



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:01 PM UTC

PDB ID : 8OQO / pdb_00008oqo
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (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

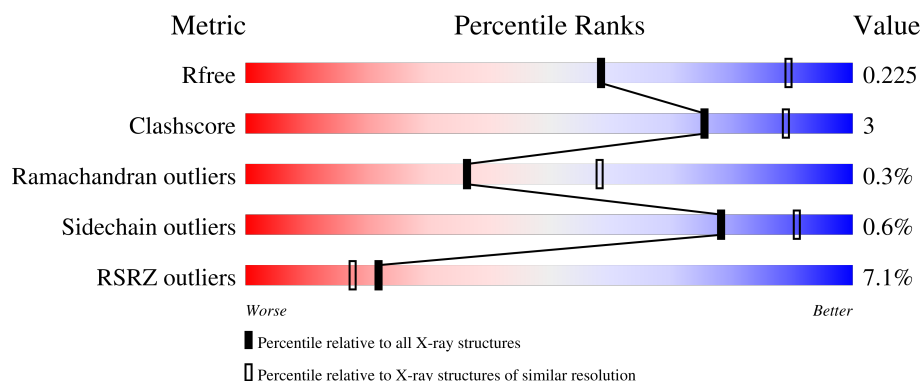
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	13% 90% 9%
1	B	736	2% 93% 6%
2	C	403	6% 90% 8%
2	D	403	5% 88% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17006 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 Probable fatty oxidation protein FadB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5421	3428	934	1038	21			
1	B	726	Total	C	N	O	S	0	0	0
			5406	3419	929	1037	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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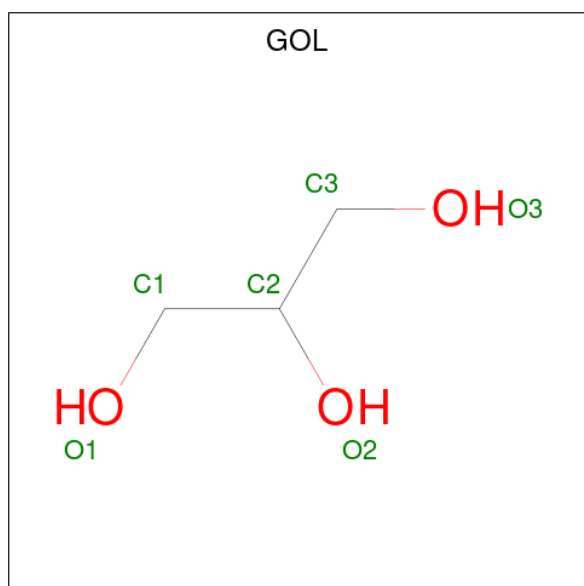
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP O53872
B	-5	SER	-	expression tag	UNP O53872
B	-4	GLN	-	expression tag	UNP O53872
B	-3	ASP	-	expression tag	UNP O53872
B	-2	PRO	-	expression tag	UNP O53872
B	-1	ASN	-	expression 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	396	Total	C	N	O	S	0	0	0
			2921	1822	519	565	15			
2	D	394	Total	C	N	O	S	0	0	0
			2909	1816	517	561	15			

- Molecule 3 is GLYCEROL (CCD ID: 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 (CCD ID: SO4) (formula: O_4S).



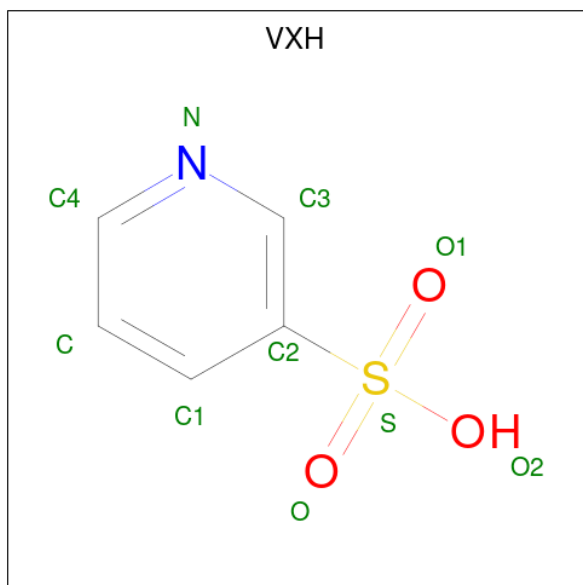
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total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

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

- Molecule 5 is pyridine-3-sulfonic acid (CCD ID: 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	0	0
			10	5	1	3	1		
5	A	1	Total	C	N	O	S	0	0
			10	5	1	3	1		
5	B	1	Total	C	N	O	S	0	0
			10	5	1	3	1		
5	B	1	Total	C	N	O	S	0	0
			10	5	1	3	1		
5	B	1	Total	C	N	O	S	0	0
			10	5	1	3	1		
5	C	1	Total	C	N	O	S	0	0
			10	5	1	3	1		
5	D	1	Total	C	N	O	S	0	1
			20	10	2	6	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	41	Total	O	0	0
			41	41		

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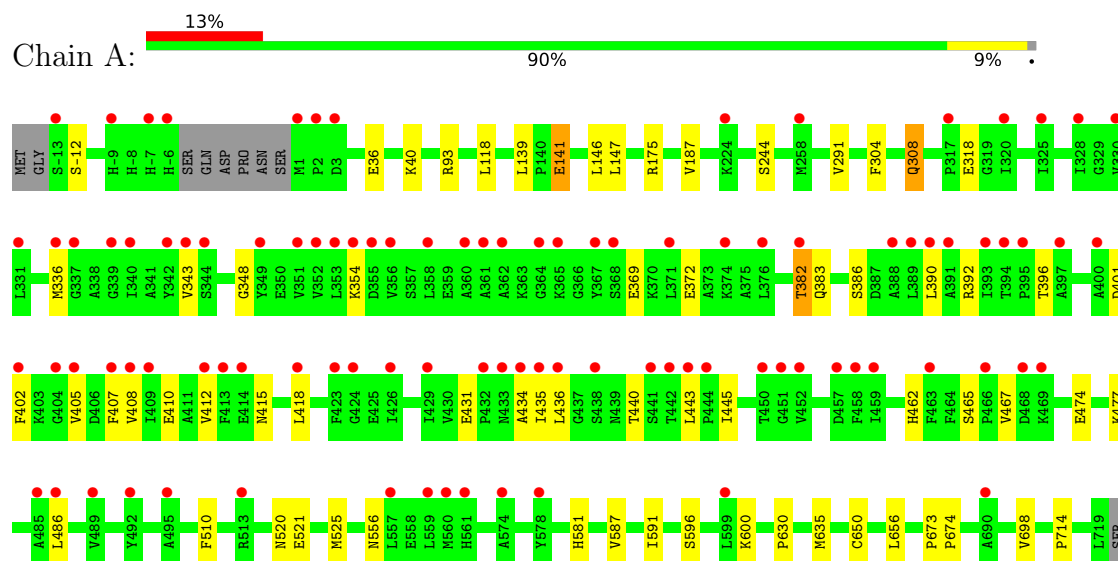
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	62	Total 62	O 62	0	0
6	C	39	Total 39	O 39	0	0
6	D	40	Total 40	O 40	0	0

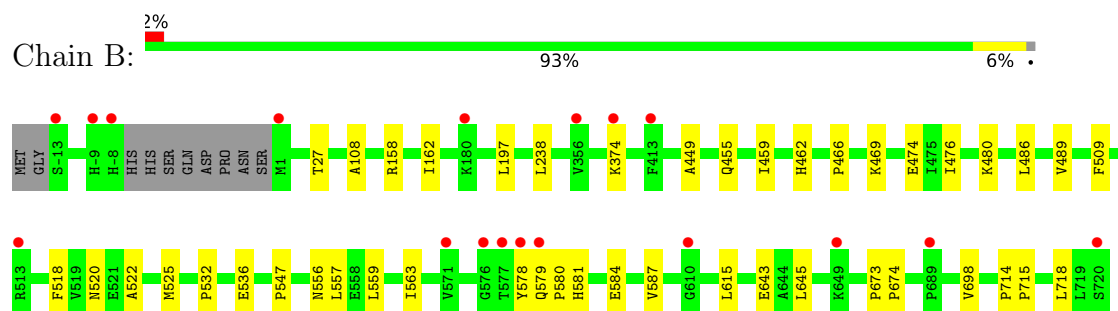
3 Residue-property plots [i](#)

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.

