



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 06:43 PM UTC

PDB ID : 6SHH / pdb_00006shh
Title : Human kallikrein 7 with aromatic coumarinic ester compound 1 covalently bound to H57
Authors : Hanke, S.; Straeter, N.
Deposited on : 2019-08-06
Resolution : 2.00 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

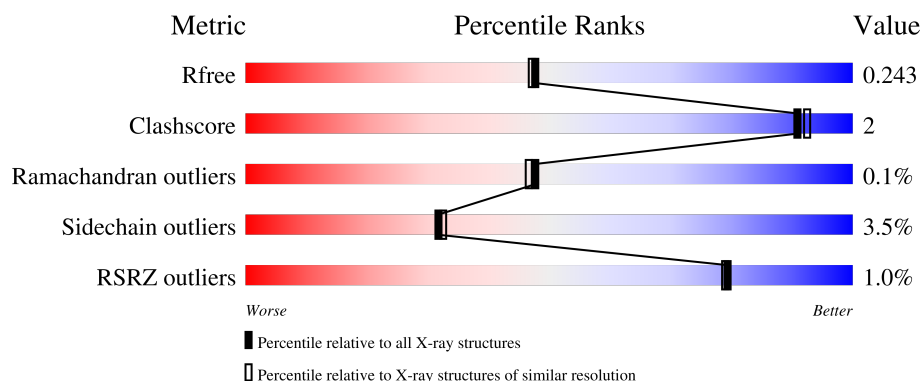
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	224	 95% .
1	B	224	 91% 9%
1	C	224	 92% 7%
1	D	224	 88% 11% .
1	E	224	 90% 10%

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Mol	Chain	Length	Quality of chain
1	F	224	95% 5%
1	G	224	2% 88% 10% •
1	H	224	% 91% 8%

2 Entry composition

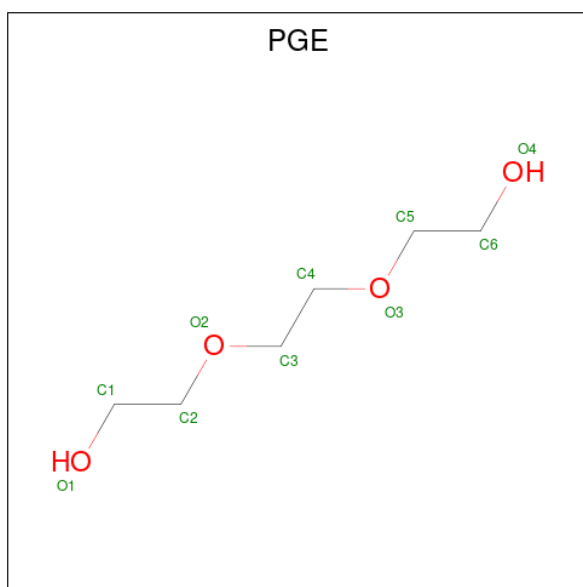
There are 6 unique types of molecules in this entry. The entry contains 15559 atoms, of which 56 are hydrogens and 0 are deuteriums.

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 Kallikrein-7.

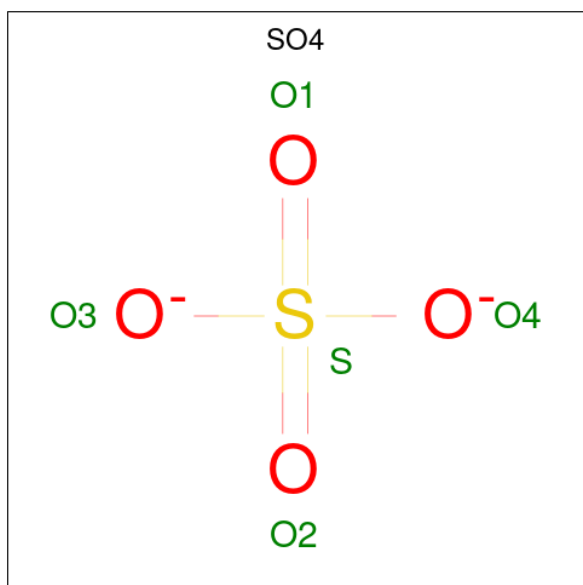
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	4	0
			1724	1074	312	320	18			
1	B	224	Total	C	N	O	S	0	4	0
			1699	1059	303	319	18			
1	C	224	Total	C	N	O	S	0	2	0
			1701	1057	308	318	18			
1	D	224	Total	C	N	O	S	0	2	0
			1709	1064	309	318	18			
1	E	224	Total	C	N	O	S	0	3	0
			1701	1062	304	317	18			
1	F	224	Total	C	N	O	S	0	2	0
			1696	1057	305	316	18			
1	G	224	Total	C	N	O	S	0	1	0
			1702	1059	309	316	18			
1	H	224	Total	C	N	O	S	0	1	0
			1697	1054	307	318	18			

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			24	6	14	4		
2	D	1	Total	C	H	O	0	0
			24	6	14	4		
2	E	1	Total	C	H	O	0	0
			24	6	14	4		
2	F	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

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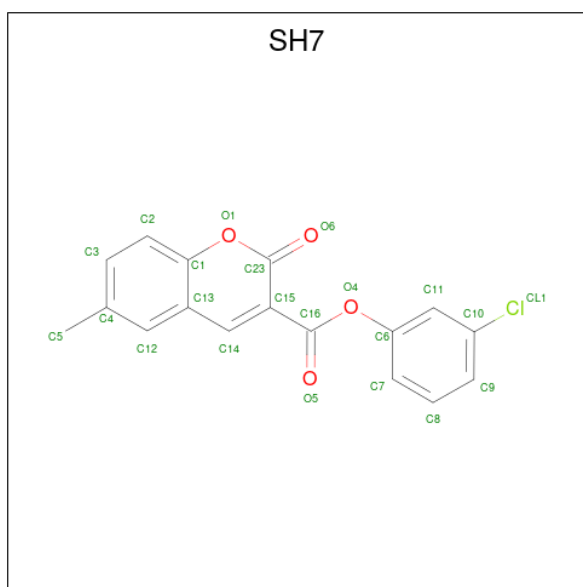
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

