



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:32 PM UTC

PDB ID : 8OPY / pdb_00008opy
Title : Structure of Mycobacterium tuberculosis beta-oxidation trifunctional enzyme
in complex with Fragment-B-DNQ
Authors : Dalwani, S.; Wierenga, R.K.; Venkatesan, R.
Deposited on : 2023-04-10
Resolution : 2.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

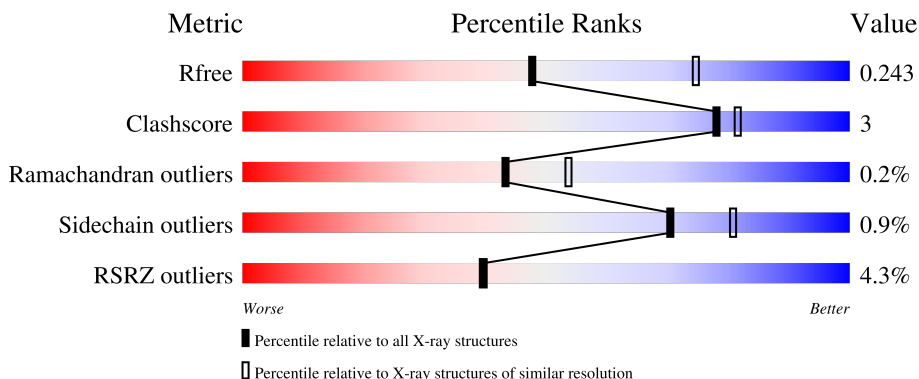
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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

Mol	Chain	Length	Quality of chain
1	A	736	
1	B	736	
2	C	403	
2	D	403	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17024 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
			Total	C	N	O	S			
1	A	731	5448	3445	939	1042	22	0	1	0
1	B	728	5425	3432	934	1037	22	0	1	0

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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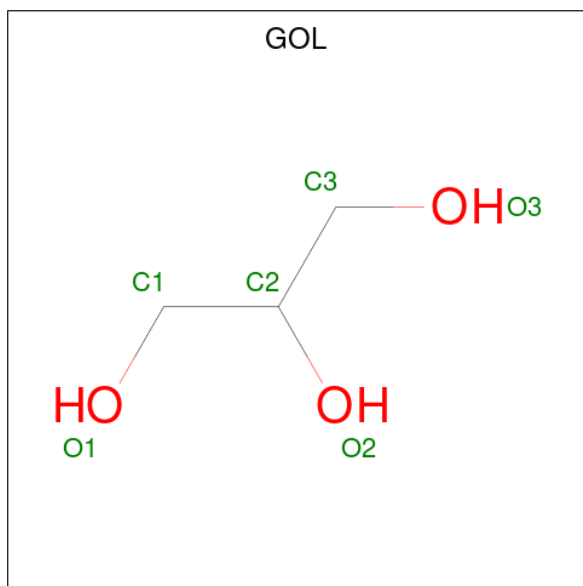
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP O53872
B	-5	SER	-	expression tag	UNP O53872
B	-4	GLN	-	expression tag	UNP O53872
B	-3	ASP	-	expression tag	UNP O53872
B	-2	PRO	-	expression tag	UNP O53872
B	-1	ASN	-	expression 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	395	Total	C	N	O	S	0	1	0
			2921	1822	518	566	15			
2	D	399	Total	C	N	O	S	0	0	0
			2939	1834	522	568	15			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



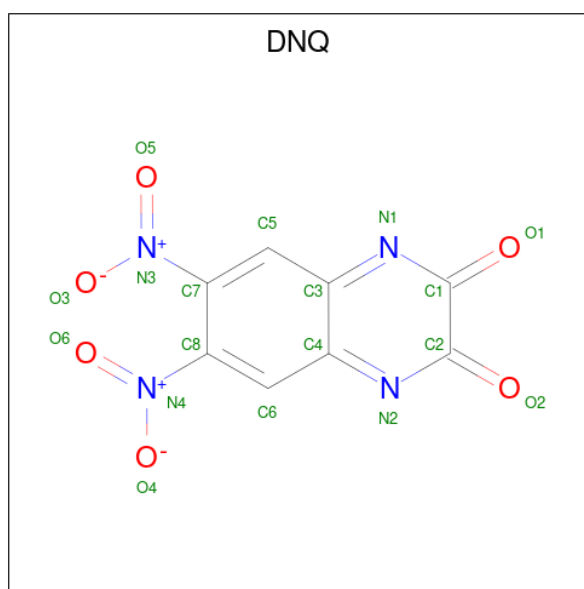
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total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

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

- Molecule 5 is 6,7-DINITROQUINOXALINE-2,3-DIONE (CCD ID: DNQ) (formula: $C_8H_2N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	1
			18	8	4	6		
5	D	1	Total	C	N	O	0	1
			18	8	4	6		