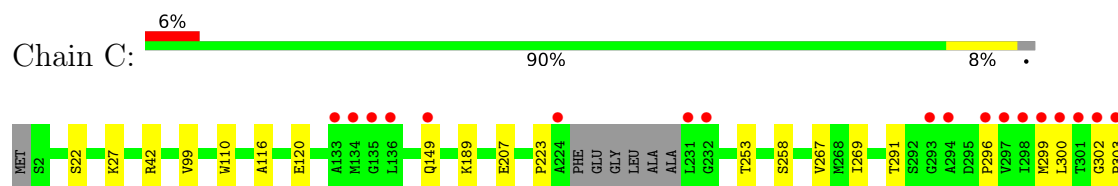
- Molecule 1: Probable fatty oxidation protein FadB

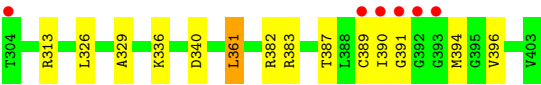


- Molecule 1: Probable fatty oxidation protein FadB

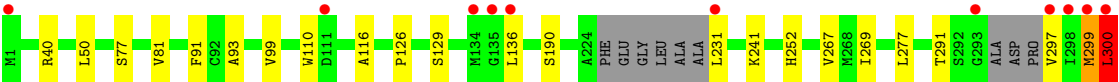
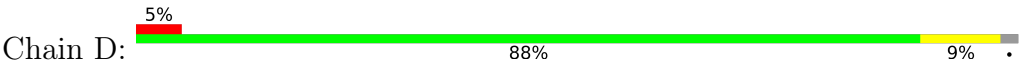


- Molecule 2: Putative acyltransferase Rv0859





● 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	250.78Å 136.14Å 121.05Å 90.00° 110.42° 90.00°	Depositor
Resolution (Å)	46.96 – 2.60 46.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.96-2.60) 99.6 (46.96-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.188 , 0.225 0.190 , 0.225	Depositor DCC
R_{free} test set	5852 reflections (4.99%)	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 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17006	wwPDB-VP
Average B, all atoms (Å ²)	85.0	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.*

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: VXH, OCS, 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	0.08	0/5514	0.23	0/7460
1	B	0.08	0/5497	0.24	0/7437
2	C	0.08	0/2964	0.26	0/4012
2	D	0.08	0/2950	0.26	0/3990
All	All	0.08	0/16925	0.24	0/22899

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	5421	0	5456	35	0
1	B	5406	0	5447	23	0
2	C	2921	0	2937	24	0
2	D	2909	0	2934	25	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	30	0	0	0	0
5	C	10	0	0	0	0
5	D	20	0	0	0	0
6	A	41	0	0	0	0
6	B	62	0	0	1	0
6	C	39	0	0	0	0
6	D	40	0	0	0	0
All	All	17006	0	16790	101	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 (101) 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:C:299:MET:HE3	2:C:391:GLY:HA2	1.73	0.70
1:A:596:SER:HB3	1:A:600:LYS:HD2	1.76	0.67
1:A:336:MET:HG2	1:A:465:SER:HB3	1.78	0.65
2:D:50:LEU:HD21	2:D:277:LEU:HD23	1.82	0.62
2:D:299:MET:O	2:D:301:THR:N	2.32	0.61
2:D:299:MET:HE2	2:D:392:GLY:H	1.64	0.61
2:C:99:VAL:HG13	2:C:269:ILE:HD11	1.83	0.61
2:D:252:HIS:HE1	2:D:332:SER:H	1.50	0.59
1:A:408:VAL:HB	1:A:436:LEU:HA	1.85	0.59
2:D:291:THR:HG22	2:D:396:VAL:HG22	1.83	0.59
2:D:99:VAL:HG13	2:D:269:ILE:HD11	1.85	0.59
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.85	0.58
1:B:459:ILE:HG21	1:B:489:VAL:HG21	1.85	0.58
1:A:415:ASN:HB3	1:A:418:LEU:HB3	1.87	0.57
2:D:390:ILE:HG21	2:D:394:MET:HE3	1.87	0.57
2:C:313:ARG:HD3	2:D:110:TRP:CD1	2.41	0.56
2:D:299:MET:C	2:D:301:THR:H	2.13	0.56
2:C:300:LEU:HA	2:C:389:CYS:HB2	1.87	0.55
1:B:520:ASN:HB3	1:B:581:HIS:CE1	2.41	0.55
1:A:354:LYS:HB2	1:A:402:PHE:HE2	1.73	0.53
1:A:-12:SER:O	1:A:93:ARG:NH1	2.39	0.53
1:A:630:PRO:HG2	1:A:635:MET:HE2	1.91	0.53
1:A:244:SER:HB3	2:D:231:LEU:HD13	1.91	0.52
2:C:296:PRO:HD3	2:D:81:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:300:LEU:HA	2:D:389:CYS:HB2	1.91	0.52
2:D:91:PHE:HB2	2:D:390:ILE:HG23	1.92	0.51
2:C:22:SER:OG	2:C:207:GLU:OE2	2.21	0.51
2:D:190:SER:OG	2:D:374:ASP:OD2	2.17	0.51
2:C:223:PRO:HA	2:C:253:THR:HG22	1.93	0.51
2:C:110:TRP:O	2:D:313:ARG:NH1	2.44	0.50
2:C:258:SER:HB3	2:C:329:ALA:HA	1.94	0.50
1:A:348:GLY:HA2	1:A:392:ARG:NH1	2.27	0.50
1:B:466:PRO:HG2	1:B:469:LYS:HE3	1.93	0.50
1:A:36:GLU:HG3	1:A:40:LYS:HE3	1.94	0.50
2:C:303:PRO:HD3	2:C:389:CYS:HA	1.92	0.50
1:A:410:GLU:OE2	1:A:412:VAL:HG22	2.12	0.49
2:C:27:LYS:NZ	2:D:136:LEU:O	2.45	0.49
1:A:440:THR:HG21	1:A:443:LEU:HB2	1.94	0.49
1:A:462:HIS:HB3	1:A:474:GLU:HB3	1.94	0.49
2:C:302:GLY:N	2:C:303:PRO:HD2	2.28	0.48
2:D:241:LYS:HD3	2:D:297:VAL:HG21	1.94	0.48
1:A:118:LEU:HD23	1:A:139:LEU:HG	1.95	0.48
1:A:141:GLU:HG3	1:A:147:LEU:C	2.39	0.48
2:D:354:ALA:HB1	2:D:359:HIS:HB2	1.96	0.48
1:A:405:VAL:O	1:A:434:ALA:HB2	2.13	0.48
1:B:532:PRO:HB2	1:B:615:LEU:HD13	1.96	0.47
1:B:579:GLN:NE2	1:B:580:PRO:O	2.47	0.47
2:C:110:TRP:CD1	2:D:313:ARG:HD3	2.49	0.47
1:B:557:LEU:HB3	1:B:587:VAL:HG13	1.97	0.47
2:C:336:LYS:NZ	2:C:340:ASP:OD2	2.46	0.47
1:A:405:VAL:N	1:A:431:GLU:HG2	2.30	0.47
1:B:578:TYR:OH	1:B:584:GLU:OE2	2.32	0.46
2:C:390:ILE:HG21	2:C:394:MET:HE3	1.97	0.46
2:D:93:ALA:HB3	2:D:390:ILE:HD11	1.97	0.46
1:B:522:ALA:HA	1:B:525:MET:HE3	1.96	0.46
2:C:149:GLN:HG2	2:C:299:MET:HE1	1.97	0.46
1:B:698:VAL:HG13	1:B:714:PRO:HG3	1.97	0.46
1:A:407:PHE:HE1	1:A:435:ILE:HD12	1.81	0.45
1:A:698:VAL:HG13	1:A:714:PRO:HG3	1.97	0.45
1:B:162:ILE:HD12	1:B:238:LEU:HD21	1.99	0.45
1:B:476:ILE:HG21	1:B:509:PHE:CE1	2.52	0.45
1:B:459:ILE:HD11	1:B:486:LEU:HD12	1.99	0.45
2:D:116:ALA:O	2:D:267:VAL:N	2.48	0.44
1:A:304:PHE:O	1:A:308:GLN:HB2	2.18	0.44
1:B:158:ARG:NH1	6:B:2501:HOH:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:99:VAL:HG11	2:D:369:LEU:HD22	2.00	0.44
1:A:369:GLU:HG2	1:A:390:LEU:HD21	2.00	0.44
1:B:715:PRO:HD2	1:B:718:LEU:HD12	1.98	0.44
2:C:390:ILE:HB	2:C:394:MET:HB2	2.00	0.44
1:A:510:PHE:CD1	1:A:656:LEU:HD11	2.53	0.43
1:B:714:PRO:HA	1:B:715:PRO:HD3	1.91	0.43
1:A:445:ILE:HD12	1:A:445:ILE:HA	1.91	0.42
2:C:390:ILE:HD11	2:C:396:VAL:HG23	2.01	0.42
2:D:126:PRO:O	2:D:129:SER:OG	2.34	0.42
1:A:354:LYS:HB2	1:A:402:PHE:CE2	2.54	0.42
1:B:673:PRO:HA	1:B:674:PRO:HD3	1.91	0.42
1:A:520:ASN:HB3	1:A:581:HIS:CE1	2.54	0.42
1:A:587:VAL:O	1:A:591:ILE:HG12	2.20	0.42
1:B:559:LEU:O	1:B:563:ILE:HG12	2.20	0.42
2:C:291:THR:HG22	2:C:396:VAL:HG22	2.01	0.42
2:C:326:LEU:HD13	2:C:387:THR:HG23	2.02	0.41
1:A:382:THR:HG22	1:A:383:GLN:H	1.85	0.41
1:A:521:GLU:O	1:A:525:MET:HG3	2.20	0.41
1:A:396:THR:HG21	1:A:401:ASP:CG	2.45	0.41
1:A:343:VAL:HG21	1:A:467:VAL:C	2.46	0.41
1:A:477:LYS:HG3	1:A:486:LEU:HD21	2.03	0.41
1:B:518:PHE:HB2	1:B:643:GLU:CD	2.46	0.41
2:C:42:ARG:NH2	2:C:189:LYS:O	2.51	0.41
2:D:302:GLY:N	2:D:303:PRO:HD2	2.35	0.41
2:C:382:ARG:HG3	2:C:383:ARG:HG3	2.02	0.41
1:A:146:LEU:HD22	1:A:291:VAL:HG22	2.02	0.41
1:A:407:PHE:CE1	1:A:435:ILE:HD12	2.55	0.41
1:B:536:GLU:CD	1:B:547:PRO:HB2	2.46	0.41
2:C:120:GLU:HG2	2:C:361:LEU:HB2	2.03	0.41
2:D:40:ARG:NH1	2:D:77:SER:O	2.45	0.41
1:A:673:PRO:HA	1:A:674:PRO:HD3	1.97	0.40
2:C:116:ALA:O	2:C:267:VAL:N	2.52	0.40
1:B:108:ALA:HB1	1:B:197:LEU:HB3	2.02	0.40
1:A:372:GLU:HB3	1:A:386:SER:OG	2.21	0.40
1:B:645:LEU:HD22	1:B:715:PRO:HD3	2.02	0.40
1:B:449:ALA:O	1:B:455:GLN:HG2	2.22	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	722/736 (98%)	693 (96%)	28 (4%)	1 (0%)	48	70
1	B	721/736 (98%)	696 (96%)	24 (3%)	1 (0%)	48	70
2	C	392/403 (97%)	379 (97%)	12 (3%)	1 (0%)	36	58
2	D	388/403 (96%)	377 (97%)	8 (2%)	3 (1%)	16	34
All	All	2223/2278 (98%)	2145 (96%)	72 (3%)	6 (0%)	36	58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	361	LEU
2	D	300	LEU
2	D	361	LEU
1	B	556	ASN
1	A	556	ASN
2	D	299	MET

