Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2024 – 01:22 am GMT

PDB ID	:	8OQO
Title	:	Structure of Mycobacterium tuberculosis beta-oxidation trifunctional enzyme in complex with Fragment-M-49
Authors	:	Dalwani, S.; Wierenga, R.K.; Venkatesan, R.
Deposited on	:	2023-04-12
Resolution	:	2.60 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:

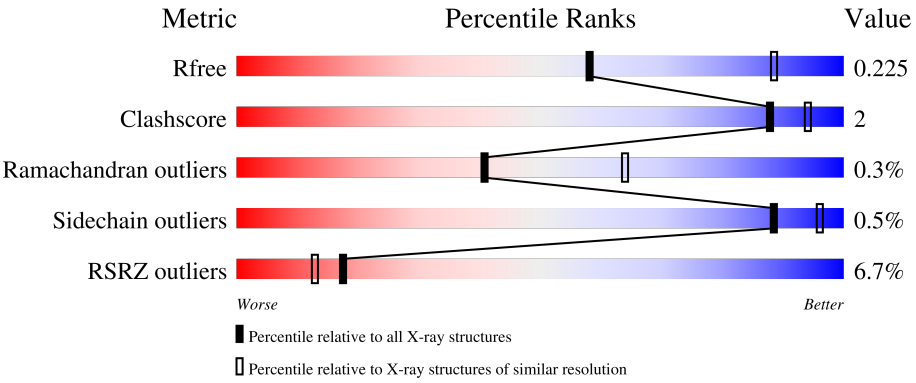
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	17% 93% 6%
1	B	736	% 94%
2	C	403	3% 91% 8%
2	D	403	2% 92% 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16676 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	727	Total	C	N	O	S	0	0	0
			5085	3195	899	972	19			
1	B	726	Total	C	N	O	S	0	0	0
			5379	3404	925	1029	21			

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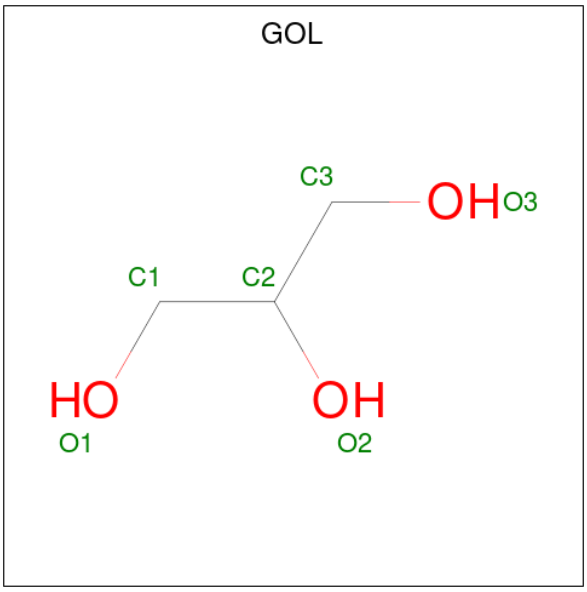
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP O53872
B	-5	SER	-	expression tag	UNP O53872
B	-4	GLN	-	expression tag	UNP O53872
B	-3	ASP	-	expression tag	UNP O53872
B	-2	PRO	-	expression tag	UNP O53872
B	-1	ASN	-	expression tag	UNP O53872
B	0	SER	-	expression tag	UNP O53872

- Molecule 2 is a protein called Putative acyltransferase Rv0859.

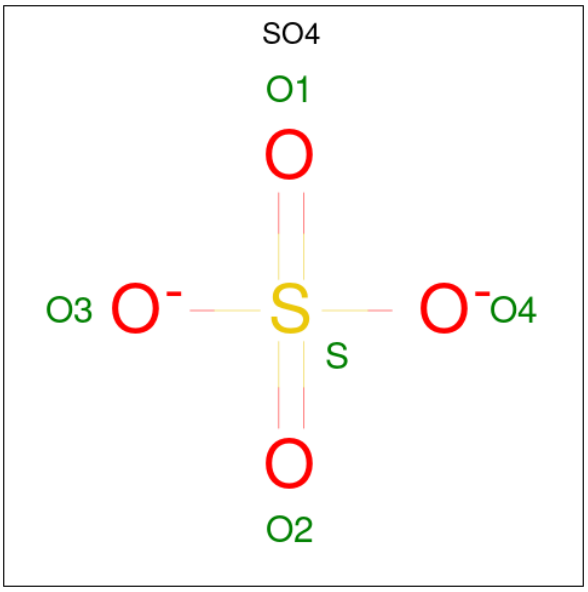
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	398	Total	C	N	O	S	0	0	0
			2942	1838	520	569	15			
2	D	393	Total	C	N	O	S	0	0	0
			2897	1807	516	560	14			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 (three-letter code: SO4) (formula: O_4S).



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

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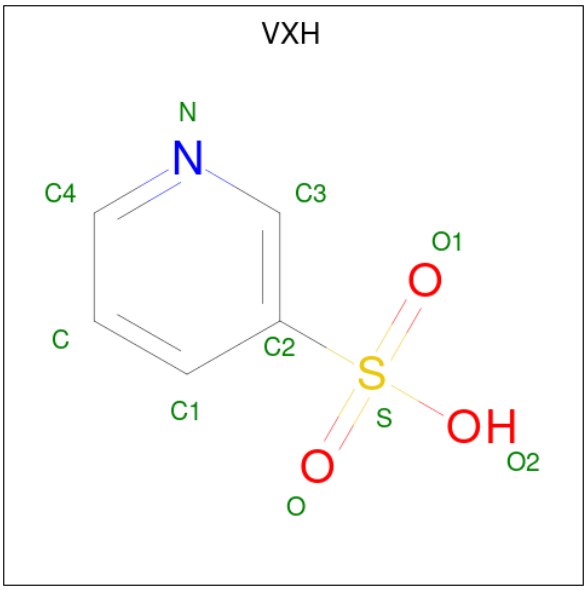
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is pyridine-3-sulfonic acid (three-letter code: VXH) (formula: $C_5H_5NO_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O S 10 5 1 3 1	0	0
5	A	1	Total C N O S 10 5 1 3 1	0	0
5	B	1	Total C N O S 10 5 1 3 1	0	0
5	B	1	Total C N O S 10 5 1 3 1	0	0
5	B	1	Total C N O S 10 5 1 3 1	0	0
5	B	1	Total C N O S 10 5 1 3 1	0	0
5	C	1	Total C N O S 10 5 1 3 1	0	0
5	D	1	Total C N O S 20 10 2 6 2	0	1

- Molecule 6 is water.

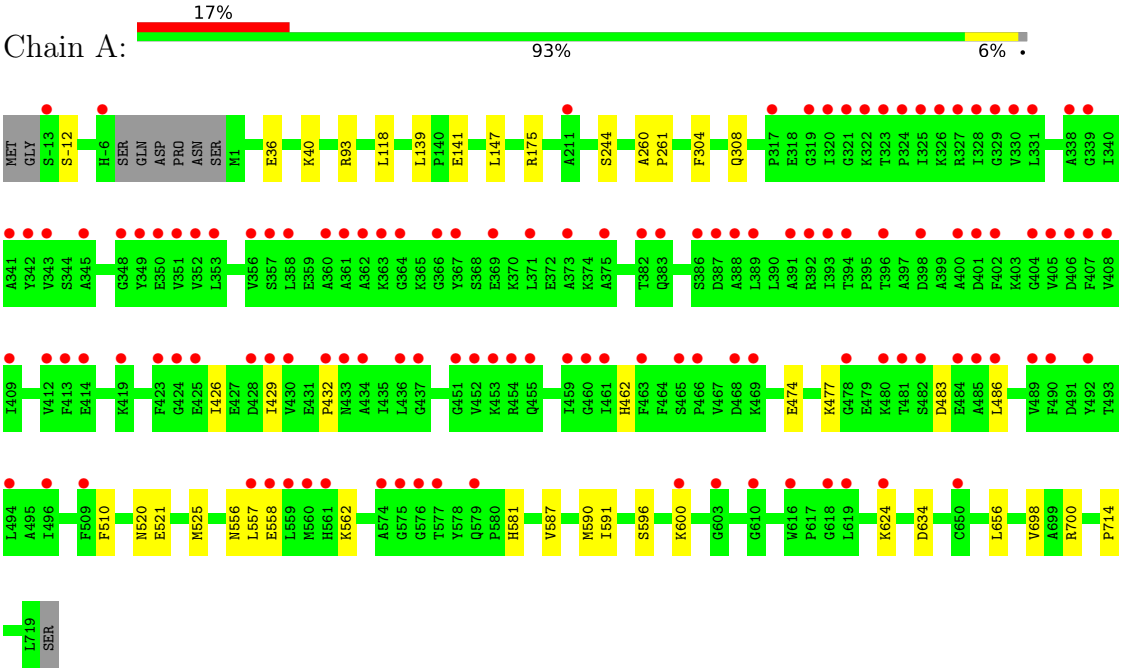
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	43	Total O 43 43	0	0
6	B	66	Total O 66 66	0	0
6	C	41	Total O 41 41	0	0
6	D	46	Total O 46 46	0	0

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.