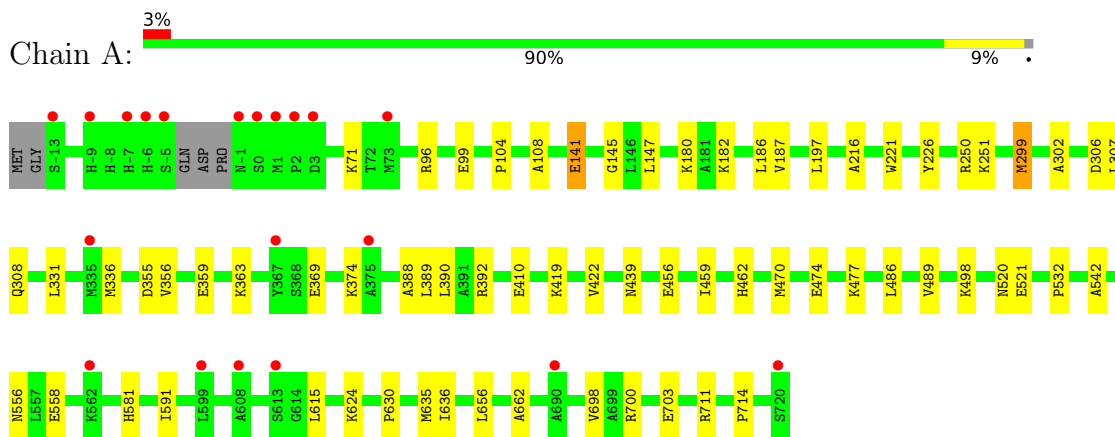
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	29	Total O 29 29	0	0
6	B	34	Total O 34 34	0	0
6	C	41	Total O 41 41	0	0
6	D	28	Total O 28 28	0	0

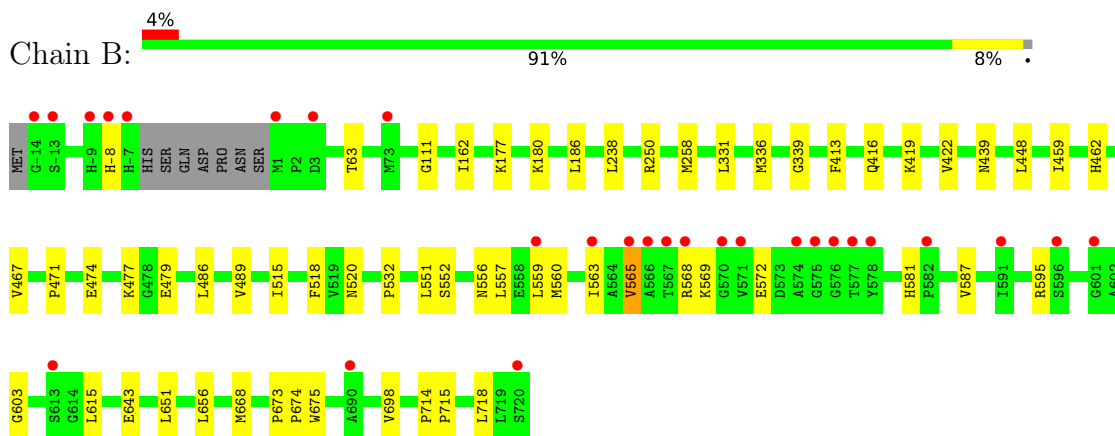
3 Residue-property plots [i](#)

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.

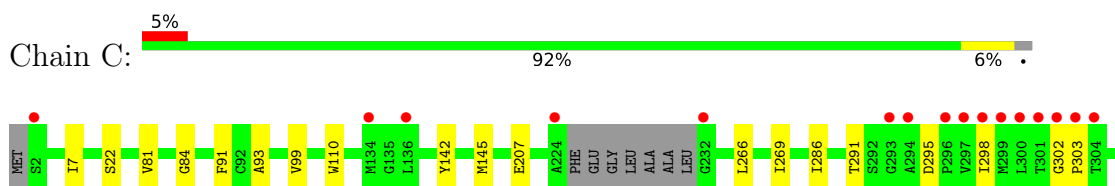
- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

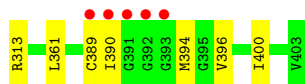


- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

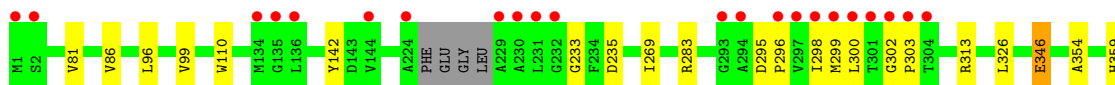
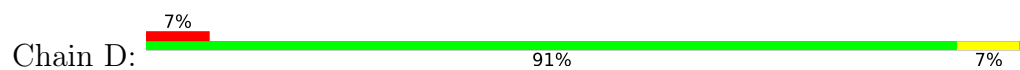


- Molecule 2: Putative acyltransferase Rv0859





● Molecule 2: Putative acyltransferase Rv0859



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	249.82Å 134.53Å 118.84Å 90.00° 110.82° 90.00°	Depositor
Resolution (Å)	47.01 – 2.45 47.01 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.7 (47.01-2.45) 98.1 (47.01-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.45Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.211 , 0.243 0.209 , 0.243	Depositor DCC
R_{free} test set	2100 reflections (1.55%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtrriage
Anisotropy	0.228	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17024	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, DNQ, SO4