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	557/565 (99%)	551 (99%)	6 (1%)	65	84
1	B	556/565 (98%)	553 (100%)	3 (0%)	81	92
2	C	305/310 (98%)	305 (100%)	0	100	100
2	D	304/310 (98%)	303 (100%)	1 (0%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1722/1750 (98%)	1712 (99%)	10 (1%)	78 91

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	GLU
1	A	175	ARG
1	A	187	VAL
1	A	308	GLN
1	A	318	GLU
1	A	382	THR
1	B	27	THR
1	B	374	LYS
1	B	480	LYS
2	D	300	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	GLN
1	A	561	HIS
1	A	681	GLN
1	B	136	GLN
1	B	163	GLN
1	B	294	GLN
1	B	383	GLN
1	B	550	GLN
1	B	681	GLN
2	D	43	HIS
2	D	49	ASN
2	D	149	GLN
2	D	327	ASN
2	D	342	ASN
2	D	380	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	OCS	B	650	1	6,8,9	0.90	0	7,11,13	1.42	0
1	OCS	A	650	1	6,8,9	0.90	0	7,11,13	1.44	1 (14%)

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
1	OCS	B	650	1	-	3/4/7/9	-
1	OCS	A	650	1	-	3/4/7/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	650	OCS	OD1-SG-CB	2.11	109.91	106.76

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	650	OCS	CA-CB-SG-OD1
1	A	650	OCS	CA-CB-SG-OD2
1	A	650	OCS	CA-CB-SG-OD3
1	B	650	OCS	CA-CB-SG-OD1
1	B	650	OCS	CA-CB-SG-OD2
1	B	650	OCS	CA-CB-SG-OD3

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

25 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	B	2402	-	4,4,4	0.24	0	6,6,6	0.05	0
4	SO4	C	504	-	4,4,4	0.24	0	6,6,6	0.07	0
5	VXH	A	2405	-	10,10,10	0.13	0	14,14,14	0.34	0
4	SO4	D	501	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	D	502	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	B	2403	-	4,4,4	0.24	0	6,6,6	0.08	0
5	VXH	B	2407	-	10,10,10	0.20	0	14,14,14	0.34	0
4	SO4	A	2404	-	4,4,4	0.23	0	6,6,6	0.06	0
5	VXH	D	506[A]	-	10,10,10	0.21	0	14,14,14	0.34	0
4	SO4	D	504	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	A	2402	-	4,4,4	0.24	0	6,6,6	0.06	0
3	GOL	B	2401	-	5,5,5	0.91	0	5,5,5	1.11	0
3	GOL	A	2401	-	5,5,5	0.91	0	5,5,5	1.11	0
5	VXH	A	2406	-	10,10,10	0.21	0	14,14,14	0.34	0
5	VXH	B	2405	-	10,10,10	0.20	0	14,14,14	0.34	0
4	SO4	C	503	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	C	501	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	D	505	-	4,4,4	0.24	0	6,6,6	0.06	0
5	VXH	B	2406	-	10,10,10	0.22	0	14,14,14	0.34	0
4	SO4	C	502	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	A	2403	-	4,4,4	0.23	0	6,6,6	0.07	0
5	VXH	D	506[B]	-	10,10,10	0.21	0	14,14,14	0.34	0
4	SO4	B	2404	-	4,4,4	0.24	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	VXH	C	505	-	10,10,10	0.22	0	14,14,14	0.34	0
4	SO4	D	503	-	4,4,4	0.24	0	6,6,6	0.08	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
5	VXH	D	506[A]	-	-	0/6/6/6	0/1/1/1
5	VXH	A	2405	-	-	0/6/6/6	0/1/1/1
5	VXH	B	2405	-	-	0/6/6/6	0/1/1/1
5	VXH	D	506[B]	-	-	0/6/6/6	0/1/1/1
3	GOL	B	2401	-	-	1/4/4/4	-
5	VXH	B	2406	-	-	1/6/6/6	0/1/1/1
3	GOL	A	2401	-	-	0/4/4/4	-
5	VXH	A	2406	-	-	0/6/6/6	0/1/1/1
5	VXH	C	505	-	-	1/6/6/6	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 (3) torsion outliers are listed below:

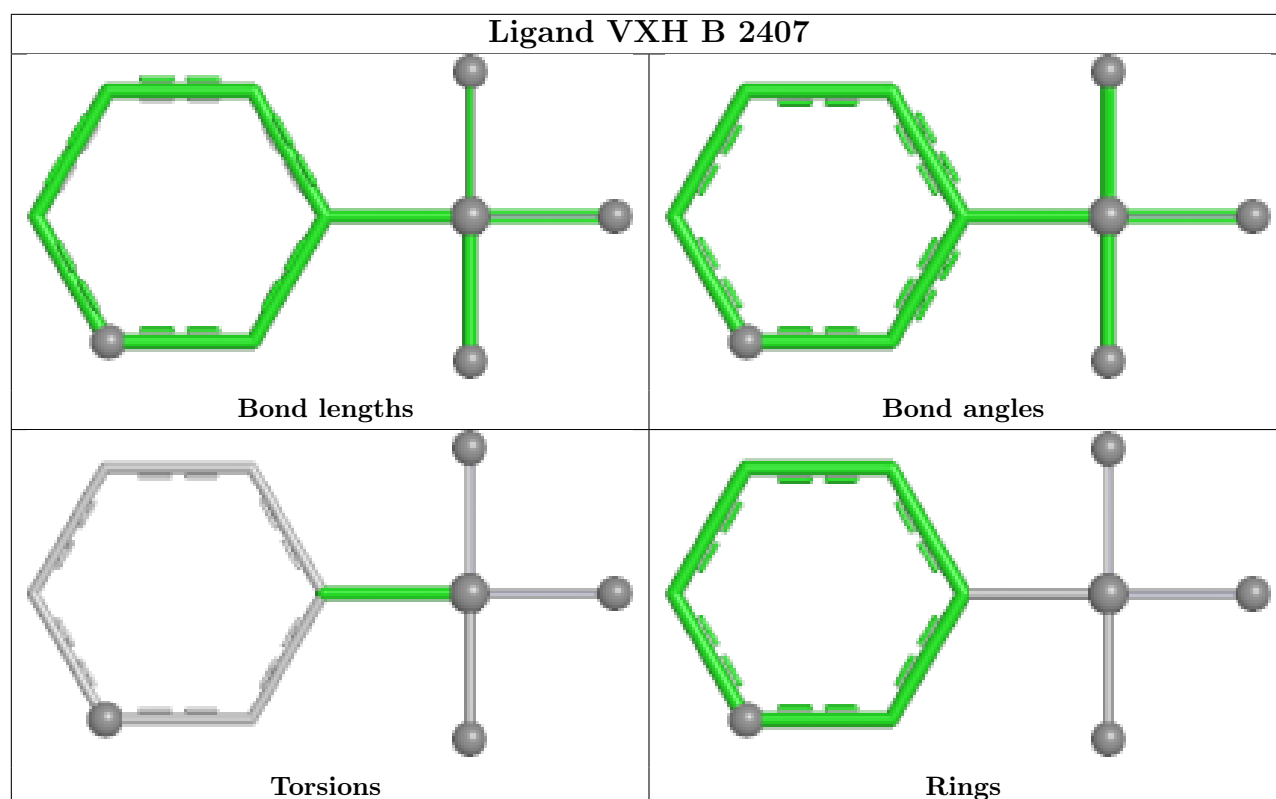
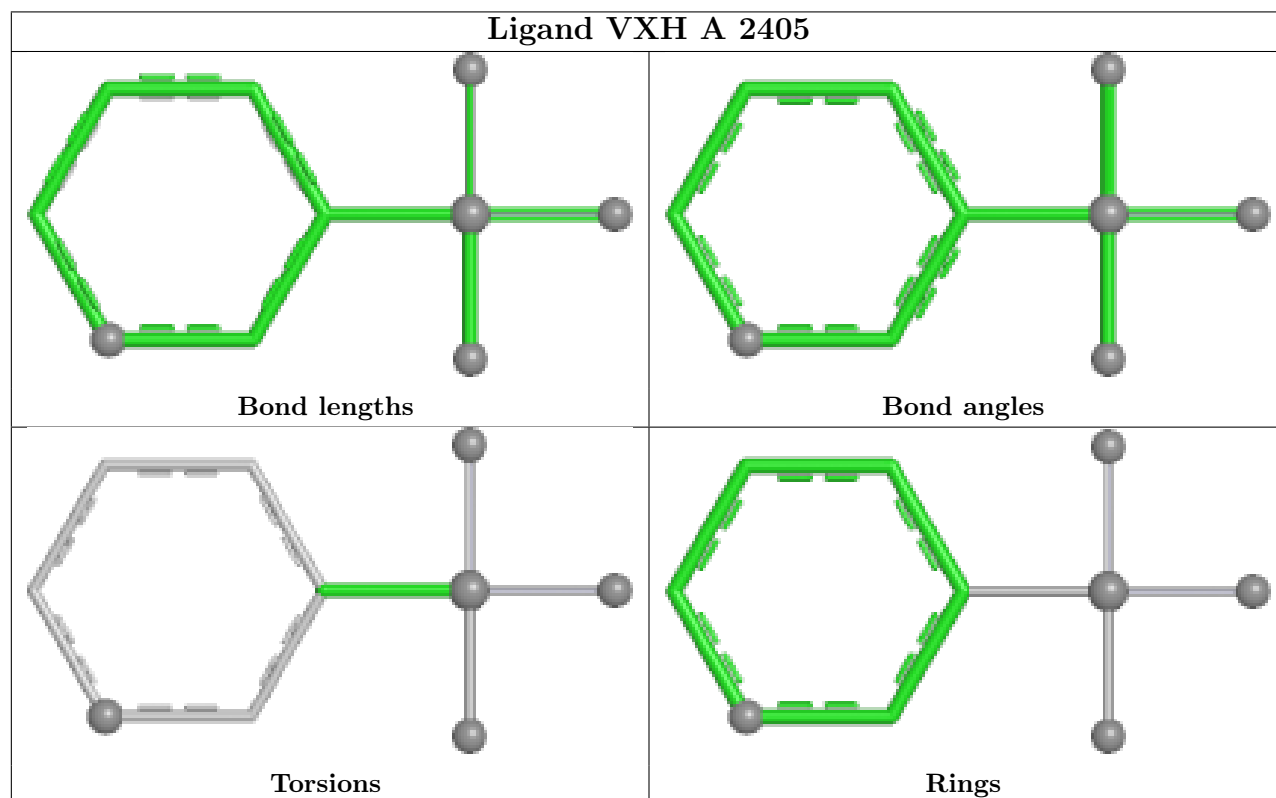
Mol	Chain	Res	Type	Atoms
3	B	2401	GOL	O1-C1-C2-O2
5	B	2406	VXH	C3-C2-S-O1
5	C	505	VXH	C3-C2-S-O1