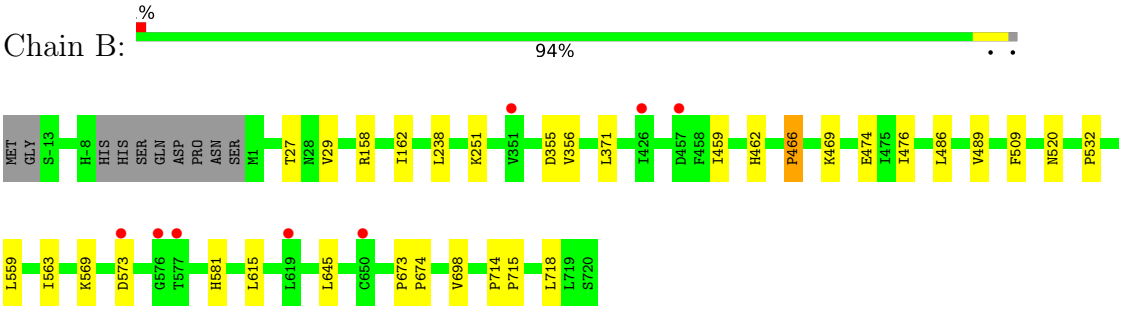
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

Chain A:



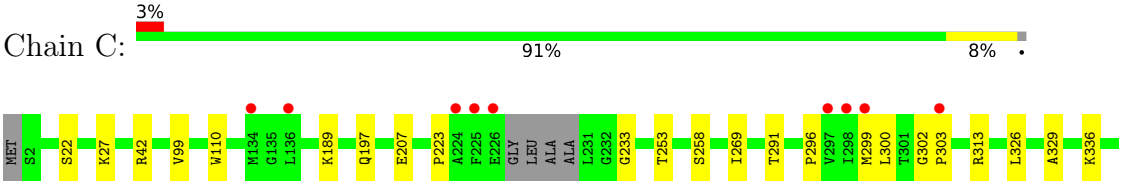
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

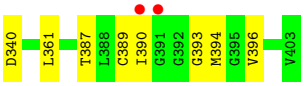
Chain B:



• Molecule 2: Putative acyltransferase Rv0859

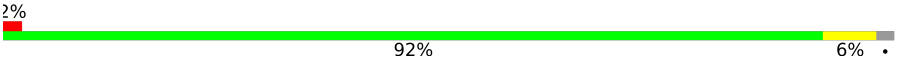
Chain C:

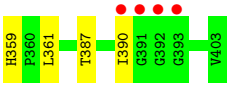




• Molecule 2: Putative acyltransferase Rv0859

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	250.78Å 136.14Å 121.05Å 90.00° 110.42° 90.00°	Depositor
Resolution (Å)	58.75 – 2.60 58.75 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (58.75-2.60) 99.4 (58.75-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.192 , 0.227 0.190 , 0.225	Depositor DCC
R_{free} test set	5842 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	71.1	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16676	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, VXH, 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	0.24	0/5176	0.45	0/7033
1	B	0.25	0/5480	0.46	0/7421
2	C	0.24	0/2986	0.50	0/4042
2	D	0.24	0/2938	0.49	0/3975
All	All	0.24	0/16580	0.47	0/22471

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	5085	0	4800	18	0
1	B	5379	0	5401	19	0
2	C	2942	0	2954	21	0
2	D	2897	0	2914	17	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
4	C	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	25	0	0	0	0
5	A	20	0	0	0	0
5	B	40	0	0	0	0
5	C	10	0	0	0	0
5	D	20	0	0	0	0
6	A	43	0	0	0	0
6	B	66	0	0	1	0
6	C	41	0	0	0	0
6	D	46	0	0	0	0
All	All	16676	0	16085	66	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 2.

All (66) 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:596:SER:HB3	1:A:600:LYS:HD2	1.80	0.64
2:D:50:LEU:HD21	2:D:277:LEU:HD23	1.81	0.63
2:D:99:VAL:HG13	2:D:269:ILE:HD11	1.82	0.61
2:C:99:VAL:HG13	2:C:269:ILE:HD11	1.82	0.61
2:C:313:ARG:HD3	2:D:110:TRP:CD1	2.37	0.59
1:B:459:ILE:HG21	1:B:489:VAL:HG21	1.85	0.59
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.86	0.57
2:D:252:HIS:HE1	2:D:332:SER:H	1.53	0.57
1:A:-12:SER:O	1:A:93:ARG:NH1	2.37	0.56
2:D:91:PHE:HB2	2:D:390:ILE:HG23	1.88	0.56
1:B:520:ASN:HB3	1:B:581:HIS:CE1	2.41	0.54
2:D:93:ALA:HB3	2:D:390:ILE:HD11	1.90	0.53
2:C:22:SER:OG	2:C:207:GLU:OE2	2.21	0.53
2:C:300:LEU:HA	2:C:389:CYS:HB2	1.90	0.52
2:C:296:PRO:HD3	2:D:81:VAL:HG21	1.92	0.51
1:A:36:GLU:HG3	1:A:40:LYS:HE3	1.93	0.51
1:A:244:SER:HB3	2:D:231:LEU:HD13	1.91	0.51
2:C:27:LYS:NZ	2:D:136:LEU:O	2.44	0.51
2:C:223:PRO:HA	2:C:253:THR:HG22	1.93	0.50
2:C:258:SER:HB3	2:C:329:ALA:HA	1.93	0.50
2:C:110:TRP:O	2:D:313:ARG:NH1	2.45	0.50
1:B:162:ILE:HD12	1:B:238:LEU:HD21	1.95	0.49
2:C:303:PRO:HD3	2:C:389:CYS:HA	1.93	0.49
2:C:299:MET:HG2	2:C:393:GLY:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:110:TRP:CD1	2:D:313:ARG:HD3	2.48	0.48
2:C:302:GLY:N	2:C:303:PRO:HD2	2.29	0.48
1:A:462:HIS:HB3	1:A:474:GLU:HB3	1.96	0.48
1:B:466:PRO:HG2	1:B:469:LYS:HE3	1.96	0.47
1:B:532:PRO:HB2	1:B:615:LEU:HD13	1.97	0.47
1:A:118:LEU:HD23	1:A:139:LEU:HG	1.96	0.47
1:B:158:ARG:NH1	6:B:2501:HOH:O	2.45	0.47
1:B:27:THR:HG22	1:B:29:VAL:HG23	1.97	0.47
1:B:459:ILE:HD11	1:B:486:LEU:HD12	1.97	0.47
2:D:354:ALA:HB1	2:D:359:HIS:HB2	1.98	0.46
1:A:510:PHE:CD1	1:A:656:LEU:HD11	2.51	0.46
1:A:304:PHE:O	1:A:308:GLN:HB2	2.16	0.46
2:C:336:LYS:NZ	2:C:340:ASP:OD2	2.48	0.45
1:B:698:VAL:HG13	1:B:714:PRO:HG3	1.98	0.45
2:C:291:THR:HG22	2:C:396:VAL:HG22	1.98	0.45
1:B:714:PRO:HA	1:B:715:PRO:HD3	1.90	0.44
1:B:251:LYS:HD2	2:C:233:GLY:HA2	2.00	0.44
2:C:326:LEU:HD13	2:C:387:THR:HG23	2.00	0.44
1:B:476:ILE:HG21	1:B:509:PHE:CE1	2.53	0.43
2:C:390:ILE:HB	2:C:394:MET:HB2	2.00	0.43
1:B:355:ASP:OD1	1:B:356:VAL:N	2.44	0.43
1:A:698:VAL:HG13	1:A:714:PRO:HG3	1.99	0.43
2:D:40:ARG:NH1	2:D:77:SER:O	2.44	0.43
1:B:569:LYS:HG2	1:B:573:ASP:OD1	2.18	0.43
2:D:276:LYS:HE2	2:D:276:LYS:HB3	1.83	0.43
1:A:557:LEU:HD22	1:A:590:MET:HB2	2.00	0.42
2:C:42:ARG:NH2	2:C:189:LYS:O	2.48	0.42
2:D:326:LEU:HD13	2:D:387:THR:HG23	2.01	0.42
1:A:477:LYS:HG3	1:A:486:LEU:HD21	2.02	0.42
1:A:587:VAL:O	1:A:591:ILE:HG12	2.19	0.42
1:B:715:PRO:HD2	1:B:718:LEU:HD12	2.00	0.42
1:B:645:LEU:HD22	1:B:715:PRO:HD3	2.01	0.42
1:B:559:LEU:O	1:B:563:ILE:HG12	2.20	0.42
1:A:141:GLU:HG3	1:A:147:LEU:C	2.40	0.42
1:A:521:GLU:O	1:A:525:MET:HG3	2.20	0.41
2:C:313:ARG:HD3	2:D:110:TRP:HD1	1.85	0.41
1:B:673:PRO:HA	1:B:674:PRO:HD3	1.93	0.41
1:A:624:LYS:HB3	1:A:624:LYS:HE2	1.85	0.40
1:A:520:ASN:HB3	1:A:581:HIS:CE1	2.56	0.40
2:C:110:TRP:CZ2	2:D:288:ALA:HA	2.57	0.40
1:A:260:ALA:HB3	1:A:261:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:ASP:OD1	1:A:700:ARG:NH2	2.49	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	723/736 (98%)	689 (95%)	30 (4%)	4 (1%)	25 47
1	B	722/736 (98%)	699 (97%)	23 (3%)	0	100 100
2	C	394/403 (98%)	382 (97%)	11 (3%)	1 (0%)	41 64
2	D	387/403 (96%)	378 (98%)	8 (2%)	1 (0%)	41 64
All	All	2226/2278 (98%)	2148 (96%)	72 (3%)	6 (0%)	41 64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	432	PRO
2	C	361	LEU
2	D	361	LEU
1	A	429	ILE
1	A	426	ILE
1	A	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	460/566 (81%)	456 (99%)	4 (1%)	78	91
1	B	551/566 (97%)	549 (100%)	2 (0%)	91	97
2	C	307/310 (99%)	306 (100%)	1 (0%)	92	98
2	D	301/310 (97%)	300 (100%)	1 (0%)	92	98
All	All	1619/1752 (92%)	1611 (100%)	8 (0%)	88	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	ARG
1	A	483	ASP
1	A	558	GLU
1	A	562	LYS
1	B	371	LEU
1	B	466	PRO
2	C	197	GLN
2	D	346	GLU

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)

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	503	-	4,4,4	0.14	0	6,6,6	0.05	0
5	VXH	A	2405	-	10,10,10	0.16	0	13,14,14	0.18	0
4	SO4	B	2403	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	A	2402	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.04	0
5	VXH	D	506[B]	-	10,10,10	0.26	0	13,14,14	0.24	0
4	SO4	A	2403	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	2404	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.05	0
5	VXH	D	506[A]	-	10,10,10	0.26	0	13,14,14	0.24	0
5	VXH	C	505	-	10,10,10	0.22	0	13,14,14	0.18	0
4	SO4	D	503	-	4,4,4	0.14	0	6,6,6	0.05	0
5	VXH	B	2408	-	10,10,10	0.27	0	13,14,14	0.24	0
5	VXH	B	2405	-	10,10,10	0.20	0	13,14,14	0.19	0
5	VXH	B	2407	-	10,10,10	0.20	0	13,14,14	0.18	0
4	SO4	D	501	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	2402	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	C	504	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	D	502	-	4,4,4	0.14	0	6,6,6	0.04	0
5	VXH	B	2406	-	10,10,10	0.26	0	13,14,14	0.24	0
3	GOL	B	2401	-	5,5,5	0.87	0	5,5,5	1.03	0
4	SO4	D	504	-	4,4,4	0.14	0	6,6,6	0.05	0
5	VXH	A	2406	-	10,10,10	0.27	0	13,14,14	0.24	0
4	SO4	A	2404	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	D	505	-	4,4,4	0.14	0	6,6,6	0.05	0
3	GOL	A	2401	-	5,5,5	0.87	0	5,5,5	1.01	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	2401	-	-	2/4/4/4	-
5	VXH	D	506[B]	-	-	0/6/6/6	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	VXH	B	2406	-	-	0/6/6/6	0/1/1/1
5	VXH	A	2406	-	-	0/6/6/6	0/1/1/1
5	VXH	A	2405	-	-	1/6/6/6	0/1/1/1
5	VXH	D	506[A]	-	-	0/6/6/6	0/1/1/1
5	VXH	C	505	-	-	0/6/6/6	0/1/1/1
3	GOL	A	2401	-	-	1/4/4/4	-
5	VXH	B	2408	-	-	0/6/6/6	0/1/1/1
5	VXH	B	2405	-	-	0/6/6/6	0/1/1/1
5	VXH	B	2407	-	-	0/6/6/6	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

