



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:52 pm BST

PDB ID : 5KEW
Title : *Vibrio parahaemolyticus* VtrA/VtrC complex bound to the bile salt tau-rodeoxycholate
Authors : Tomchick, D.R.; Orth, K.; Rivera-Cancel, G.
Deposited on : 2016-06-10
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

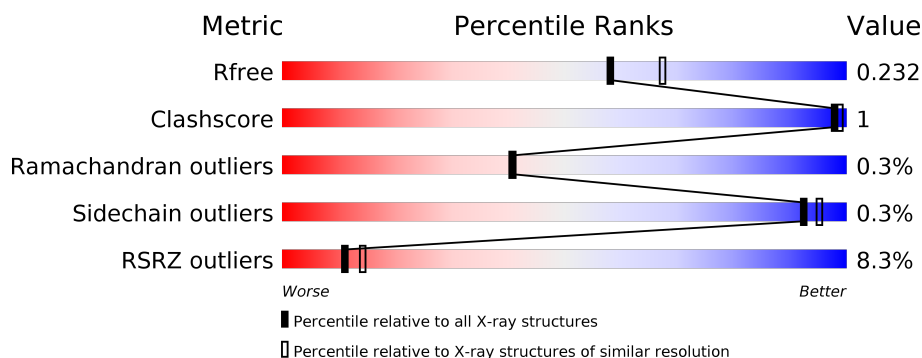
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	94	<div> <div>4%</div> <div>95% 5%</div> </div>
1	C	94	<div> <div>6%</div> <div>90% . . .</div> </div>
1	E	94	<div> <div>12%</div> <div>90% . 6%</div> </div>
2	B	144	<div> <div>%</div> <div>88% . 8%</div> </div>
2	D	144	<div> <div>13%</div> <div>84% . 13%</div> </div>
2	F	144	<div> <div>10%</div> <div>85% . 12%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11236 atoms, of which 5459 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 VtrA Protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	89	Total	C	H	N	O	S	0	0	0
			1474	477	737	115	144	1			
1	C	90	Total	C	H	N	O	S	0	0	0
			1486	481	741	116	147	1			
1	E	88	Total	C	H	N	O	S	0	0	0
			1462	473	733	114	141	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q87GI4
C	0	MET	-	initiating methionine	UNP Q87GI4
E	0	MET	-	initiating methionine	UNP Q87GI4

- Molecule 2 is a protein called VtrC Protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	132	Total	C	H	N	O	S	0	0	0
			2147	705	1049	179	212	2			
2	D	125	Total	C	H	N	O	S	0	0	0
			2040	672	996	171	199	2			
2	F	127	Total	C	H	N	O	S	0	0	0
			2073	683	1015	172	201	2			

There are 39 discrepancies between the modelled and reference sequences:

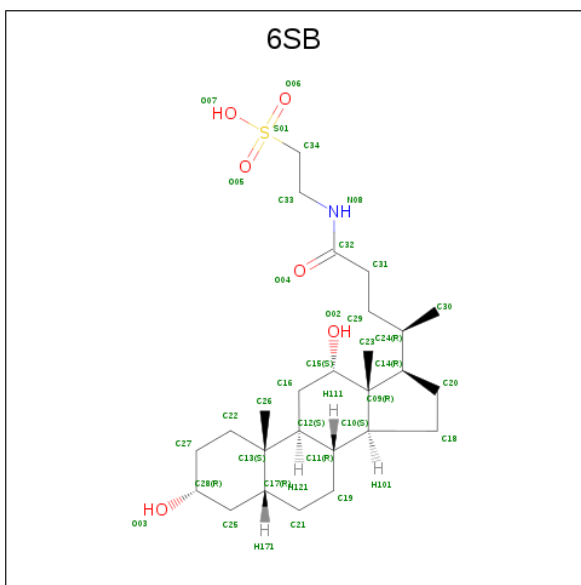
Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	MET	-	initiating methionine	UNP Q87GI3
B	-11	GLY	-	expression tag	UNP Q87GI3
B	-10	SER	-	expression tag	UNP Q87GI3
B	-9	SER	-	expression tag	UNP Q87GI3
B	-8	HIS	-	expression tag	UNP Q87GI3

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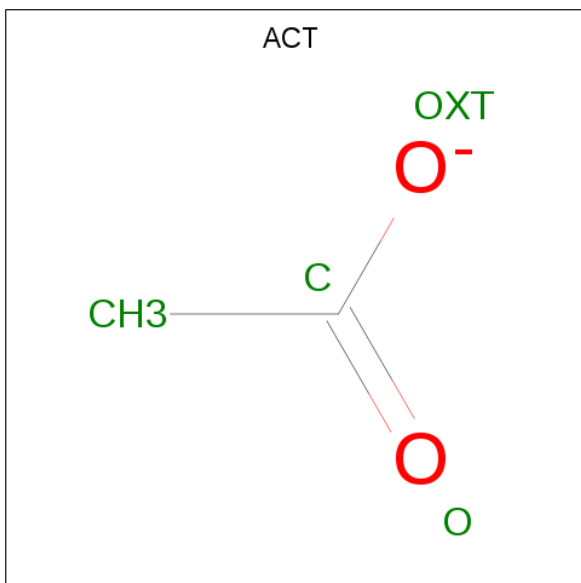
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP Q87GI3
B	-6	HIS	-	expression tag	UNP Q87GI3
B	-5	HIS	-	expression tag	UNP Q87GI3
B	-4	HIS	-	expression tag	UNP Q87GI3
B	-3	HIS	-	expression tag	UNP Q87GI3
B	-2	SER	-	expression tag	UNP Q87GI3
B	-1	GLN	-	expression tag	UNP Q87GI3
B	0	ASP	-	expression tag	UNP Q87GI3
D	-12	MET	-	initiating methionine	UNP Q87GI3
D	-11	GLY	-	expression tag	UNP Q87GI3
D	-10	SER	-	expression tag	UNP Q87GI3
D	-9	SER	-	expression tag	UNP Q87GI3
D	-8	HIS	-	expression tag	UNP Q87GI3
D	-7	HIS	-	expression tag	UNP Q87GI3
D	-6	HIS	-	expression tag	UNP Q87GI3
D	-5	HIS	-	expression tag	UNP Q87GI3
D	-4	HIS	-	expression tag	UNP Q87GI3
D	-3	HIS	-	expression tag	UNP Q87GI3
D	-2	SER	-	expression tag	UNP Q87GI3
D	-1	GLN	-	expression tag	UNP Q87GI3
D	0	ASP	-	expression tag	UNP Q87GI3
F	-12	MET	-	initiating methionine	UNP Q87GI3
F	-11	GLY	-	expression tag	UNP Q87GI3
F	-10	SER	-	expression tag	UNP Q87GI3
F	-9	SER	-	expression tag	UNP Q87GI3
F	-8	HIS	-	expression tag	UNP Q87GI3
F	-7	HIS	-	expression tag	UNP Q87GI3
F	-6	HIS	-	expression tag	UNP Q87GI3
F	-5	HIS	-	expression tag	UNP Q87GI3
F	-4	HIS	-	expression tag	UNP Q87GI3
F	-3	HIS	-	expression tag	UNP Q87GI3
F	-2	SER	-	expression tag	UNP Q87GI3
F	-1	GLN	-	expression tag	UNP Q87GI3
F	0	ASP	-	expression tag	UNP Q87GI3