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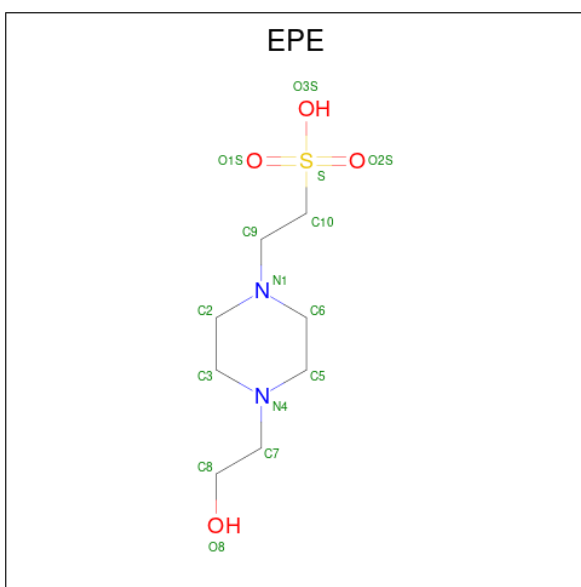
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is (3-chlorophenyl) 6-methyl-2-oxidanylidene-chromene-3-carboxylate (CCD ID: SH7) (formula: C₁₇H₁₁ClO₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			30	22	8		
4	B	1	Total	C	O	0	1
			30	22	8		
4	C	1	Total	C	O	0	1
			30	22	8		
4	D	1	Total	C	O	0	1
			30	22	8		
4	E	1	Total	C	O	0	1
			30	22	8		
4	F	1	Total	C	O	0	1
			30	22	8		
4	G	1	Total	C	O	0	1
			30	22	8		
4	H	1	Total	C	O	0	1
			30	22	8		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	157	Total	O	0	1
			157	157		
6	B	148	Total	O	0	1
			148	148		
6	C	159	Total	O	0	4
			159	159		
6	D	139	Total	O	0	2
			139	139		
6	E	162	Total	O	0	2
			162	162		
6	F	175	Total	O	0	2
			175	175		
6	G	103	Total	O	0	2
			103	103		
6	H	106	Total	O	0	1
			106	106		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

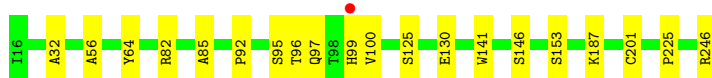
- Molecule 1: Kallikrein-7

Chain A:  95%



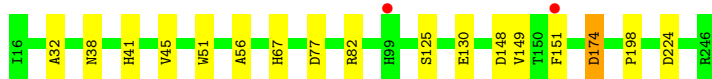
- Molecule 1: Kallikrein-7

Chain B:  91%

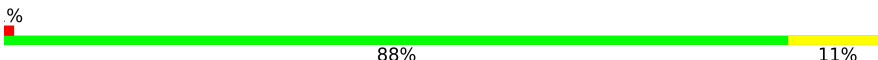


- Molecule 1: Kallikrein-7

Chain C:  92%

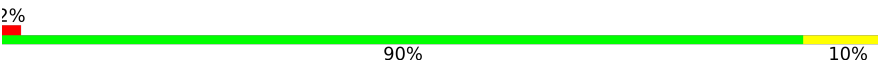


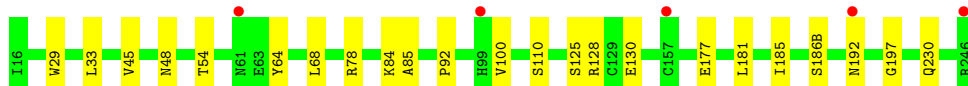
- Molecule 1: Kallikrein-7

Chain D:  88%

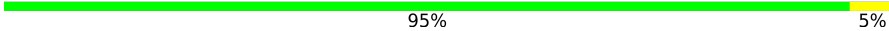


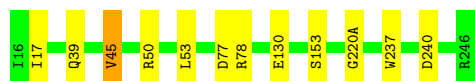
- Molecule 1: Kallikrein-7

Chain E:  90%



- Molecule 1: Kallikrein-7

Chain F:  95% 5%

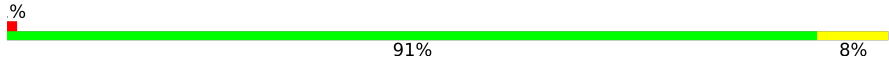


• Molecule 1: Kallikrein-7

Chain G:  88% 10% 2%



• Molecule 1: Kallikrein-7

Chain H:  91% 8% 1%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.63Å 116.41Å 290.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.03 – 2.00 47.03 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.03-2.00) 99.1 (47.03-2.00)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.189 , 0.226 0.202 , 0.243	Depositor DCC
R_{free} test set	2107 reflections (1.18%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15559	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: EPE, SO4, PGE, SH7

