



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:46 PM UTC

PDB ID : 7OFX / pdb_00007ofx
Title : Crystal structure of a GH31 family sulfoquinovosidase mutant D455N from *Agrobacterium tumefaciens* in complex with sulfoquinovosyl glycerol (SQGro)
Authors : Sharma, M.; Davies, G.J.
Deposited on : 2021-05-05
Resolution : 2.15 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

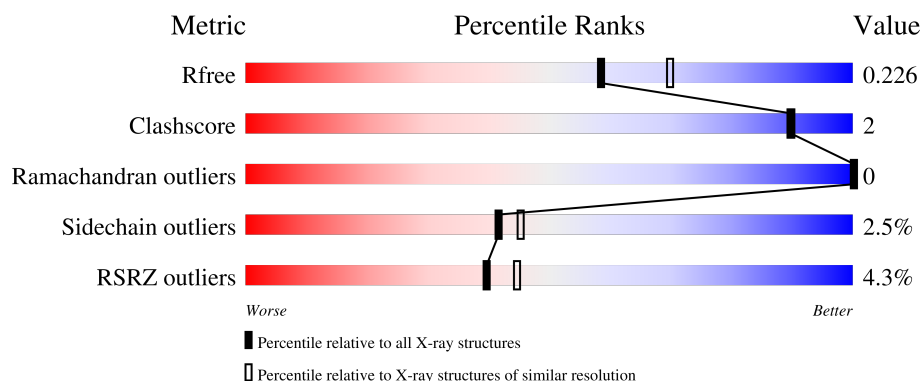
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	672	2% 92% 6% .
1	B	672	3% 93% 6% .
1	C	672	7% 92% 6% ..
1	D	672	6% 92% 6% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20924 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 Alpha-glucosidase yihQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	0	0
			5097	3265	869	942	21			
1	C	661	Total	C	N	O	S	0	0	0
			5071	3249	871	931	20			
1	D	663	Total	C	N	O	S	0	0	0
			5101	3267	881	933	20			
1	B	665	Total	C	N	O	S	0	0	0
			5136	3289	880	946	21			

There are 44 discrepancies between the modelled and reference sequences:

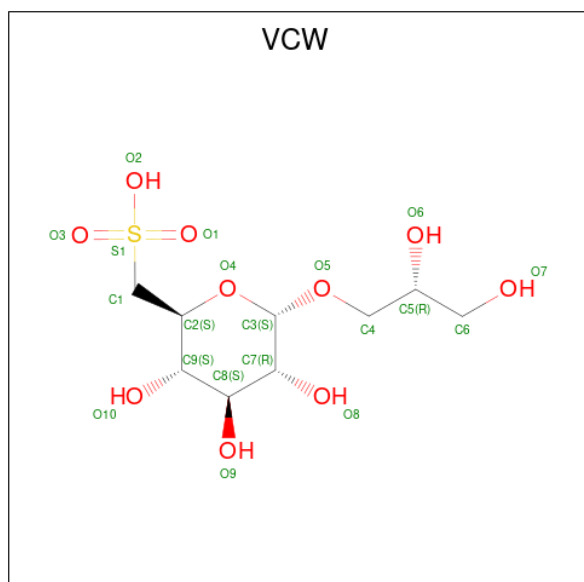
Chain	Residue	Modelled	Actual	Comment	Reference
A	370	ALA	GLU	engineered mutation	UNP A0A083ZKV2
A	371	ALA	GLU	engineered mutation	UNP A0A083ZKV2
A	455	ASN	ASP	engineered mutation	UNP A0A083ZKV2
A	665	LEU	-	expression tag	UNP A0A083ZKV2
A	666	GLU	-	expression tag	UNP A0A083ZKV2
A	667	HIS	-	expression tag	UNP A0A083ZKV2
A	668	HIS	-	expression tag	UNP A0A083ZKV2
A	669	HIS	-	expression tag	UNP A0A083ZKV2
A	670	HIS	-	expression tag	UNP A0A083ZKV2
A	671	HIS	-	expression tag	UNP A0A083ZKV2
A	672	HIS	-	expression tag	UNP A0A083ZKV2
C	370	ALA	GLU	engineered mutation	UNP A0A083ZKV2
C	371	ALA	GLU	engineered mutation	UNP A0A083ZKV2
C	455	ASN	ASP	engineered mutation	UNP A0A083ZKV2
C	665	LEU	-	expression tag	UNP A0A083ZKV2
C	666	GLU	-	expression tag	UNP A0A083ZKV2
C	667	HIS	-	expression tag	UNP A0A083ZKV2
C	668	HIS	-	expression tag	UNP A0A083ZKV2
C	669	HIS	-	expression tag	UNP A0A083ZKV2
C	670	HIS	-	expression tag	UNP A0A083ZKV2
C	671	HIS	-	expression tag	UNP A0A083ZKV2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	672	HIS	-	expression tag	UNP A0A083ZKV2
D	370	ALA	GLU	engineered mutation	UNP A0A083ZKV2
D	371	ALA	GLU	engineered mutation	UNP A0A083ZKV2
D	455	ASN	ASP	engineered mutation	UNP A0A083ZKV2
D	665	LEU	-	expression tag	UNP A0A083ZKV2
D	666	GLU	-	expression tag	UNP A0A083ZKV2
D	667	HIS	-	expression tag	UNP A0A083ZKV2
D	668	HIS	-	expression tag	UNP A0A083ZKV2
D	669	HIS	-	expression tag	UNP A0A083ZKV2
D	670	HIS	-	expression tag	UNP A0A083ZKV2
D	671	HIS	-	expression tag	UNP A0A083ZKV2
D	672	HIS	-	expression tag	UNP A0A083ZKV2
B	370	ALA	GLU	engineered mutation	UNP A0A083ZKV2
B	371	ALA	GLU	engineered mutation	UNP A0A083ZKV2
B	455	ASN	ASP	engineered mutation	UNP A0A083ZKV2
B	665	LEU	-	expression tag	UNP A0A083ZKV2
B	666	GLU	-	expression tag	UNP A0A083ZKV2
B	667	HIS	-	expression tag	UNP A0A083ZKV2
B	668	HIS	-	expression tag	UNP A0A083ZKV2
B	669	HIS	-	expression tag	UNP A0A083ZKV2
B	670	HIS	-	expression tag	UNP A0A083ZKV2
B	671	HIS	-	expression tag	UNP A0A083ZKV2
B	672	HIS	-	expression tag	UNP A0A083ZKV2

- Molecule 2 is [(2S,3S,4S,5R,6S)-6-[(2R)-2,3-bis(oxidanyl)propoxy]-3,4,5-tris(oxidanyl)oxan-2-yl]methanesulfonic acid (CCD ID: VCW) (formula: C₉H₁₈O₁₀S) (labeled as "Ligand of Interest" by depositor).