- Molecule 3 is Taurodeoxycholate (three-letter code: 6SB) (formula: C₂₆H₄₅NO₆S).



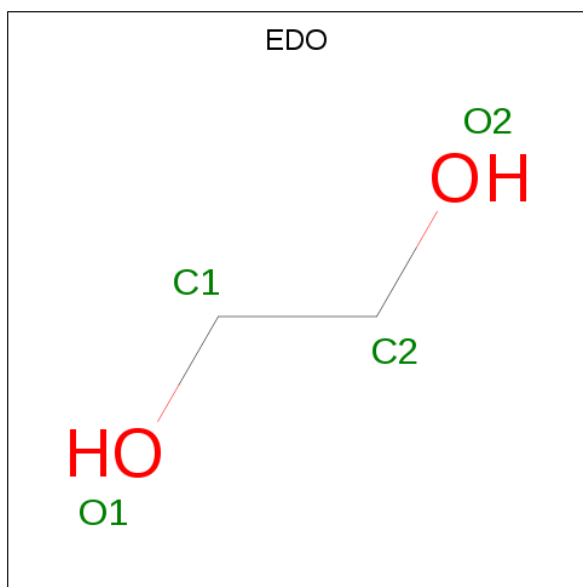
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 78	C 26	H 44	N 1	O 6	S 1	0	0
3	B	1	Total 78	C 26	H 44	N 1	O 6	S 1	0	0
3	D	1	Total 78	C 26	H 44	N 1	O 6	S 1	0	0
3	F	1	Total 78	C 26	H 44	N 1	O 6	S 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



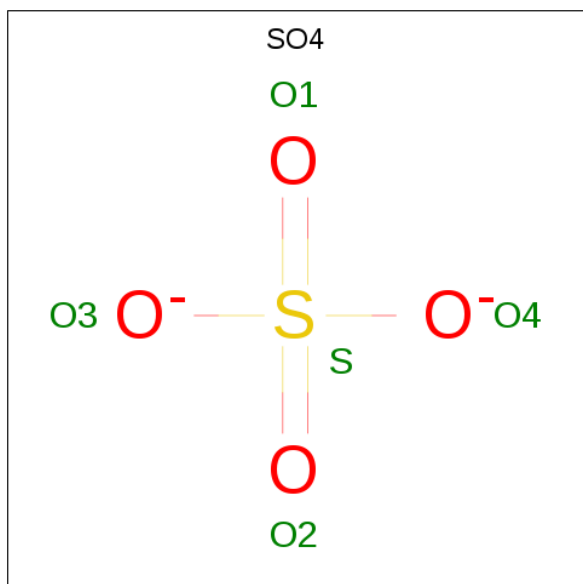
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	B	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

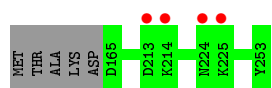
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	37	Total O 37 37	0	0
7	B	39	Total O 39 39	0	0
7	C	23	Total O 23 23	0	0
7	D	37	Total O 37 37	0	0
7	E	21	Total O 21 21	0	0
7	F	36	Total O 36 36	0	0

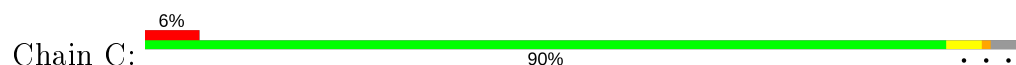
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

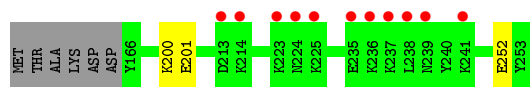
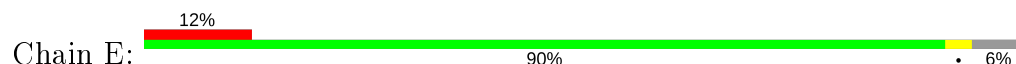
• Molecule 1: VtrA Protein