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	0.11	0/5551	0.27	0/7511
1	B	0.12	0/5527	0.27	0/7478
2	C	0.12	0/2967	0.30	0/4016
2	D	0.13	0/2982	0.31	0/4037
All	All	0.12	0/17027	0.28	0/23042

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5448	0	5482	34	0
1	B	5425	0	5466	29	0
2	C	2921	0	2939	18	0
2	D	2939	0	2961	22	0
3	A	12	0	16	0	0
3	B	6	0	8	0	0
4	A	25	0	0	0	0
4	B	35	0	0	0	0
4	C	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	20	0	0	0	0
5	D	36	0	4	0	0
6	A	29	0	0	0	0
6	B	34	0	0	0	0
6	C	41	0	0	0	0
6	D	28	0	0	1	0
All	All	17024	0	16876	95	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 (95) 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)
2:D:382:ARG:HG3	2:D:383:ARG:HG3	1.74	0.69
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.75	0.67
1:A:251:LYS:HD2	2:D:233:GLY:HA2	1.80	0.64
1:A:250:ARG:NH1	2:D:142:TYR:O	2.32	0.63
2:D:382:ARG:NH2	2:D:401:GLU:OE2	2.27	0.62
2:D:99:VAL:HG13	2:D:269:ILE:HD11	1.82	0.61
1:B:250:ARG:NH1	2:C:142:TYR:O	2.34	0.61
1:A:462:HIS:HB3	1:A:474:GLU:HB3	1.84	0.59
1:B:698:VAL:HG13	1:B:714:PRO:HG3	1.84	0.58
2:C:91:PHE:HB2	2:C:390:ILE:HG23	1.86	0.58
1:B:520:ASN:HB3	1:B:581:HIS:CE1	2.38	0.58
1:B:532:PRO:HB2	1:B:615:LEU:HD13	1.86	0.57
2:C:84:GLY:HA2	2:D:394:MET:HE3	1.85	0.57
1:A:369:GLU:HG2	1:A:390:LEU:HD13	1.87	0.56
1:A:470:MET:O	1:A:498:LYS:NZ	2.34	0.56
1:A:520:ASN:HB3	1:A:581:HIS:CE1	2.40	0.55
2:C:295:ASP:HB3	2:C:298:ILE:HG22	1.88	0.55
2:C:81:VAL:HG11	2:D:296:PRO:HD3	1.88	0.55
2:D:302:GLY:N	2:D:303:PRO:HD2	2.22	0.54
1:A:410:GLU:OE2	1:A:419:LYS:NZ	2.36	0.53
1:B:565:VAL:HG23	1:B:569:LYS:HE2	1.91	0.53
1:B:331:LEU:HD13	1:B:422:VAL:HG12	1.89	0.53
1:A:359:GLU:HG2	1:A:363:LYS:HE2	1.91	0.52
2:C:22:SER:OG	2:C:207:GLU:OE2	2.23	0.52
1:A:698:VAL:HG13	1:A:714:PRO:HG3	1.91	0.52
2:D:295:ASP:HB3	2:D:298:ILE:HG22	1.92	0.51
2:D:390:ILE:HD12	2:D:394:MET:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:LEU:HB3	1:B:587:VAL:HG13	1.93	0.51
1:B:471:PRO:HG2	1:B:668:MET:HB3	1.94	0.50
2:C:302:GLY:N	2:C:303:PRO:HD2	2.27	0.50
2:C:110:TRP:CD1	2:D:313:ARG:HD3	2.47	0.50
2:C:390:ILE:HG21	2:C:394:MET:HE3	1.94	0.50
1:A:459:ILE:HG21	1:A:489:VAL:HG21	1.94	0.50
1:B:459:ILE:HD13	1:B:489:VAL:HG21	1.94	0.49
1:B:250:ARG:NH1	2:C:145:MET:HG2	2.27	0.49
1:B:413:PHE:O	1:B:419:LYS:NZ	2.45	0.49
1:A:477:LYS:HG3	1:A:486:LEU:HD21	1.95	0.48
1:B:515:ILE:HD11	1:B:551:LEU:HD21	1.94	0.48
2:C:291:THR:HG22	2:C:396:VAL:HG22	1.94	0.48
2:C:93:ALA:HB2	2:C:390:ILE:HD11	1.95	0.47
2:C:303:PRO:HD3	2:C:389:CYS:HA	1.97	0.47
1:A:302:ALA:HA	1:A:306:ASP:HB2	1.96	0.47
2:C:99:VAL:HG13	2:C:269:ILE:HD11	1.96	0.47
1:A:700:ARG:NH1	1:A:703:GLU:OE1	2.48	0.47