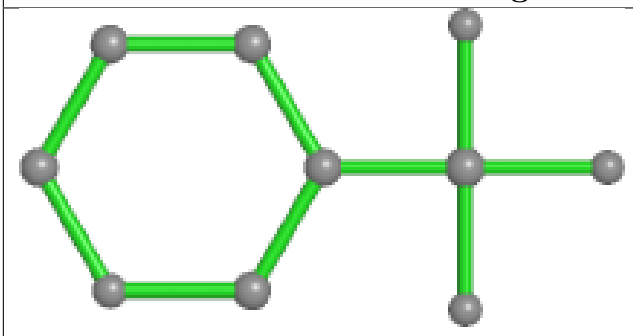
Mol	Chain	Res	Type	Atoms
3	B	2401	GOL	O1-C1-C2-O2
3	B	2401	GOL	O1-C1-C2-C3
3	A	2401	GOL	C1-C2-C3-O3
5	A	2405	VXH	C3-C2-S-O

There are no ring outliers.

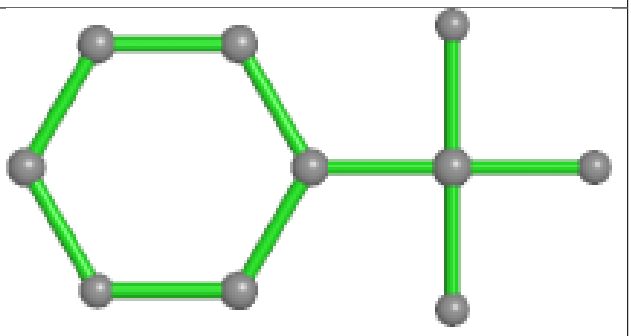
No monomer is involved in short contacts.

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 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.

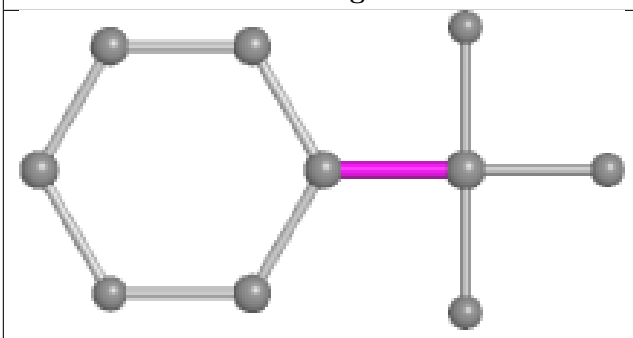
Ligand VXH A 2405



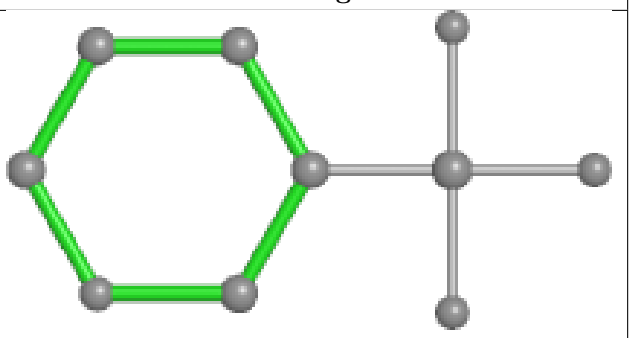
Bond lengths



Bond angles

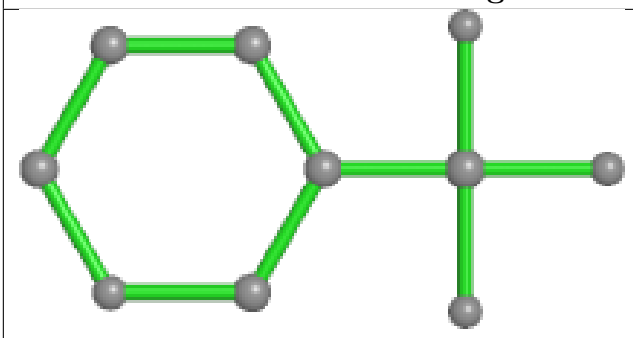


Torsions

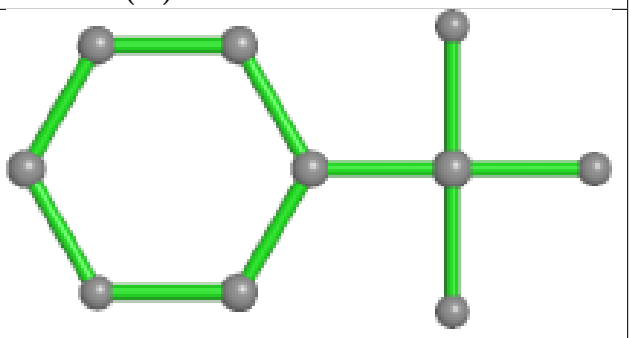


Rings

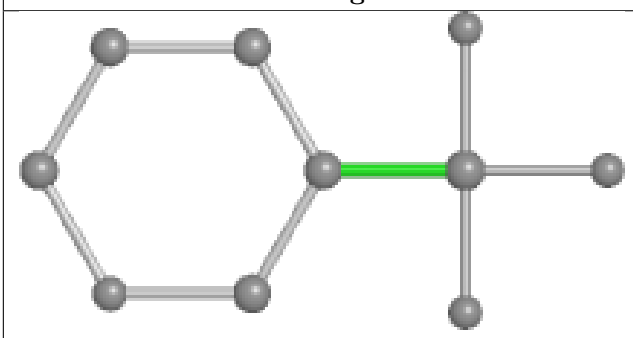
Ligand VXH D 506 (B)



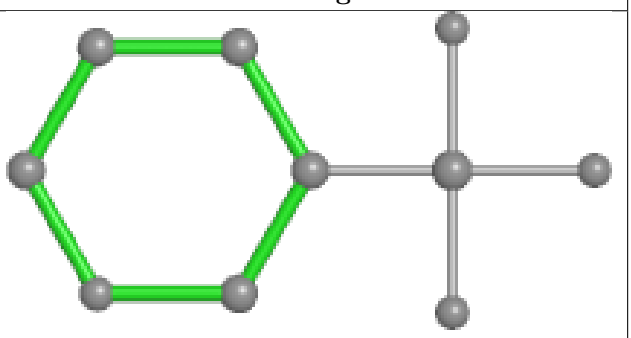
Bond lengths



Bond angles

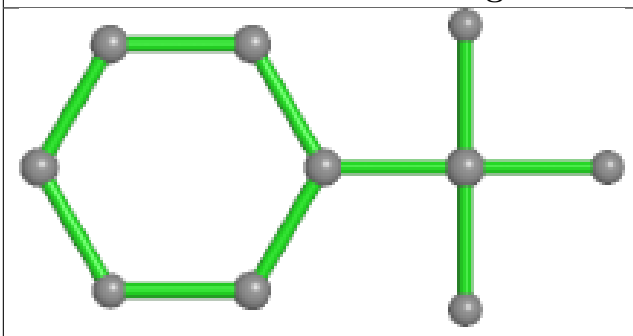


Torsions

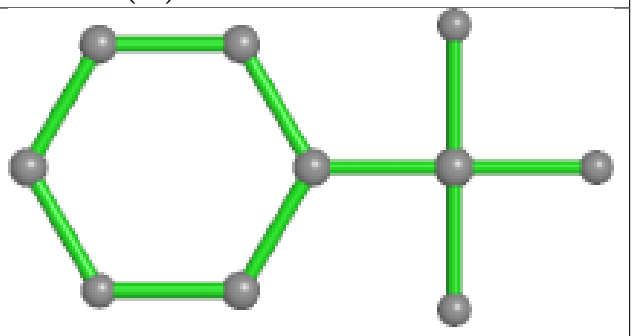


Rings

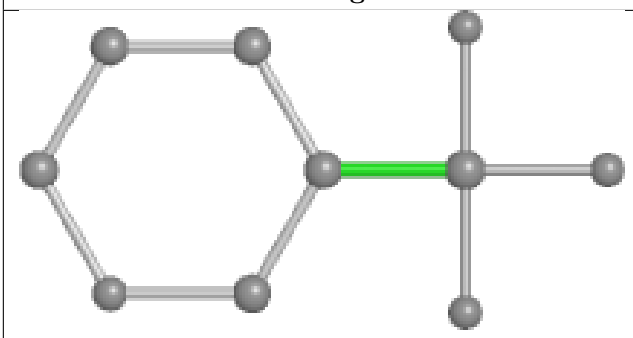
Ligand VXH D 506 (A)