• Molecule 1: VtrA Protein



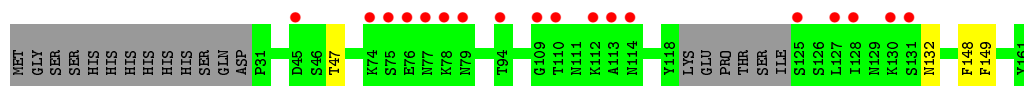
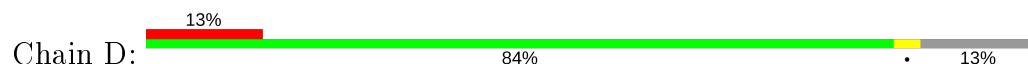
• Molecule 1: VtrA Protein



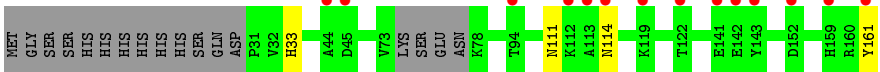
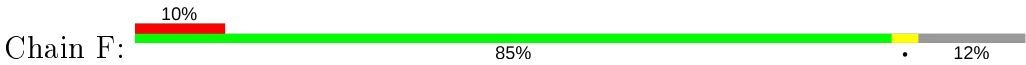
• Molecule 2: VtrC Protein



• Molecule 2: VtrC Protein



• Molecule 2: VtrC Protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.38 Å 71.28 Å 203.73 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.64 – 2.10 35.64 – 2.10	Depositor EDS
% Data completeness (in resolution range)	86.3 (35.64-2.10) 86.3 (35.64-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.46 (at 2.10 Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.197 , 0.231 0.198 , 0.232	Depositor DCC
R_{free} test set	2000 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11236	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: 6SB, ACT, EDO, 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	0.25	0/751	0.40	0/1010
1	C	0.24	0/759	0.41	0/1021
1	E	0.25	0/743	0.40	0/999
2	B	0.24	0/1126	0.44	0/1527
2	D	0.24	0/1070	0.43	0/1448
2	F	0.25	0/1085	0.45	0/1470
All	All	0.24	0/5534	0.43	0/7475

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	737	737	737	0	0
1	C	745	741	741	2	0
1	E	729	733	733	1	1
2	B	1098	1049	1052	2	0
2	D	1044	996	996	1	1
2	F	1058	1015	1015	2	0
3	A	34	44	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	34	44	0	0	0
3	D	34	44	0	0	0
3	F	34	44	0	0	0
4	A	4	3	3	0	0
4	B	4	3	3	0	0
5	A	4	6	6	0	0
6	B	5	0	0	0	0
6	C	10	0	0	0	0
6	D	5	0	0	0	0
6	E	5	0	0	0	0
7	A	37	0	0	0	0
7	B	39	0	0	0	0
7	C	23	0	0	0	0
7	D	37	0	0	0	0
7	E	21	0	0	0	0
7	F	36	0	0	0	0
All	All	5777	5459	5286	8	1

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 1.

All (8) 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:B:51:ASP:OD2	2:B:70:ARG:NH2	2.30	0.64
2:F:111:ASN:ND2	2:F:114:ASN:OD1	2.37	0.58
2:B:34:PHE:HB2	2:B:161:TYR:HB2	1.96	0.48
1:E:200:LYS:NZ	1:E:252:GLU:OE1	2.41	0.47
1:C:228:LYS:NZ	1:C:253:TYR:O	2.48	0.47
1:C:223:LYS:O	1:C:224:ASN:CB	2.63	0.46
2:F:33:HIS:HA	2:F:161:TYR:HE1	1.81	0.45
2:D:132:ASN:HB3	2:D:149:PHE:CD1	2.54	0.43

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:THR:H	1:E:201:GLU:OE2[1_545]	1.59	0.01

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	87/94 (93%)	86 (99%)	1 (1%)	0	100	100
1	C	88/94 (94%)	83 (94%)	3 (3%)	2 (2%)	6	2
1	E	86/94 (92%)	83 (96%)	3 (4%)	0	100	100
2	B	130/144 (90%)	126 (97%)	4 (3%)	0	100	100
2	D	121/144 (84%)	114 (94%)	7 (6%)	0	100	100
2	F	123/144 (85%)	121 (98%)	2 (2%)	0	100	100
All	All	635/714 (89%)	613 (96%)	20 (3%)	2 (0%)	41	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	224	ASN
1	C	235	GLU

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	85/89 (96%)	85 (100%)	0	100	100
1	C	86/89 (97%)	86 (100%)	0	100	100
1	E	84/89 (94%)	84 (100%)	0	100	100
2	B	123/134 (92%)	122 (99%)	1 (1%)	81	86
2	D	116/134 (87%)	115 (99%)	1 (1%)	78	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	118/134 (88%)	118 (100%)	0	100	100
All	All	612/669 (92%)	610 (100%)	2 (0%)	92	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	0	ASP
2	D	148	PHE

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
6	SO4	D	302	-	4,4,4	0.14	0	6,6,6	0.05	0
4	ACT	A	302	-	1,3,3	1.17	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6SB	D	301	-	37,37,37	3.95	19 (51%)	57,58,58	1.82	14 (24%)
6	SO4	E	302	-	4,4,4	0.13	0	6,6,6	0.05	0
3	6SB	B	301	-	37,37,37	3.99	18 (48%)	57,58,58	1.96	13 (22%)
3	6SB	F	301	-	37,37,37	4.01	19 (51%)	57,58,58	1.90	13 (22%)
6	SO4	C	303	-	4,4,4	0.14	0	6,6,6	0.04	0
6	SO4	B	302	-	4,4,4	0.14	0	6,6,6	0.06	0
3	6SB	A	301	-	37,37,37	4.02	19 (51%)	57,58,58	1.95	14 (24%)
5	EDO	A	303	-	3,3,3	0.43	0	2,2,2	0.38	0
6	SO4	C	302	-	4,4,4	0.15	0	6,6,6	0.04	0
4	ACT	B	303	-	1,3,3	1.32	0	0,3,3	0.00	-