1:A:96:ARG:NH1	1:A:99:GLU:OE1	2.45	0.46
2:C:313:ARG:HD3	2:D:110:TRP:CD1	2.49	0.46
1:A:656:LEU:HD13	1:A:662:ALA:HB2	1.97	0.46
1:B:258:MET:HG2	1:B:675:TRP:HB3	1.97	0.46
1:B:518:PHE:HB2	1:B:643:GLU:CD	2.41	0.46
2:C:7:ILE:HD11	2:C:286:ILE:HD11	1.96	0.46
1:A:331:LEU:HD13	1:A:422:VAL:HG12	1.99	0.45
1:A:355:ASP:OD1	1:A:356:VAL:N	2.43	0.45
1:A:71:LYS:HE3	1:A:71:LYS:HB2	1.83	0.45
2:D:96:LEU:HD23	2:D:396:VAL:HG12	2.00	0.44
1:B:162:ILE:HD12	1:B:238:LEU:HD21	1.99	0.44
1:A:104:PRO:HG3	1:A:216:ALA:HB1	1.99	0.44
2:D:326:LEU:HD13	2:D:387:THR:HG23	2.00	0.44
2:D:382:ARG:CG	2:D:383:ARG:HG3	2.47	0.44
1:A:630:PRO:HG2	1:A:635:MET:HE2	2.00	0.43
1:B:651:LEU:HD23	1:B:656:LEU:HB2	2.00	0.43
2:D:299:MET:O	2:D:393:GLY:HA2	2.18	0.43
1:A:521:GLU:OE2	1:A:711:ARG:NE	2.35	0.43
2:D:354:ALA:HB1	2:D:359:HIS:HB2	2.01	0.43
1:A:145:GLY:HA2	1:A:299:MET:HE3	2.00	0.43
2:D:390:ILE:HD11	2:D:396:VAL:HG23	1.99	0.43
1:A:141:GLU:HG3	1:A:147:LEU:C	2.44	0.43
1:A:336:MET:HE2	1:A:439:ASN:HD21	1.84	0.43
1:B:336:MET:HE2	1:B:439:ASN:HD21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:PRO:HD2	1:B:718:LEU:HD12	2.00	0.43
1:B:416:GLN:HG3	1:B:448:LEU:HD23	2.00	0.42
1:A:542:ALA:HB2	1:A:636:ILE:HG23	2.01	0.42
1:A:532:PRO:HB2	1:A:615:LEU:HD13	2.01	0.42
1:B:477:LYS:HB2	1:B:486:LEU:HD11	2.00	0.42
1:A:624:LYS:HB3	1:A:624:LYS:HE2	1.84	0.42
2:D:298:ILE:O	2:D:300:LEU:N	2.47	0.42
1:A:108:ALA:HB1	1:A:197:LEU:HB3	2.01	0.42
1:A:389:LEU:HA	1:A:392:ARG:NH1	2.35	0.42
1:A:558:GLU:HG3	1:A:591:ILE:HD12	2.01	0.42
1:A:388:ALA:O	1:A:392:ARG:HG3	2.20	0.41
1:B:63:THR:HA	1:B:111:GLY:HA3	2.01	0.41
1:B:177:LYS:HB2	1:B:180:LYS:HD3	2.03	0.41
1:B:552:SER:HB3	1:B:560:MET:HE1	2.02	0.41
2:C:266:LEU:HD23	2:C:266:LEU:HA	1.94	0.41
1:B:595:ARG:HB3	1:B:603:GLY:HA2	2.03	0.41
1:B:673:PRO:HA	1:B:674:PRO:HD3	1.94	0.41
2:D:390:ILE:HB	2:D:394:MET:HB2	2.03	0.41
1:A:182:LYS:HA	1:A:187:VAL:O	2.20	0.41
1:A:221:TRP:HA	1:A:226:TYR:CG	2.56	0.41
2:D:346:GLU:CD	2:D:346:GLU:H	2.29	0.41
2:D:283:ARG:NH2	6:D:602:HOH:O	2.54	0.40
1:B:568:ARG:NH1	1:B:572:GLU:OE2	2.54	0.40
2:C:286:ILE:HD13	2:C:400:ILE:HG22	2.02	0.40
1:A:331:LEU:HB2	1:A:410:GLU:HA	2.04	0.40
1:B:339:GLY:HA3	1:B:467:VAL:HB	2.02	0.40
1:B:559:LEU:O	1:B:563:ILE:HG13	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	728/736 (99%)	703 (97%)	24 (3%)	1 (0%)	48	61
1	B	725/736 (98%)	703 (97%)	20 (3%)	2 (0%)	36	45
2	C	392/403 (97%)	382 (97%)	9 (2%)	1 (0%)	36	45
2	D	395/403 (98%)	381 (96%)	13 (3%)	1 (0%)	36	45
All	All	2240/2278 (98%)	2169 (97%)	66 (3%)	5 (0%)	43	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	361	LEU
1	B	-8	HIS
2	D	361	LEU
1	A	556	ASN
1	B	556	ASN