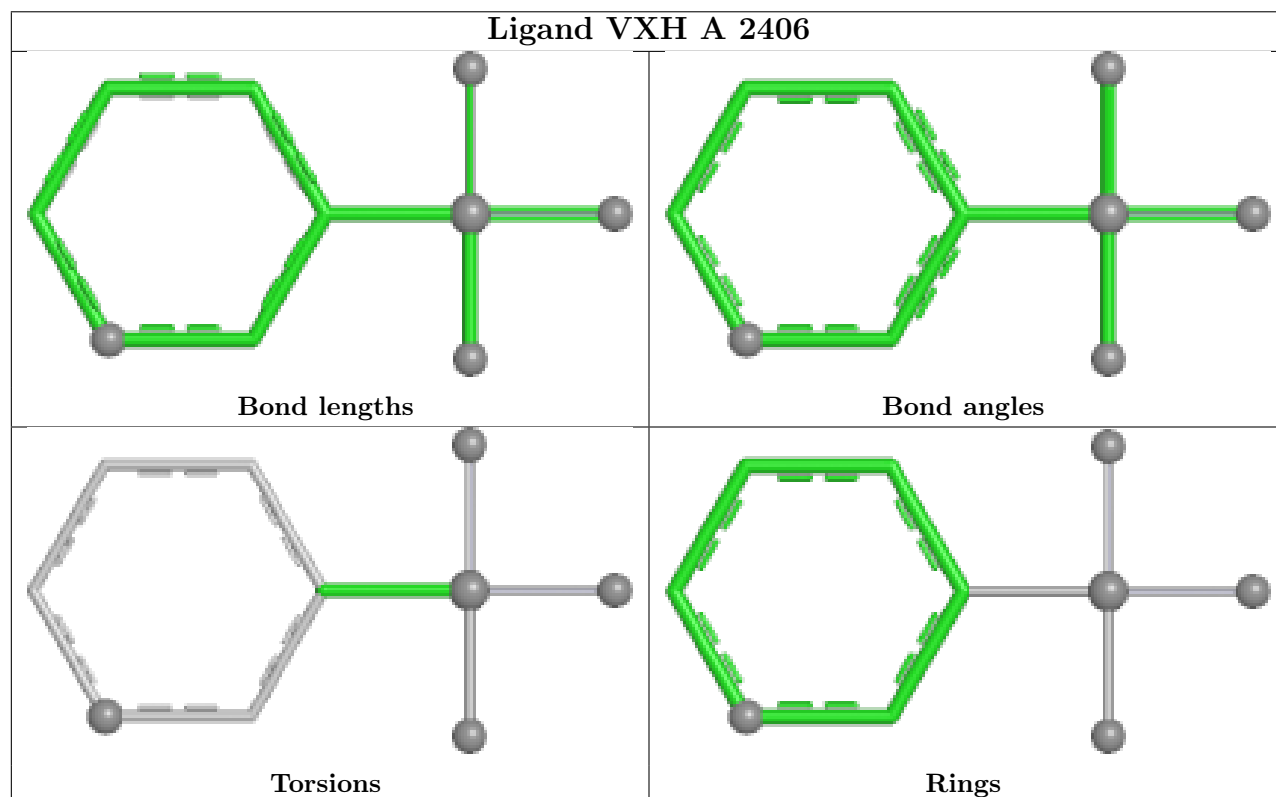
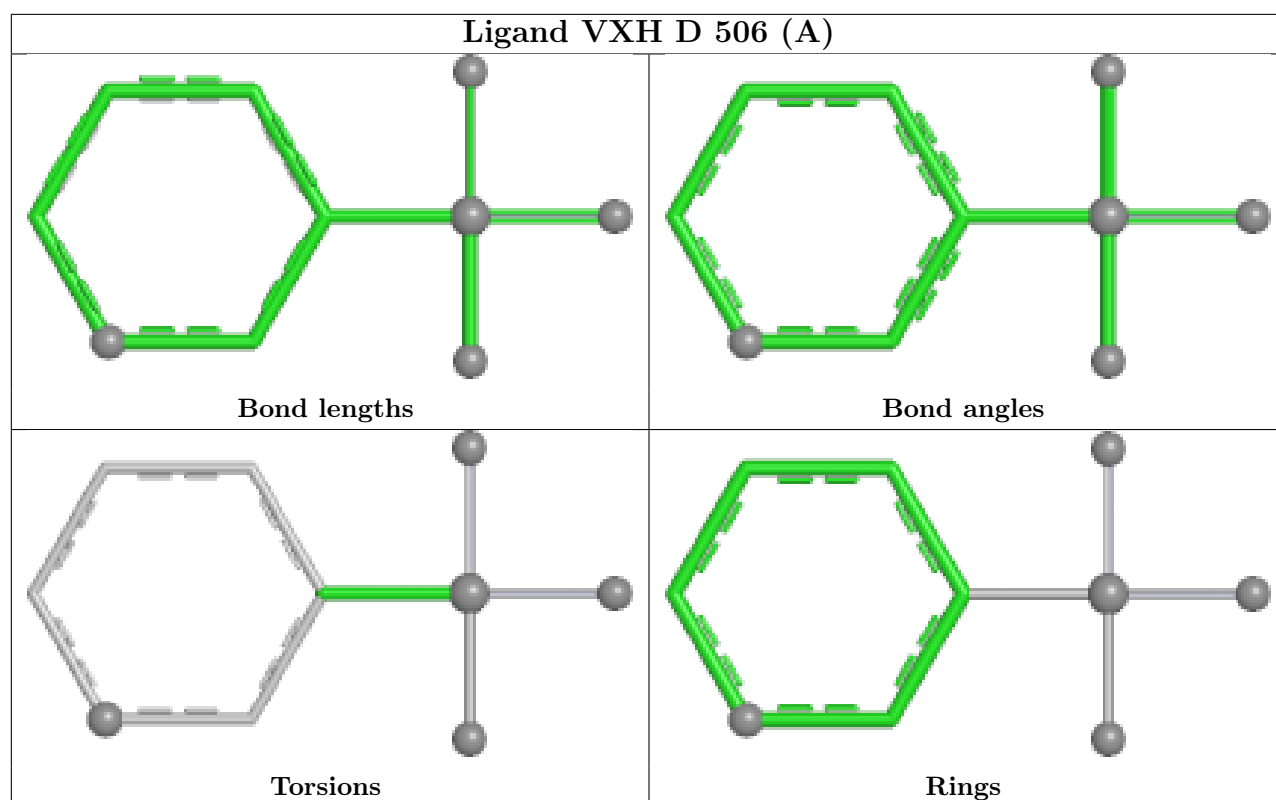
There are no ring outliers.