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	6SB	F	301	-	-	4/16/78/78	0/4/4/4
3	6SB	A	301	-	-	2/16/78/78	0/4/4/4
3	6SB	D	301	-	-	0/16/78/78	0/4/4/4
3	6SB	B	301	-	-	3/16/78/78	0/4/4/4
5	EDO	A	303	-	-	1/1/1/1	-

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	6SB	C16-C15	11.86	1.73	1.53
3	F	301	6SB	C16-C15	11.85	1.73	1.53
3	A	301	6SB	C16-C15	11.81	1.73	1.53
3	D	301	6SB	C16-C15	11.79	1.73	1.53
3	A	301	6SB	C24-C14	-9.94	1.37	1.54
3	B	301	6SB	C24-C14	-9.71	1.37	1.54
3	D	301	6SB	C24-C14	-9.65	1.37	1.54
3	F	301	6SB	C24-C14	-9.65	1.37	1.54
3	A	301	6SB	C20-C14	9.34	1.73	1.54
3	F	301	6SB	C20-C14	9.29	1.73	1.54
3	D	301	6SB	C20-C14	9.26	1.73	1.54
3	B	301	6SB	C20-C14	9.20	1.73	1.54
3	D	301	6SB	C11-C12	6.80	1.66	1.53
3	A	301	6SB	C11-C12	6.75	1.66	1.53
3	F	301	6SB	C32-N08	6.75	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	301	6SB	C11-C12	6.74	1.66	1.53
3	A	301	6SB	C32-N08	6.72	1.48	1.33
3	B	301	6SB	C32-N08	6.69	1.48	1.33
3	B	301	6SB	C11-C12	6.63	1.66	1.53
3	A	301	6SB	O02-C15	-6.61	1.32	1.43
3	F	301	6SB	O02-C15	-6.53	1.32	1.43
3	B	301	6SB	O02-C15	-6.53	1.32	1.43
3	D	301	6SB	O02-C15	-6.44	1.32	1.43
3	D	301	6SB	C32-N08	6.39	1.47	1.33
3	F	301	6SB	C09-C14	3.78	1.62	1.55
3	A	301	6SB	C09-C14	3.69	1.61	1.55
3	B	301	6SB	C09-C14	3.65	1.61	1.55
3	F	301	6SB	C29-C24	3.65	1.63	1.54
3	B	301	6SB	C29-C24	3.61	1.63	1.54
3	F	301	6SB	C34-S01	3.57	1.82	1.77
3	A	301	6SB	C21-C17	3.56	1.62	1.53
3	A	301	6SB	C34-S01	3.56	1.82	1.77
3	B	301	6SB	C34-S01	3.51	1.82	1.77
3	D	301	6SB	C29-C24	3.49	1.63	1.54
3	F	301	6SB	C21-C17	3.49	1.61	1.53
3	D	301	6SB	C21-C17	3.47	1.61	1.53
3	A	301	6SB	C29-C24	3.46	1.63	1.54
3	D	301	6SB	C09-C14	3.44	1.61	1.55
3	B	301	6SB	C21-C17	3.43	1.61	1.53
3	D	301	6SB	C09-C15	-3.43	1.49	1.54
3	A	301	6SB	C18-C10	3.40	1.61	1.54
3	D	301	6SB	C18-C10	3.39	1.61	1.54
3	F	301	6SB	C18-C10	3.35	1.61	1.54
3	B	301	6SB	C18-C10	3.34	1.61	1.54
3	B	301	6SB	C09-C15	-3.19	1.49	1.54
3	F	301	6SB	C31-C32	3.18	1.57	1.51
3	D	301	6SB	C34-S01	3.13	1.82	1.77
3	B	301	6SB	C31-C32	3.10	1.57	1.51
3	F	301	6SB	C09-C10	3.04	1.60	1.55
3	A	301	6SB	C31-C32	3.01	1.57	1.51
3	A	301	6SB	C09-C15	-3.01	1.49	1.54
3	A	301	6SB	C21-C19	2.99	1.60	1.52
3	F	301	6SB	C09-C15	-2.96	1.49	1.54
3	F	301	6SB	C21-C19	2.90	1.60	1.52
3	D	301	6SB	C21-C19	2.90	1.60	1.52
3	B	301	6SB	C09-C10	2.90	1.60	1.55
3	A	301	6SB	C09-C10	2.89	1.60	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	6SB	C21-C19	2.88	1.60	1.52
3	D	301	6SB	C09-C10	2.80	1.60	1.55
3	D	301	6SB	C31-C32	2.70	1.56	1.51
3	A	301	6SB	O04-C32	-2.23	1.18	1.23
3	B	301	6SB	O04-C32	-2.22	1.18	1.23
3	A	301	6SB	O06-S01	2.21	1.51	1.45
3	B	301	6SB	O06-S01	2.21	1.51	1.45
3	B	301	6SB	O05-S01	2.19	1.51	1.45
3	F	301	6SB	O04-C32	-2.18	1.18	1.23
3	D	301	6SB	O06-S01	2.18	1.51	1.45
3	F	301	6SB	O05-S01	2.18	1.51	1.45
3	A	301	6SB	O05-S01	2.17	1.51	1.45
3	F	301	6SB	O06-S01	2.17	1.51	1.45
3	D	301	6SB	O05-S01	2.16	1.51	1.45
3	D	301	6SB	O04-C32	-2.16	1.18	1.23
3	A	301	6SB	C25-C28	2.15	1.55	1.51
3	D	301	6SB	C25-C28	2.10	1.55	1.51
3	F	301	6SB	C25-C28	2.09	1.55	1.51

