



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:10 PM UTC

PDB ID : 6PSM / pdb_00006psm
Title : Crystal structure of PsS1_19B C77S in complex with kappa-neocarrabiose
Authors : Hettle, A.G.; Boraston, A.B.
Deposited on : 2019-07-12
Resolution : 1.95 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

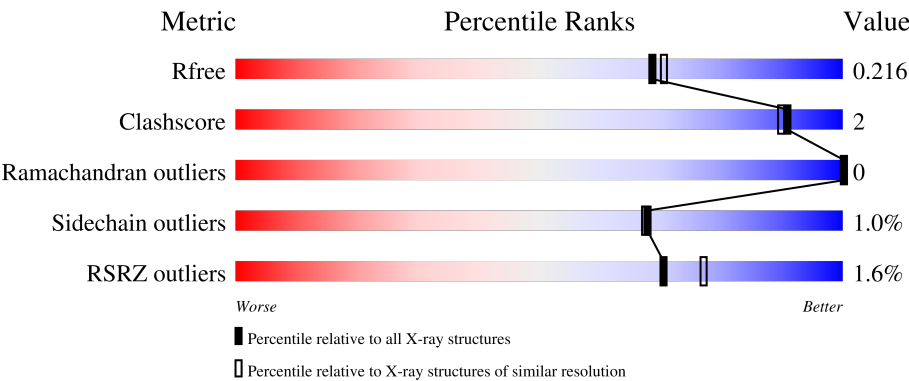
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	469	% 91%5%5%
1	B	469	2% 90%5%5%
1	C	469	2% 91%5%.
1	D	469	3% 90%.5%
1	E	469	% 91%. .

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Mol	Chain	Length	Quality of chain
1	F	469	% 91% 5%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22255 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.

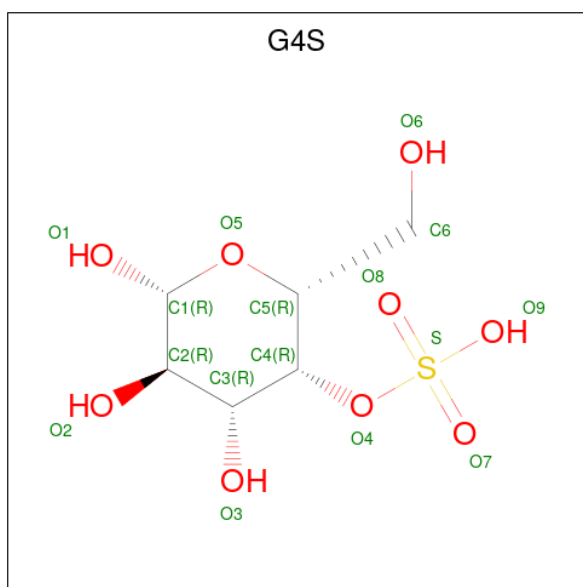
- Molecule 1 is a protein called exo-4S-kappa carrageenan S1 sulfatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	2	0
			3537	2259	594	674	10			
1	B	447	Total	C	N	O	S	0	0	0
			3526	2254	593	670	9			
1	C	448	Total	C	N	O	S	0	0	0
			3540	2260	599	672	9			
1	D	444	Total	C	N	O	S	0	1	0
			3505	2240	591	666	8			
1	E	448	Total	C	N	O	S	0	1	0
			3545	2264	599	673	9			
1	F	447	Total	C	N	O	S	0	0	1
			3522	2249	593	671	9			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

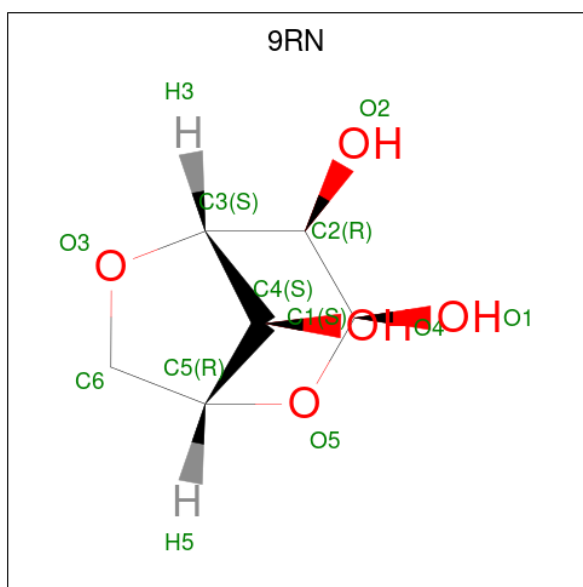
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	E	1	Total	Ca	0	0
			1	1		
2	F	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 4-O-sulfo-beta-D-galactopyranose (CCD ID: G4S) (formula: C₆H₁₂O₉S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			16	6	9	1		
3	B	1	Total	C	O	S	0	0
			16	6	9	1		
3	C	1	Total	C	O	S	0	0
			16	6	9	1		
3	D	1	Total	C	O	S	0	0
			16	6	9	1		
3	E	1	Total	C	O	S	0	0
			16	6	9	1		
3	F	1	Total	C	O	S	0	0
			16	6	9	1		

- Molecule 4 is 3,6-anhydro-D-galactose (CCD ID: 9RN) (formula: $C_6H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		
4	E	1	Total	C	O	0	0
			10	6	4		
4	F	1	Total	C	O	0	0
			10	6	4		

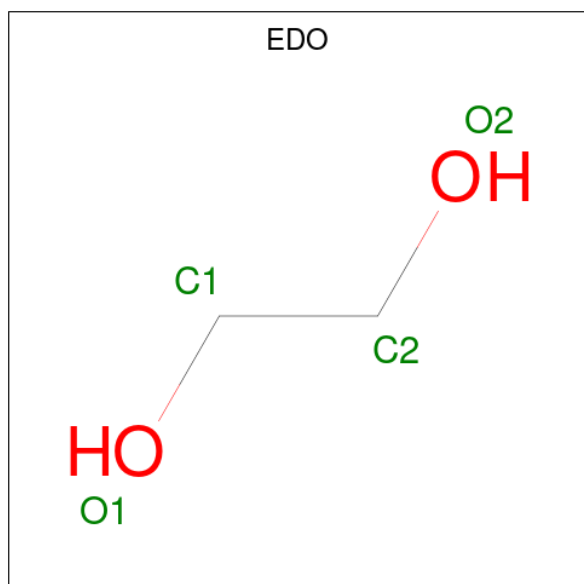
- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		
5	C	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		
5	E	1	Total	Cl	0	0
			1	1		
5	F	1	Total	Cl	0	0
			1	1		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	Zn 2	0	0
6	D	2	Total 2	Zn 2	0	0
6	E	2	Total 2	Zn 2	0	0

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	140	Total 140	O 140	0	0

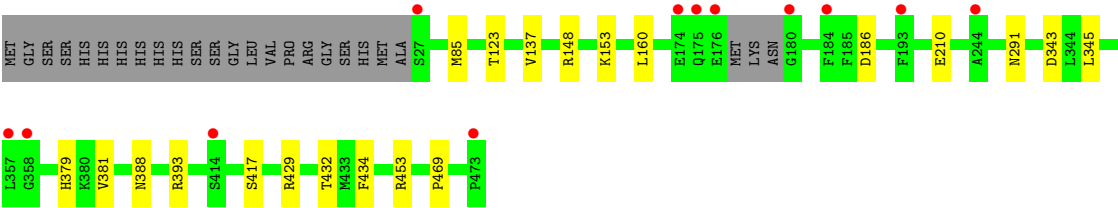
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	121	Total 121	O 121	0	0
8	C	163	Total 163	O 163	0	0
8	D	131	Total 131	O 131	0	0
8	E	145	Total 145	O 145	0	0
8	F	186	Total 186	O 186	0	0

- Molecule 1: exo-4S-kappa carrageenan S1 sulfatase

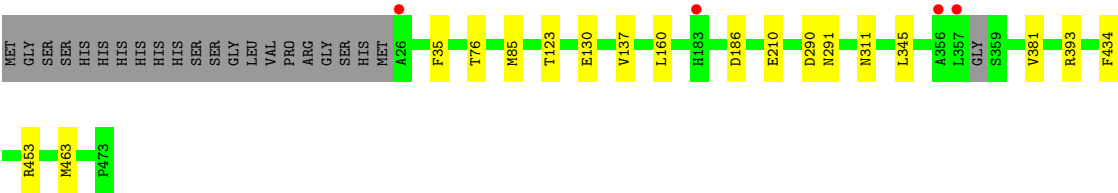
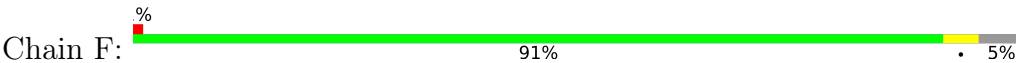