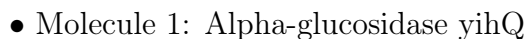


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O S 20 9 10 1	0	0
2	C	1	Total C O S 20 9 10 1	0	0
2	D	1	Total C O S 20 9 10 1	0	0
2	B	1	Total C O S 20 9 10 1	0	0

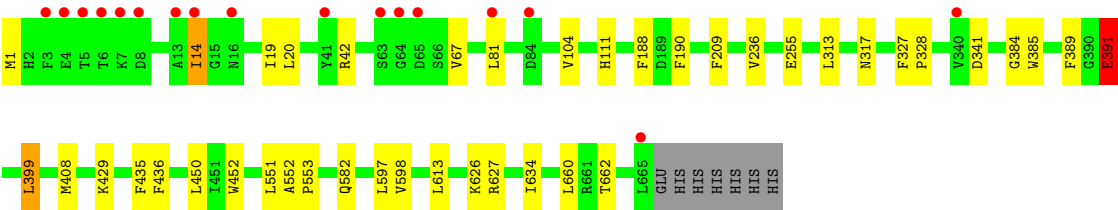
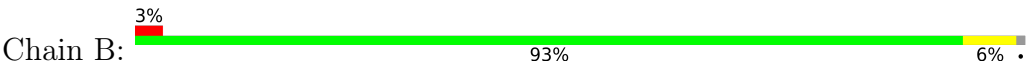
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	125	Total O 125 125	0	0
3	C	90	Total O 90 90	0	0
3	D	100	Total O 100 100	0	0
3	B	124	Total O 124 124	0	0

- Molecule 1: Alpha-glucosidase yihQ



● Molecule 1: Alpha-glucosidase yihQ



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.53Å 168.40Å 100.69Å 90.00° 116.53° 90.00°	Depositor
Resolution (Å)	61.01 – 2.15 61.01 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.4 (61.01-2.15) 97.4 (61.01-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.194 , 0.224 0.199 , 0.226	Depositor DCC
R_{free} test set	7734 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20924	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: VCW

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	1.07	1/5244 (0.0%)	1.26	5/7147 (0.1%)
1	B	1.08	1/5283 (0.0%)	1.28	5/7194 (0.1%)
1	C	1.05	1/5219 (0.0%)	1.28	7/7115 (0.1%)
1	D	1.08	2/5249 (0.0%)	1.26	3/7153 (0.0%)
All	All	1.07	5/20995 (0.0%)	1.27	20/28609 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	484	HIS	CE1-NE2	6.40	1.39	1.32
1	D	654	HIS	CE1-NE2	5.57	1.38	1.32
1	A	465	GLY	C-O	5.32	1.29	1.24
1	C	520	HIS	CE1-NE2	5.11	1.37	1.32
1	B	111	HIS	CE1-NE2	5.06	1.37	1.32

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	CYS	CB-CA-C	7.01	121.50	109.51
1	B	391	GLU	CB-CG-CD	6.73	124.05	112.60
1	C	321	CYS	CA-CB-SG	-5.72	101.24	114.40
1	C	317	ASN	CB-CA-C	5.68	118.15	110.37
1	B	627	ARG	CB-CA-C	5.59	119.06	109.51
1	C	531	ILE	CA-C-O	-5.55	114.64	120.57
1	D	317	ASN	CB-CA-C	5.44	117.82	110.37
1	D	391	GLU	CB-CG-CD	5.41	121.80	112.60
1	A	660	LEU	CA-C-O	-5.39	115.91	122.64
1	D	432	GLU	CB-CG-CD	5.38	121.75	112.60
1	C	399	LEU	CA-C-N	5.24	127.56	120.38
1	C	399	LEU	C-N-CA	5.24	127.56	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	317	ASN	CB-CA-C	5.23	117.53	110.37
1	B	399	LEU	CA-C-N	5.17	127.47	120.38
1	B	399	LEU	C-N-CA	5.17	127.47	120.38
1	C	391	GLU	CB-CG-CD	5.15	121.35	112.60
1	A	317	ASN	CB-CA-C	5.07	117.31	110.37
1	A	399	LEU	CA-C-N	5.05	127.30	120.38
1	A	399	LEU	C-N-CA	5.05	127.30	120.38
1	A	391	GLU	CB-CG-CD	5.05	121.19	112.60