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	6SB	C10-C09-C15	6.15	113.12	107.40
3	B	301	6SB	C10-C09-C15	6.08	113.06	107.40
3	F	301	6SB	C10-C09-C15	5.84	112.84	107.40
3	D	301	6SB	C10-C09-C15	5.66	112.67	107.40
3	A	301	6SB	C14-C09-C15	5.07	122.29	117.67
3	F	301	6SB	C14-C09-C15	4.74	121.99	117.67
3	B	301	6SB	C14-C09-C15	4.48	121.75	117.67
3	B	301	6SB	C23-C09-C15	-4.24	104.75	109.07
3	F	301	6SB	C23-C09-C15	-3.98	105.01	109.07
3	A	301	6SB	C23-C09-C15	-3.93	105.06	109.07
3	F	301	6SB	O06-S01-C34	3.77	111.46	106.92
3	A	301	6SB	O05-S01-C34	3.77	111.45	106.92
3	D	301	6SB	O05-S01-C34	3.68	111.35	106.92
3	B	301	6SB	O06-S01-O05	-3.68	101.23	113.95
3	F	301	6SB	O06-S01-O05	-3.66	101.29	113.95
3	B	301	6SB	O06-S01-C34	3.64	111.30	106.92
3	D	301	6SB	O06-S01-C34	3.64	111.30	106.92
3	A	301	6SB	O06-S01-O05	-3.63	101.39	113.95
3	D	301	6SB	O06-S01-O05	-3.60	101.50	113.95
3	A	301	6SB	O06-S01-C34	3.55	111.19	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	301	6SB	O05-S01-C34	3.54	111.18	106.92
3	B	301	6SB	C09-C14-C24	-3.46	115.36	119.50
3	D	301	6SB	C23-C09-C15	-3.45	105.56	109.07
3	D	301	6SB	C09-C14-C24	-3.40	115.44	119.50
3	A	301	6SB	C12-C11-C10	3.36	113.59	109.09
3	B	301	6SB	O05-S01-C34	3.33	110.92	106.92
3	A	301	6SB	C09-C14-C24	-3.17	115.71	119.50
3	A	301	6SB	C23-C09-C10	-3.13	106.31	111.21
3	D	301	6SB	C14-C09-C15	3.11	120.50	117.67
3	F	301	6SB	C23-C09-C10	-3.04	106.45	111.21
3	B	301	6SB	C23-C09-C10	-3.03	106.47	111.21
3	F	301	6SB	C09-C14-C24	-2.99	115.93	119.50
3	D	301	6SB	C23-C09-C10	-2.83	106.78	111.21
3	B	301	6SB	O07-S01-C34	2.81	110.32	105.77
3	F	301	6SB	O07-S01-C34	2.76	110.23	105.77
3	A	301	6SB	O07-S01-C34	2.74	110.20	105.77
3	D	301	6SB	C12-C16-C15	-2.70	110.74	114.30
3	B	301	6SB	C12-C13-C17	2.45	112.02	108.58
3	B	301	6SB	C31-C32-N08	2.44	120.53	116.42
3	B	301	6SB	C12-C16-C15	-2.41	111.11	114.30
3	B	301	6SB	C19-C11-C12	2.38	113.44	110.49
3	D	301	6SB	C33-N08-C32	-2.31	118.54	122.84
3	F	301	6SB	C12-C13-C17	2.31	111.82	108.58
3	F	301	6SB	C23-C09-C14	-2.30	107.61	111.21
3	D	301	6SB	O07-S01-C34	2.24	109.40	105.77
3	A	301	6SB	C25-C17-C21	-2.20	107.71	111.74
3	A	301	6SB	C23-C09-C14	-2.17	107.81	111.21
3	D	301	6SB	C14-C09-C10	2.17	102.28	100.09
3	F	301	6SB	C12-C16-C15	-2.15	111.46	114.30
3	D	301	6SB	C12-C13-C17	2.12	111.56	108.58
3	D	301	6SB	C12-C11-C10	2.11	111.92	109.09
3	A	301	6SB	C12-C13-C17	2.02	111.42	108.58
3	F	301	6SB	C12-C11-C10	2.02	111.80	109.09
3	A	301	6SB	C30-C24-C29	-2.01	107.22	110.36

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	6SB	C33-C34-S01-O05
3	B	301	6SB	C33-C34-S01-O07
3	F	301	6SB	C14-C24-C29-C31