● Molecule 1: exo-4S-kappa carrageenan S1 sulfatase



● Molecule 1: exo-4S-kappa carrageenan S1 sulfatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	93.05Å 93.05Å 300.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.19 – 1.95 48.19 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.19-1.95) 99.7 (48.19-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.192 , 0.212 0.198 , 0.216	Depositor DCC
R_{free} test set	10434 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.703	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.110 for -h,-k,l 0.114 for h,-h-k,-l 0.178 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22255	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.74% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G4S, CL, EDO, 9RN, CA, ZN

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	0.98	0/3630	1.22	3/4909 (0.1%)
1	B	0.99	0/3616	1.22	3/4889 (0.1%)
1	C	1.00	0/3630	1.22	3/4904 (0.1%)
1	D	0.99	0/3594	1.21	1/4856 (0.0%)
1	E	1.01	0/3635	1.22	1/4912 (0.0%)
1	F	1.00	0/3611	1.22	3/4882 (0.1%)
All	All	0.99	0/21716	1.22	14/29352 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	186	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	186	ASP	CA-CB-CG	5.93	118.53	112.60
1	B	186	ASP	CA-CB-CG	5.61	118.21	112.60
1	D	186	ASP	CA-CB-CG	5.54	118.14	112.60
1	F	186	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	76	THR	CA-C-N	5.27	127.60	120.65
1	B	76	THR	C-N-CA	5.27	127.60	120.65
1	F	76	THR	CA-C-N	5.16	127.46	120.65
1	F	76	THR	C-N-CA	5.16	127.46	120.65
1	E	186	ASP	CA-CB-CG	5.13	117.73	112.60
1	C	76	THR	CA-C-N	5.03	127.29	120.65
1	C	76	THR	C-N-CA	5.03	127.29	120.65
1	A	76	THR	CA-C-N	5.00	127.25	120.65
1	A	76	THR	C-N-CA	5.00	127.25	120.65

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	3537	0	3383	11	0
1	B	3526	0	3374	13	0
1	C	3540	0	3412	15	0
1	D	3505	0	3359	11	0
1	E	3545	0	3406	13	0
1	F	3522	0	3370	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	16	0	10	0	0
3	B	16	0	10	0	0
3	C	16	0	10	0	0
3	D	16	0	10	0	0
3	E	16	0	10	0	0
3	F	16	0	10	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
4	E	10	0	0	0	0
4	F	10	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	2	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
7	A	4	0	6	0	0
7	C	4	0	6	0	0
7	D	4	0	6	0	0
7	E	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	4	0	6	0	0
8	A	140	0	0	1	0
8	B	121	0	0	0	0
8	C	163	0	0	0	0
8	D	131	0	0	0	0
8	E	145	0	0	1	0
8	F	186	0	0	0	0
All	All	22255	0	20394	72	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 (72) 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:C:248:ASN:HB3	1:F:130:GLU:OE1	1.76	0.85
1:A:85[A]:MET:HE3	1:A:123:THR:HB	1.62	0.80
1:B:177:MET:HE2	1:B:188:LYS:HG2	1.67	0.77
1:B:85:MET:HE3	1:B:123:THR:HB	1.67	0.76
1:C:85:MET:HE3	1:C:123:THR:HB	1.68	0.76
1:F:85:MET:HE3	1:F:123:THR:HB	1.66	0.76
1:D:85:MET:HE3	1:D:123:THR:HB	1.67	0.75
1:E:85:MET:HE3	1:E:123:THR:HB	1.69	0.75
1:B:85:MET:CE	1:B:123:THR:HB	2.28	0.63
1:D:85:MET:CE	1:D:123:THR:HB	2.29	0.63
1:C:85:MET:CE	1:C:123:THR:HB	2.28	0.63
1:F:85:MET:CE	1:F:123:THR:HB	2.29	0.62
1:A:85[A]:MET:CE	1:A:123:THR:HB	2.30	0.60
1:E:85:MET:CE	1:E:123:THR:HB	2.31	0.60
1:C:129:LYS:HD2	1:C:133:TYR:O	2.03	0.57
1:C:160:LEU:CD2	1:C:210:GLU:HG3	2.37	0.54
1:E:429:ARG:HA	1:E:432:THR:HG22	1.88	0.54
1:A:160:LEU:CD2	1:A:210:GLU:HG3	2.37	0.54
1:D:160:LEU:CD2	1:D:210:GLU:HG3	2.38	0.54
1:B:160:LEU:CD2	1:B:210:GLU:HG3	2.39	0.53
1:D:429:ARG:HA	1:D:432[A]:THR:HG22	1.90	0.53
1:F:160:LEU:CD2	1:F:210:GLU:HG3	2.39	0.52
1:B:429:ARG:HA	1:B:432:THR:HG22	1.90	0.52
1:E:160:LEU:CD2	1:E:210:GLU:HG3	2.39	0.52
1:C:272:ASP:O	1:C:276:GLU:HG3	2.13	0.48
1:F:311:ASN:HB2	1:F:463:MET:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:LEU:HD23	1:B:210:GLU:HG3	1.95	0.47
1:E:432:THR:HG23	8:E:736:HOH:O	2.14	0.47
1:C:160:LEU:HD23	1:C:210:GLU:HG3	1.96	0.47
1:E:160:LEU:HD23	1:E:210:GLU:HG3	1.96	0.47
1:C:248:ASN:CB	1:F:130:GLU:OE1	2.58	0.47
1:E:453:ARG:NE	1:E:453:ARG:HA	2.31	0.46
1:C:453:ARG:NE	1:C:453:ARG:HA	2.31	0.46
1:F:345:LEU:C	1:F:345:LEU:HD23	2.41	0.46
1:A:160:LEU:HD23	1:A:210:GLU:HG3	1.98	0.46
1:C:345:LEU:C	1:C:345:LEU:HD23	2.41	0.45
1:B:177:MET:CE	1:B:188:LYS:HG2	2.44	0.45
1:F:453:ARG:NE	1:F:453:ARG:HA	2.32	0.45
1:A:345:LEU:C	1:A:345:LEU:HD23	2.42	0.45
1:B:345:LEU:C	1:B:345:LEU:HD23	2.42	0.45
1:D:453:ARG:NE	1:D:453:ARG:HA	2.32	0.44
1:E:345:LEU:C	1:E:345:LEU:HD23	2.43	0.44
1:D:148:ARG:HA	1:D:153:LYS:HD2	2.00	0.44
1:A:453:ARG:NE	1:A:453:ARG:HA	2.33	0.44
1:D:160:LEU:HD23	1:D:210:GLU:HG3	2.00	0.44
1:B:453:ARG:HA	1:B:453:ARG:NE	2.33	0.43
1:F:381:VAL:HA	1:F:393:ARG:O	2.18	0.43
1:D:345:LEU:HD23	1:D:345:LEU:C	2.43	0.43
1:E:381:VAL:HA	1:E:393:ARG:O	2.19	0.43
8:A:669:HOH:O	1:C:200:LYS:HE2	2.18	0.43
1:F:160:LEU:HD23	1:F:210:GLU:HG3	2.01	0.42
1:A:381:VAL:HA	1:A:393:ARG:O	2.19	0.42
1:C:381:VAL:HA	1:C:393:ARG:O	2.20	0.42
1:D:381:VAL:HA	1:D:393:ARG:O	2.19	0.42
1:E:386[A]:LYS:HD2	1:E:389:ARG:NH2	2.35	0.41
1:B:381:VAL:HA	1:B:393:ARG:O	2.20	0.41
1:D:343:ASP:CG	1:D:379:HIS:HE2	2.29	0.41
1:A:113:ALA:HA	1:A:145:ASP:HB2	2.02	0.41
1:C:292:GLY:HA3	1:C:315:GLY:O	2.21	0.41
1:A:231:ALA:HA	1:A:232:VAL:HA	1.90	0.41
1:E:343:ASP:CG	1:E:379:HIS:HE2	2.28	0.40
1:A:343:ASP:CG	1:A:379:HIS:HE2	2.30	0.40
1:E:292:GLY:HA3	1:E:315:GLY:O	2.21	0.40
1:B:243:LEU:HD23	1:B:243:LEU:HA	1.98	0.40
1:B:343:ASP:CG	1:B:379:HIS:HE2	2.29	0.40
1:F:35:PHE:CZ	1:F:290:ASP:HA	2.56	0.40
1:A:292:GLY:HA3	1:A:315:GLY:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ALA:HA	1:B:145:ASP:HB2	2.01	0.40
1:C:35:PHE:CZ	1:C:290:ASP:HA	2.56	0.40
1:C:129:LYS:HD2	1:C:129:LYS:HA	1.87	0.40
1:D:417:SER:HB3	1:D:469:PRO:HG3	2.04	0.40
1:E:238:SER:OG	1:E:243:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	447/469 (95%)	433 (97%)	14 (3%)	0	100	100
1	B	445/469 (95%)	432 (97%)	13 (3%)	0	100	100
1	C	446/469 (95%)	429 (96%)	17 (4%)	0	100	100
1	D	441/469 (94%)	426 (97%)	15 (3%)	0	100	100
1	E	447/469 (95%)	433 (97%)	14 (3%)	0	100	100
1	F	443/469 (94%)	428 (97%)	15 (3%)	0	100	100
All	All	2669/2814 (95%)	2581 (97%)	88 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	365/398 (92%)	361 (99%)	4 (1%)	65	64
1	B	361/398 (91%)	356 (99%)	5 (1%)	59	56
1	C	367/398 (92%)	364 (99%)	3 (1%)	73	74
1	D	362/398 (91%)	358 (99%)	4 (1%)	65	64
1	E	366/398 (92%)	364 (100%)	2 (0%)	81	82
1	F	363/398 (91%)	360 (99%)	3 (1%)	73	74
All	All	2184/2388 (92%)	2163 (99%)	21 (1%)	68	67