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	5097	0	4765	18	0
1	B	5136	0	4825	19	0
1	C	5071	0	4716	19	0
1	D	5101	0	4765	15	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
2	C	20	0	0	0	0
2	D	20	0	0	0	0
3	A	125	0	0	0	0
3	B	124	0	0	3	0
3	C	90	0	0	0	0
3	D	100	0	0	0	0
All	All	20924	0	19071	71	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 (71) 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:B:1:MET:HE1	1:B:209:PHE:CD1	2.27	0.68
1:C:286:TRP:HB2	1:C:321:CYS:SG	2.40	0.62
1:D:399:LEU:HD13	1:D:408:MET:HG3	1.81	0.62
1:C:592:TYR:HD2	1:C:596:MET:HE3	1.66	0.60
1:C:613:LEU:HD22	1:C:634:ILE:HD13	1.85	0.58
1:C:399:LEU:HD13	1:C:408:MET:HG3	1.87	0.57
1:B:399:LEU:HD13	1:B:408:MET:HG3	1.87	0.57
1:A:592:TYR:HD2	1:A:596:MET:HE3	1.70	0.56
1:C:632:ARG:HG3	1:C:634:ILE:HD11	1.88	0.56
1:A:399:LEU:HD13	1:A:408:MET:HG3	1.88	0.55
1:B:327:PHE:HB3	1:B:328:PRO:HD3	1.89	0.54
1:A:327:PHE:HB3	1:A:328:PRO:HD3	1.90	0.54
1:A:613:LEU:HD22	1:A:634:ILE:HD13	1.89	0.53
1:B:67:VAL:HG13	1:B:81:LEU:HB2	1.90	0.53
1:D:291:ASN:OD1	1:D:293:THR:HB	2.08	0.52
1:A:592:TYR:CD2	1:A:596:MET:HE3	2.44	0.52
1:C:592:TYR:CD2	1:C:596:MET:HE3	2.44	0.52
1:A:68:THR:CG2	1:A:77:PRO:HB3	2.40	0.52
1:D:327:PHE:HB3	1:D:328:PRO:HD3	1.93	0.50
1:D:651:SER:O	1:D:654:HIS:HD2	1.94	0.48
1:A:17:ARG:HD3	1:A:174:ARG:O	2.13	0.48
1:C:327:PHE:HB3	1:C:328:PRO:HD3	1.94	0.48
1:D:19:ILE:HG22	1:D:20:LEU:HD13	1.96	0.47
1:B:551:LEU:HD21	1:B:660:LEU:HD11	1.96	0.47
1:B:1:MET:HE1	1:B:209:PHE:CG	2.50	0.47
1:C:389:PHE:HA	1:C:391:GLU:OE2	2.15	0.47
1:A:554:TYR:CD2	1:A:596:MET:HE2	2.49	0.46
1:B:42:ARG:HE	1:B:42:ARG:HB3	1.50	0.46
1:C:188:PHE:HB3	1:C:190:PHE:CE2	2.51	0.46
1:D:17:ARG:HD3	1:D:174:ARG:O	2.16	0.46
1:B:597:LEU:HD23	1:B:598:VAL:N	2.32	0.45
1:C:479:MET:HA	1:C:479:MET:HE2	1.98	0.45
1:D:237:TYR:CD2	1:D:556:LYS:HD2	2.52	0.45
1:A:1:MET:HE2	1:A:12:ILE:HG22	1.97	0.45
1:A:389:PHE:HA	1:A:391:GLU:OE2	2.16	0.45
1:B:255:GLU:HG2	3:B:904:HOH:O	2.17	0.44
1:A:68:THR:HG23	1:A:77:PRO:HB3	2.00	0.44
1:C:92:ALA:HB2	1:C:203:VAL:HG21	1.99	0.44
1:A:479:MET:HA	1:A:479:MET:HE2	2.00	0.43
1:B:188:PHE:HB3	1:B:190:PHE:CE2	2.53	0.43
1:D:479:MET:HA	1:D:479:MET:HE2	1.99	0.43
1:A:597:LEU:HD23	1:A:598:VAL:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLU:CB	3:B:914:HOH:O	2.66	0.43
1:D:634:ILE:HD11	1:D:646:PHE:CZ	2.53	0.43
1:B:436:PHE:HA	1:B:450:LEU:O	2.18	0.43
1:C:554:TYR:CD2	1:C:596:MET:HE2	2.54	0.43
1:D:389:PHE:HA	1:D:391:GLU:OE2	2.19	0.43
1:C:436:PHE:HA	1:C:450:LEU:O	2.19	0.43
1:D:582:GLN:H	1:D:582:GLN:CD	2.26	0.42
1:B:385:TRP:O	1:B:435:PHE:HA	2.20	0.42
1:B:551:LEU:CD2	1:B:660:LEU:HD11	2.49	0.42
1:A:436:PHE:HA	1:A:450:LEU:O	2.19	0.42
1:B:429:LYS:HD3	3:B:922:HOH:O	2.18	0.42
1:B:552:ALA:HB3	1:B:553:PRO:HD3	2.01	0.42
1:A:385:TRP:O	1:A:435:PHE:HA	2.20	0.42
1:C:385:TRP:O	1:C:435:PHE:HA	2.19	0.42
1:C:551:LEU:CD2	1:C:660:LEU:HD21	2.50	0.42
1:C:597:LEU:HD23	1:C:598:VAL:N	2.35	0.41
1:C:633:ASP:C	1:C:634:ILE:HD12	2.45	0.41
1:B:313:LEU:HA	1:B:384:GLY:O	2.19	0.41
1:C:337:ALA:HB1	1:C:397:ILE:HD12	2.03	0.41
1:A:188:PHE:HB3	1:A:190:PHE:CE2	2.56	0.41
1:B:1:MET:HE2	1:B:14:ILE:HG12	2.03	0.41
1:B:19:ILE:HG22	1:B:20:LEU:HD13	2.03	0.41
1:A:313:LEU:HA	1:A:384:GLY:O	2.21	0.40
1:D:385:TRP:O	1:D:435:PHE:HA	2.21	0.40
1:D:188:PHE:HB3	1:D:190:PHE:CE2	2.55	0.40
1:D:552:ALA:HB3	1:D:553:PRO:HD3	2.03	0.40
1:D:436:PHE:HA	1:D:450:LEU:O	2.22	0.40
1:B:389:PHE:HA	1:B:391:GLU:OE2	2.22	0.40
1:C:313:LEU:HA	1:C:384:GLY:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	659/672 (98%)	636 (96%)	23 (4%)	0	100	100
1	B	663/672 (99%)	642 (97%)	21 (3%)	0	100	100
1	C	659/672 (98%)	638 (97%)	21 (3%)	0	100	100
1	D	661/672 (98%)	638 (96%)	23 (4%)	0	100	100
All	All	2642/2688 (98%)	2554 (97%)	88 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	502/545 (92%)	491 (98%)	11 (2%)	45	51
1	B	506/545 (93%)	495 (98%)	11 (2%)	45	51
1	C	493/545 (90%)	479 (97%)	14 (3%)	38	40
1	D	497/545 (91%)	483 (97%)	14 (3%)	38	40
All	All	1998/2180 (92%)	1948 (98%)	50 (2%)	42	45

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	14	ILE
1	A	20	LEU
1	A	75	GLN
1	A	83	LEU
1	A	104	VAL
1	A	128	ARG
1	A	236	VAL
1	A	391	GLU
1	A	452	TRP
1	A	613	LEU
1	C	75	GLN
1	C	83	LEU