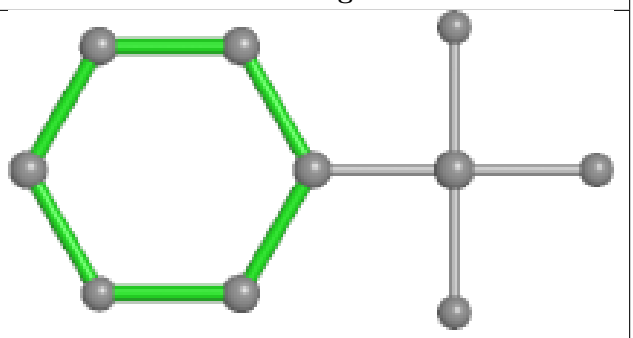
Bond lengths



Bond angles

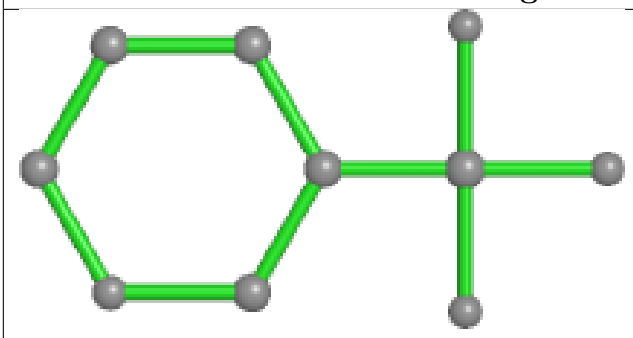


Torsions

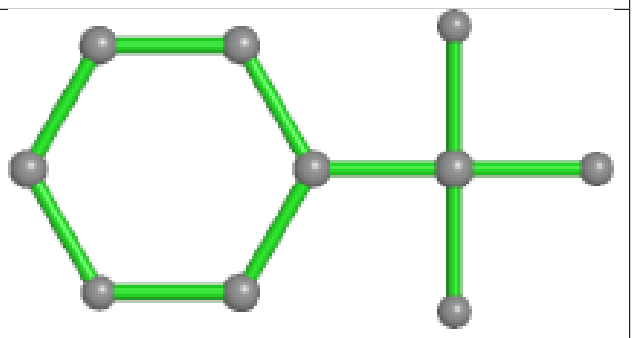


Rings

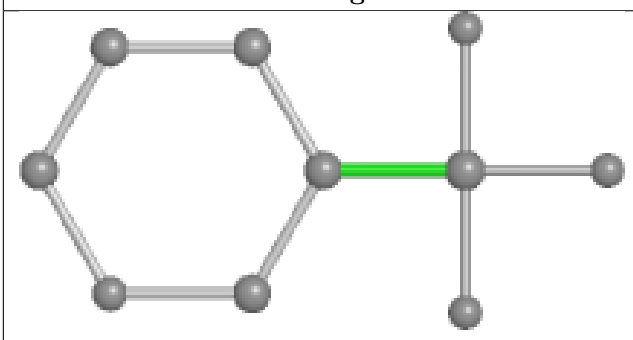
Ligand VXH C 505



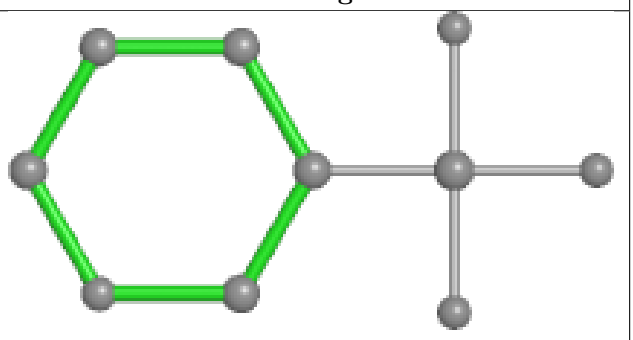
Bond lengths



Bond angles

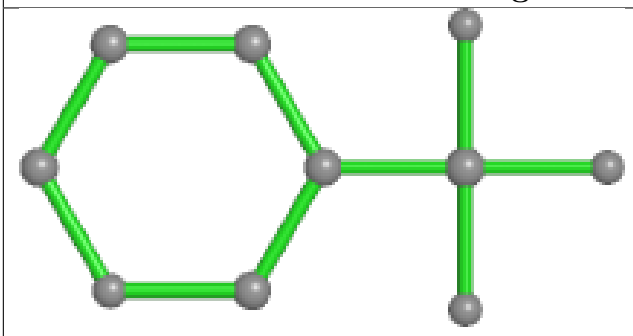


Torsions

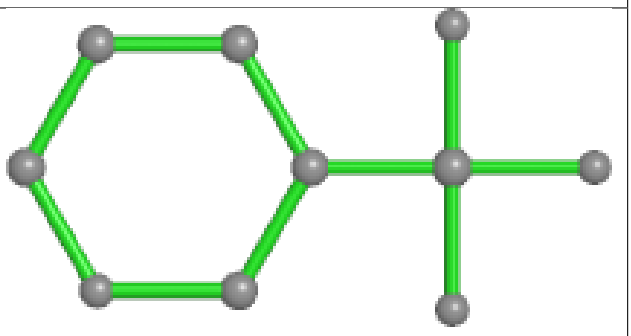


Rings

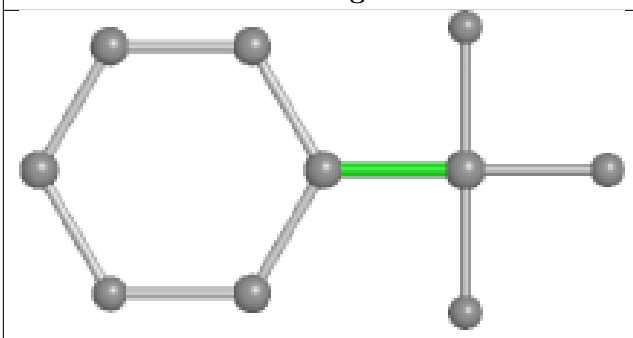
Ligand VXH B 2408



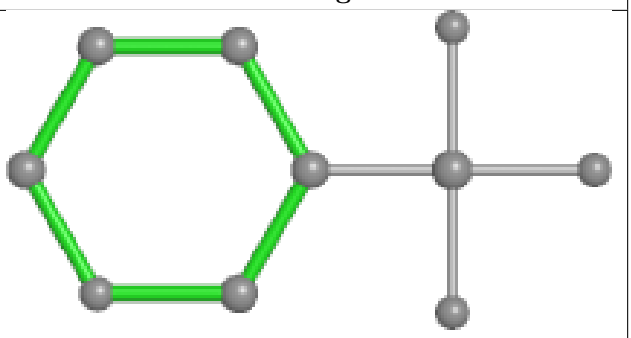
Bond lengths



Bond angles

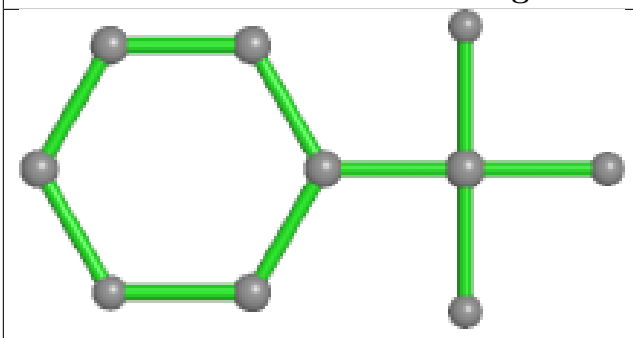


Torsions

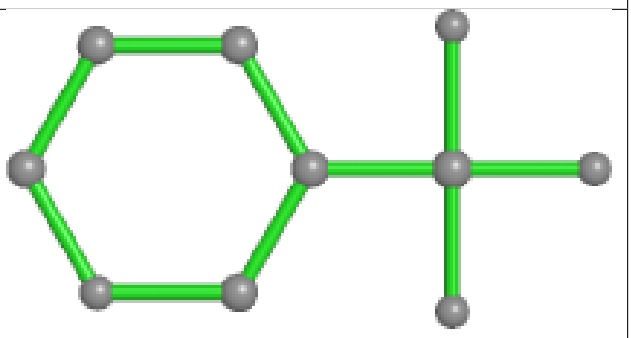


Rings

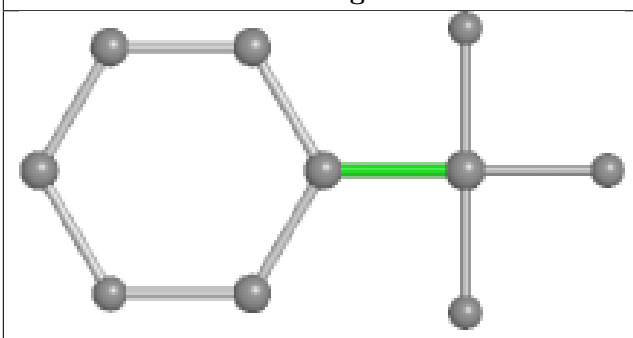
Ligand VXH B 2405



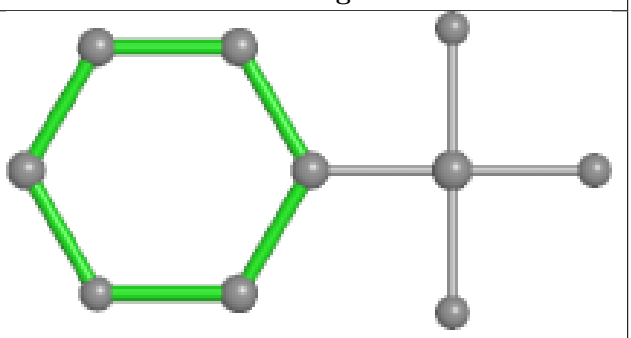
Bond lengths



Bond angles

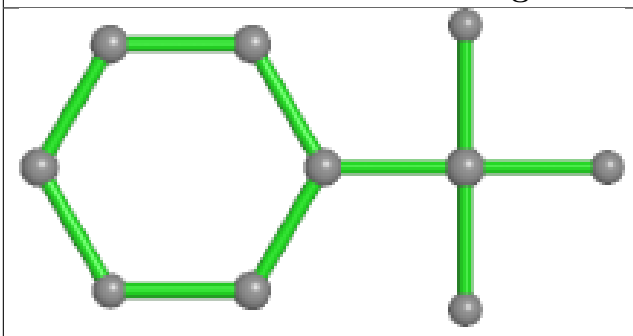


Torsions

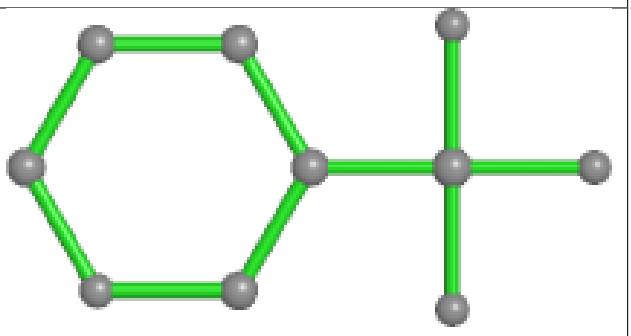


Rings

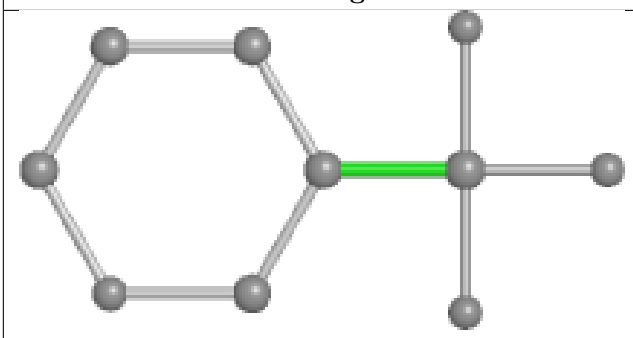
Ligand VXH B 2407



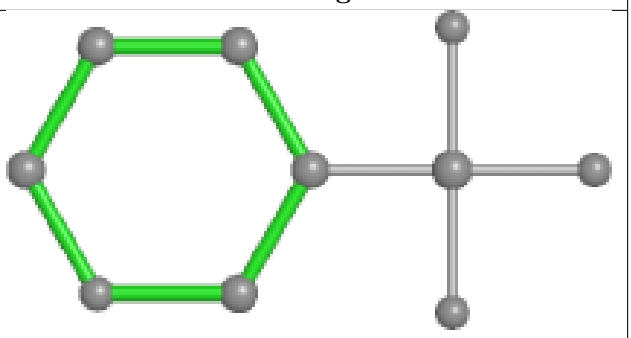
Bond lengths



Bond angles

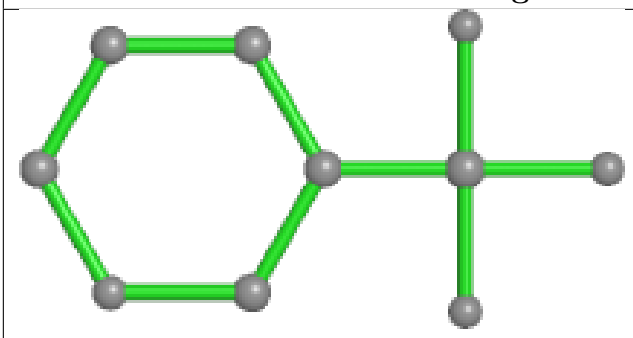


Torsions

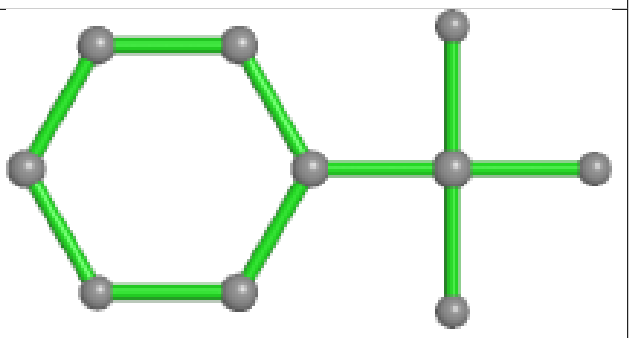


Rings

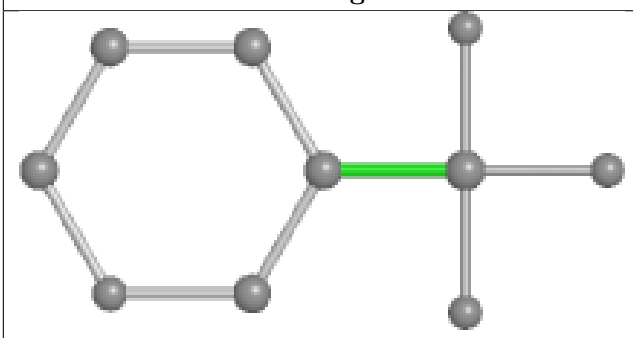
Ligand VXH B 2406



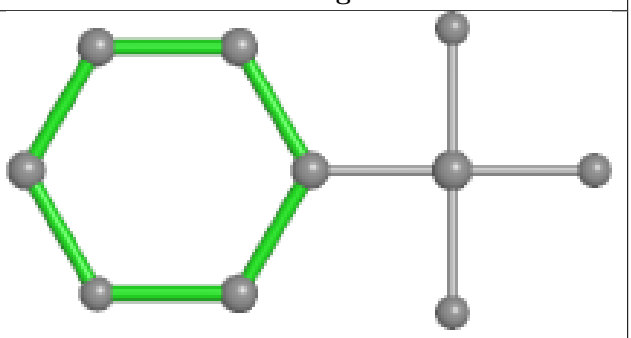
Bond lengths



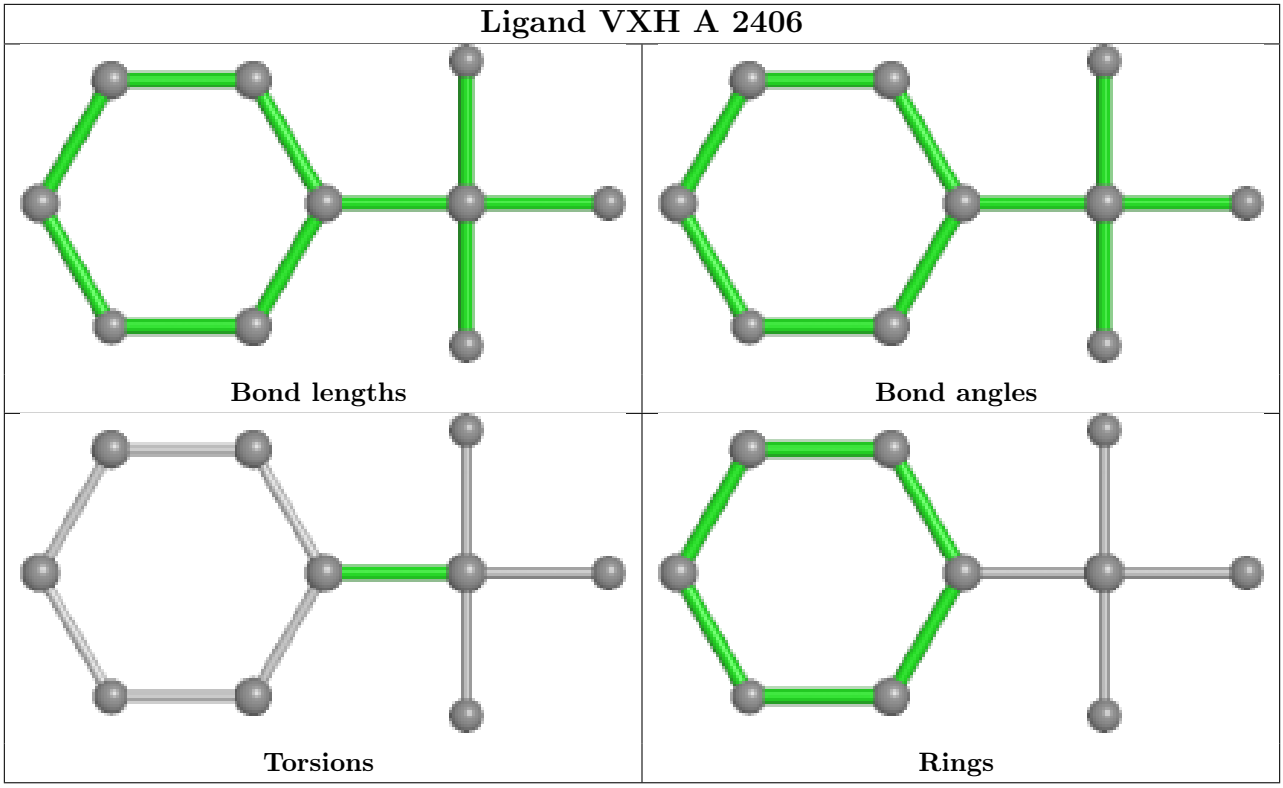
Bond angles



Torsions



Rings



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	727/736 (98%)	0.84	123 (16%) 1 1	52, 86, 175, 258	0
1	B	726/736 (98%)	0.05	8 (1%) 80 78	48, 74, 122, 151	0
2	C	398/403 (98%)	0.21	11 (2%) 53 46	43, 65, 107, 156	0
2	D	393/403 (97%)	0.23	8 (2%) 65 60	47, 67, 101, 160	0
All	All	2244/2278 (98%)	0.37	150 (6%) 17 13	43, 74, 150, 258	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	349	TYR	22.8
1	A	351	VAL	13.7
1	A	325	ILE	11.2
1	A	405	VAL	9.0
1	A	434	ALA	8.9
1	A	352	VAL	8.4
1	A	391	ALA	7.5
1	A	367	TYR	7.3
1	A	362	ALA	7.3
1	A	328	ILE	7.1
1	A	429	ILE	7.0
1	A	343	VAL	6.6
1	A	394	THR	6.2
1	A	320	ILE	6.0
2	D	301	THR	5.9
1	A	371	LEU	5.9
1	A	402	PHE	5.8
1	A	486	LEU	5.7
1	A	459	ILE	5.7
1	A	387	ASP	5.6
1	A	321	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	345	ALA	5.5