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	137	VAL
1	A	291	ASN
1	A	434	PHE
1	B	137	VAL
1	B	171	ASN
1	B	291	ASN
1	B	388	ASN
1	B	434	PHE
1	C	137	VAL
1	C	388	ASN
1	C	434	PHE
1	D	137	VAL
1	D	291	ASN
1	D	388	ASN
1	D	434	PHE
1	E	137	VAL
1	E	434	PHE
1	F	137	VAL
1	F	291	ASN
1	F	434	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	419	GLN
1	B	388	ASN
1	C	195	ASN

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Mol	Chain	Res	Type
1	C	388	ASN
1	C	419	GLN
1	D	328	HIS
1	D	419	GLN
1	F	328	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 35 ligands modelled in this entry, 18 are monoatomic - leaving 17 for Mogul analysis.

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	9RN	E	507	3	11,11,12	0.48	0	13,16,18	1.42	2 (15%)
3	G4S	B	503	4,2	16,16,16	0.83	0	21,24,24	0.71	0
3	G4S	A	502	4,2	16,16,16	1.26	1 (6%)	21,24,24	0.71	0
3	G4S	D	506	4,2	16,16,16	0.86	0	21,24,24	0.74	0
4	9RN	A	503	3	11,11,12	0.55	0	13,16,18	1.39	3 (23%)
4	9RN	B	504	3	11,11,12	0.51	0	13,16,18	1.30	2 (15%)
7	EDO	C	503	-	3,3,3	0.29	0	2,2,2	0.53	0
7	EDO	D	505	-	3,3,3	0.19	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	9RN	C	505	3	11,11,12	0.50	0	13,16,18	1.30	2 (15%)
4	9RN	D	507	3	11,11,12	0.48	0	13,16,18	1.27	2 (15%)
3	G4S	F	504	4,2	16,16,16	1.22	1 (6%)	21,24,24	0.66	0
4	9RN	F	505	3	11,11,12	0.51	0	13,16,18	1.31	2 (15%)
7	EDO	A	507	-	3,3,3	0.19	0	2,2,2	0.23	0
3	G4S	E	506	4,2	16,16,16	0.86	0	21,24,24	0.78	0
7	EDO	F	503	-	3,3,3	0.13	0	2,2,2	0.34	0
3	G4S	C	504	4,2	16,16,16	1.26	1 (6%)	21,24,24	0.68	0
7	EDO	E	505	-	3,3,3	0.30	0	2,2,2	0.06	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
4	9RN	E	507	3	-	-	0/3/2/2
3	G4S	B	503	4,2	-	0/7/27/27	0/1/1/1
3	G4S	A	502	4,2	-	0/7/27/27	0/1/1/1
3	G4S	D	506	4,2	-	0/7/27/27	0/1/1/1
7	EDO	C	503	-	-	0/1/1/1	-
7	EDO	D	505	-	-	0/1/1/1	-
4	9RN	A	503	3	-	-	0/3/2/2
4	9RN	B	504	3	-	-	0/3/2/2
4	9RN	C	505	3	-	-	0/3/2/2
4	9RN	D	507	3	-	-	0/3/2/2
3	G4S	F	504	4,2	-	0/7/27/27	0/1/1/1
7	EDO	A	507	-	-	0/1/1/1	-
7	EDO	F	503	-	-	0/1/1/1	-
3	G4S	E	506	4,2	-	0/7/27/27	0/1/1/1
4	9RN	F	505	3	-	-	0/3/2/2
3	G4S	C	504	4,2	-	0/7/27/27	0/1/1/1
7	EDO	E	505	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	G4S	O7-S	3.94	1.62	1.45
3	C	504	G4S	O8-S	3.91	1.62	1.45
3	F	504	G4S	O7-S	3.88	1.62	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	507	9RN	O5-C5-C6	-3.33	108.47	113.33
4	D	507	9RN	C2-C3-C4	-3.12	106.12	113.85
4	F	505	9RN	C2-C3-C4	-3.09	106.21	113.85
4	A	503	9RN	O5-C5-C6	-3.06	108.87	113.33
4	B	504	9RN	O5-C5-C6	-3.03	108.91	113.33
4	E	507	9RN	C2-C3-C4	-2.86	106.78	113.85
4	B	504	9RN	C2-C3-C4	-2.70	107.16	113.85
4	F	505	9RN	O5-C5-C6	-2.70	109.39	113.33
4	C	505	9RN	O5-C5-C6	-2.61	109.51	113.33
4	D	507	9RN	O5-C5-C6	-2.60	109.54	113.33
4	C	505	9RN	C2-C3-C4	-2.54	107.56	113.85
4	A	503	9RN	C2-C3-C4	-2.51	107.65	113.85
4	A	503	9RN	C1-C2-C3	2.08	112.14	109.29

There are no chirality outliers.

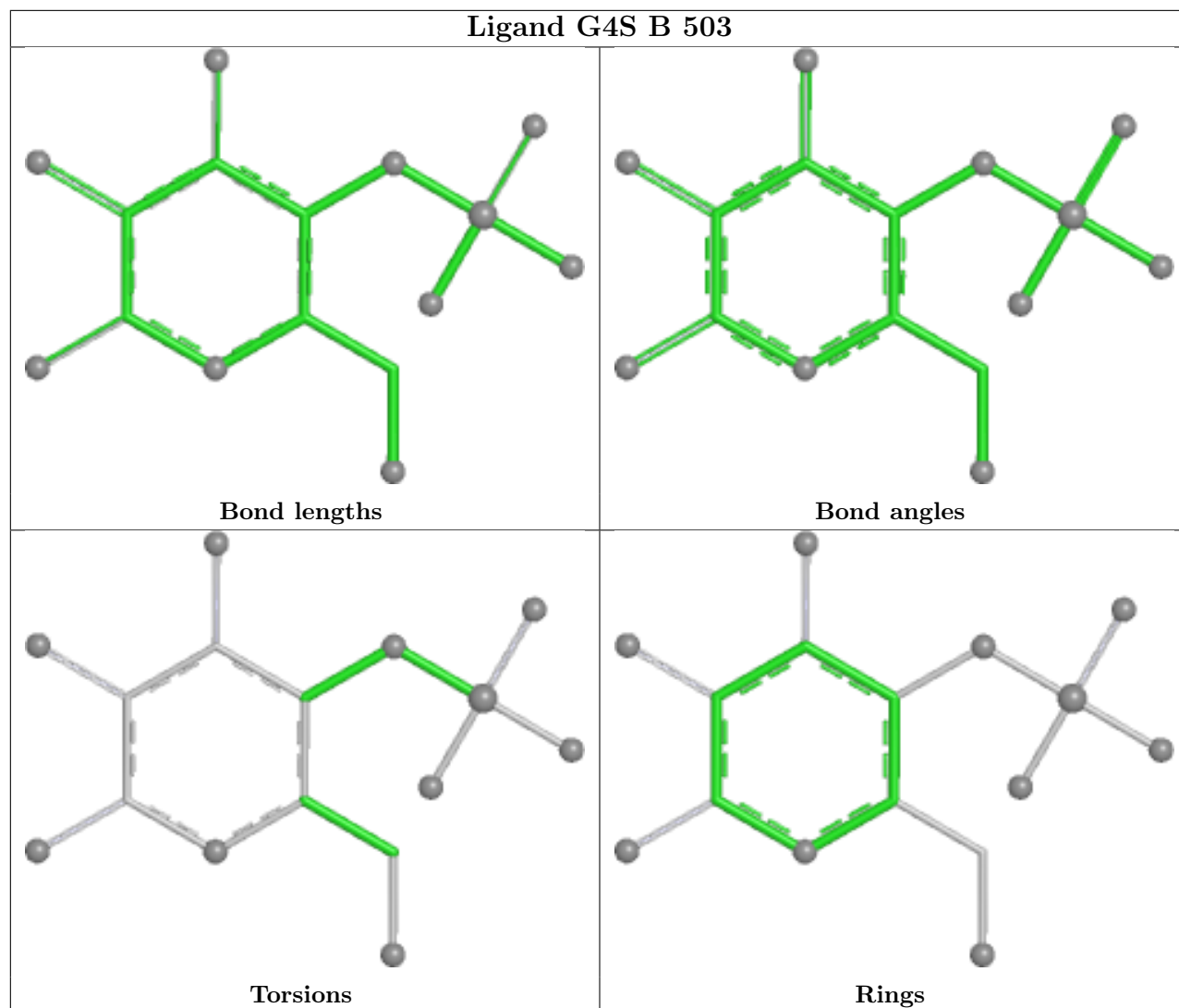
There are no torsion outliers.