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Mol	Chain	Res	Type
1	C	104	VAL
1	C	128	ARG
1	C	299	ARG
1	C	307	ASP
1	C	341	ASP
1	C	391	GLU
1	C	452	TRP
1	C	556	LYS
1	C	582	GLN
1	C	613	LEU
1	C	634	ILE
1	C	660	LEU
1	D	14	ILE
1	D	25	ASP
1	D	104	VAL
1	D	128	ARG
1	D	175	LYS
1	D	236	VAL
1	D	301	LYS
1	D	391	GLU
1	D	400	SER
1	D	452	TRP
1	D	556	LYS
1	D	582	GLN
1	D	613	LEU
1	D	662	THR
1	B	14	ILE
1	B	104	VAL
1	B	236	VAL
1	B	341	ASP
1	B	391	GLU
1	B	452	TRP
1	B	582	GLN
1	B	613	LEU
1	B	626	LYS
1	B	634	ILE
1	B	662	THR

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	22	HIS

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Mol	Chain	Res	Type
1	A	456	GLN
1	A	653	HIS
1	C	22	HIS
1	C	75	GLN
1	C	277	GLN
1	C	653	HIS
1	D	22	HIS
1	D	456	GLN
1	D	654	HIS
1	B	2	HIS
1	B	22	HIS
1	B	225	HIS
1	B	456	GLN
1	B	653	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](#)

4 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
2	VCW	A	701	-	18,20,20	0.56	0	26,29,29	1.20	1 (3%)
2	VCW	B	701	-	18,20,20	0.83	1 (5%)	26,29,29	1.33	4 (15%)
2	VCW	D	701	-	18,20,20	0.85	1 (5%)	26,29,29	0.98	2 (7%)
2	VCW	C	701	-	18,20,20	0.97	1 (5%)	26,29,29	1.07	1 (3%)

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
2	VCW	A	701	-	-	0/12/32/32	0/1/1/1
2	VCW	B	701	-	-	0/12/32/32	0/1/1/1
2	VCW	D	701	-	-	1/12/32/32	0/1/1/1
2	VCW	C	701	-	-	1/12/32/32	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	VCW	O3-S1	3.35	1.54	1.45
2	D	701	VCW	O3-S1	2.89	1.53	1.45
2	B	701	VCW	O3-S1	2.64	1.52	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	VCW	O3-S1-C1	-3.44	101.62	106.76
2	A	701	VCW	O3-S1-C1	-3.43	101.63	106.76
2	C	701	VCW	O2-S1-O1	3.03	118.98	111.40
2	B	701	VCW	O2-S1-O1	2.80	118.40	111.40
2	D	701	VCW	O3-S1-C1	-2.62	102.85	106.76
2	B	701	VCW	O2-S1-O3	-2.51	105.11	111.40
2	B	701	VCW	C3-O4-C2	2.03	117.69	113.72
2	D	701	VCW	O2-S1-O1	2.00	116.40	111.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	701	VCW	O4-C3-O5-C4