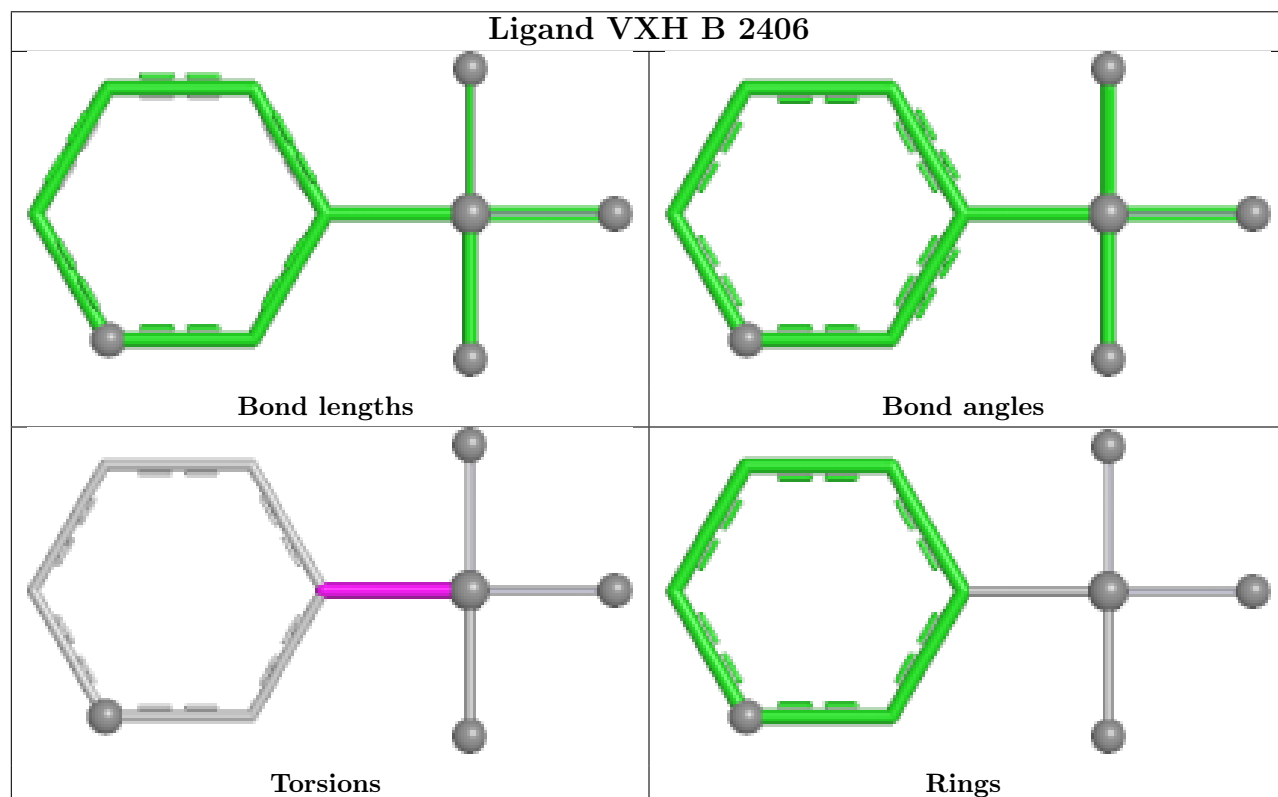
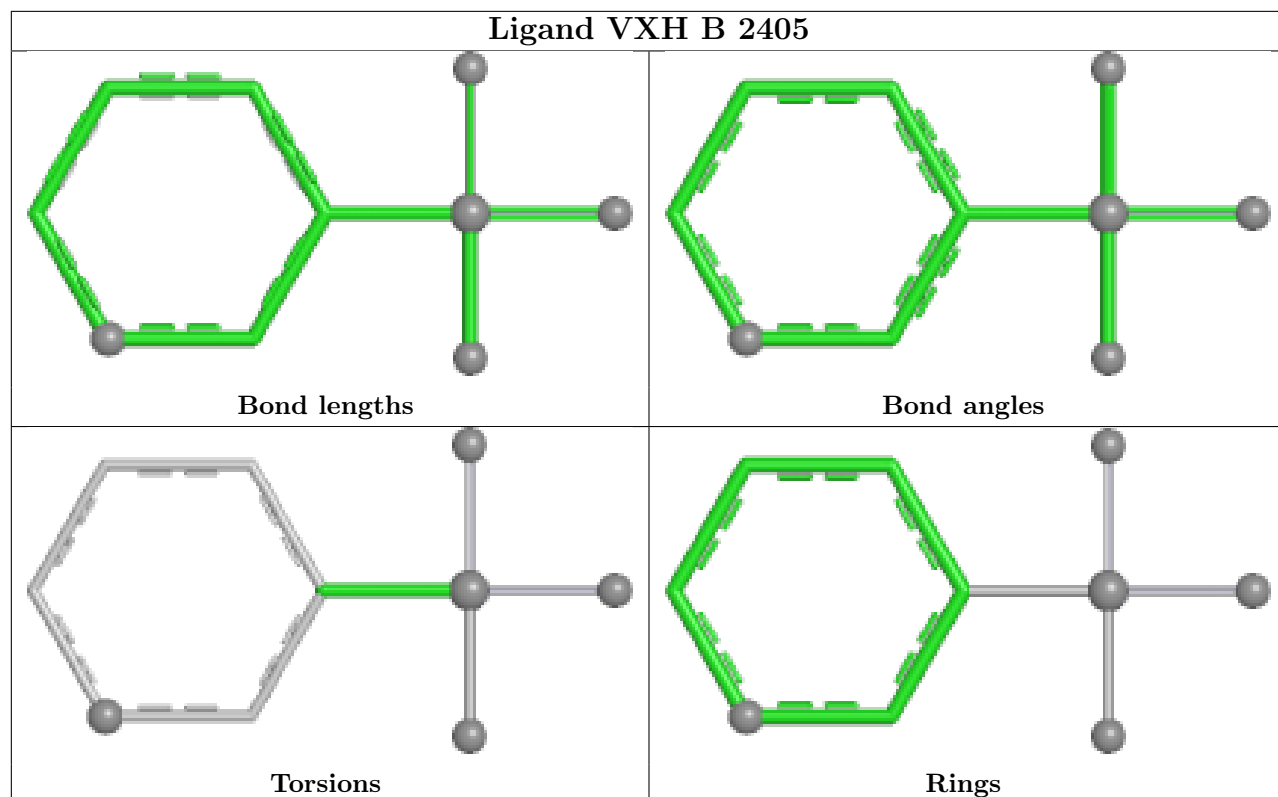
No monomer is involved in short contacts.

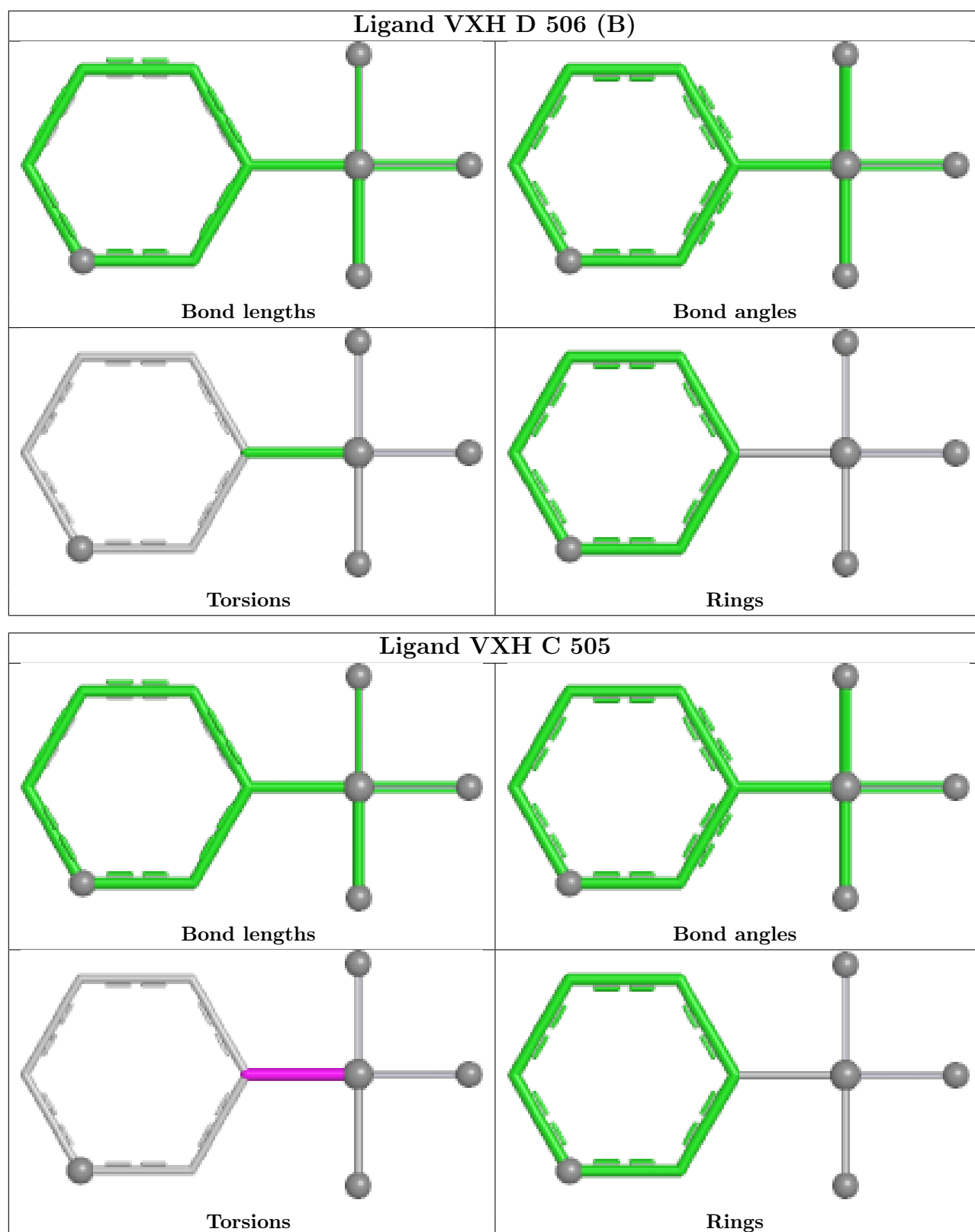
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ⓘ