There are no ring outliers.

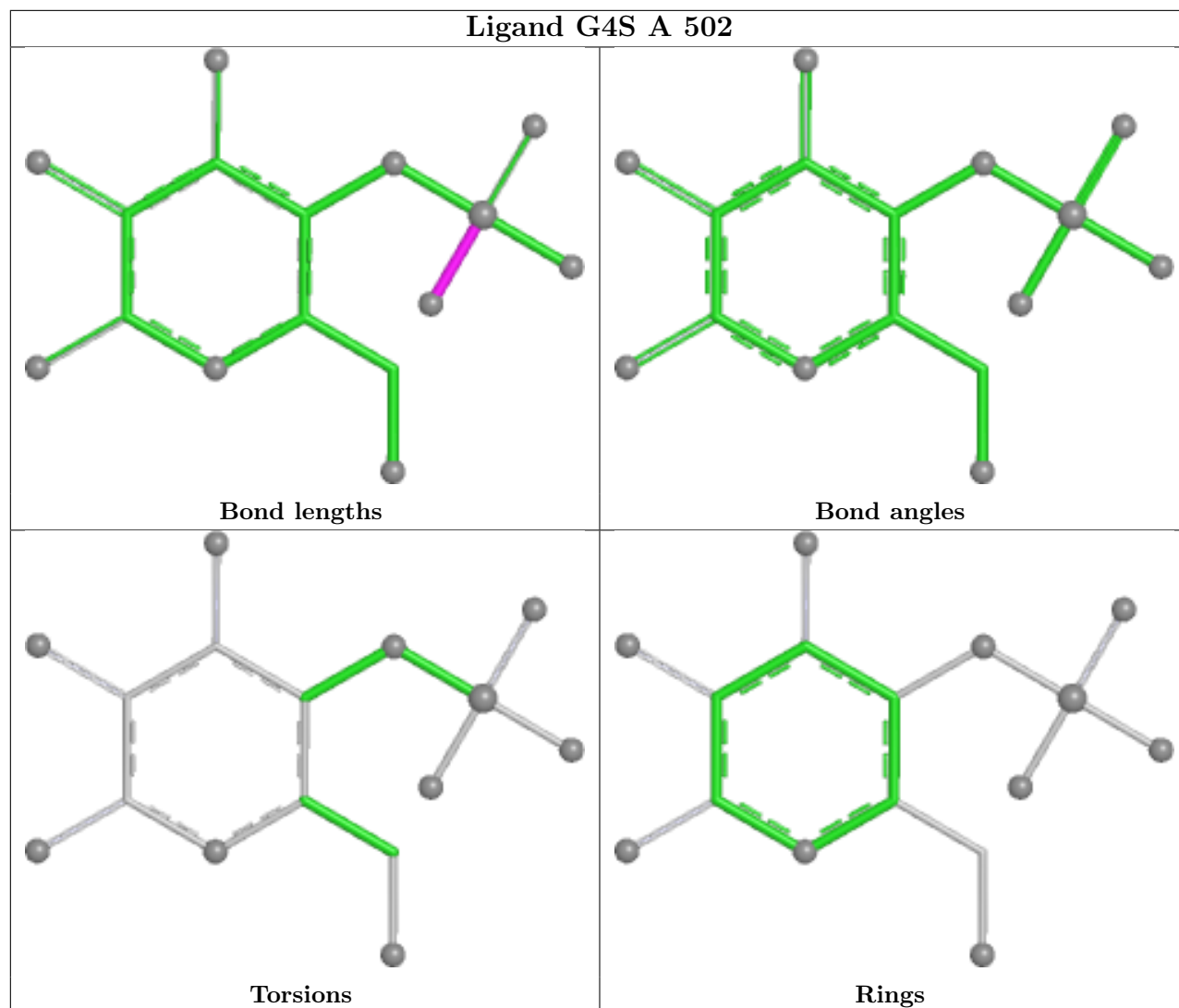
No monomer is involved in short contacts.

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.