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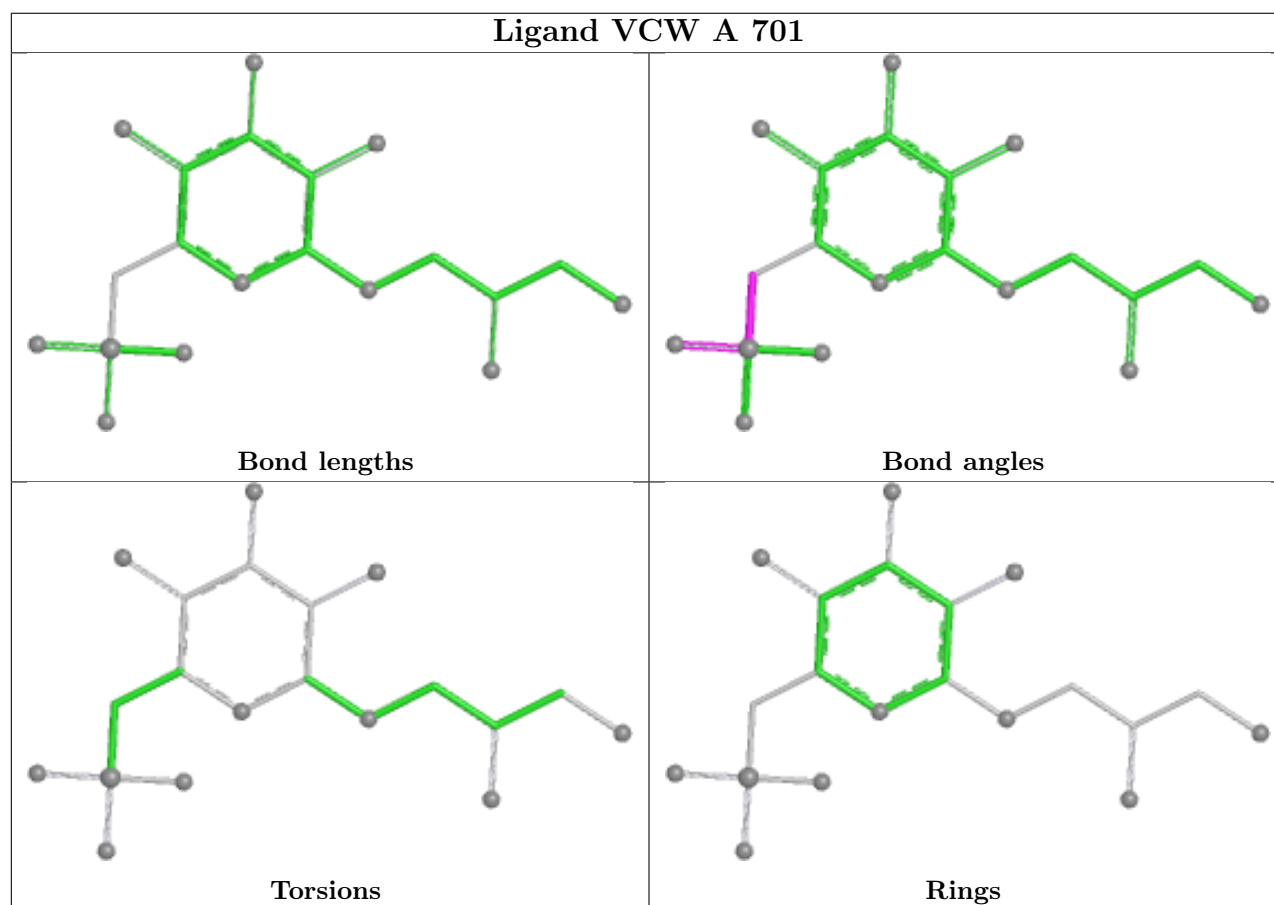
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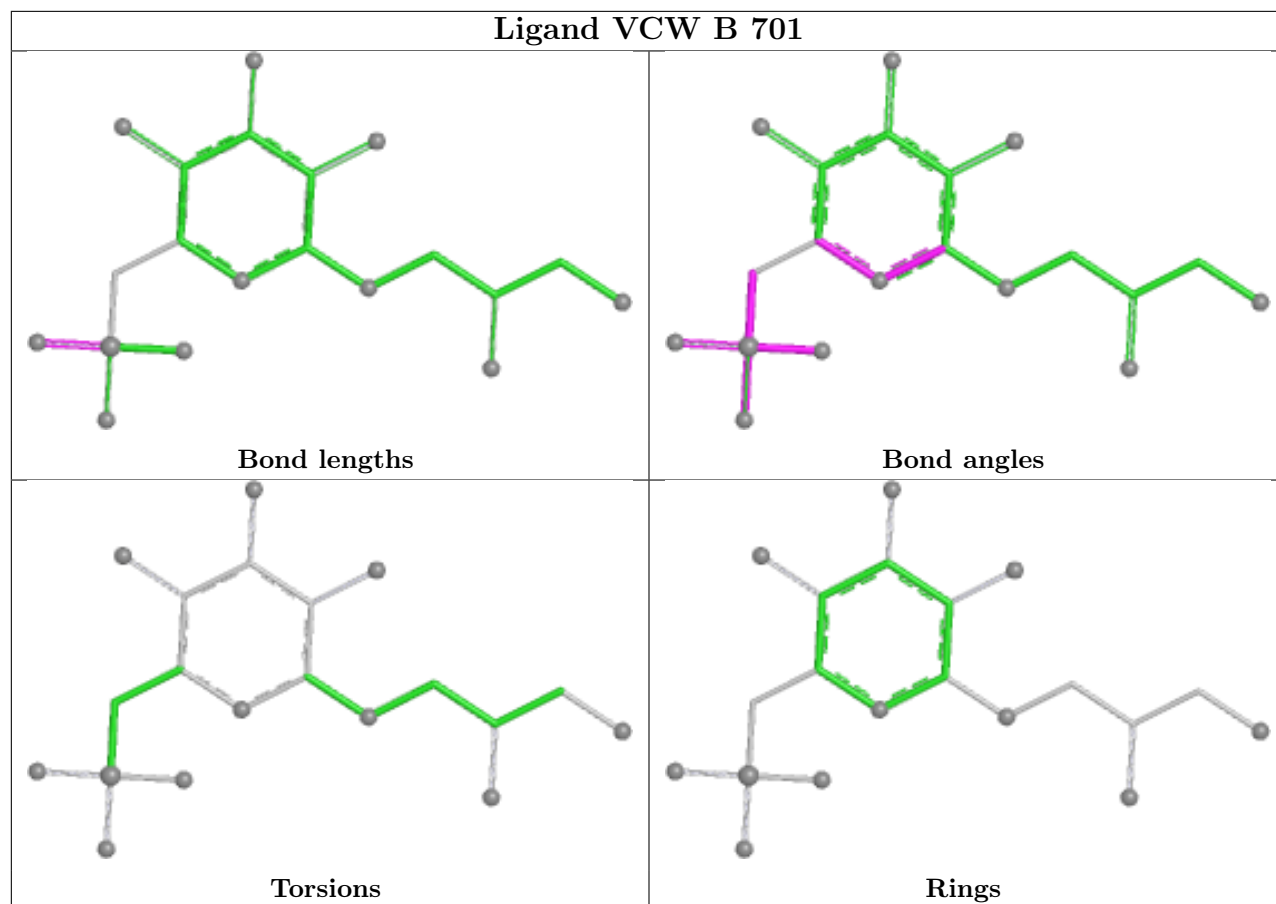
Mol	Chain	Res	Type	Atoms
2	C	701	VCW	C5-C4-O5-C3