1	A	428	ASP	5.5
2	D	229	ALA	5.3
1	A	338	ALA	5.3
1	A	404	GLY	5.1
1	A	430	VAL	5.0
1	A	327	ARG	5.0
1	A	436	LEU	5.0
1	A	408	VAL	4.8
1	A	353	LEU	4.8
1	A	331	LEU	4.6
1	A	424	GLY	4.6
1	A	557	LEU	4.6
1	A	407	PHE	4.6
2	C	297	VAL	4.6
1	A	386	SER	4.5
1	A	400	ALA	4.5
2	C	303	PRO	4.5
1	A	423	PHE	4.4
1	A	413	PHE	4.3
2	C	299	MET	4.3
1	A	452	VAL	4.2
1	A	468	ASP	4.2
1	A	392	ARG	4.1
1	A	382	THR	4.1
1	A	-6	HIS	4.1
1	A	406	ASP	4.1
1	A	437	GLY	4.1
1	A	455	GLN	4.0
1	A	560	MET	4.0
1	A	375	ALA	4.0
1	A	409	ILE	3.9
1	A	357	SER	3.8
1	A	364	GLY	3.8
1	A	388	ALA	3.8
1	A	360	ALA	3.8
2	D	391	GLY	3.7
1	A	425	GLU	3.7
2	C	225	PHE	3.6
1	B	577	THR	3.6
1	A	574	ALA	3.6
1	A	577	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	453	LYS	3.5
2	D	392	GLY	3.5
1	A	358	LEU	3.5
2	D	390	ILE	3.5
1	A	322	LYS	3.5
1	A	356	VAL	3.5
1	A	509	PHE	3.4
1	A	432	PRO	3.4
1	A	610	GLY	3.4
1	A	401	ASP	3.4
1	A	576	GLY	3.4
1	A	393	ILE	3.3
1	A	485	ALA	3.3
1	A	366	GLY	3.2
1	A	600	LYS	3.2
1	A	463	PHE	3.2
1	A	561	HIS	3.2
1	A	348	GLY	3.1
1	A	339	GLY	3.1
1	A	492	TYR	3.1
1	A	490	PHE	3.0
1	A	480	LYS	3.0
1	A	461	ILE	3.0
2	D	1	MET	3.0
1	A	650	CYS	3.0
1	A	466	PRO	3.0
1	A	396	THR	3.0
1	A	383	GLN	3.0
1	A	489	VAL	2.9
1	A	324	PRO	2.9
1	A	342	TYR	2.9
1	A	478	GLY	2.8
2	C	134	MET	2.8
1	A	482	SER	2.8
1	A	398	ASP	2.8
1	A	373	ALA	2.8
2	C	226	GLU	2.8
1	A	603	GLY	2.8
1	A	361	ALA	2.8
1	A	330	VAL	2.7
2	C	391	GLY	2.7
1	A	341	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	451	GLY	2.7
1	A	559	LEU	2.7
1	B	576	GLY	2.7
1	A	323	THR	2.7
1	A	496	ILE	2.6
2	C	224	ALA	2.6
1	B	573	ASP	2.6
1	A	317	PRO	2.6
1	A	433	ASN	2.6
1	B	457	ASP	2.6
1	A	454	ARG	2.6
2	D	303	PRO	2.5
1	A	575	GLY	2.5
1	A	484	GLU	2.5
2	C	390	ILE	2.5
1	A	412	VAL	2.5
1	A	494	LEU	2.4
1	A	579	GLN	2.4
1	A	389	LEU	2.4
1	A	326	LYS	2.4
2	C	298	ILE	2.3
1	B	426	ILE	2.3
1	A	558	GLU	2.3
1	B	650	CYS	2.3
1	A	369	GLU	2.2
1	A	618	GLY	2.2
1	A	469	LYS	2.2
1	A	481	THR	2.2
1	B	619	LEU	2.2
1	A	350	GLU	2.2
1	B	351	VAL	2.2
1	A	-13	SER	2.1
1	A	616	TRP	2.1
1	A	363	LYS	2.1
2	C	136	LEU	2.1
1	A	329	GLY	2.1
1	A	319	GLY	2.1
1	A	619	LEU	2.1
2	D	393	GLY	2.1
1	A	419	LYS	2.1