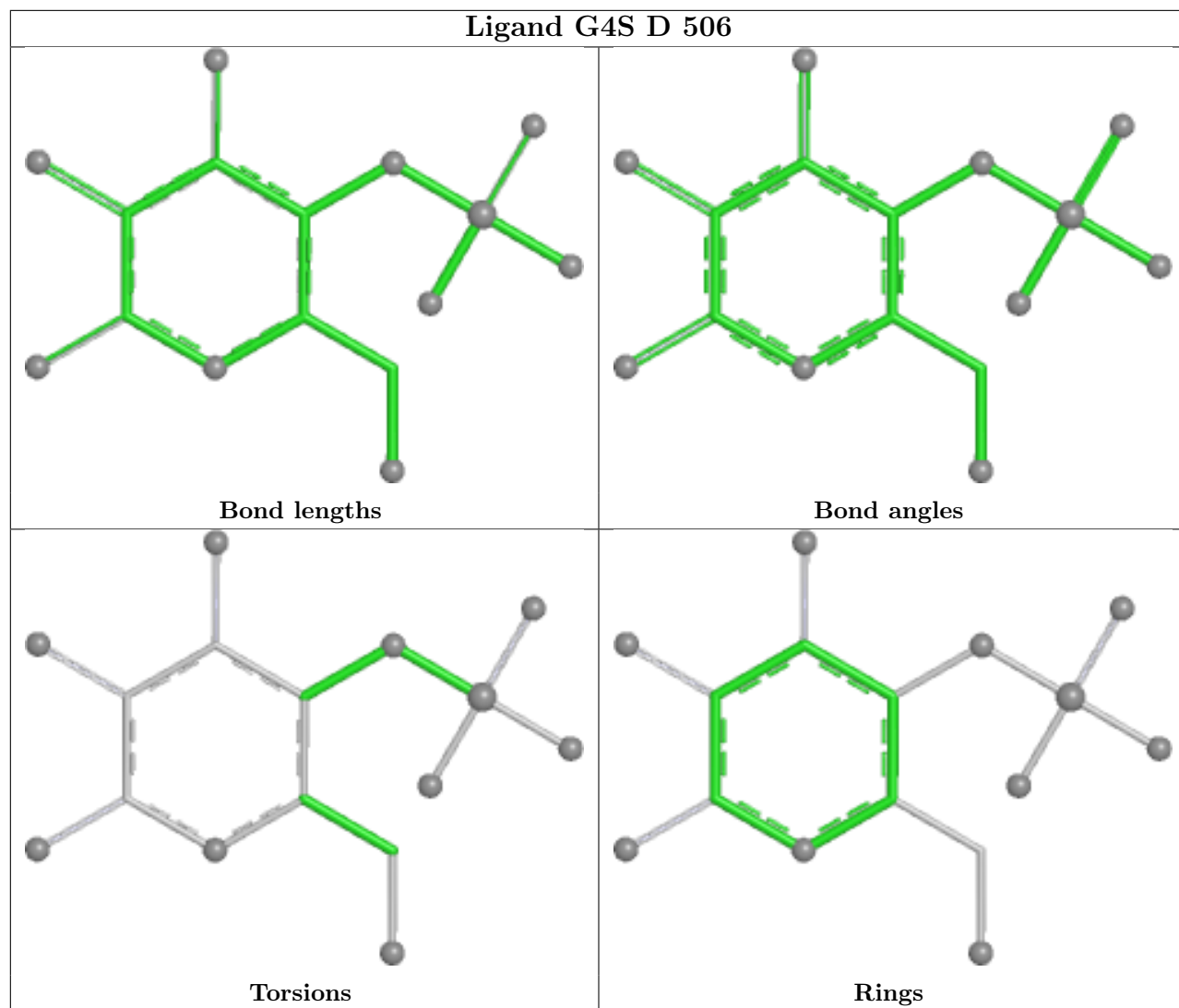
Ligand G4S B 503



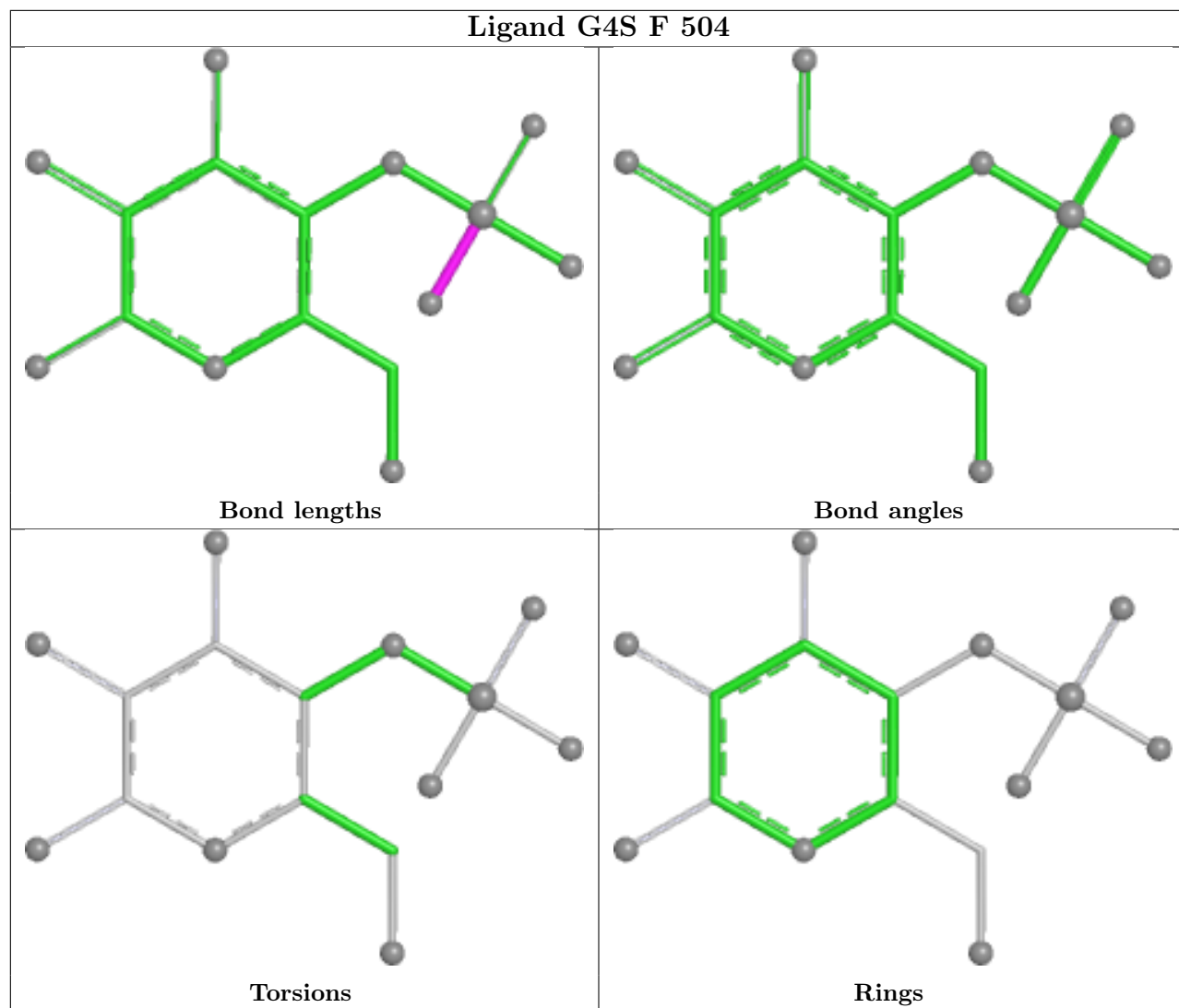
Ligand G4S A 502



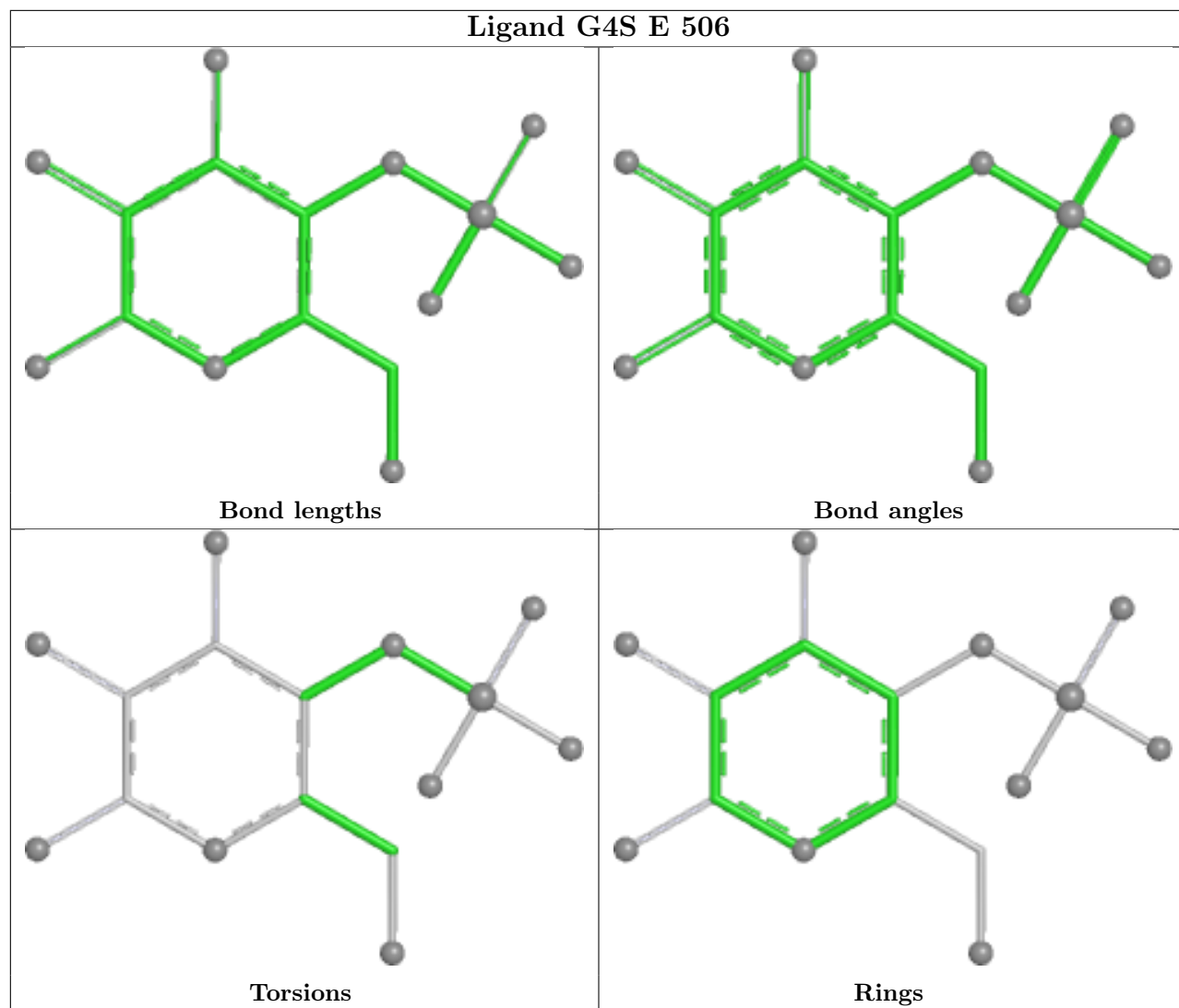
Ligand G4S D 506

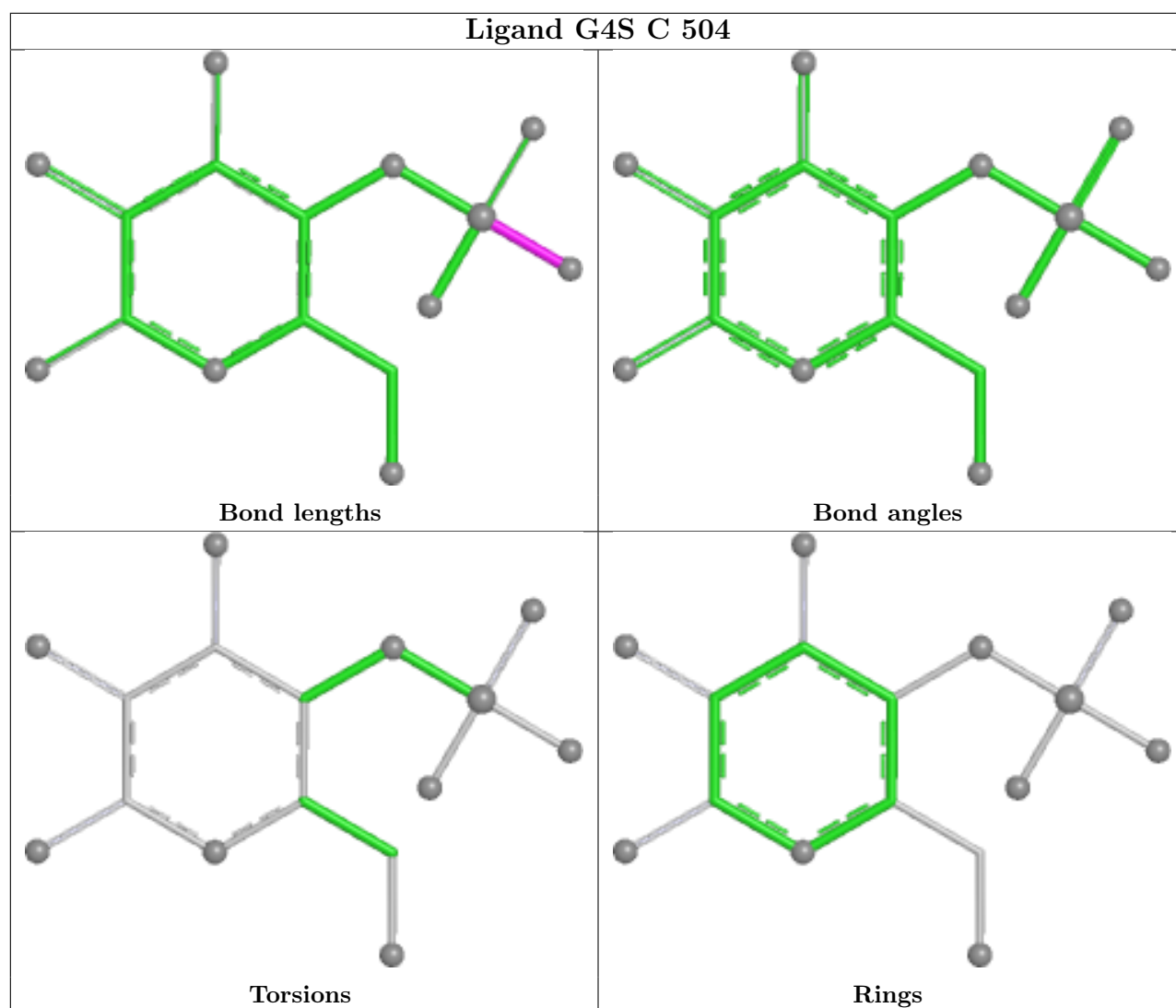


Ligand G4S F 504



Ligand G4S E 506





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	447/469 (95%)	-0.05	3 (0%) 84 88	9, 19, 32, 47	2 (0%)
1	B	447/469 (95%)	0.15	8 (1%) 67 75	11, 21, 36, 47	0
1	C	448/469 (95%)	-0.10	10 (2%) 62 69	11, 18, 32, 60	0
1	D	444/469 (94%)	0.12	12 (2%) 56 62	10, 21, 38, 57	1 (0%)
1	E	448/469 (95%)	-0.01	5 (1%) 78 83	8, 20, 34, 48	1 (0%)
1	F	447/469 (95%)	-0.21	4 (0%) 81 85	11, 17, 29, 56	0
All	All	2681/2814 (95%)	-0.02	42 (1%) 70 77	8, 19, 35, 60	4 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	26	ALA	5.3
1	F	26	ALA	4.5
1	C	180	GLY	4.3
1	C	26	ALA	4.0
1	A	50	THR	3.7
1	D	244	ALA	3.5
1	C	183	HIS	3.4
1	D	414	SER	3.3
1	D	180	GLY	3.0
1	D	27	SER	2.9
1	F	357	LEU	2.9
1	C	179	ASN	2.8
1	D	358	GLY	2.8
1	E	357	LEU	2.7
1	C	50	THR	2.6
1	B	332	GLY	2.6
1	D	357	LEU	2.6
1	E	248	ASN	2.4
1	F	356	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	183	HIS	2.4
1	A	428	GLU	2.4
1	E	356	ALA	2.3
1	D	176	GLU	2.3
1	E	221	GLU	2.3
1	B	243	LEU	2.3
1	B	473	PRO	2.3
1	D	473	PRO	2.3
1	A	330	LYS	2.3
1	D	184	PHE	2.2
1	D	175	GLN	2.2
1	C	184	PHE	2.2
1	D	193	PHE	2.2
1	D	174	GLU	2.1
1	B	242	ASP	2.1
1	C	181	ASN	2.1
1	B	432	THR	2.1
1	C	178	LYS	2.1
1	C	182	LYS	2.1
1	B	468	LEU	2.1
1	B	49	SER	2.0
1	C	359	SER	2.0
1	B	428	GLU	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.

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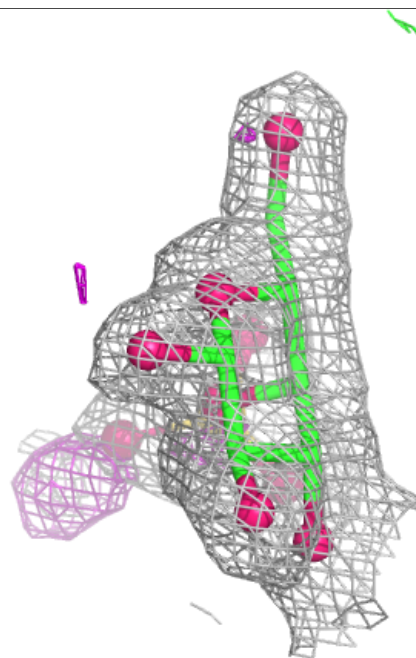