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	562/566 (99%)	554 (99%)	8 (1%)	59	72
1	B	559/566 (99%)	556 (100%)	3 (0%)	81	87
2	C	306/310 (99%)	306 (100%)	0	100	100
2	D	306/310 (99%)	301 (98%)	5 (2%)	55	69
All	All	1733/1752 (99%)	1717 (99%)	16 (1%)	70	81

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	GLU
1	A	180	LYS
1	A	186	LEU
1	A	299	MET
1	A	307	LEU
1	A	308	GLN

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Mol	Chain	Res	Type
1	A	374	LYS
1	A	456	GLU
1	B	186	LEU
1	B	479	GLU
1	B	565	VAL
2	D	81	VAL
2	D	86	VAL
2	D	235	ASP
2	D	346	GLU
2	D	382	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	416	GLN
1	A	561	HIS
1	B	633	GLN
1	B	681	GLN
2	D	43	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

26 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
4	SO4	C	501	-	4,4,4	0.25	0	6,6,6	0.12	0
4	SO4	D	503	-	4,4,4	0.22	0	6,6,6	0.10	0
5	DNQ	D	501[A]	-	19,19,19	1.90	4 (21%)	10,28,28	1.04	0
5	DNQ	D	502[B]	-	19,19,19	1.91	4 (21%)	10,28,28	1.03	0
4	SO4	A	807	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	B	804	-	4,4,4	0.23	0	6,6,6	0.11	0
3	GOL	A	801	-	5,5,5	0.94	0	5,5,5	0.98	0
4	SO4	B	806	-	4,4,4	0.24	0	6,6,6	0.11	0
4	SO4	A	806	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	C	504	-	4,4,4	0.22	0	6,6,6	0.12	0
4	SO4	C	505	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	D	506	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	B	808	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	A	803	-	4,4,4	0.24	0	6,6,6	0.05	0
4	SO4	B	802	-	4,4,4	0.23	0	6,6,6	0.11	0
4	SO4	A	805	-	4,4,4	0.22	0	6,6,6	0.10	0
4	SO4	B	807	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	C	503	-	4,4,4	0.25	0	6,6,6	0.07	0
4	SO4	D	505	-	4,4,4	0.23	0	6,6,6	0.12	0
4	SO4	A	804	-	4,4,4	0.23	0	6,6,6	0.09	0
3	GOL	B	801	-	5,5,5	0.81	0	5,5,5	1.05	0
4	SO4	D	504	-	4,4,4	0.22	0	6,6,6	0.10	0
3	GOL	A	802	-	5,5,5	1.00	0	5,5,5	1.01	0
4	SO4	B	805	-	4,4,4	0.26	0	6,6,6	0.10	0
4	SO4	B	803	-	4,4,4	0.25	0	6,6,6	0.10	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	B	801	-	-	1/4/4/4	-
3	GOL	A	801	-	-	0/4/4/4	-
3	GOL	A	802	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DNQ	D	501[A]	-	-	0/4/20/20	0/2/2/2
5	DNQ	D	502[B]	-	-	3/4/20/20	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501[A]	DNQ	C3-N1	3.85	1.37	1.33
5	D	502[B]	DNQ	C4-N2	3.85	1.37	1.33
5	D	501[A]	DNQ	C4-N2	3.84	1.37	1.33
5	D	502[B]	DNQ	C3-N1	3.84	1.37	1.33
5	D	502[B]	DNQ	C1-N1	3.37	1.43	1.38
5	D	502[B]	DNQ	C2-N2	3.36	1.43	1.38
5	D	501[A]	DNQ	C1-N1	3.34	1.43	1.38
5	D	501[A]	DNQ	C2-N2	3.33	1.43	1.38

There are no bond angle outliers.

There are no chirality outliers.

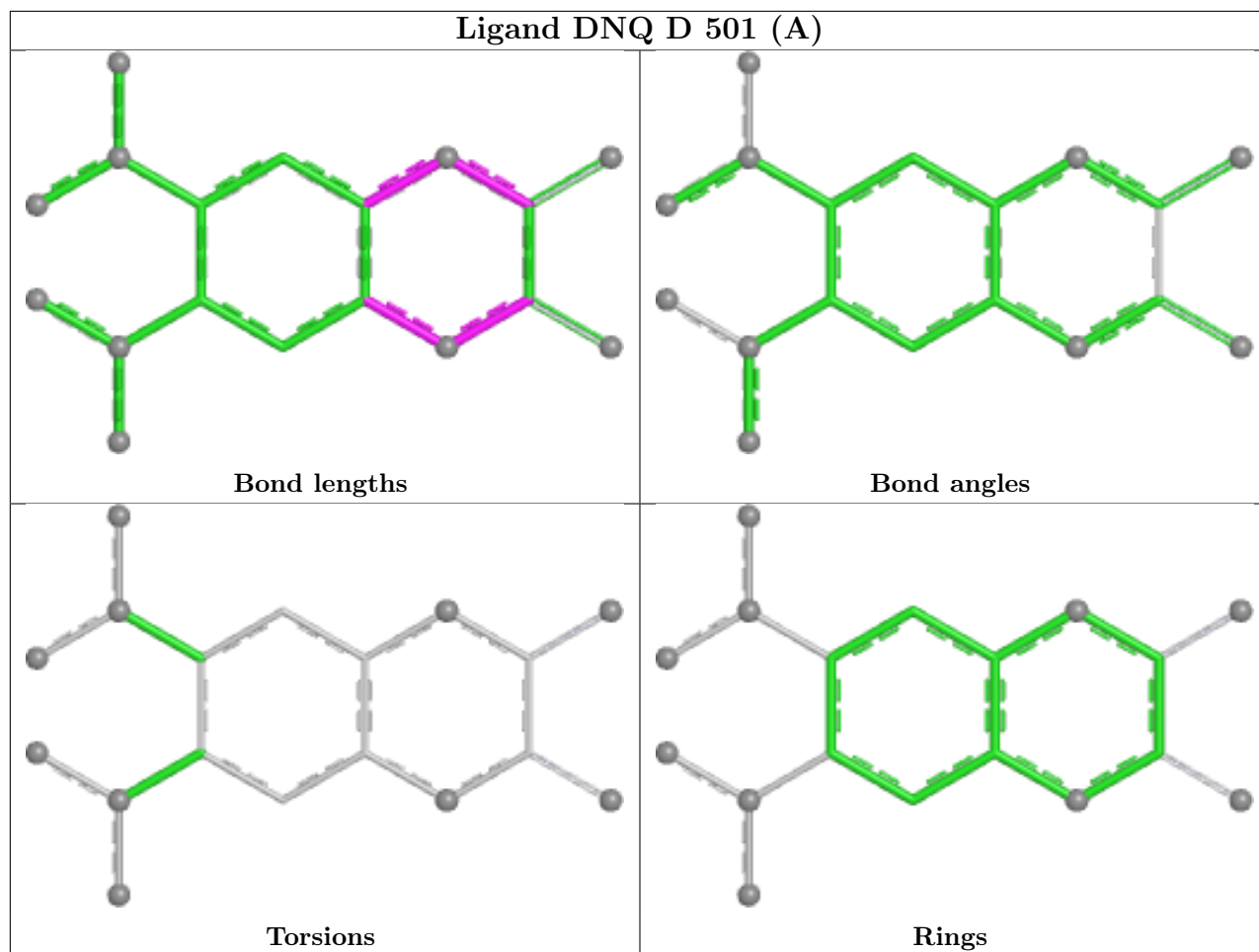
All (4) torsion outliers are listed below:

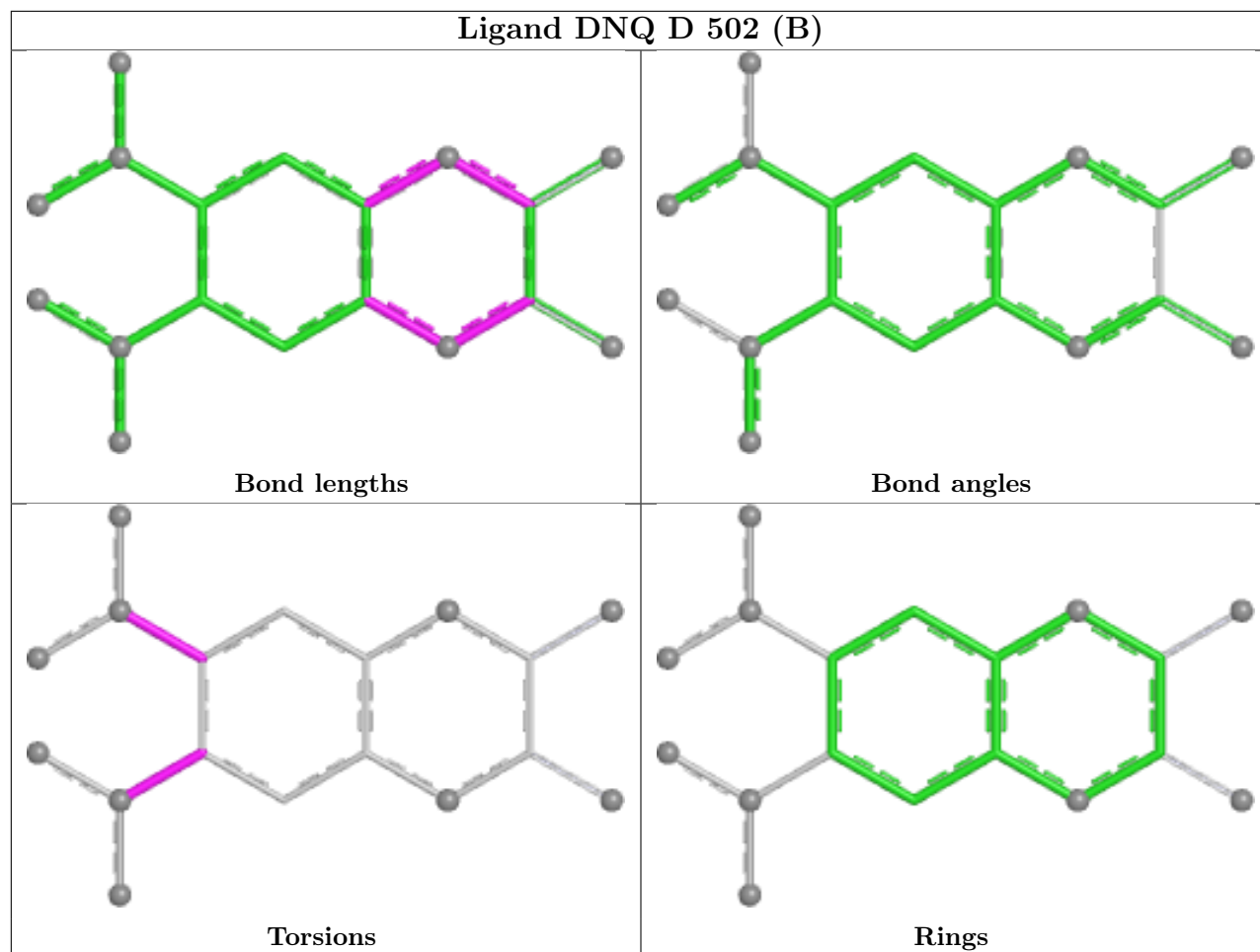
Mol	Chain	Res	Type	Atoms
5	D	502[B]	DNQ	C6-C8-N4-O6
5	D	502[B]	DNQ	C7-C8-N4-O6
5	D	502[B]	DNQ	C5-C7-N3-O5
3	B	801	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	731/736 (99%)	0.14	20 (2%) 56 57	32, 67, 101, 137	1 (0%)
1	B	728/736 (98%)	0.06	28 (3%) 44 44	35, 62, 100, 153	1 (0%)
2	C	395/403 (98%)	-0.04	21 (5%) 32 30	41, 55, 89, 115	1 (0%)
2	D	399/403 (99%)	0.07	27 (6%) 23 21	41, 57, 97, 139	0
All	All	2253/2278 (98%)	0.07	96 (4%) 40 39	32, 61, 99, 153	3 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-14	GLY	7.2
2	D	391	GLY	7.0
1	B	575	GLY	5.4
2	D	301	THR	5.3
2	D	136	LEU	5.3
2	D	300	LEU	5.2
2	C	300	LEU	5.0
2	D	302	GLY	4.7
2	D	296	PRO	4.7
2	D	390	ILE	4.7
1	B	571	VAL	4.6
1	B	574	ALA	4.6
2	C	390	ILE	4.6
2	C	392	GLY	4.5
2	D	303	PRO	4.5
2	C	391	GLY	4.3
2	C	224	ALA	4.3
1	B	-8	HIS	4.3
2	C	296	PRO	4.3
2	C	303	PRO	4.3
2	D	232	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
2	C	301	THR	4.1
2	D	135	GLY	3.9
2	C	389	CYS	3.8
2	D	393	GLY	3.7
1	A	-5	SER	3.7
1	B	565	VAL	3.7
2	D	294	ALA	3.7
2	C	294	ALA	3.6
2	D	299	MET	3.6
1	B	577	THR	3.6
1	A	1	MET	3.5
2	D	297	VAL	3.5
2	D	389	CYS	3.5
1	A	-1	ASN	3.4
2	D	1	MET	3.4
2	C	299	MET	3.4
2	D	392	GLY	3.3
1	B	-13	SER	3.2
2	D	304	THR	3.2
2	C	136	LEU	3.2
1	A	-7	HIS	3.1
2	D	2	SER	3.1
2	C	293	GLY	3.1
2	C	302	GLY	3.1
1	B	-7	HIS	3.1
1	B	566	ALA	3.0
2	D	231	LEU	3.0
2	D	134	MET	3.0
1	B	720	SER	3.0
1	A	73[A]	MET	3.0
1	A	-13	SER	2.9
1	B	-9	HIS	2.9
1	B	578	TYR	2.9
1	B	1	MET	2.9
1	A	720	SER	2.9
1	A	367	TYR	2.8
2	C	297	VAL	2.8
2	D	298	ILE	2.7
1	B	567	THR	2.7
2	D	229	ALA	2.7
1	A	-6	HIS	2.7
1	B	576	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	393	GLY	2.6
2	C	232	GLY	2.6
1	B	73[A]	MET	2.6
2	C	134	MET	2.6
1	B	3	ASP	2.6
2	C	298	ILE	2.6
1	B	591	ILE	2.6
1	B	559	LEU	2.5
1	A	562	LYS	2.4
2	C	2	SER	2.4
1	A	599	LEU	2.4
1	B	563	ILE	2.3
2	D	144	VAL	2.3
1	A	690	ALA	2.2
1	B	690	ALA	2.2
1	A	613	SER	2.2
1	A	2	PRO	2.2
1	A	375	ALA	2.2
2	D	224	ALA	2.2
1	B	613	SER	2.2
1	B	570	GLY	2.1
1	B	568	ARG	2.1
1	B	601	GLY	2.1
1	B	582	PRO	2.1
2	D	230	ALA	2.1
2	C	304	THR	2.1
1	A	3	ASP	2.1
1	A	0	SER	2.1
1	A	335	MET	2.0
1	A	-9	HIS	2.0
1	A	608	ALA	2.0
2	D	293	GLY	2.0
1	B	596	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