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	1.02	3/1772 (0.2%)	1.31	11/2406 (0.5%)
1	B	1.06	3/1744 (0.2%)	1.25	6/2371 (0.3%)
1	C	1.02	2/1740 (0.1%)	1.27	10/2365 (0.4%)
1	D	0.99	1/1751 (0.1%)	1.26	8/2379 (0.3%)
1	E	1.02	1/1743 (0.1%)	1.27	5/2371 (0.2%)
1	F	0.99	1/1738 (0.1%)	1.24	5/2364 (0.2%)
1	G	1.04	3/1741 (0.2%)	1.37	10/2365 (0.4%)
1	H	0.95	1/1736 (0.1%)	1.24	5/2361 (0.2%)
All	All	1.01	15/13965 (0.1%)	1.28	60/18982 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	2
All	All	0	4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	124	PRO	N-CA	16.63	1.67	1.47
1	H	130	GLU	C-N	13.82	1.49	1.33
1	B	130	GLU	C-N	13.42	1.49	1.33
1	C	130	GLU	C-N	13.40	1.49	1.33
1	D	130	GLU	C-N	13.40	1.49	1.33
1	A	130	GLU	C-N	13.35	1.49	1.33
1	F	130	GLU	C-N	13.32	1.49	1.33
1	E	130	GLU	C-N	13.30	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	130	GLU	C-N	13.21	1.49	1.33
1	G	123	LEU	C-N	9.15	1.44	1.33
1	A	235[A]	THR	C-O	6.76	1.32	1.24
1	A	235[B]	THR	C-O	6.76	1.32	1.24
1	B	225	PRO	C-O	-5.63	1.17	1.23
1	B	92	PRO	C-O	-5.50	1.17	1.24
1	C	41	HIS	C-O	-5.09	1.18	1.23

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	123	LEU	CA-C-N	16.56	137.29	119.90
1	G	123	LEU	C-N-CA	16.56	137.29	119.90
1	H	130	GLU	CA-C-N	11.52	132.24	120.38
1	H	130	GLU	C-N-CA	11.52	132.24	120.38
1	G	130	GLU	CA-C-N	10.61	131.31	120.38
1	G	130	GLU	C-N-CA	10.61	131.31	120.38
1	D	130	GLU	CA-C-N	10.26	130.94	120.38
1	D	130	GLU	C-N-CA	10.26	130.94	120.38
1	A	130	GLU	CA-C-N	10.00	130.68	120.38
1	A	130	GLU	C-N-CA	10.00	130.68	120.38
1	E	130	GLU	CA-C-N	9.98	130.66	120.38
1	E	130	GLU	C-N-CA	9.98	130.66	120.38
1	F	130	GLU	CA-C-N	9.83	130.51	120.38
1	F	130	GLU	C-N-CA	9.83	130.51	120.38
1	C	130	GLU	CA-C-N	9.82	130.49	120.38
1	C	130	GLU	C-N-CA	9.82	130.49	120.38
1	A	235[A]	THR	N-CA-C	9.38	123.76	111.75
1	A	235[B]	THR	N-CA-C	9.38	123.76	111.75
1	A	235[A]	THR	CA-C-O	8.67	129.91	120.20
1	A	235[B]	THR	CA-C-O	8.67	129.91	120.20
1	B	130	GLU	CA-C-N	8.55	129.18	120.38
1	B	130	GLU	C-N-CA	8.55	129.18	120.38
1	G	124	PRO	CA-N-CD	-7.17	101.96	112.00
1	D	174	ASP	CA-CB-CG	7.05	119.65	112.60
1	G	125	SER	N-CA-C	-7.01	104.36	113.12
1	B	99[A]	HIS	CB-CA-C	6.45	122.67	110.35
1	C	130	GLU	O-C-N	-6.30	114.37	121.43
1	B	130	GLU	O-C-N	-6.12	114.58	121.43
1	G	130	GLU	O-C-N	-6.04	115.08	121.30
1	C	51	TRP	N-CA-C	5.90	119.09	109.24
1	D	125	SER	N-CA-C	-5.84	106.19	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	192	ASN	CA-CB-CG	5.80	118.40	112.60
1	E	48	ASN	CA-CB-CG	5.79	118.39	112.60
1	C	174	ASP	CA-CB-CG	5.66	118.26	112.60
1	G	124	PRO	CB-CA-C	5.63	118.28	111.46
1	C	149	VAL	N-CA-C	5.56	116.99	108.71
1	C	224	ASP	CA-CB-CG	5.50	118.10	112.60
1	D	77	ASP	CA-CB-CG	5.49	118.09	112.60
1	H	240	ASP	CA-CB-CG	5.46	118.06	112.60
1	C	125	SER	N-CA-C	-5.45	107.17	113.88
1	G	77	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	125	SER	N-CA-C	-5.41	106.81	113.41
1	D	65	THR	N-CA-C	-5.38	99.64	108.41
1	A	235[A]	THR	O-C-N	-5.37	116.08	122.20
1	A	235[B]	THR	O-C-N	-5.37	116.08	122.20
1	A	130	GLU	O-C-N	-5.35	115.44	121.43
1	H	130	GLU	O-C-N	-5.30	115.84	121.30
1	E	125	SER	N-CA-C	-5.28	106.97	113.41
1	F	77	ASP	CA-CB-CG	5.25	117.85	112.60
1	E	130	GLU	O-C-N	-5.23	115.57	121.43
1	B	99[A]	HIS	N-CA-CB	5.21	122.81	114.27
1	D	131	PRO	N-CA-C	5.19	117.03	110.70
1	A	131	PRO	N-CA-C	5.15	116.99	110.70
1	C	77	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	151	PHE	N-CA-C	5.12	116.82	109.04
1	G	240	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	198	PRO	N-CA-C	5.06	120.13	111.68
1	F	240	ASP	CA-C-N	5.05	127.00	120.44
1	F	240	ASP	C-N-CA	5.05	127.00	120.44
1	H	140	GLY	N-CA-C	5.01	117.99	110.18

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	56	ALA	Mainchain
1	C	56	ALA	Mainchain