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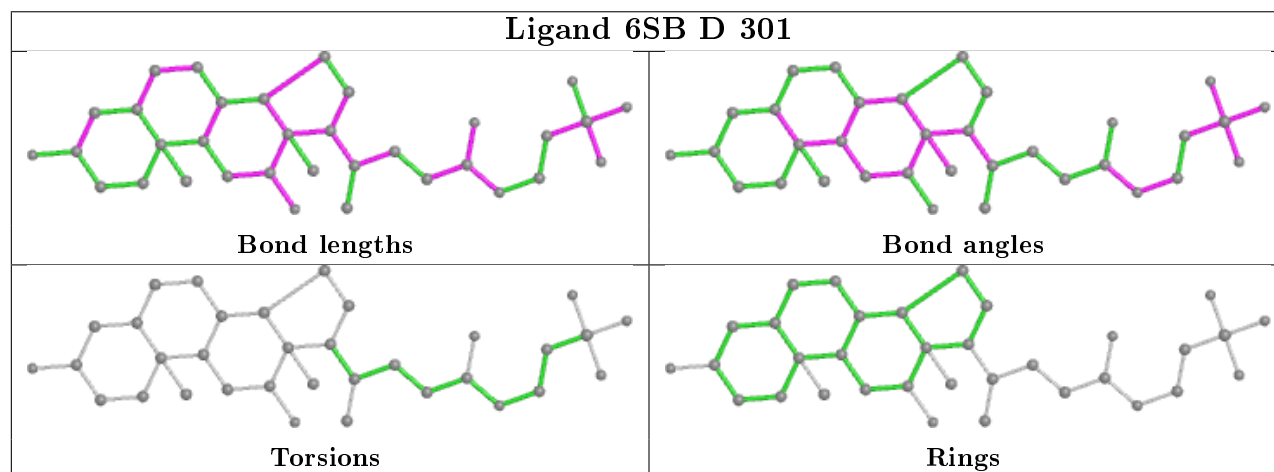
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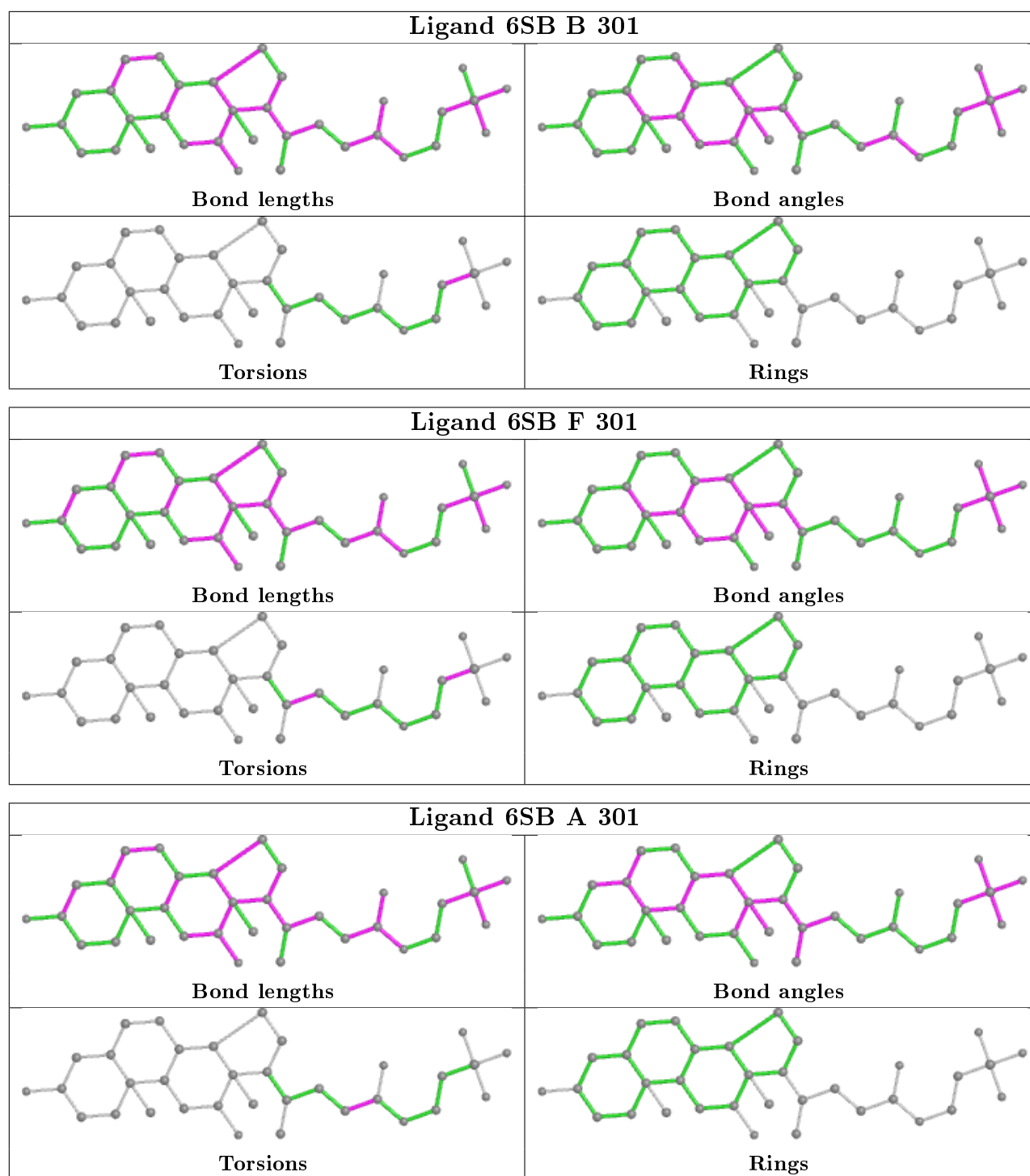
Mol	Chain	Res	Type	Atoms
5	A	303	EDO	O1-C1-C2-O2
3	F	301	6SB	C30-C24-C29-C31
3	B	301	6SB	C33-C34-S01-O06
3	F	301	6SB	C33-C34-S01-O05
3	A	301	6SB	C29-C31-C32-O04
3	A	301	6SB	C29-C31-C32-N08
3	F	301	6SB	C33-C34-S01-O07