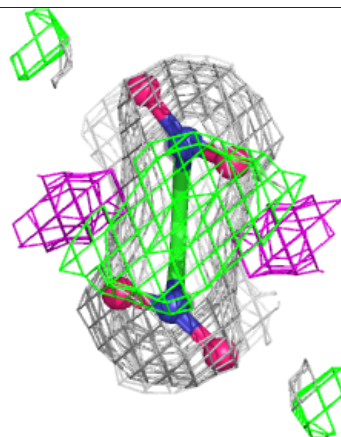
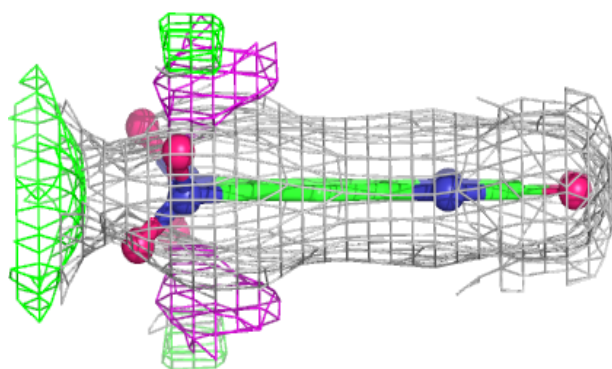
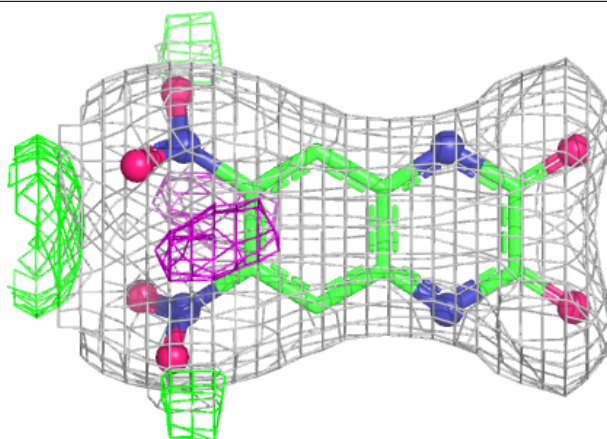
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DNQ	D	502[B]	18/18	0.60	0.22	99,101,103,103	18
4	SO4	A	807	5/5	0.62	0.10	132,137,151,156	0
4	SO4	B	806	5/5	0.67	0.11	105,109,119,142	0
4	SO4	B	807	5/5	0.67	0.10	127,127,141,150	0
4	SO4	B	805	5/5	0.67	0.08	85,93,123,126	0
4	SO4	B	808	5/5	0.71	0.09	116,121,136,152	0
5	DNQ	D	501[A]	18/18	0.81	0.20	94,100,100,100	18
4	SO4	D	506	5/5	0.81	0.08	88,101,110,120	0
3	GOL	A	801	6/6	0.82	0.20	65,69,72,76	0
3	GOL	B	801	6/6	0.82	0.18	61,63,69,71	0
4	SO4	D	505	5/5	0.85	0.09	85,88,97,102	0
4	SO4	C	505	5/5	0.85	0.10	86,103,118,127	0
4	SO4	B	804	5/5	0.86	0.09	81,82,104,109	0
4	SO4	A	806	5/5	0.86	0.06	112,113,123,123	0
4	SO4	C	504	5/5	0.87	0.06	89,99,106,118	0
4	SO4	A	805	5/5	0.87	0.08	80,87,99,102	0
4	SO4	C	503	5/5	0.88	0.07	91,103,109,110	0
4	SO4	D	504	5/5	0.88	0.08	81,86,92,93	0
4	SO4	C	502	5/5	0.88	0.08	80,87,92,104	0
3	GOL	A	802	6/6	0.89	0.19	74,79,82,86	0
4	SO4	A	804	5/5	0.90	0.07	70,92,96,103	0
4	SO4	A	803	5/5	0.90	0.08	85,88,100,102	0
4	SO4	D	503	5/5	0.91	0.07	84,85,98,100	0
4	SO4	B	803	5/5	0.91	0.08	66,78,104,105	0
4	SO4	B	802	5/5	0.91	0.07	89,93,100,108	0
4	SO4	C	501	5/5	0.92	0.11	74,75,88,90	0