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	1724	0	1710	6	0
1	B	1699	0	1659	3	0
1	C	1701	0	1661	3	0
1	D	1709	0	1683	8	0
1	E	1701	0	1667	8	0
1	F	1696	0	1659	4	0
1	G	1702	0	1672	11	0
1	H	1697	0	1652	4	0
2	A	10	14	14	0	0
2	D	10	14	14	1	0
2	E	10	14	14	0	0
2	F	10	14	14	1	0
3	A	45	0	0	1	0
3	B	65	0	0	0	0
3	C	65	0	0	0	0
3	D	50	0	0	0	0
3	E	40	0	0	0	0
3	F	50	0	0	0	0
3	G	45	0	0	0	0
3	H	55	0	0	0	0
4	A	30	0	0	0	0
4	B	30	0	0	0	0
4	C	30	0	0	0	0
4	D	30	0	0	0	0
4	E	30	0	0	0	0
4	F	30	0	0	0	0
4	G	30	0	0	0	0
4	H	30	0	0	0	0
5	G	15	0	17	0	0
5	H	15	0	17	0	0
6	A	157	0	0	0	0
6	B	148	0	0	1	0
6	C	159	0	0	0	0
6	D	139	0	0	1	0
6	E	162	0	0	1	0
6	F	175	0	0	0	0
6	G	103	0	0	0	0
6	H	106	0	0	0	0
All	All	15503	56	13453	46	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 (46) 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:G:124:PRO:N	1:G:124:PRO:CA	1.67	1.44
1:D:82:ARG:HE	2:D:301:PGE:H62	1.58	0.69
1:F:50:ARG:O	1:F:50:ARG:HG3	2.00	0.61
1:G:124:PRO:N	1:G:124:PRO:C	2.55	0.59
1:D:38:ASN:OD1	1:D:82:ARG:NH2	2.33	0.58
1:D:167:ASP:HA	1:D:170:LYS:HD3	1.86	0.57
1:G:100:VAL:HG23	1:G:177:GLU:HG2	1.87	0.57
1:G:24:ARG:HE	1:G:24:ARG:H	1.53	0.56
1:G:64:TYR:HB2	1:G:85:ALA:HB3	1.90	0.53
1:H:64:TYR:HB2	1:H:85:ALA:HB3	1.92	0.52
1:F:45:VAL:HG23	1:F:53:LEU:HB3	1.91	0.52
1:E:64:TYR:HB2	1:E:85:ALA:HB3	1.93	0.51
1:F:237:TRP:HB2	2:F:301:PGE:H5	1.92	0.50
1:E:100:VAL:HG23	1:E:177:GLU:HG3	1.94	0.49
1:D:50:ARG:O	1:D:50:ARG:HG3	2.13	0.48
1:G:32:ALA:HB3	1:G:67:HIS:HB3	1.96	0.47
6:B:488:HOH:O	1:E:78:ARG:HG2	2.14	0.47
1:D:163:ILE:HD12	1:D:225:PRO:HB3	1.96	0.46
1:A:45[A]:VAL:HG23	1:A:53:LEU:HB3	1.97	0.46
1:A:64:TYR:HB2	1:A:85:ALA:HB3	1.98	0.46
1:D:197:GLY:HA3	6:D:421:HOH:O	2.16	0.45
1:C:32:ALA:HB3	1:C:67:HIS:HB3	1.99	0.45
1:E:92:PRO:HG2	1:G:92:PRO:HG2	1.98	0.44
1:A:45[A]:VAL:CG1	1:A:198:PRO:HB3	2.48	0.44
1:G:24:ARG:H	1:G:24:ARG:NE	2.16	0.44
1:H:48:ASN:HA	1:H:120:LYS:HD3	1.99	0.44
1:A:45[A]:VAL:HG11	1:A:198:PRO:HB3	2.00	0.44
1:F:17:ILE:HG21	1:F:220(A):GLY:HA3	2.00	0.43
1:E:33:LEU:HD11	1:E:54:THR:HG21	1.99	0.43
1:E:197:GLY:HA3	6:E:404:HOH:O	2.19	0.43
1:C:45:VAL:CG1	1:C:198:PRO:HB3	2.48	0.42
1:G:50:ARG:HH21	1:G:111:GLN:HG3	1.84	0.42
1:B:64:TYR:HB2	1:B:85:ALA:HB3	2.00	0.42
1:E:181:LEU:HD22	1:E:230:GLN:HG3	2.01	0.42
1:G:70:SER:HB3	1:G:80:ALA:HB2	2.02	0.42
1:A:128:ARG:HD2	3:A:304:SO4:O1	2.20	0.41
1:H:218:PHE:HA	1:H:219:PRO:C	2.44	0.41
1:D:218:PHE:HA	1:D:219:PRO:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:172:TYR:HB2	1:H:176:LEU:HD13	2.02	0.41
1:B:32:ALA:HB2	1:B:141:TRP:CZ3	2.56	0.41
1:G:100:VAL:CG2	1:G:177:GLU:HG2	2.50	0.41
1:D:230:GLN:HG2	1:D:232:CYS:SG	2.61	0.40
1:A:45[B]:VAL:HG12	1:A:53:LEU:HB3	2.03	0.40
1:B:95:SER:HB3	1:B:100:VAL:HG12	2.03	0.40
1:C:38:ASN:OD1	1:C:82:ARG:NH2	2.55	0.40
1:E:185:ILE:HB	1:E:186(B):SER:HB3	2.04	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	226/224 (101%)	221 (98%)	5 (2%)	0	100	100
1	B	225/224 (100%)	217 (96%)	8 (4%)	0	100	100
1	C	223/224 (100%)	218 (98%)	5 (2%)	0	100	100
1	D	224/224 (100%)	221 (99%)	3 (1%)	0	100	100
1	E	225/224 (100%)	221 (98%)	4 (2%)	0	100	100
1	F	224/224 (100%)	220 (98%)	4 (2%)	0	100	100
1	G	223/224 (100%)	217 (97%)	6 (3%)	0	100	100
1	H	223/224 (100%)	217 (97%)	5 (2%)	1 (0%)	30	27
All	All	1793/1792 (100%)	1752 (98%)	40 (2%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	188	LYS