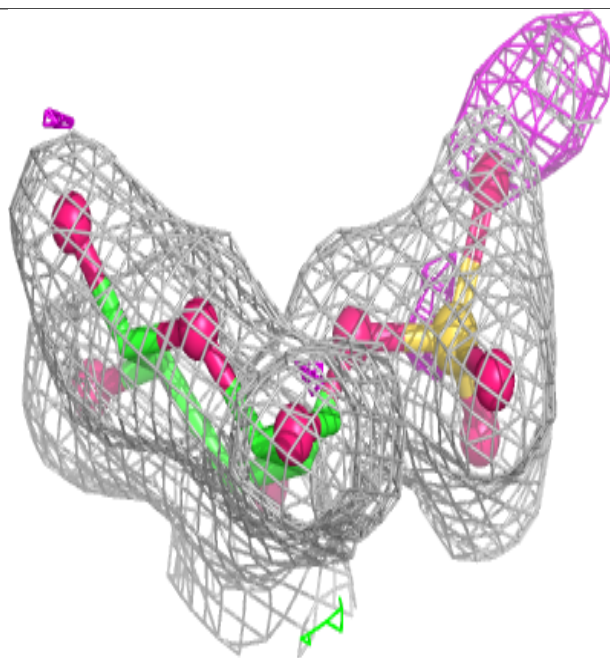
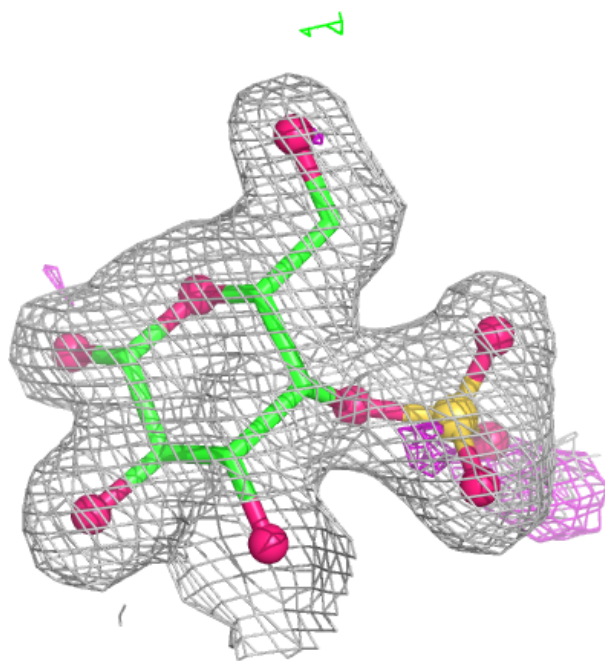
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	9RN	C	505	10/11	0.94	0.08	15,16,16,17	0
4	9RN	B	504	10/11	0.95	0.06	16,16,17,18	0
2	CA	A	501	1/1	0.95	0.14	26,26,26,26	1
7	EDO	C	503	4/4	0.95	0.08	19,23,23,23	0
7	EDO	D	505	4/4	0.95	0.09	27,29,30,31	0
4	9RN	D	507	10/11	0.96	0.06	18,19,20,20	0
4	9RN	E	507	10/11	0.96	0.06	15,17,18,20	0
7	EDO	A	507	4/4	0.96	0.06	23,25,25,26	0
2	CA	D	501	1/1	0.96	0.19	37,37,37,37	0
3	G4S	E	506	16/16	0.96	0.07	16,18,22,22	0
7	EDO	E	505	4/4	0.96	0.08	24,28,28,31	0
7	EDO	F	503	4/4	0.96	0.07	24,28,28,30	0
3	G4S	C	504	16/16	0.97	0.06	15,17,20,20	0
3	G4S	D	506	16/16	0.97	0.06	20,23,25,27	0
4	9RN	F	505	10/11	0.97	0.05	14,15,16,17	0
2	CA	E	501	1/1	0.97	0.13	24,24,24,24	1
3	G4S	F	504	16/16	0.97	0.06	13,15,17,17	0
4	9RN	A	503	10/11	0.97	0.05	15,17,17,18	0
3	G4S	A	502	16/16	0.97	0.06	16,17,20,23	0
3	G4S	B	503	16/16	0.97	0.06	17,19,22,23	0
5	CL	A	504	1/1	0.98	0.04	20,20,20,20	0
2	CA	C	501	1/1	0.98	0.13	28,28,28,28	1
2	CA	F	501	1/1	0.98	0.10	27,27,27,27	0
6	ZN	A	506	1/1	0.99	0.02	23,23,23,23	0
2	CA	B	501	1/1	0.99	0.17	27,27,27,27	1
5	CL	B	502	1/1	0.99	0.03	21,21,21,21	0
5	CL	C	502	1/1	0.99	0.04	17,17,17,17	0
5	CL	D	502	1/1	0.99	0.05	22,22,22,22	0
6	ZN	A	505	1/1	0.99	0.02	22,22,22,22	0
6	ZN	E	504	1/1	1.00	0.04	21,21,21,21	0
5	CL	E	502	1/1	1.00	0.02	17,17,17,17	0
5	CL	F	502	1/1	1.00	0.04	15,15,15,15	0
6	ZN	D	503	1/1	1.00	0.03	20,20,20,20	0
6	ZN	D	504	1/1	1.00	0.04	22,22,22,22	0
6	ZN	E	503	1/1	1.00	0.04	22,22,22,22	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.