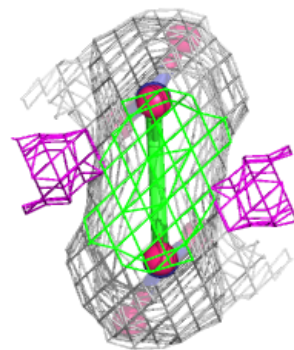
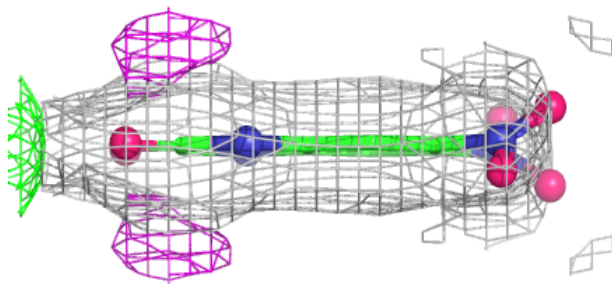
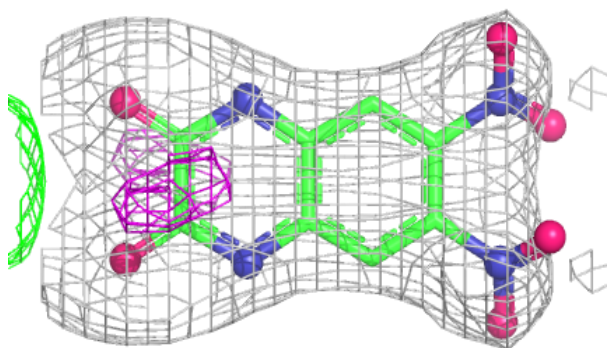
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DNQ D 502 (B):

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

**Electron density around DNQ D 501 (A):**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.