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	197/194 (102%)	195 (99%)	2 (1%)	68	75
1	B	192/194 (99%)	184 (96%)	8 (4%)	26	25
1	C	192/194 (99%)	190 (99%)	2 (1%)	68	75
1	D	194/194 (100%)	183 (94%)	11 (6%)	18	15
1	E	192/194 (99%)	184 (96%)	8 (4%)	26	25
1	F	191/194 (98%)	187 (98%)	4 (2%)	47	52
1	G	192/194 (99%)	182 (95%)	10 (5%)	21	18
1	H	191/194 (98%)	182 (95%)	9 (5%)	23	22
All	All	1541/1552 (99%)	1487 (96%)	54 (4%)	32	32

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	178	ASN
1	B	82	ARG
1	B	96	THR
1	B	97	GLN
1	B	146	SER
1	B	153	SER
1	B	187	LYS
1	B	201	CYS
1	B	246	ARG
1	C	148	ASP
1	C	174	ASP
1	D	39	GLN
1	D	68	LEU
1	D	78	ARG
1	D	81	GLN
1	D	82	ARG
1	D	84	LYS
1	D	96	THR

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Mol	Chain	Res	Type
1	D	153	SER
1	D	167	ASP
1	D	169	THR
1	D	174	ASP
1	E	29	TRP
1	E	45[A]	VAL
1	E	45[B]	VAL
1	E	68	LEU
1	E	84	LYS
1	E	110	SER
1	E	128	ARG
1	E	192	ASN
1	F	39	GLN
1	F	45	VAL
1	F	78	ARG
1	F	153	SER
1	G	24	ARG
1	G	29	TRP
1	G	45	VAL
1	G	82	ARG
1	G	96	THR
1	G	122	ARG
1	G	163	ILE
1	G	177	GLU
1	G	189	ASN
1	G	235	THR
1	H	29	TRP
1	H	45	VAL
1	H	49	GLU
1	H	67	HIS
1	H	96	THR
1	H	116	SER
1	H	153	SER
1	H	176	LEU
1	H	178	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	A	230	GLN
1	B	41	HIS

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Mol	Chain	Res	Type
1	B	192	ASN
1	C	97	GLN
1	C	99[A]	HIS
1	C	245	HIS
1	D	41	HIS
1	E	41	HIS
1	E	192	ASN
1	E	245	HIS
1	F	97	GLN
1	G	41	HIS
1	G	111	GLN
1	G	178	ASN
1	H	192	ASN

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](#)