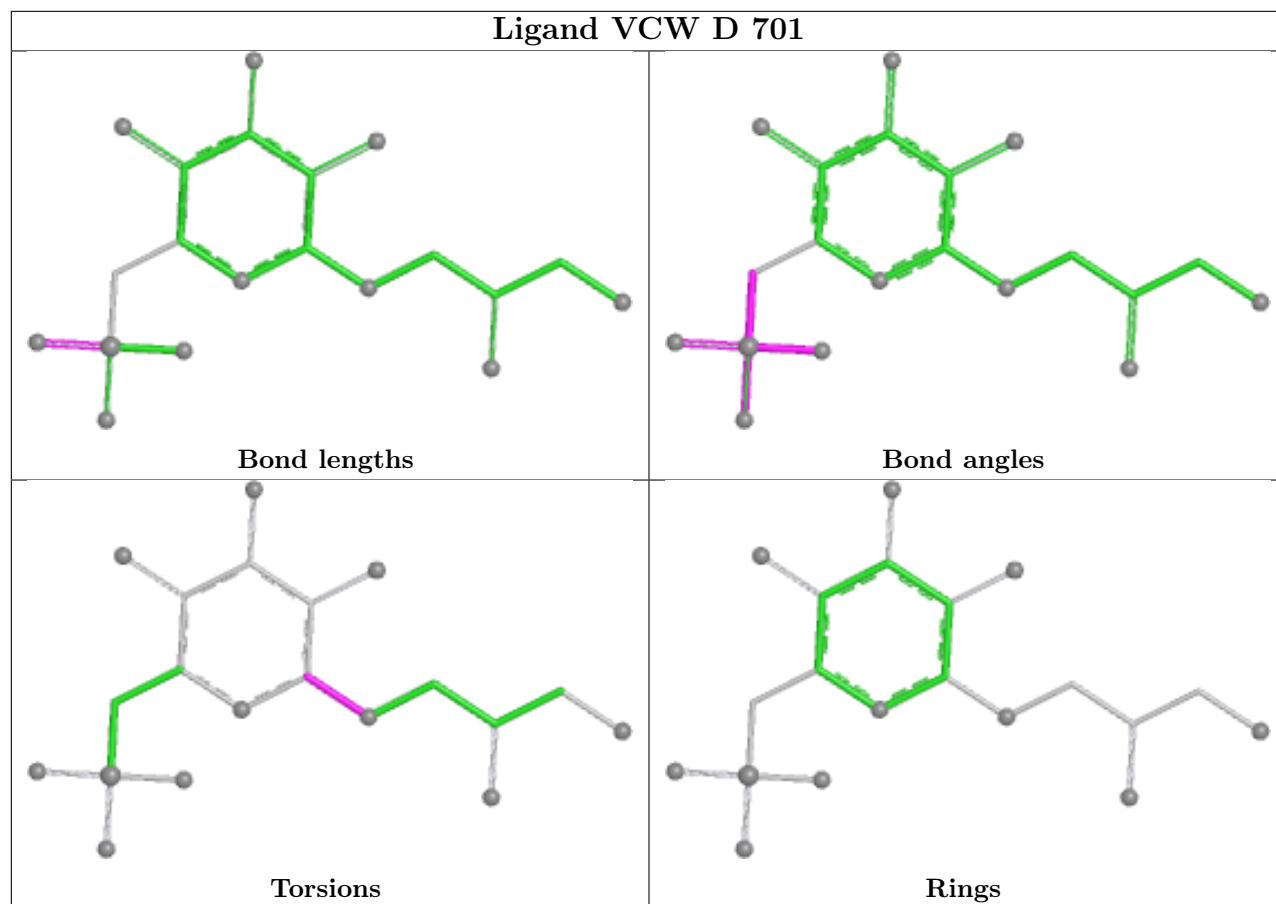
There are no ring outliers.