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	726/736 (98%)	0.57	98 (13%) 7 5	52, 88, 186, 251	0
1	B	725/736 (98%)	0.01	18 (2%) 58 52	48, 75, 123, 154	0
2	C	396/403 (98%)	-0.06	24 (6%) 27 22	44, 65, 105, 142	0
2	D	394/403 (97%)	-0.01	20 (5%) 33 28	47, 68, 105, 169	0
All	All	2241/2278 (98%)	0.18	160 (7%) 22 17	44, 74, 161, 251	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	303	PRO	5.9
1	A	356	VAL	5.8
1	B	577	THR	5.8
1	A	434	ALA	5.8
2	D	391	GLY	5.7
2	C	389	CYS	5.7
2	D	389	CYS	5.7
1	A	358	LEU	5.6
1	A	353	LEU	5.4
2	D	390	ILE	5.3
2	D	392	GLY	5.3
1	A	352	VAL	5.2
2	C	136	LEU	5.1
1	A	349	TYR	5.1
1	A	426	ILE	4.9
2	D	393	GLY	4.9
1	A	407	PHE	4.8
1	A	413	PHE	4.8
2	D	1	MET	4.7
2	C	390	ILE	4.6
1	A	393	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	409	ILE	4.3
2	D	303	PRO	4.2
1	A	388	ALA	4.2
1	A	343	VAL	4.2
2	C	299	MET	4.2
1	A	342	TYR	4.1
1	A	574	ALA	4.1
2	C	300	LEU	4.1
1	A	367	TYR	4.0
1	A	423	PHE	4.0
1	B	576	GLY	4.0
1	A	432	PRO	4.0
2	C	134	MET	3.9
1	A	408	VAL	3.9
2	D	231	LEU	3.8
1	A	351	VAL	3.8
1	B	578	TYR	3.7
2	C	301	THR	3.7
1	A	468	ASP	3.7
2	C	224	ALA	3.7
1	A	-13	SER	3.7
2	C	231	LEU	3.6
1	A	492	TYR	3.6
2	D	302	GLY	3.6
2	C	391	GLY	3.6
1	A	414	GLU	3.5
2	D	299	MET	3.5
1	A	330	VAL	3.5
2	D	134	MET	3.5
1	A	389	LEU	3.5
2	D	135	GLY	3.4
1	A	394	THR	3.4
2	C	392	GLY	3.4
2	D	297	VAL	3.4
1	B	579	GLN	3.4
2	D	298	ILE	3.3
2	C	135	GLY	3.3
2	C	393	GLY	3.3
1	A	405	VAL	3.2
1	A	438	SER	3.2
2	D	301	THR	3.2
1	B	413	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	376	LEU	3.1
1	A	391	ALA	3.0
2	C	297	VAL	3.0
2	C	133	ALA	3.0
1	B	720	SER	3.0
1	A	-6	HIS	3.0
1	A	354	LYS	3.0
1	A	429	ILE	3.0
2	C	296	PRO	3.0
1	A	371	LEU	2.9
1	A	436	LEU	2.9
1	A	559	LEU	2.9
2	D	136	LEU	2.9
2	D	300	LEU	2.9
2	C	302	GLY	2.9
1	A	368	SER	2.9
1	A	328	ILE	2.9
2	C	304	THR	2.9
1	A	458	PHE	2.9
1	A	466	PRO	2.9
1	A	424	GLY	2.9
1	A	557	LEU	2.9
1	A	339	GLY	2.9
1	A	340	ILE	2.8
1	A	355	ASP	2.8
1	A	485	ALA	2.8
1	A	418	LEU	2.8
1	A	402	PHE	2.8
1	A	452	VAL	2.8
2	C	294	ALA	2.8
1	A	599	LEU	2.7
1	A	360	ALA	2.7
1	A	400	ALA	2.7
1	A	412	VAL	2.7
2	D	111	ASP	2.7
1	A	362	ALA	2.7
1	A	457	ASP	2.7
1	A	325	ILE	2.7
1	A	395	PRO	2.7
1	A	337	GLY	2.6
2	C	293	GLY	2.6
1	A	690	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	364	GLY	2.6
1	A	390	LEU	2.6
1	A	444	PRO	2.6
1	A	1	MET	2.5
1	A	2	PRO	2.5
2	C	298	ILE	2.5
1	A	560	MET	2.5
1	B	1	MET	2.5
1	A	442	THR	2.5
2	D	293	GLY	2.5
1	A	469	LYS	2.4
1	A	513	ARG	2.4
1	A	443	LEU	2.4
1	B	-13	SER	2.4
1	B	-8	HIS	2.4
1	A	336	MET	2.4
1	A	3	ASP	2.4
1	A	258	MET	2.4
1	A	317	PRO	2.4
1	A	382	THR	2.4
1	B	356	VAL	2.4
1	A	361	ALA	2.4
1	A	489	VAL	2.3
1	A	331	LEU	2.3
1	A	-7	HIS	2.3
1	B	-9	HIS	2.3
1	A	441	SER	2.3
1	A	451	GLY	2.3
1	A	495	ALA	2.3
1	A	374	LYS	2.3
1	A	463	PHE	2.3
1	A	320	ILE	2.2
1	A	459	ILE	2.2
1	A	433	ASN	2.2
1	A	561	HIS	2.2
1	B	610	GLY	2.2
1	A	224	LYS	2.2
1	A	-9	HIS	2.2
1	A	344	SER	2.2
1	B	374	LYS	2.2
1	B	689	PRO	2.1
1	B	180	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	435	ILE	2.1
1	B	649	LYS	2.1
1	A	486	LEU	2.1
1	A	578	TYR	2.1
2	C	232	GLY	2.1
1	A	397	ALA	2.1
1	B	513	ARG	2.1
1	A	450	THR	2.0
2	C	149	GLN	2.0
1	A	404	GLY	2.0
1	B	571	VAL	2.0
1	A	365	LYS	2.0
2	D	304	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	OCS	A	650	9/10	0.89	0.18	71,83,103,106	0
1	OCS	B	650	9/10	0.90	0.16	57,61,92,108	0

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
4	SO4	B	2403	5/5	0.62	0.12	114,133,167,181	0
4	SO4	D	504	5/5	0.68	0.14	123,133,137,141	5
4	SO4	A	2404	5/5	0.70	0.09	141,144,174,177	0