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	89/94 (94%)	0.08	4 (4%) 33 38	12, 21, 62, 82	0
1	C	90/94 (95%)	0.13	6 (6%) 17 22	15, 30, 77, 93	0
1	E	88/94 (93%)	0.58	11 (12%) 3 5	16, 36, 73, 92	0
2	B	132/144 (91%)	0.11	1 (0%) 86 88	11, 27, 57, 84	0
2	D	125/144 (86%)	0.53	18 (14%) 2 3	16, 34, 73, 97	0
2	F	127/144 (88%)	0.41	14 (11%) 5 7	17, 32, 62, 100	0
All	All	651/714 (91%)	0.31	54 (8%) 11 14	11, 30, 71, 100	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	161	TYR	7.7
2	F	45	ASP	6.8
2	D	75	SER	6.4
1	E	235	GLU	6.1
1	C	225	LYS	5.3
2	F	141	GLU	4.8
1	E	213	ASP	4.8
2	D	77	ASN	4.6
2	D	110	THR	4.6
1	E	223	LYS	4.2
1	C	164	ASP	3.9
1	C	223	LYS	3.8
2	D	114	ASN	3.8
1	E	237	LYS	3.8
2	D	76	GLU	3.6
2	D	131	SER	3.6
2	F	44	ALA	3.5
2	D	78	LYS	3.5
1	E	225	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	236	LYS	3.5
1	C	224	ASN	3.4
2	D	94	THR	3.3
2	B	141	GLU	3.3
2	F	113	ALA	3.3
2	D	112	LYS	3.2
2	F	152	ASP	3.1
2	D	45	ASP	3.1
2	D	74	LYS	3.1
2	F	114	ASN	3.1
2	F	143	TYR	3.0
1	C	235	GLU	2.9
1	E	214	LYS	2.9
1	E	224	ASN	2.8
2	F	122	THR	2.7
2	D	113	ALA	2.7
2	D	79	ASN	2.7
1	A	224	ASN	2.7
2	F	94	THR	2.5
1	C	236	LYS	2.5
1	E	238	LEU	2.4
2	F	159	HIS	2.3
1	E	239	ASN	2.3
2	D	109	GLY	2.2
2	F	112	LYS	2.2
2	F	142	GLU	2.2
2	D	130	LYS	2.1
2	F	119	LYS	2.1
1	A	213	ASP	2.1
2	D	127	LEU	2.1
1	E	241	LYS	2.1
2	D	125	SER	2.1
1	A	225	LYS	2.1
2	D	128	ILE	2.1
1	A	214	LYS	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

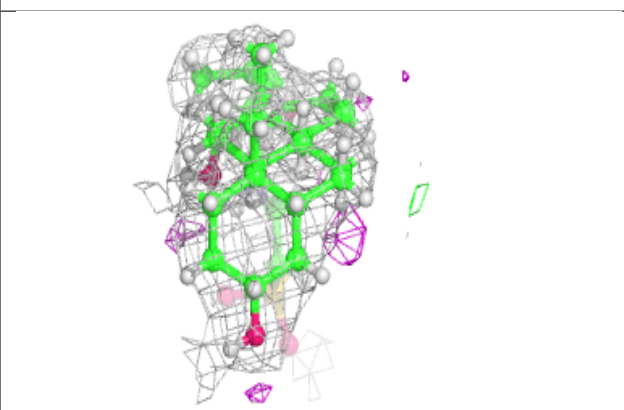
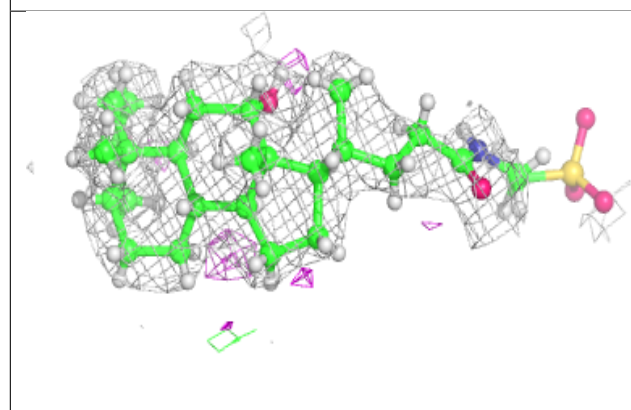
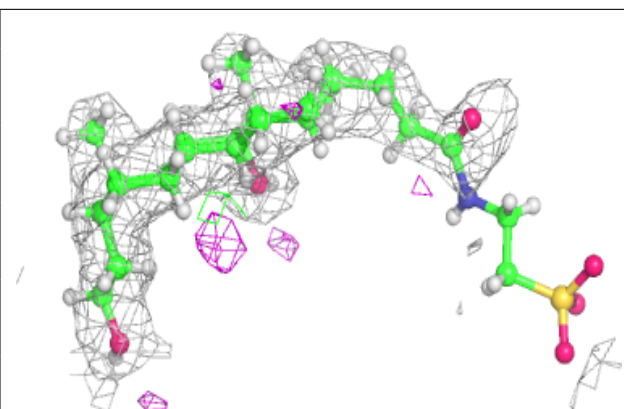
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	D	302	5/5	0.78	0.34	91,91,94,94	0
4	ACT	B	303	4/4	0.79	0.16	55,56,66,66	0
6	SO4	B	302	5/5	0.84	0.18	81,83,84,88	0
3	6SB	F	301	34/34	0.84	0.19	17,28,132,142	0
5	EDO	A	303	4/4	0.88	0.11	35,49,55,59	0
3	6SB	A	301	34/34	0.89	0.17	23,36,116,119	0
3	6SB	B	301	34/34	0.90	0.15	17,27,103,113	0
6	SO4	C	302	5/5	0.92	0.13	79,83,84,85	0
6	SO4	E	302	5/5	0.92	0.15	50,54,56,57	0
3	6SB	D	301	34/34	0.93	0.12	19,28,44,49	0
6	SO4	C	303	5/5	0.95	0.15	77,77,78,80	0
4	ACT	A	302	4/4	0.95	0.19	34,35,42,42	0