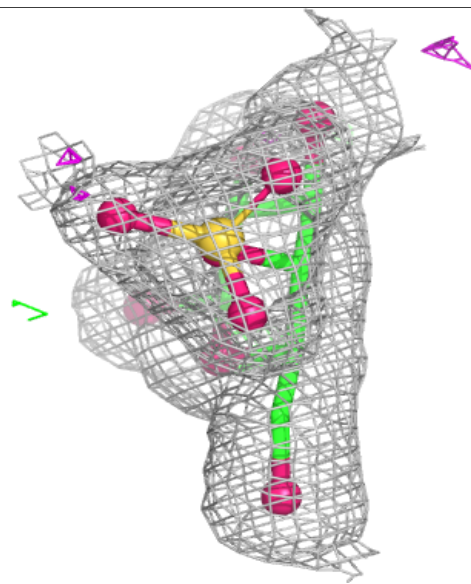
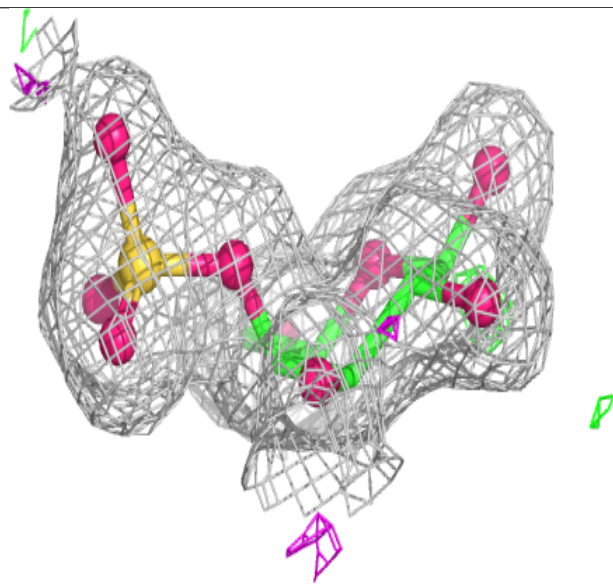
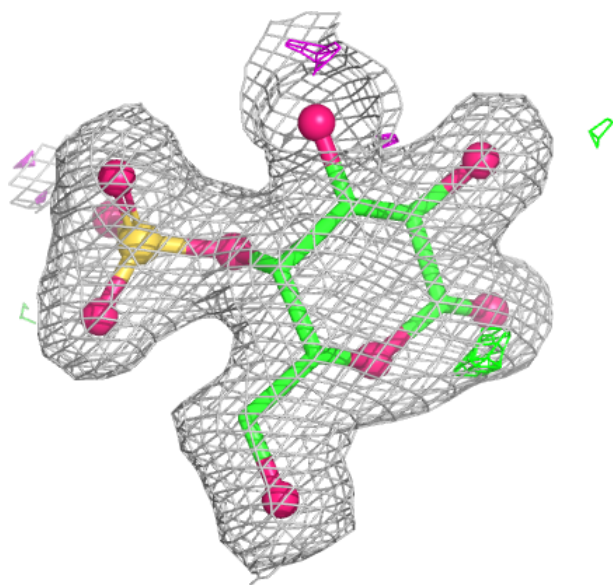
Electron density around G4S E 506:

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



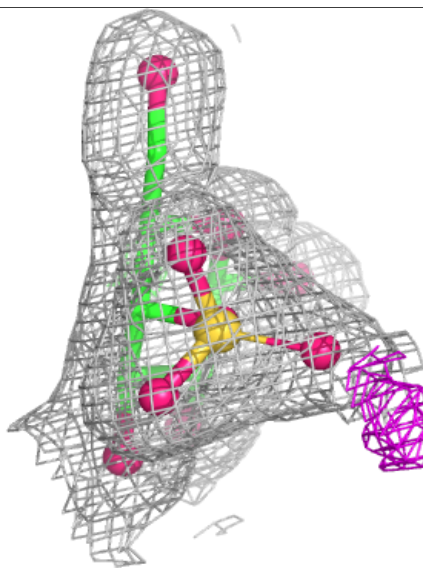
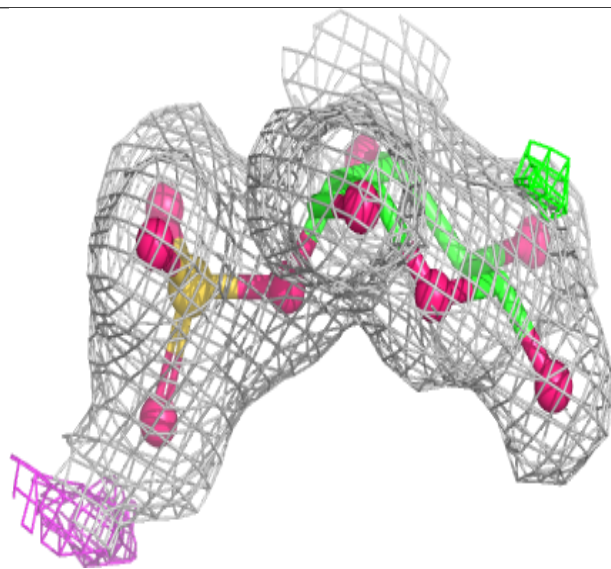
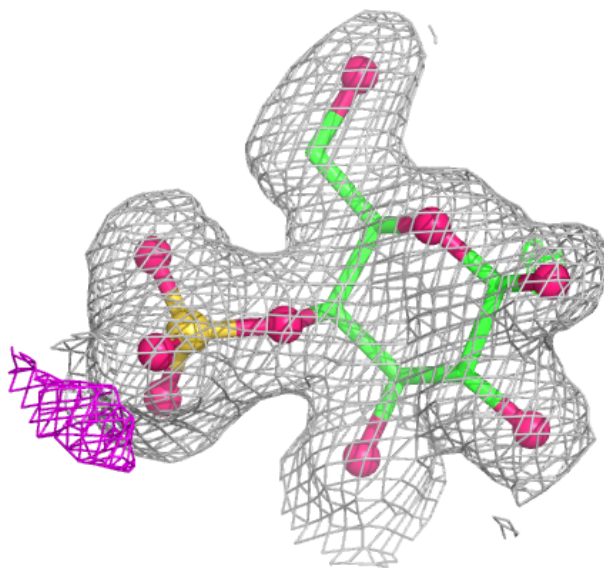
Electron density around G4S C 504:

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



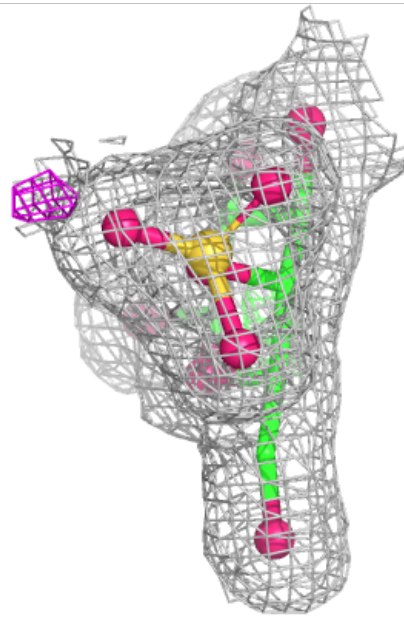
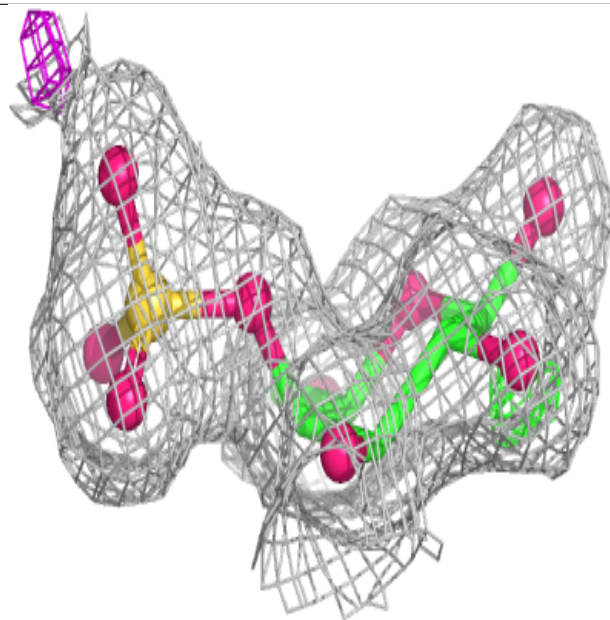
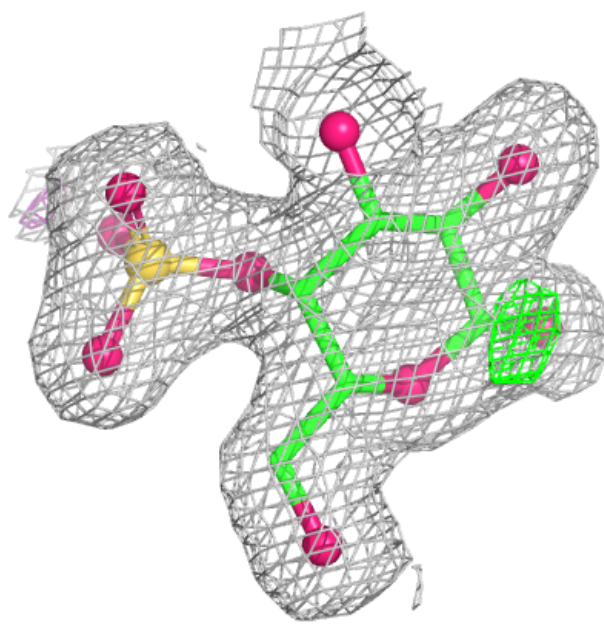
Electron density around G4S D 506:

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



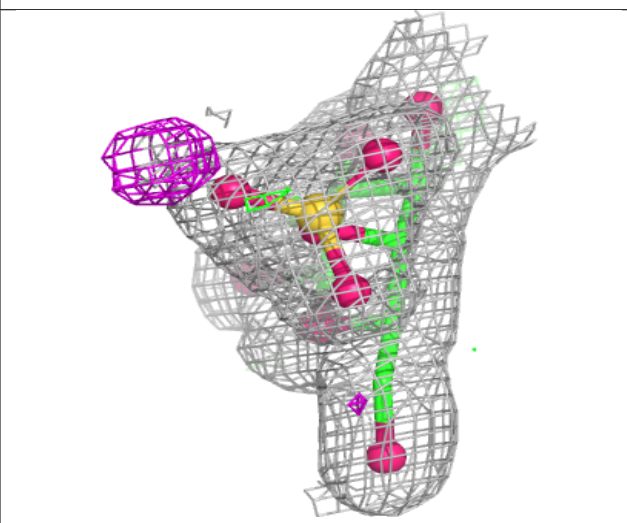
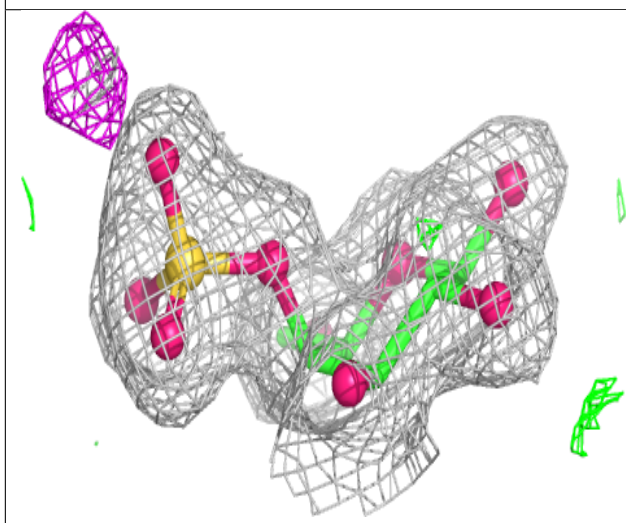
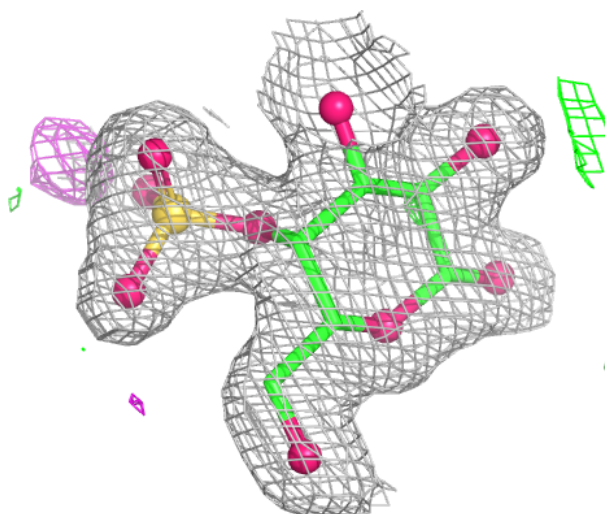
Electron density around G4S F 504:

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



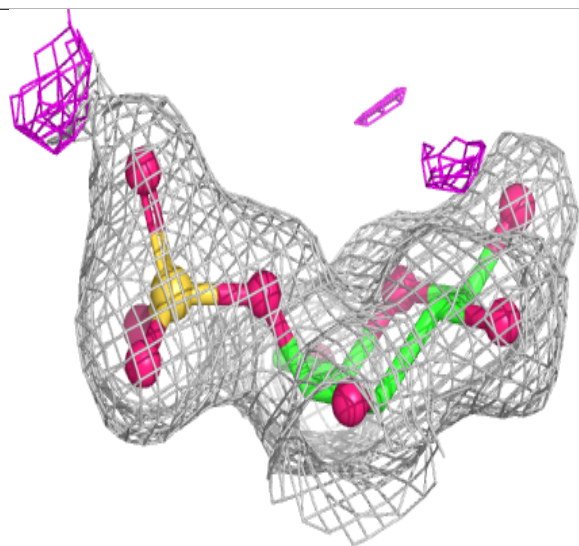
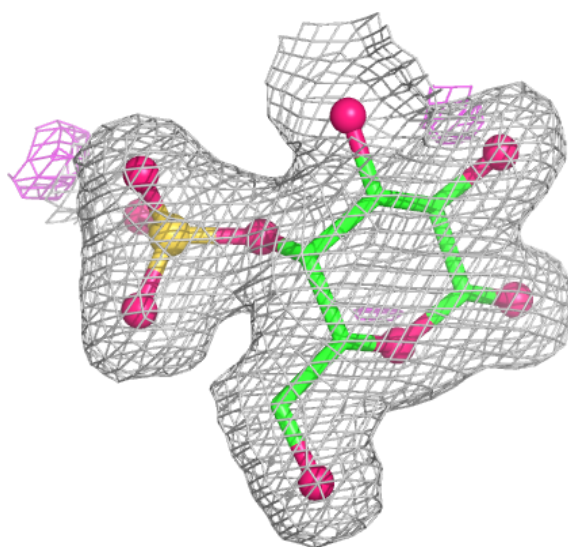
Electron density around G4S A 502:

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



Electron density around G4S B 503:

$2mF_o-DF_c$ (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.