1	A	211	ALA	2.1
1	A	414	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	465	SER	2.1
1	A	460	GLY	2.0
1	A	624	LYS	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	SO4	C	504	5/5	0.76	0.26	129,135,144,187	0
4	SO4	B	2404	5/5	0.77	0.26	120,127,139,164	0
4	SO4	D	505	5/5	0.82	0.13	102,107,122,152	0
5	VXH	B	2407	10/10	0.83	0.37	106,127,137,147	0
4	SO4	C	503	5/5	0.87	0.18	113,121,138,142	0
5	VXH	D	506[A]	10/10	0.87	0.36	71,80,96,96	10
5	VXH	D	506[B]	10/10	0.87	0.36	78,86,96,106	10
5	VXH	B	2408	10/10	0.88	0.30	112,128,152,181	0
4	SO4	D	503	5/5	0.88	0.23	94,116,141,169	0
4	SO4	D	504	5/5	0.88	0.13	122,131,134,140	5
4	SO4	C	502	5/5	0.89	0.25	107,117,137,149	0
4	SO4	B	2403	5/5	0.89	0.39	117,130,161,178	0
4	SO4	A	2403	5/5	0.90	0.20	115,123,157,159	0
4	SO4	B	2402	5/5	0.90	0.15	84,89,100,113	0
4	SO4	A	2402	5/5	0.91	0.22	98,101,107,121	0
5	VXH	A	2406	10/10	0.91	0.23	103,126,145,171	0
4	SO4	A	2404	5/5	0.91	0.13	141,141,169,175	0
4	SO4	D	502	5/5	0.93	0.27	101,110,130,132	0
3	GOL	B	2401	6/6	0.93	0.23	74,83,88,91	0
4	SO4	D	501	5/5	0.93	0.12	115,122,138,142	0

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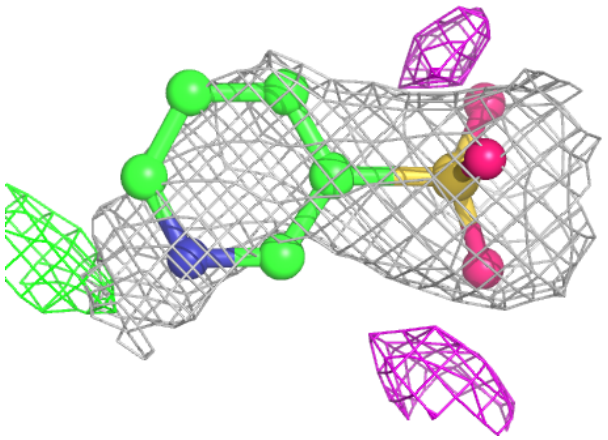
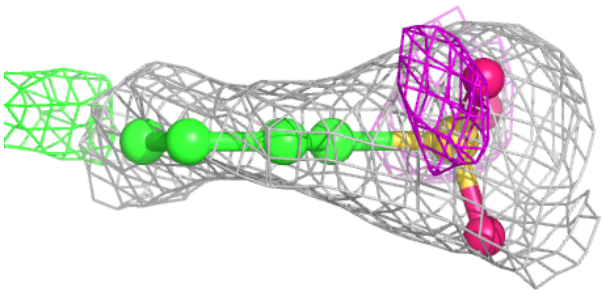
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	VXH	B	2406	10/10	0.94	0.25	101,119,133,139	0
5	VXH	C	505	10/10	0.94	0.26	91,100,114,132	0
5	VXH	B	2405	10/10	0.95	0.19	95,103,114,121	0
5	VXH	A	2405	10/10	0.96	0.19	94,109,118,123	0
3	GOL	A	2401	6/6	0.96	0.20	78,81,85,88	0
4	SO4	C	501	5/5	0.96	0.29	95,107,111,124	0

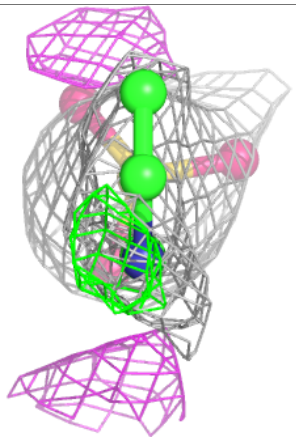
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VXH B 2407:

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

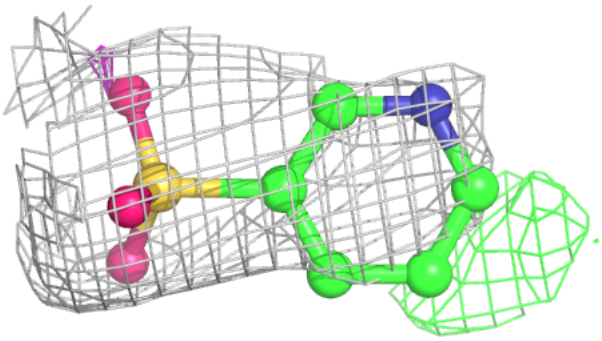


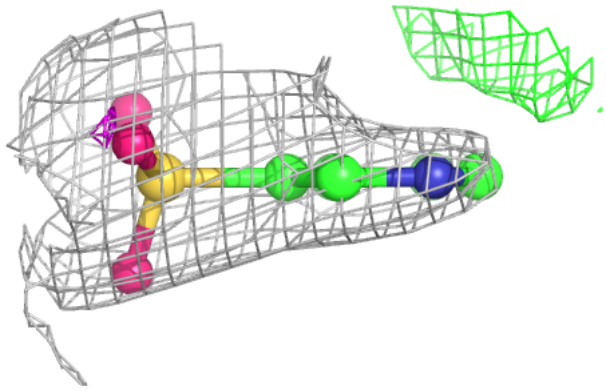


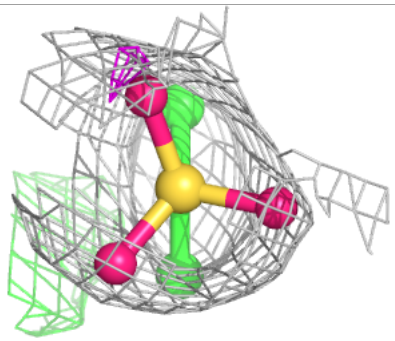


Electron density around VXH D 506 (A):

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

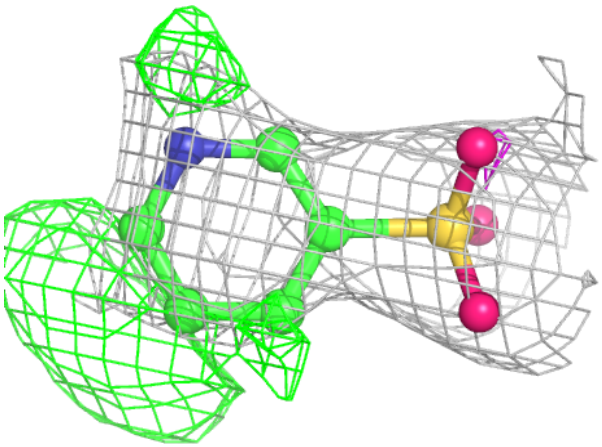


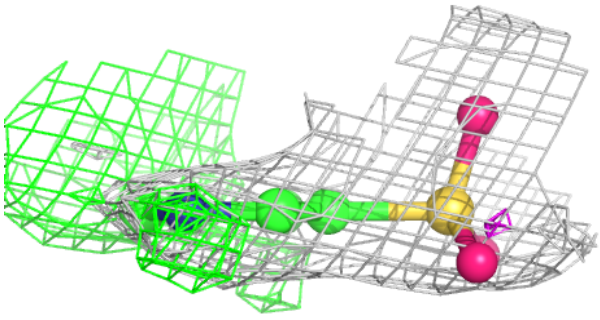


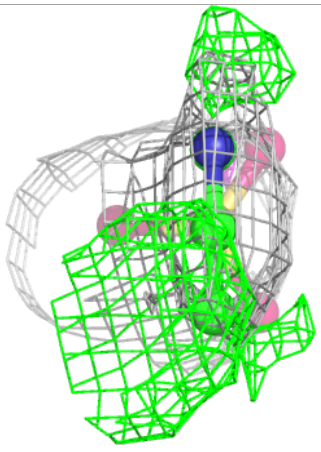


Electron density around VXH D 506 (B):