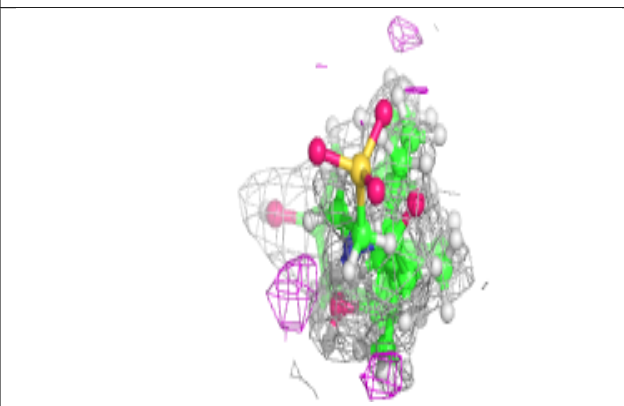
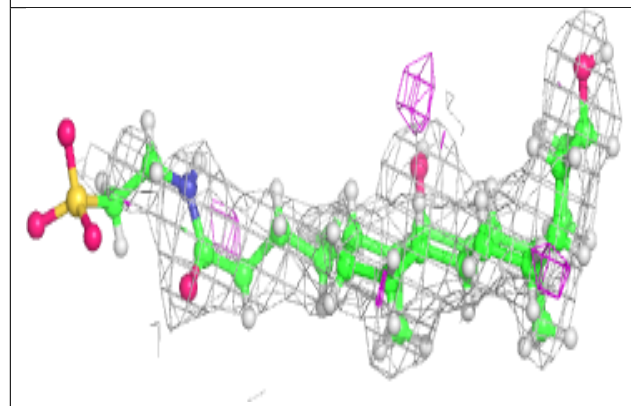
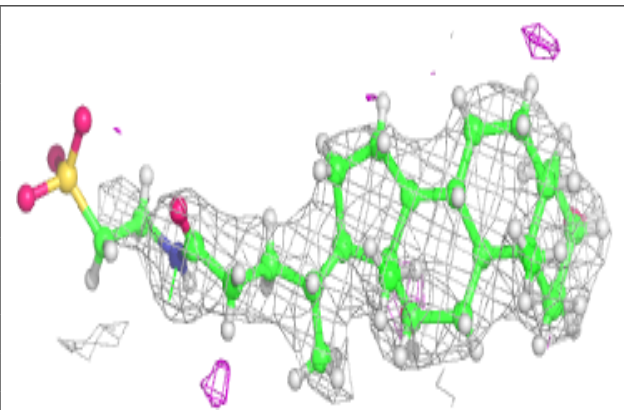
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6SB F 301:

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

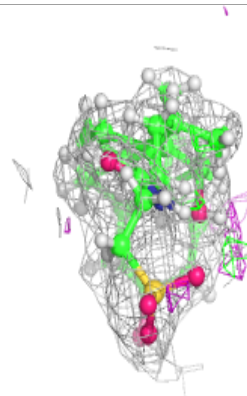
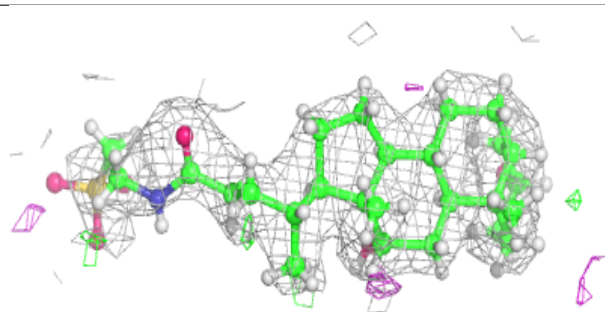
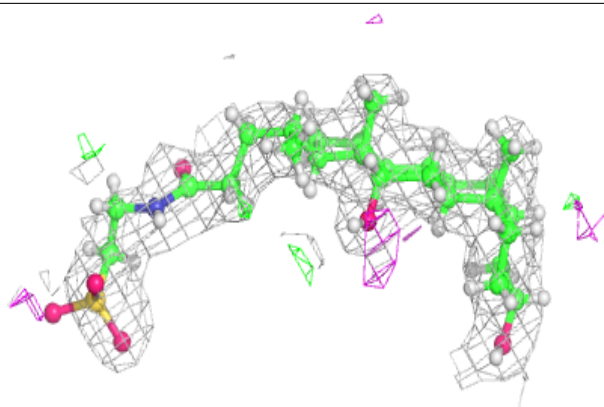
**Electron density around 6SB A 301:**

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

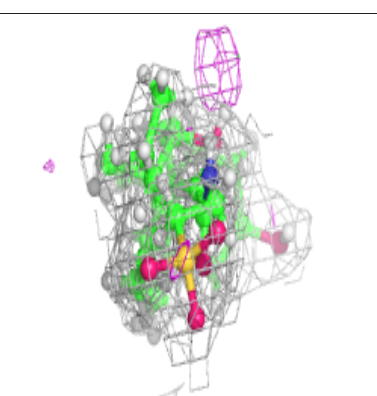
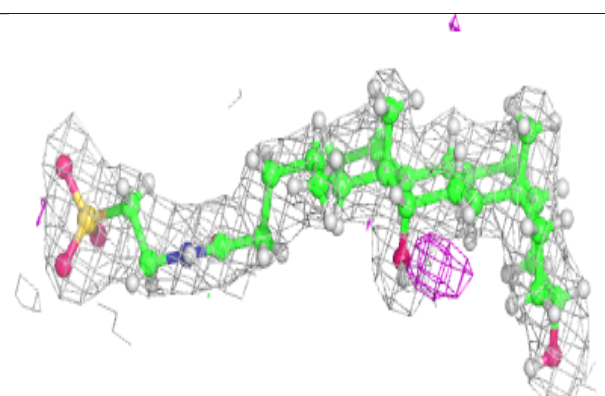
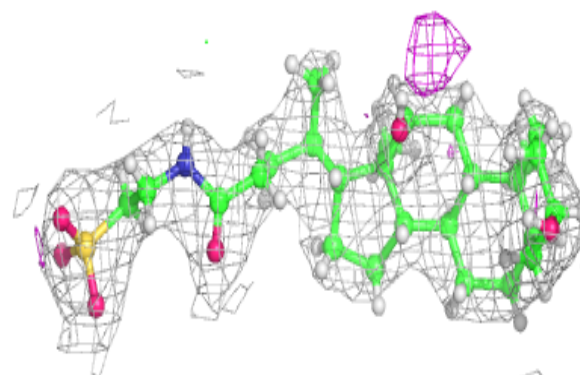


Electron density around 6SB B 301:

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

**Electron density around 6SB D 301:**

$2mF_o-DF_c$ (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.