105 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	$\# Z > 2$
3	SO4	H	310	-	4,4,4	0.28	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	E	302	-	4,4,4	0.44	0	6,6,6	0.14	0
3	SO4	D	306	-	4,4,4	0.51	0	6,6,6	0.67	0
3	SO4	D	310	-	4,4,4	0.57	0	6,6,6	0.13	0
3	SO4	A	310	-	4,4,4	0.31	0	6,6,6	0.46	0
3	SO4	H	311	-	4,4,4	0.37	0	6,6,6	0.11	0
4	SH7	E	350[A]	1	16,16,24	1.63	2 (12%)	23,23,34	1.94	4 (17%)
3	SO4	B	304	-	4,4,4	0.47	0	6,6,6	0.86	0
3	SO4	H	308	-	4,4,4	0.23	0	6,6,6	0.22	0
3	SO4	F	303	-	4,4,4	0.39	0	6,6,6	0.27	0
3	SO4	F	307	-	4,4,4	0.77	0	6,6,6	0.22	0
3	SO4	A	306	-	4,4,4	0.22	0	6,6,6	0.12	0
3	SO4	F	309	-	4,4,4	0.64	0	6,6,6	0.17	0
3	SO4	C	308	-	4,4,4	0.26	0	6,6,6	0.19	0
4	SH7	F	350[A]	1	16,16,24	0.65	0	23,23,34	1.34	3 (13%)
2	PGE	D	301	-	9,9,9	0.25	0	8,8,8	0.17	0
3	SO4	B	308	-	4,4,4	0.28	0	6,6,6	0.16	0
3	SO4	D	305	-	4,4,4	0.83	0	6,6,6	0.12	0
3	SO4	G	310	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	C	307	-	4,4,4	0.26	0	6,6,6	0.17	0
2	PGE	A	301	-	9,9,9	0.45	0	8,8,8	0.25	0
3	SO4	F	306	-	4,4,4	0.69	0	6,6,6	0.21	0
3	SO4	B	307	-	4,4,4	0.38	0	6,6,6	0.13	0
4	SH7	A	350[A]	1	16,16,24	0.61	0	23,23,34	0.80	0
3	SO4	D	308	-	4,4,4	0.23	0	6,6,6	0.98	0
4	SH7	C	350[A]	1	16,16,24	0.70	0	23,23,34	1.25	2 (8%)
5	EPE	H	301	-	15,15,15	1.12	1 (6%)	19,20,20	0.39	0
3	SO4	A	308	-	4,4,4	0.28	0	6,6,6	0.23	0
4	SH7	F	350[B]	1	16,16,24	0.61	1 (6%)	23,23,34	1.15	2 (8%)
3	SO4	H	306	-	4,4,4	0.29	0	6,6,6	0.19	0
3	SO4	D	307	-	4,4,4	0.68	0	6,6,6	0.08	0
3	SO4	B	310	-	4,4,4	0.31	0	6,6,6	0.26	0
3	SO4	E	306	-	4,4,4	0.30	0	6,6,6	0.20	0
4	SH7	B	350[B]	1	16,16,24	0.66	0	23,23,34	1.12	2 (8%)
3	SO4	A	302	-	4,4,4	0.49	0	6,6,6	0.27	0
3	SO4	E	309	-	4,4,4	0.38	0	6,6,6	0.41	0
4	SH7	D	350[A]	1	16,16,24	0.62	1 (6%)	23,23,34	1.05	3 (13%)
3	SO4	G	303	-	4,4,4	0.29	0	6,6,6	0.13	0
5	EPE	G	301	-	15,15,15	1.22	1 (6%)	19,20,20	0.49	0
3	SO4	G	304	-	4,4,4	0.27	0	6,6,6	0.09	0
3	SO4	H	309	-	4,4,4	0.26	0	6,6,6	0.20	0
4	SH7	G	350[A]	1	16,16,24	0.64	0	23,23,34	1.28	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	F	311	-	4,4,4	0.28	0	6,6,6	0.16	0
3	SO4	B	305	-	4,4,4	0.36	0	6,6,6	0.14	0
3	SO4	G	308	-	4,4,4	0.29	0	6,6,6	0.11	0
4	SH7	E	350[B]	1	16,16,24	1.64	2 (12%)	23,23,34	1.58	2 (8%)
3	SO4	G	305	-	4,4,4	0.26	0	6,6,6	0.12	0
3	SO4	F	308	-	4,4,4	0.46	0	6,6,6	0.22	0
3	SO4	B	301	-	4,4,4	0.41	0	6,6,6	0.31	0
3	SO4	C	303	-	4,4,4	0.25	0	6,6,6	0.47	0
3	SO4	E	305	-	4,4,4	0.25	0	6,6,6	0.12	0
3	SO4	G	302	-	4,4,4	0.31	0	6,6,6	0.24	0
3	SO4	A	305	-	4,4,4	0.67	0	6,6,6	0.16	0
3	SO4	C	305	-	4,4,4	0.73	0	6,6,6	0.08	0
2	PGE	E	301	-	9,9,9	0.38	0	8,8,8	0.43	0
3	SO4	C	310	-	4,4,4	0.35	0	6,6,6	0.16	0
3	SO4	B	312	-	4,4,4	0.67	0	6,6,6	0.27	0
3	SO4	D	304	-	4,4,4	0.38	0	6,6,6	0.33	0
3	SO4	E	303	-	4,4,4	0.25	0	6,6,6	0.33	0
3	SO4	D	309	-	4,4,4	0.61	0	6,6,6	0.11	0
3	SO4	H	305	-	4,4,4	0.34	0	6,6,6	0.20	0
3	SO4	C	306	-	4,4,4	0.27	0	6,6,6	0.11	0
4	SH7	A	350[B]	1	16,16,24	0.61	1 (6%)	23,23,34	0.79	1 (4%)
3	SO4	D	311	-	4,4,4	0.28	0	6,6,6	0.11	0
4	SH7	C	350[B]	1	16,16,24	0.66	1 (6%)	23,23,34	1.56	3 (13%)
3	SO4	B	306	-	4,4,4	0.32	0	6,6,6	0.21	0
3	SO4	C	304	-	4,4,4	0.81	0	6,6,6	0.29	0
3	SO4	E	307	-	4,4,4	0.63	0	6,6,6	0.10	0
3	SO4	C	313	-	4,4,4	0.28	0	6,6,6	0.37	0
3	SO4	G	307	-	4,4,4	0.25	0	6,6,6	0.07	0
3	SO4	E	308	-	4,4,4	0.25	0	6,6,6	0.24	0
3	SO4	C	301	-	4,4,4	0.22	0	6,6,6	0.39	0
3	SO4	A	309	-	4,4,4	0.29	0	6,6,6	0.35	0
3	SO4	H	304	-	4,4,4	0.35	0	6,6,6	0.52	0
4	SH7	D	350[B]	1	16,16,24	0.72	0	23,23,34	0.89	0
3	SO4	H	307	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	C	309	-	4,4,4	0.33	0	6,6,6	0.10	0
3	SO4	G	306	-	4,4,4	0.56	0	6,6,6	0.09	0
4	SH7	G	350[B]	1	16,16,24	0.62	1 (6%)	23,23,34	0.79	1 (4%)
3	SO4	C	312	-	4,4,4	0.31	0	6,6,6	0.23	0
3	SO4	H	312	-	4,4,4	0.22	0	6,6,6	0.19	0
3	SO4	F	304	-	4,4,4	0.30	0	6,6,6	0.20	0
3	SO4	B	309	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	C	311	-	4,4,4	0.48	0	6,6,6	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	H	302	-	4,4,4	0.31	0	6,6,6	0.21	0
4	SH7	H	350[A]	1	16,16,24	1.65	2 (12%)	23,23,34	1.61	2 (8%)
3	SO4	B	313	-	4,4,4	0.48	0	6,6,6	0.42	0
3	SO4	B	311	-	4,4,4	0.28	0	6,6,6	0.09	0
3	SO4	H	303	-	4,4,4	0.32	0	6,6,6	0.15	0
3	SO4	C	302	-	4,4,4	0.44	0	6,6,6	0.29	0
3	SO4	F	302	-	4,4,4	0.31	0	6,6,6	0.33	0
3	SO4	B	302	-	4,4,4	0.43	0	6,6,6	0.28	0
3	SO4	D	303	-	4,4,4	0.36	0	6,6,6	0.14	0
3	SO4	F	305	-	4,4,4	0.73	0	6,6,6	0.11	0
3	SO4	A	303	-	4,4,4	0.28	0	6,6,6	0.21	0
3	SO4	G	309	-	4,4,4	0.25	0	6,6,6	0.19	0
3	SO4	E	304	-	4,4,4	0.65	0	6,6,6	0.17	0
3	SO4	F	310	-	4,4,4	0.43	0	6,6,6	0.11	0
3	SO4	B	303	-	4,4,4	0.23	0	6,6,6	0.27	0
3	SO4	A	304	-	4,4,4	0.21	0	6,6,6	0.23	0
4	SH7	H	350[B]	1	16,16,24	1.65	2 (12%)	23,23,34	1.61	2 (8%)
3	SO4	A	307	-	4,4,4	0.49	0	6,6,6	0.64	0
2	PGE	F	301	-	9,9,9	0.19	0	8,8,8	0.37	0
4	SH7	B	350[A]	1	16,16,24	0.68	0	23,23,34	0.87	1 (4%)
3	SO4	D	302	-	4,4,4	0.29	0	6,6,6	0.21	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	SH7	E	350[B]	1	-	4/4/4/8	0/2/2/3
2	PGE	A	301	-	-	4/7/7/7	-
4	SH7	A	350[A]	1	-	4/4/4/8	0/2/2/3
4	SH7	D	350[B]	1	-	0/4/4/8	0/2/2/3
4	SH7	C	350[A]	1	-	4/4/4/8	0/2/2/3
5	EPE	H	301	-	-	2/9/19/19	0/1/1/1
4	SH7	F	350[B]	1	-	4/4/4/8	0/2/2/3
4	SH7	G	350[B]	1	-	4/4/4/8	0/2/2/3
2	PGE	E	301	-	-	4/7/7/7	-
4	SH7	H	350[A]	1	-	4/4/4/8	0/2/2/3
4	SH7	B	350[B]	1	-	2/4/4/8	0/2/2/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SH7	E	350[A]	1	-	4/4/4/8	0/2/2/3
4	SH7	D	350[A]	1	-	4/4/4/8	0/2/2/3
5	EPE	G	301	-	-	8/9/19/19	0/1/1/1
4	SH7	A	350[B]	1	-	4/4/4/8	0/2/2/3
4	SH7	C	350[B]	1	-	1/4/4/8	0/2/2/3
4	SH7	F	350[A]	1	-	4/4/4/8	0/2/2/3
4	SH7	G	350[A]	1	-	4/4/4/8	0/2/2/3
2	PGE	D	301	-	-	3/7/7/7	-
4	SH7	H	350[B]	1	-	4/4/4/8	0/2/2/3
2	PGE	F	301	-	-	2/7/7/7	-
4	SH7	B	350[A]	1	-	4/4/4/8	0/2/2/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	350[A]	SH7	O5-C16	5.45	1.36	1.22
4	H	350[B]	SH7	O5-C16	5.43	1.36	1.22
4	E	350[B]	SH7	O5-C16	5.38	1.35	1.22
4	E	350[A]	SH7	O5-C16	5.29	1.35	1.22
5	G	301	EPE	C10-S	-4.67	1.71	1.77
5	H	301	EPE	C10-S	-4.25	1.71	1.77
4	H	350[A]	SH7	O4-C16	-3.48	1.21	1.30
4	E	350[A]	SH7	O4-C16	-3.45	1.21	1.30
4	H	350[B]	SH7	O4-C16	-3.44	1.21	1.30
4	E	350[B]	SH7	O4-C16	-3.43	1.21	1.30
4	C	350[B]	SH7	O4-C16	2.08	1.36	1.30
4	G	350[B]	SH7	O4-C16	2.06	1.36	1.30
4	D	350[A]	SH7	O4-C16	2.03	1.36	1.30
4	A	350[B]	SH7	O4-C16	2.03	1.36	1.30
4	F	350[B]	SH7	O4-C16	2.02	1.36	1.30