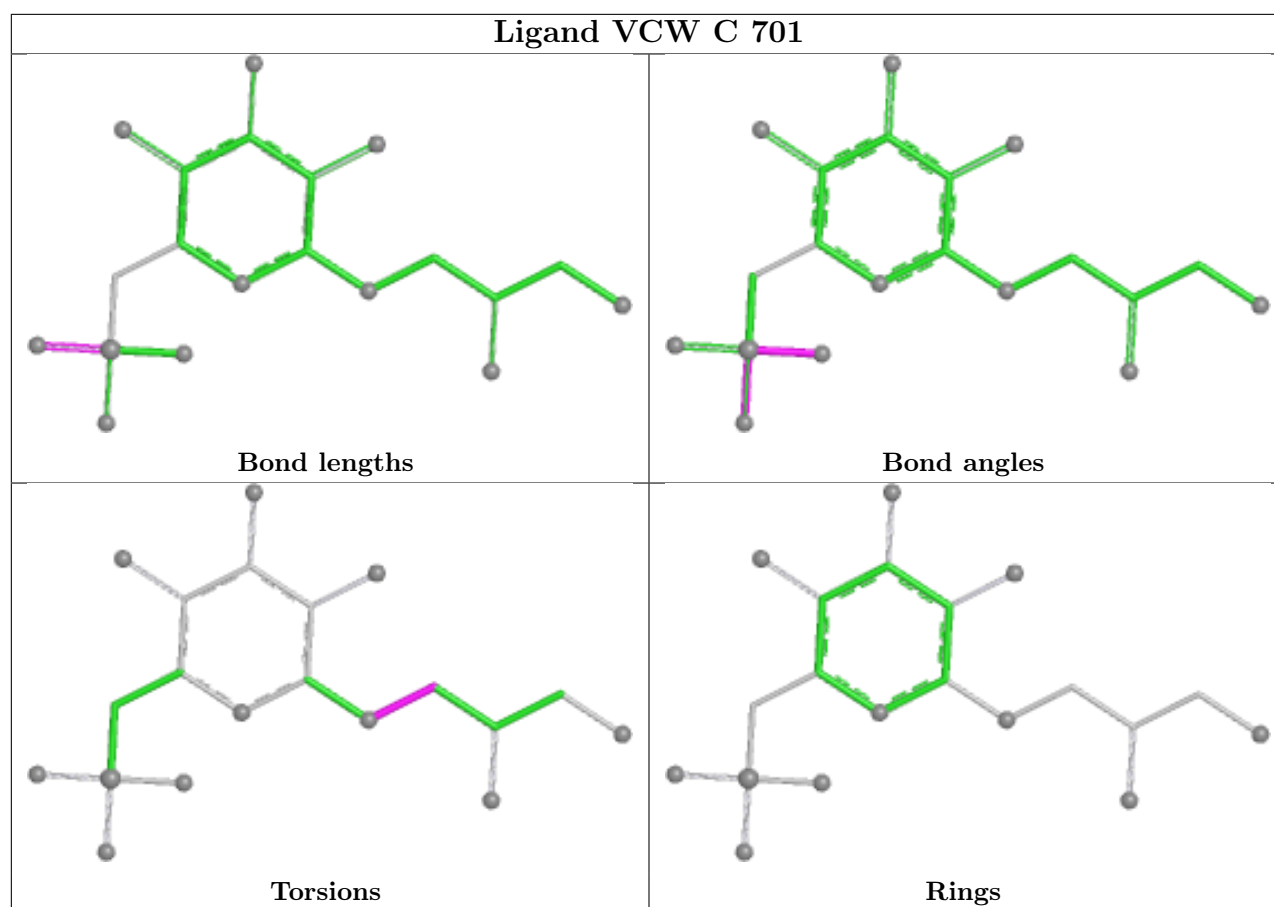
No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	661/672 (98%)	0.01	12 (1%) 67 71	15, 28, 47, 71	0
1	B	665/672 (98%)	-0.06	17 (2%) 57 61	16, 25, 48, 88	0
1	C	661/672 (98%)	0.39	45 (6%) 23 26	19, 33, 63, 101	1 (0%)
1	D	663/672 (98%)	0.21	41 (6%) 26 30	17, 28, 59, 101	0
All	All	2650/2688 (98%)	0.14	115 (4%) 40 45	15, 29, 55, 101	1 (0%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	660	LEU	6.2
1	D	65	ASP	5.6
1	D	62	VAL	5.6
1	D	340	VAL	5.4
1	B	8	ASP	5.1
1	D	6	THR	5.0
1	C	3	PHE	5.0
1	D	75	GLN	4.9
1	D	5	THR	4.9
1	D	7	LYS	4.6
1	D	83	LEU	4.6
1	D	63	SER	4.6
1	D	8	ASP	4.4
1	C	321	CYS	4.4
1	C	8	ASP	4.3
1	C	83	LEU	4.3
1	D	1	MET	4.3
1	D	86	ASN	4.2
1	B	665	LEU	4.2
1	C	2	HIS	4.1
1	C	62	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	340	VAL	4.0
1	D	9	GLY	3.9
1	D	76	ALA	3.9
1	C	63	SER	3.9
1	A	16	ASN	3.9
1	C	72	ALA	3.9
1	C	7	LYS	3.9
1	B	6	THR	3.9
1	C	6	THR	3.8
1	D	66	SER	3.8
1	A	14	ILE	3.8
1	D	64	GLY	3.7
1	D	3	PHE	3.7
1	C	616	HIS	3.6
1	D	663	ILE	3.6
1	D	16	ASN	3.6
1	C	65	ASP	3.5
1	C	9	GLY	3.4
1	C	18	ILE	3.3
1	C	14	ILE	3.3
1	D	82	THR	3.2
1	B	41	TYR	3.2
1	D	60	ALA	3.2
1	C	88	ILE	3.2
1	D	14	ILE	3.1
1	A	340	VAL	3.1
1	B	65	ASP	3.1
1	B	3	PHE	3.1
1	C	66	SER	3.1
1	C	662	THR	3.1
1	B	64	GLY	2.9
1	C	64	GLY	2.9
1	B	16	ASN	2.8
1	A	661	ARG	2.8
1	C	5	THR	2.8
1	C	13	ALA	2.8
1	B	4	GLU	2.7
1	C	86	ASN	2.7
1	B	14	ILE	2.7
1	D	59	HIS	2.7
1	C	70	SER	2.7
1	C	11	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	5	THR	2.6
1	C	631	GLY	2.6
1	C	16	ASN	2.6
1	C	87	ALA	2.6
1	C	15	GLY	2.6
1	D	10	PHE	2.6
1	B	340	VAL	2.6
1	D	15	GLY	2.6
1	C	76	ALA	2.6
1	D	81	LEU	2.5
1	D	18	ILE	2.5
1	D	634	ILE	2.5
1	C	77	PRO	2.5
1	A	83	LEU	2.5
1	C	69	LEU	2.5
1	D	61	GLU	2.4
1	D	85	GLY	2.4
1	C	634	ILE	2.4
1	C	579	ASN	2.4
1	C	84	ASP	2.4
1	A	3	PHE	2.4
1	D	25	ASP	2.3
1	C	629	ALA	2.3
1	D	2	HIS	2.3
1	D	329	VAL	2.3
1	A	15	GLY	2.3
1	D	84	ASP	2.3
1	B	84	ASP	2.3
1	C	20	LEU	2.3
1	C	4	GLU	2.2
1	C	632	ARG	2.2
1	C	12	ILE	2.2
1	C	108	THR	2.2
1	A	1	MET	2.2
1	D	95	GLU	2.2
1	D	67	VAL	2.2
1	C	95	GLU	2.2
1	B	13	ALA	2.2
1	D	91	THR	2.2
1	D	33	PHE	2.1
1	C	329	VAL	2.1
1	A	616	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	205	GLU	2.1
1	C	24	PRO	2.1
1	A	224	LEU	2.1
1	B	81	LEU	2.1
1	A	397	ILE	2.1
1	B	7	LYS	2.1
1	B	63	SER	2.1
1	D	582	GLN	2.0
1	D	4	GLU	2.0
1	C	79	LEU	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](#)

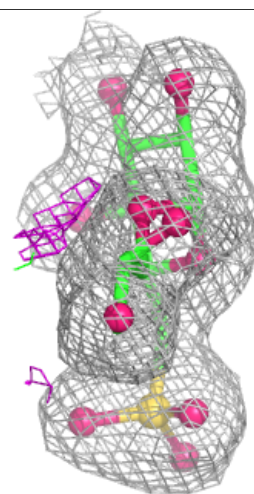
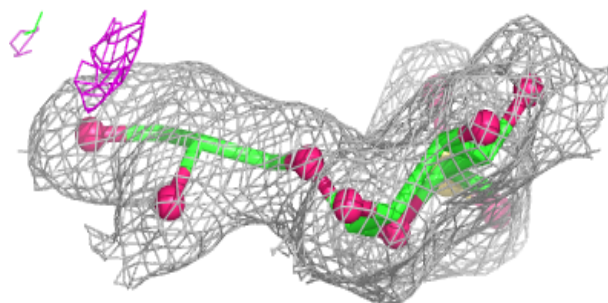
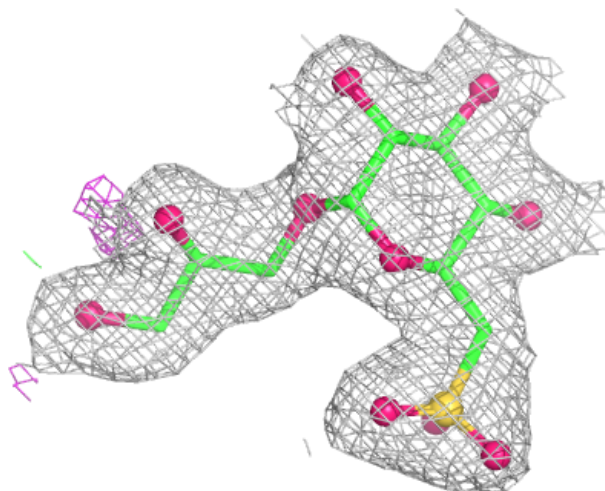
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	VCW	A	701	20/20	0.98	0.04	18,21,24,27	0
2	VCW	C	701	20/20	0.98	0.05	20,24,27,31	0
2	VCW	D	701	20/20	0.98	0.05	16,22,27,27	0
2	VCW	B	701	20/20	0.98	0.05	17,19,24,24	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.

