
3	SO4	C	505	5/5	0.95	0.25	102,107,117,130	0
3	SO4	A	801	5/5	0.96	0.12	79,82,100,122	0
3	SO4	D	505	5/5	0.96	0.08	103,106,113,115	5
3	SO4	D	506	5/5	0.96	0.28	88,94,116,128	0
3	SO4	B	803	5/5	0.96	0.14	65,84,98,117	0
3	SO4	D	502	5/5	0.97	0.17	84,85,98,101	0
3	SO4	B	802	5/5	0.98	0.10	79,86,102,107	0
3	SO4	C	502	5/5	0.98	0.08	73,73,86,89	0
3	SO4	D	503	5/5	0.98	0.17	89,91,96,109	0

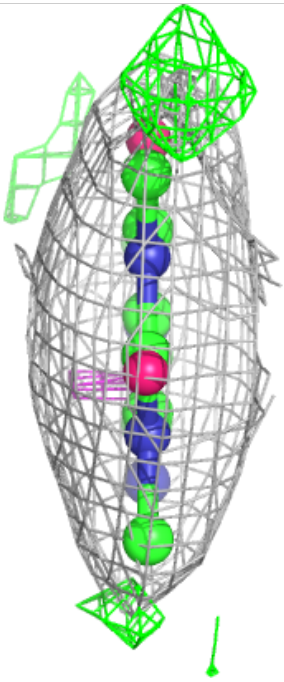
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CFF B 801:

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

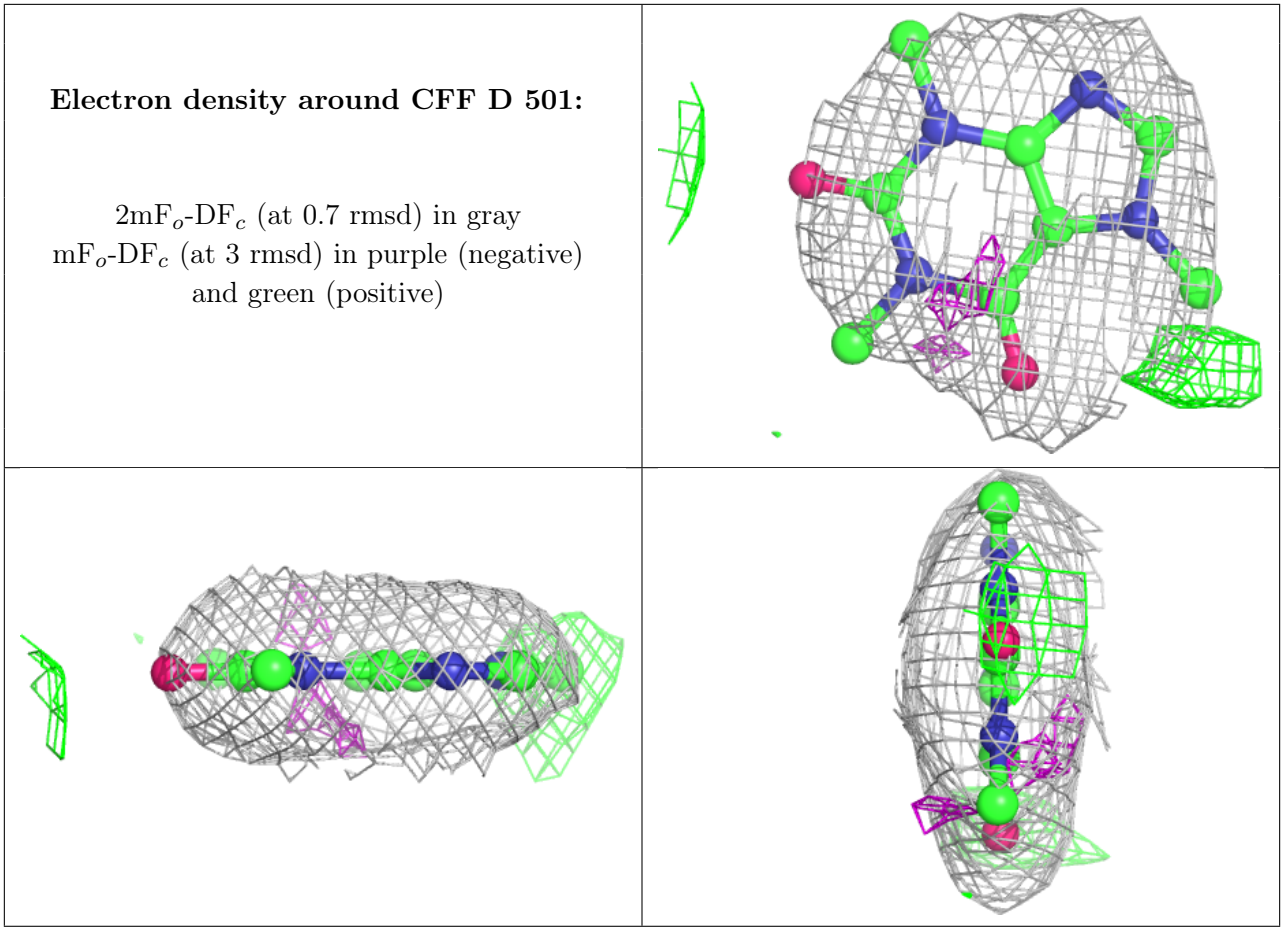






Electron density around CFF D 501:

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



6.5 Other polymers

There are no such residues in this entry.