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	350[A]	SH7	O5-C16-C15	-5.71	110.86	122.67
4	H	350[B]	SH7	O5-C16-C15	-5.67	110.95	122.67
4	E	350[B]	SH7	O5-C16-C15	-5.61	111.06	122.67
4	E	350[A]	SH7	O5-C16-C15	-5.50	111.28	122.67
4	C	350[B]	SH7	C23-C15-C16	-5.19	116.82	120.33
4	E	350[A]	SH7	C23-C15-C16	-4.36	117.38	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	350[A]	SH7	C23-C15-C16	-4.21	117.48	120.33
4	H	350[B]	SH7	O4-C16-C15	4.10	125.29	115.69
4	E	350[B]	SH7	O4-C16-C15	4.09	125.27	115.69
4	H	350[A]	SH7	O4-C16-C15	4.05	125.16	115.69
4	E	350[A]	SH7	O4-C16-C15	3.97	124.99	115.69
4	C	350[B]	SH7	C14-C15-C16	3.93	123.27	119.72
4	G	350[A]	SH7	C23-C15-C16	-3.88	117.71	120.33
4	C	350[A]	SH7	C23-C15-C16	-3.82	117.75	120.33
4	E	350[A]	SH7	C14-C15-C16	3.36	122.76	119.72
4	F	350[B]	SH7	C23-C15-C16	-3.23	118.15	120.33
4	F	350[A]	SH7	C14-C15-C16	3.16	122.58	119.72
4	B	350[B]	SH7	C23-C15-C16	-3.14	118.21	120.33
4	G	350[A]	SH7	C14-C15-C16	2.89	122.33	119.72
4	C	350[A]	SH7	C14-C15-C16	2.65	122.11	119.72
4	D	350[A]	SH7	C23-C15-C16	-2.61	118.57	120.33
4	F	350[B]	SH7	C14-C15-C16	2.52	122.00	119.72
4	B	350[B]	SH7	C14-C15-C16	2.35	121.85	119.72
4	B	350[A]	SH7	O4-C16-C15	-2.20	110.54	115.69
4	A	350[B]	SH7	O4-C16-C15	-2.07	110.85	115.69
4	D	350[A]	SH7	C14-C15-C16	2.06	121.58	119.72
4	C	350[B]	SH7	C2-C1-C13	2.05	121.70	118.18
4	G	350[B]	SH7	O4-C16-C15	-2.03	110.93	115.69
4	F	350[A]	SH7	C2-C1-C13	2.01	121.64	118.18
4	D	350[A]	SH7	O4-C16-C15	-2.00	111.00	115.69