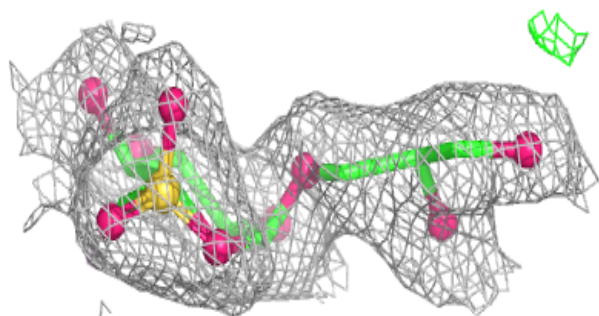
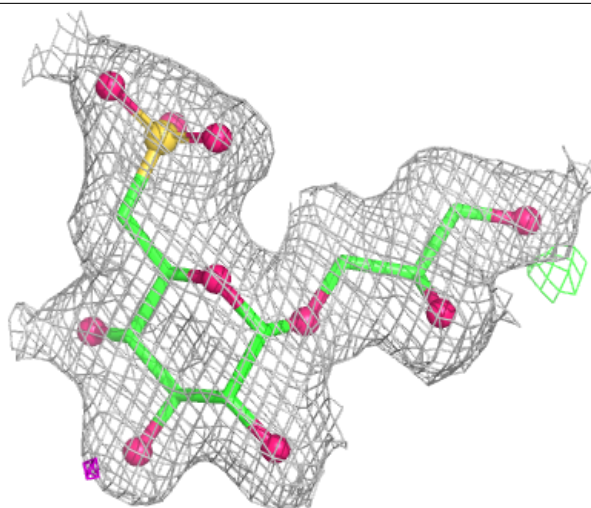
Electron density around VCW A 701:

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



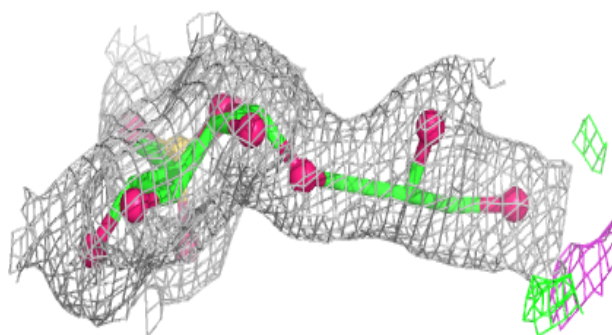
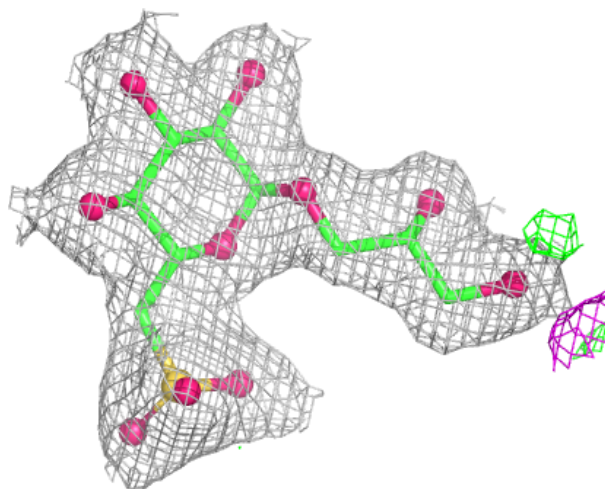
Electron density around VCW C 701:

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



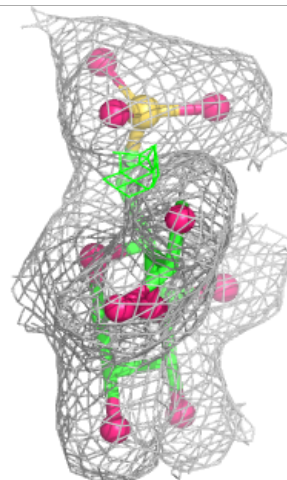
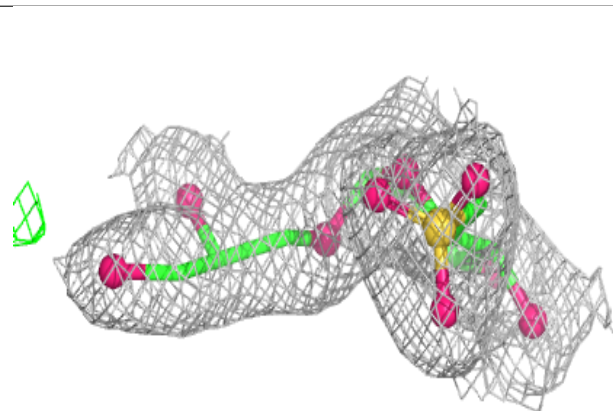
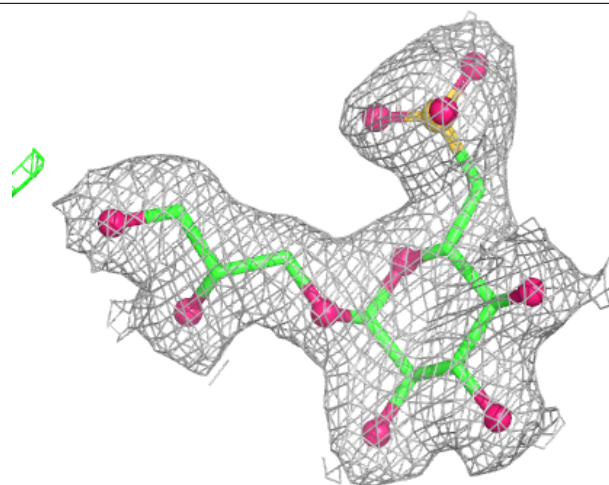
Electron density around VCW D 701:

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



Electron density around VCW B 701:

$2mF_o-DF_c$ (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.