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

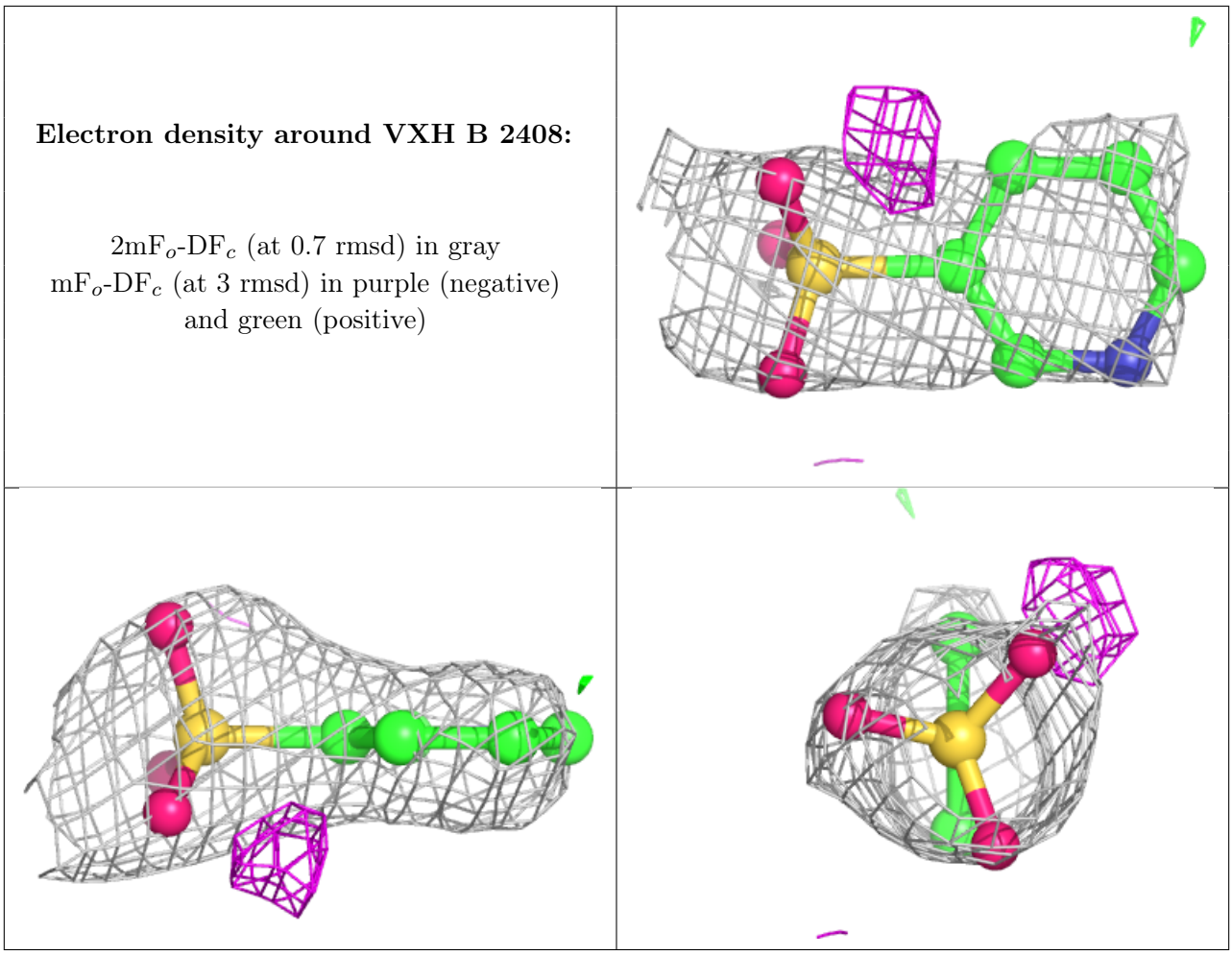






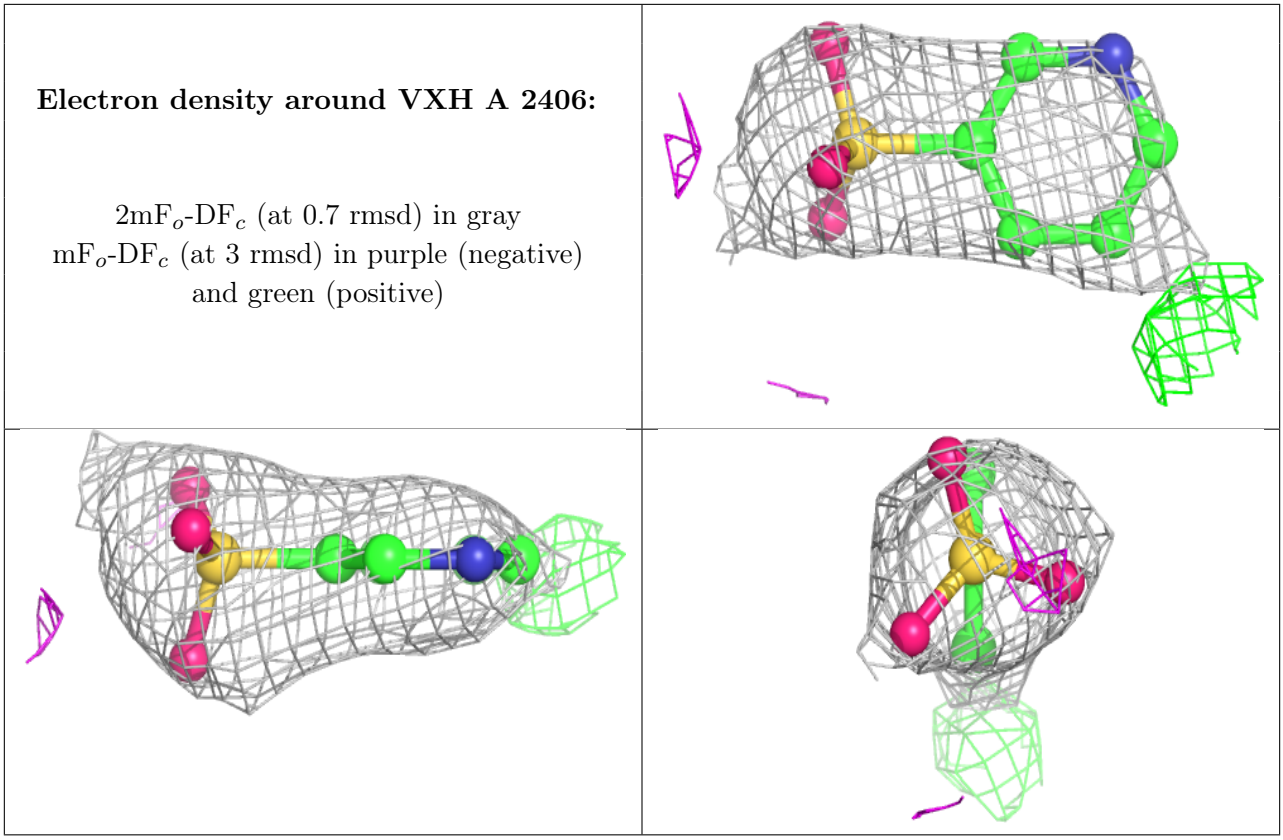
Electron density around VXH B 2408:

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



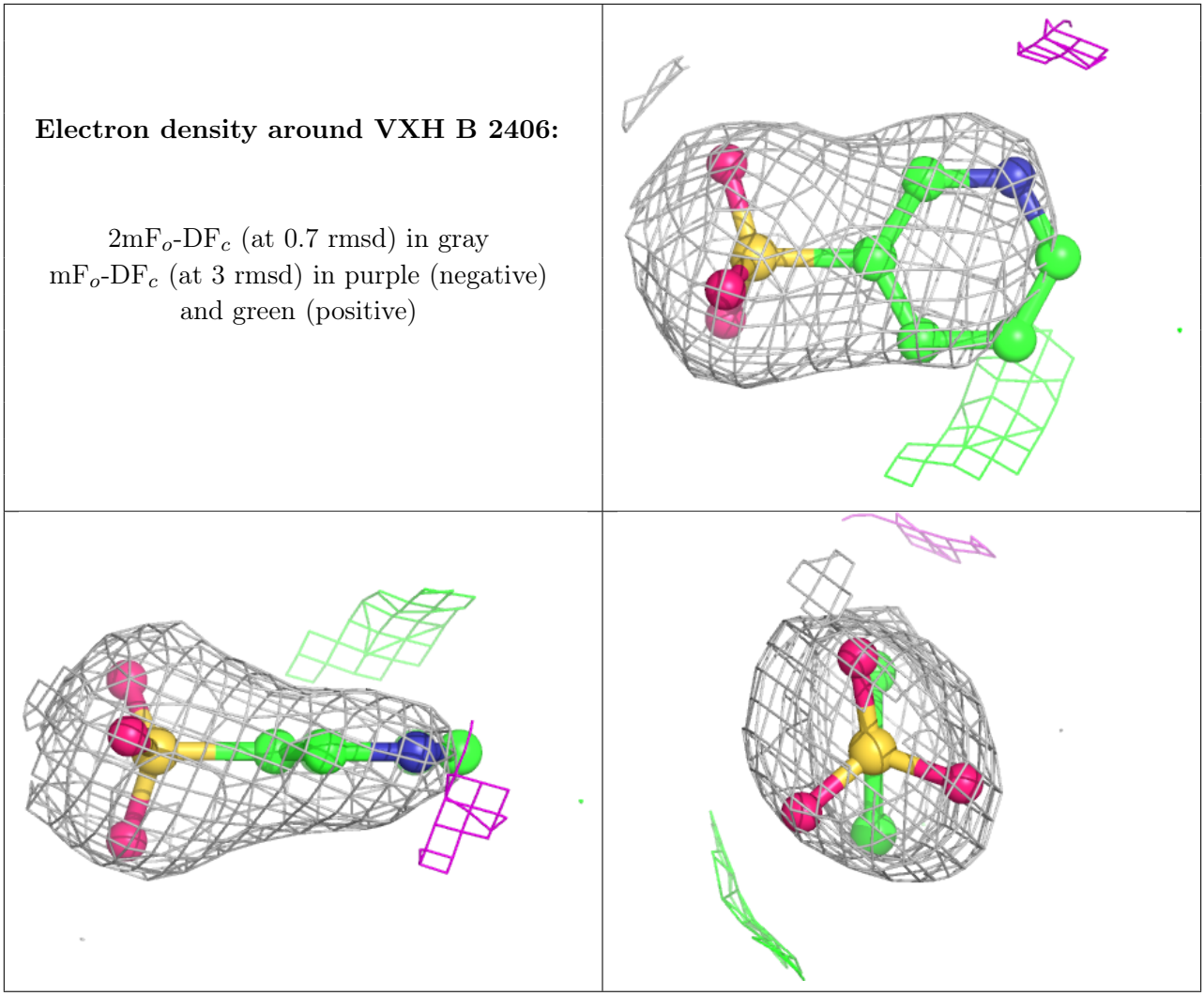
Electron density around VXH A 2406:

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



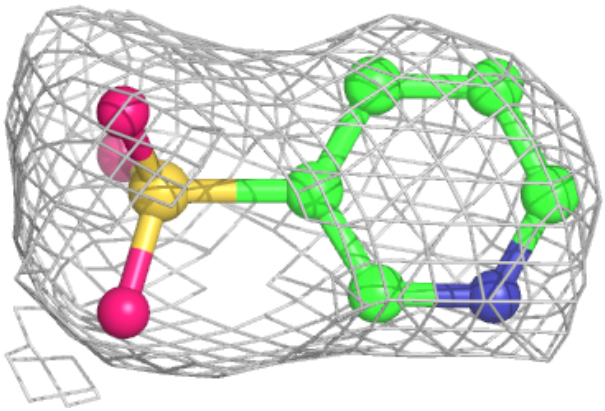
Electron density around VXH B 2406:

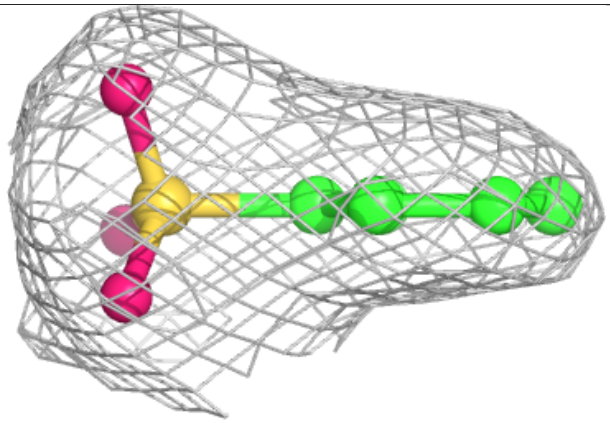
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

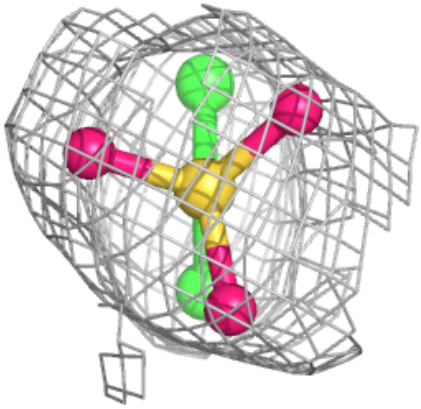


Electron density around VXH C 505:

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

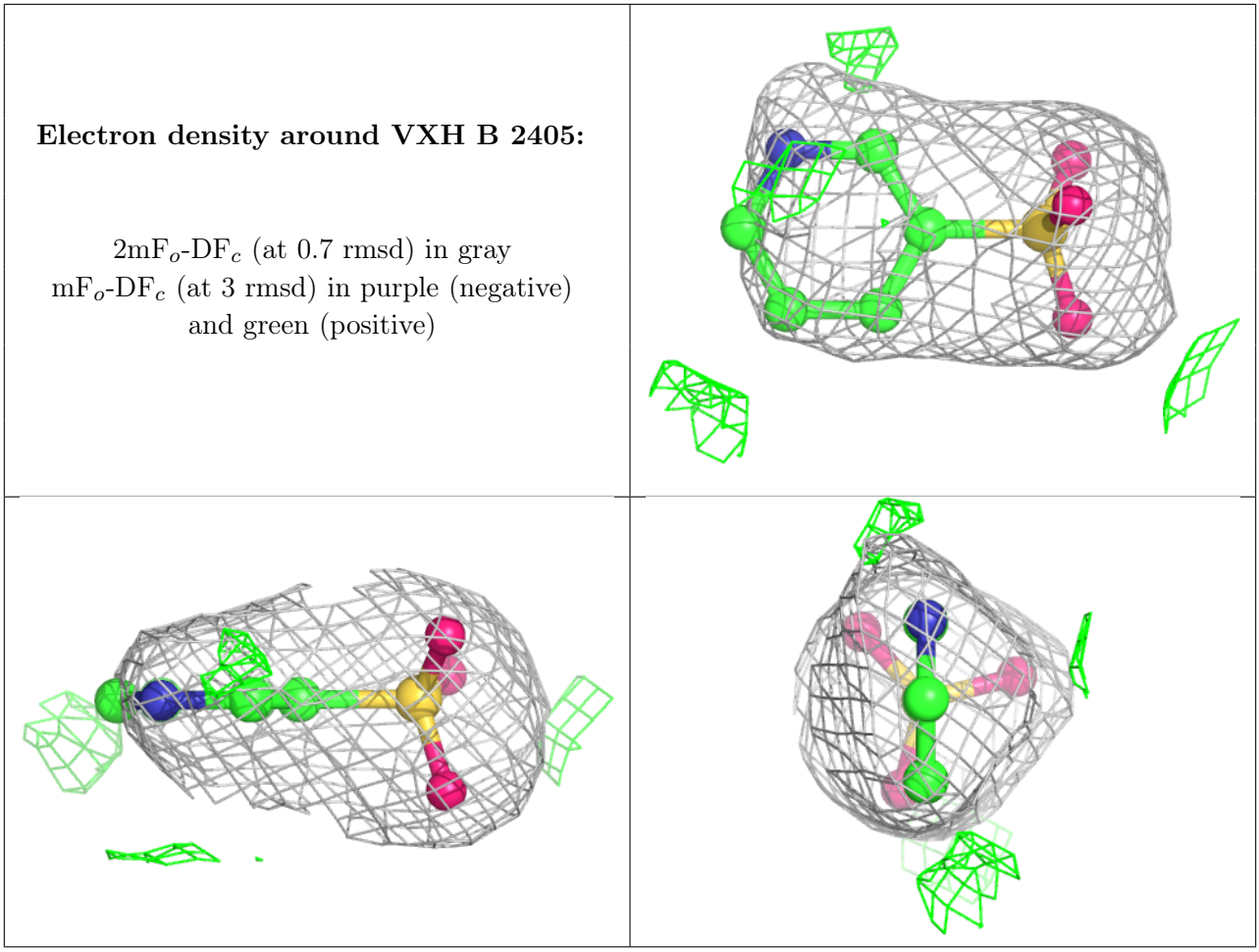






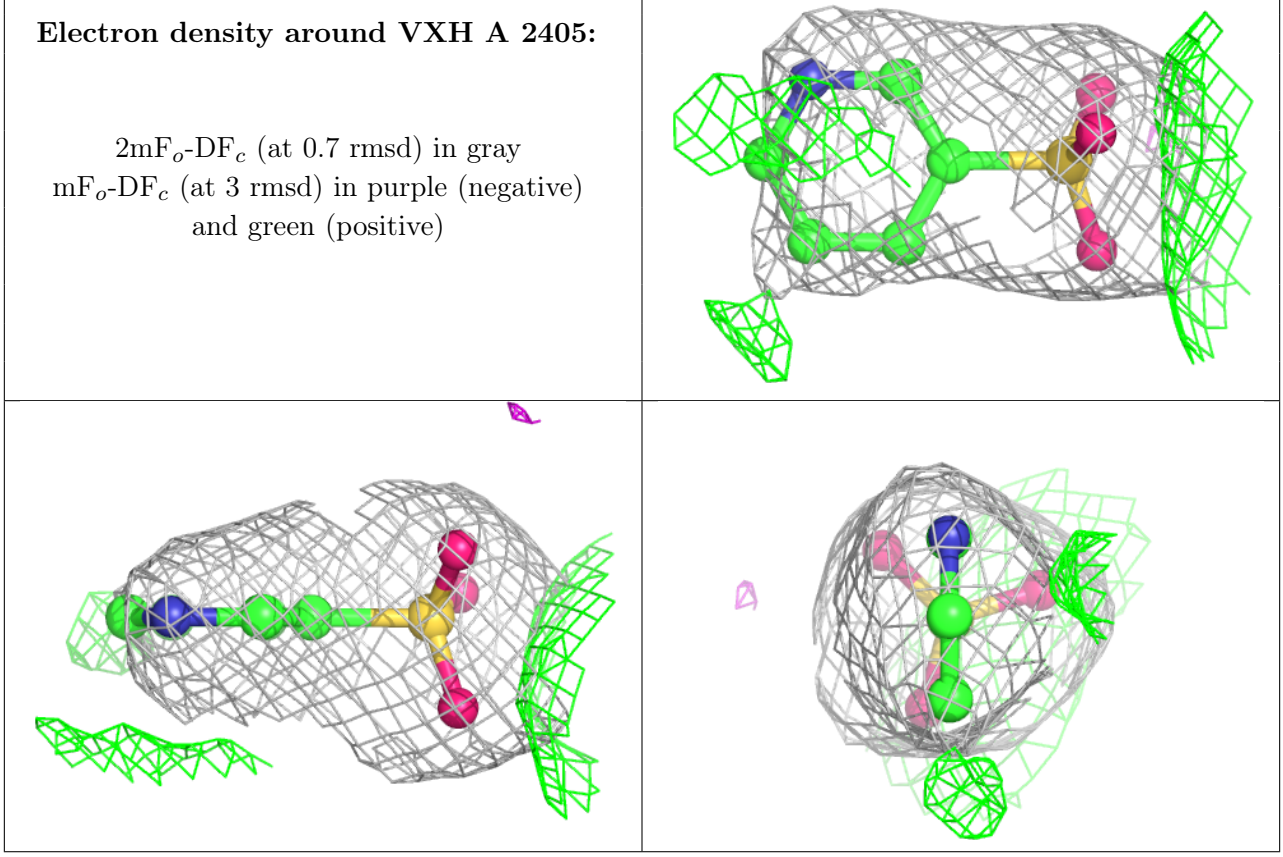
Electron density around VXH B 2405:

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



Electron density around VXH A 2405:

$2mF_o$-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.