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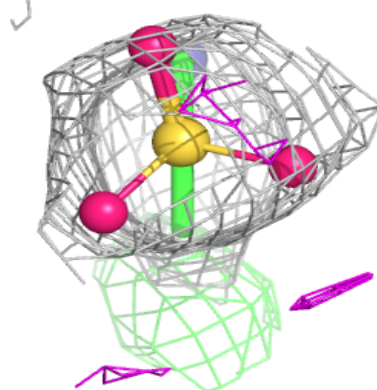
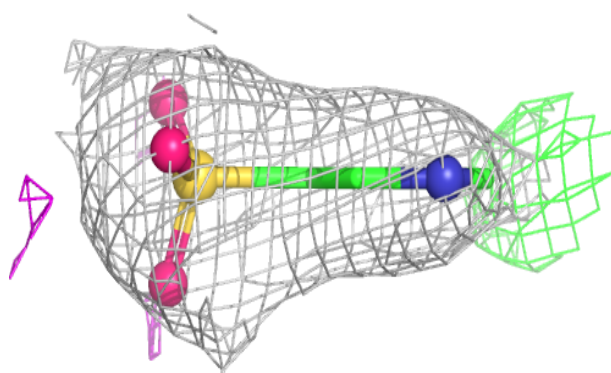
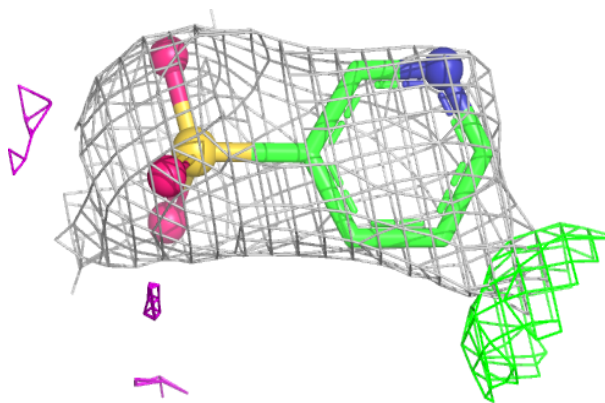
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	C	502	5/5	0.72	0.09	115,121,145,153	0
4	SO4	C	503	5/5	0.78	0.08	115,124,140,140	0
4	SO4	D	505	5/5	0.81	0.12	104,106,131,152	0
4	SO4	D	502	5/5	0.82	0.08	103,110,133,138	0
4	SO4	C	501	5/5	0.83	0.09	97,108,112,126	0
4	SO4	D	503	5/5	0.83	0.08	97,118,144,166	0
5	VXH	A	2406	10/10	0.83	0.16	109,131,153,171	0
4	SO4	B	2404	5/5	0.84	0.11	122,135,142,166	0
4	SO4	C	504	5/5	0.85	0.11	121,134,148,185	0
4	SO4	A	2402	5/5	0.86	0.10	96,104,114,125	0
4	SO4	D	501	5/5	0.87	0.07	115,121,133,135	0
4	SO4	A	2403	5/5	0.87	0.07	120,123,156,156	0
5	VXH	B	2406	10/10	0.87	0.14	106,125,132,143	0
5	VXH	B	2407	10/10	0.87	0.18	113,128,156,182	0
5	VXH	B	2405	10/10	0.90	0.15	92,102,115,125	0
4	SO4	B	2402	5/5	0.91	0.16	84,88,102,114	0
5	VXH	C	505	10/10	0.91	0.12	91,105,118,133	0
5	VXH	D	506[A]	10/10	0.91	0.22	71,79,97,99	10
5	VXH	D	506[B]	10/10	0.91	0.22	76,86,98,111	10
5	VXH	A	2405	10/10	0.92	0.16	91,106,112,115	0
3	GOL	B	2401	6/6	0.93	0.16	73,86,90,96	0
3	GOL	A	2401	6/6	0.96	0.11	79,81,86,88	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.

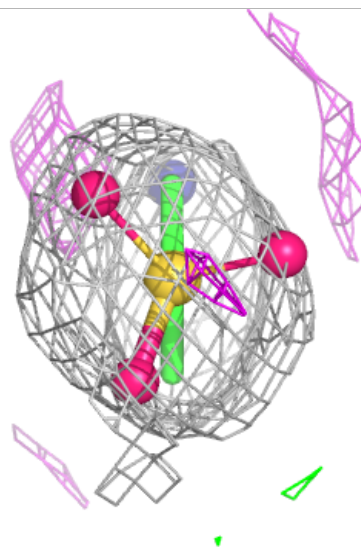
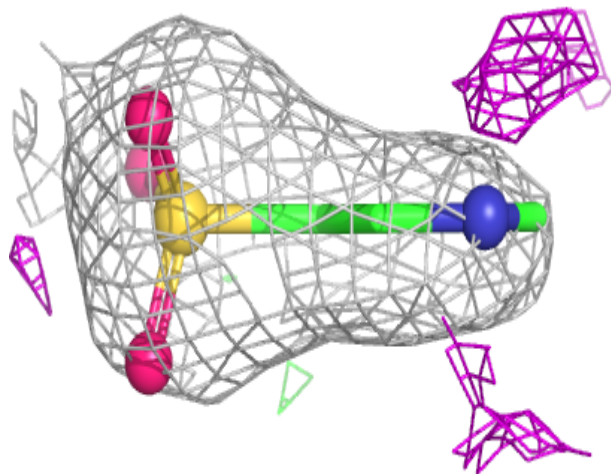
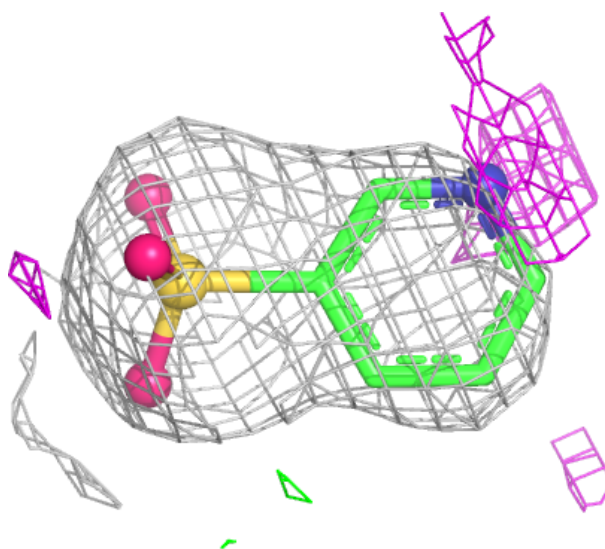
Electron density around VXH A 2406:

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



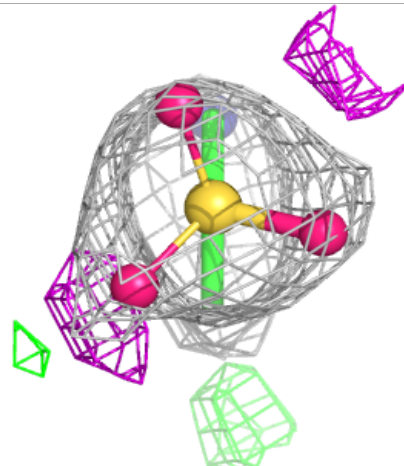
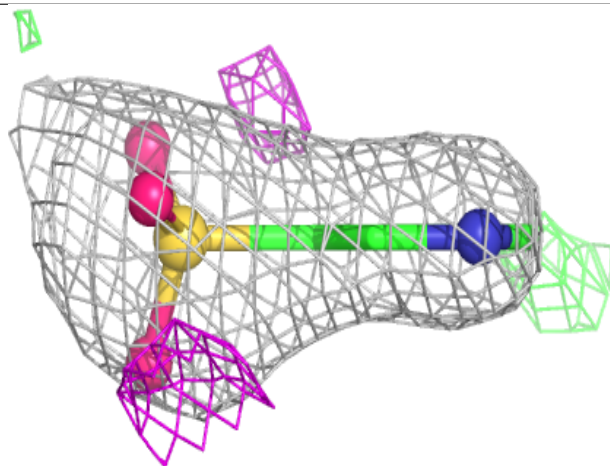
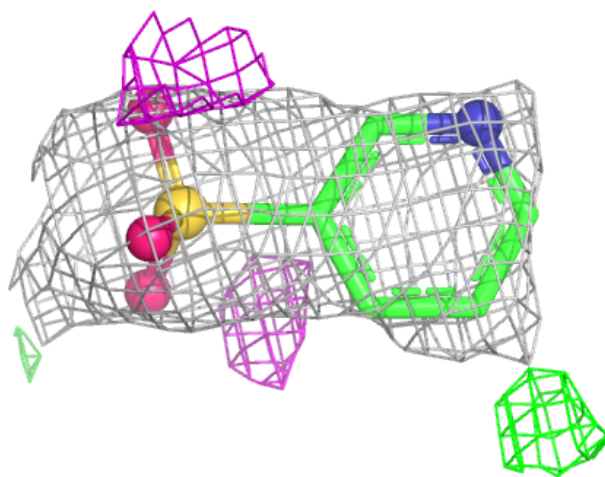
Electron density around VXH B 2406:

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



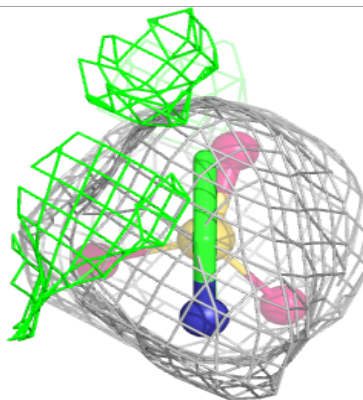
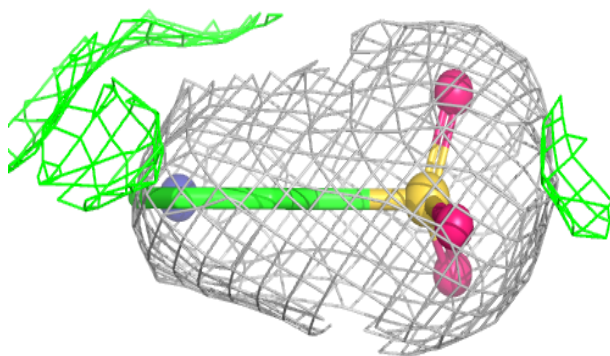
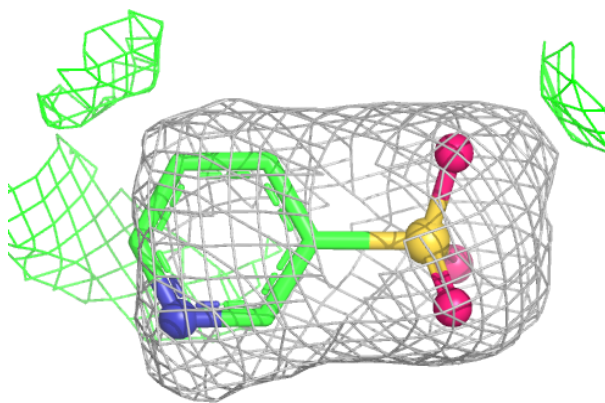
Electron density around VXH B 2407:

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

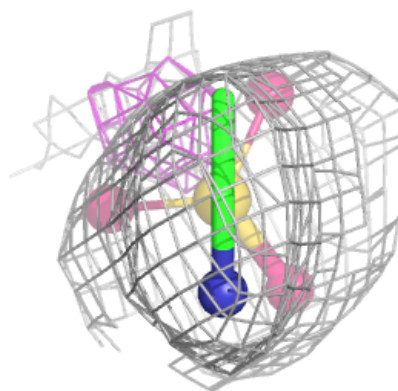
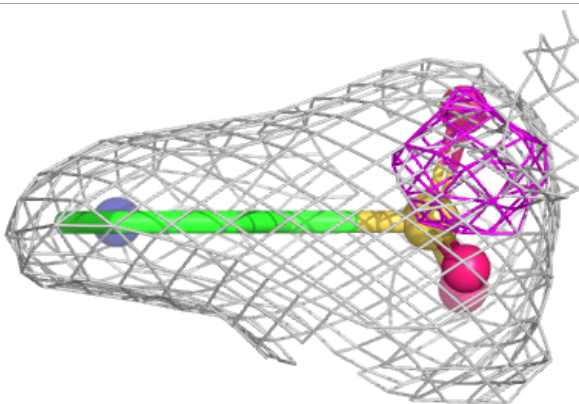
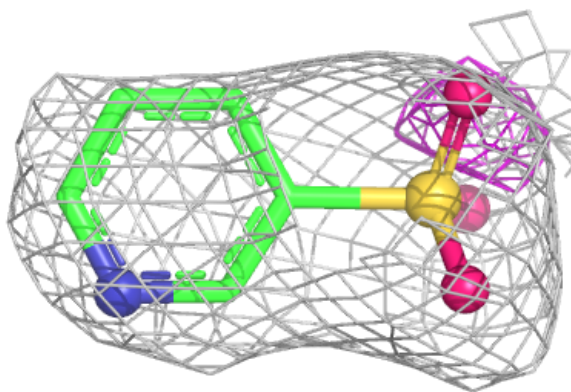


Electron density around VXH B 2405:

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

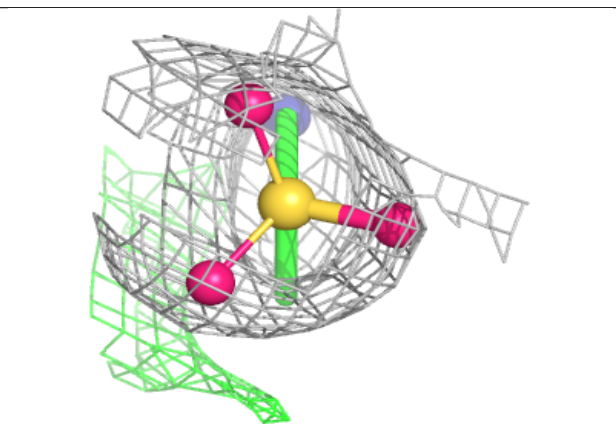
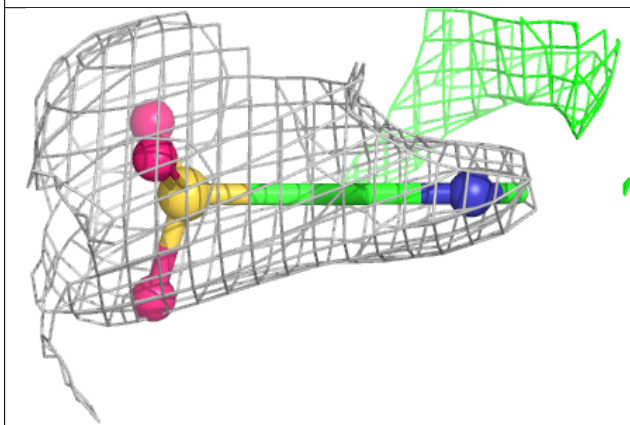
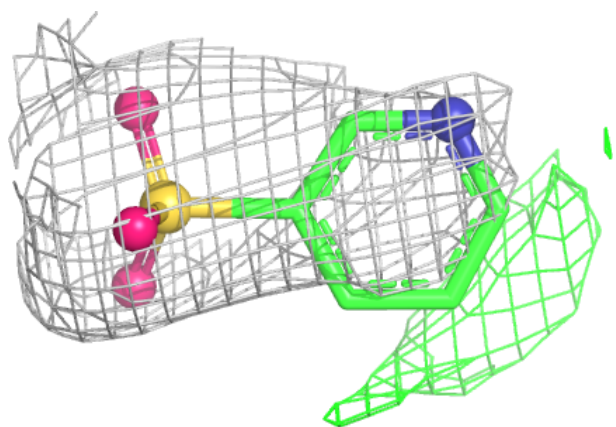
**Electron density around VXH C 505:**

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



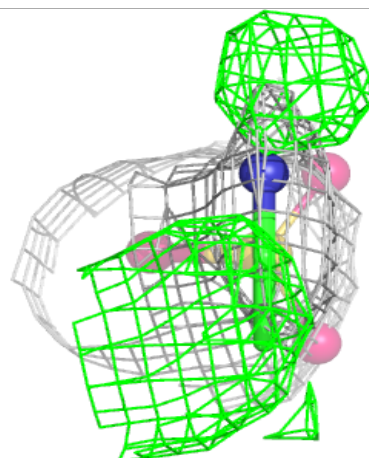
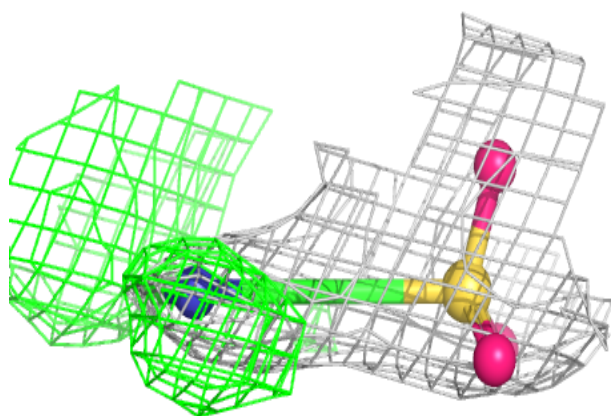
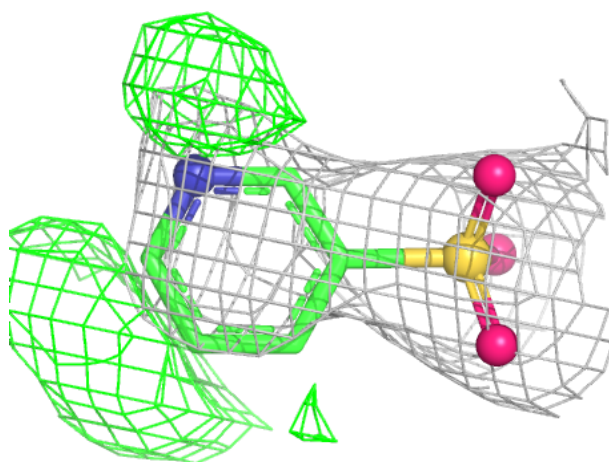
Electron density around VXH D 506 (A):

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



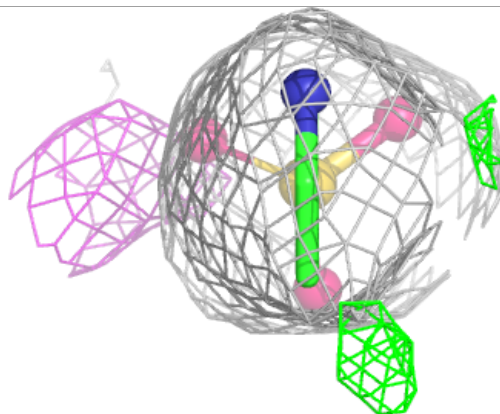
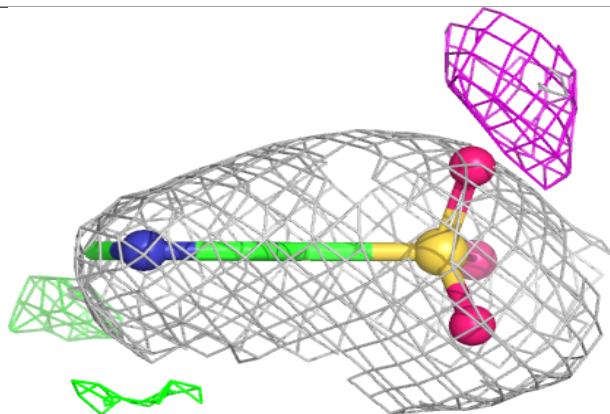
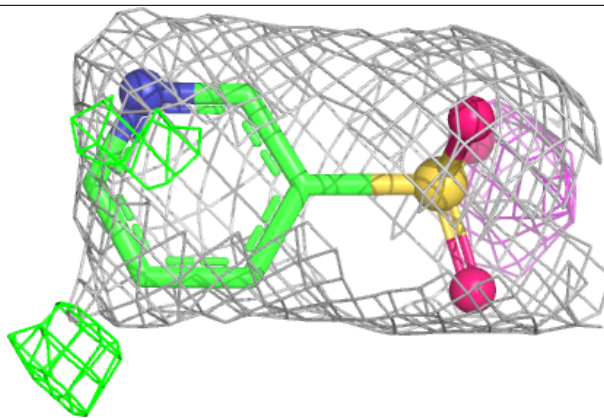
Electron density around VXH D 506 (B):

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



Electron density around VXH 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.