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	350[A]	SH7	C23-C15-C16-O5
4	A	350[A]	SH7	C14-C15-C16-O5
4	A	350[A]	SH7	C23-C15-C16-O4
4	A	350[A]	SH7	C14-C15-C16-O4
4	A	350[B]	SH7	C23-C15-C16-O5
4	A	350[B]	SH7	C14-C15-C16-O5
4	A	350[B]	SH7	C23-C15-C16-O4
4	A	350[B]	SH7	C14-C15-C16-O4
4	B	350[A]	SH7	C23-C15-C16-O5
4	B	350[A]	SH7	C14-C15-C16-O5
4	B	350[A]	SH7	C23-C15-C16-O4
4	B	350[A]	SH7	C14-C15-C16-O4
4	C	350[A]	SH7	C23-C15-C16-O5

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Mol	Chain	Res	Type	Atoms
4	C	350[A]	SH7	C14-C15-C16-O5
4	C	350[A]	SH7	C23-C15-C16-O4
4	C	350[A]	SH7	C14-C15-C16-O4
4	D	350[A]	SH7	C23-C15-C16-O5
4	D	350[A]	SH7	C14-C15-C16-O5
4	D	350[A]	SH7	C23-C15-C16-O4
4	D	350[A]	SH7	C14-C15-C16-O4
4	E	350[A]	SH7	C23-C15-C16-O5
4	E	350[A]	SH7	C14-C15-C16-O5
4	E	350[A]	SH7	C23-C15-C16-O4
4	E	350[A]	SH7	C14-C15-C16-O4
4	E	350[B]	SH7	C23-C15-C16-O5
4	E	350[B]	SH7	C23-C15-C16-O4
4	F	350[A]	SH7	C23-C15-C16-O5
4	F	350[A]	SH7	C14-C15-C16-O5
4	F	350[A]	SH7	C23-C15-C16-O4
4	F	350[A]	SH7	C14-C15-C16-O4
4	F	350[B]	SH7	C23-C15-C16-O5
4	F	350[B]	SH7	C23-C15-C16-O4
4	G	350[A]	SH7	C23-C15-C16-O5
4	G	350[A]	SH7	C14-C15-C16-O5
4	G	350[A]	SH7	C23-C15-C16-O4
4	G	350[A]	SH7	C14-C15-C16-O4
4	G	350[B]	SH7	C23-C15-C16-O5
4	G	350[B]	SH7	C14-C15-C16-O5
4	G	350[B]	SH7	C23-C15-C16-O4
4	G	350[B]	SH7	C14-C15-C16-O4
4	H	350[A]	SH7	C23-C15-C16-O5
4	H	350[A]	SH7	C14-C15-C16-O5
4	H	350[A]	SH7	C23-C15-C16-O4
4	H	350[A]	SH7	C14-C15-C16-O4
4	H	350[B]	SH7	C23-C15-C16-O5
4	H	350[B]	SH7	C14-C15-C16-O5
4	H	350[B]	SH7	C23-C15-C16-O4
4	H	350[B]	SH7	C14-C15-C16-O4
5	G	301	EPE	C9-C10-S-O1S
5	G	301	EPE	C9-C10-S-O2S
2	A	301	PGE	O2-C3-C4-O3
5	G	301	EPE	C9-C10-S-O3S
2	F	301	PGE	O3-C5-C6-O4
2	A	301	PGE	O3-C5-C6-O4
2	D	301	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
5	G	301	EPE	C10-C9-N1-C2
5	G	301	EPE	C10-C9-N1-C6
5	H	301	EPE	C10-C9-N1-C2
5	H	301	EPE	C10-C9-N1-C6
4	F	350[B]	SH7	C14-C15-C16-O5
4	F	350[B]	SH7	C14-C15-C16-O4
5	G	301	EPE	C8-C7-N4-C3
5	G	301	EPE	C8-C7-N4-C5
5	G	301	EPE	S-C10-C9-N1
2	E	301	PGE	C4-C3-O2-C2
2	F	301	PGE	O2-C3-C4-O3
2	E	301	PGE	C3-C4-O3-C5
2	E	301	PGE	O2-C3-C4-O3
2	D	301	PGE	C1-C2-O2-C3
4	E	350[B]	SH7	C14-C15-C16-O5
4	E	350[B]	SH7	C14-C15-C16-O4
2	E	301	PGE	C6-C5-O3-C4
2	A	301	PGE	O1-C1-C2-O2
2	A	301	PGE	C1-C2-O2-C3
2	D	301	PGE	O1-C1-C2-O2
4	B	350[B]	SH7	C14-C15-C16-O4
4	C	350[B]	SH7	C14-C15-C16-O5
4	B	350[B]	SH7	C23-C15-C16-O4

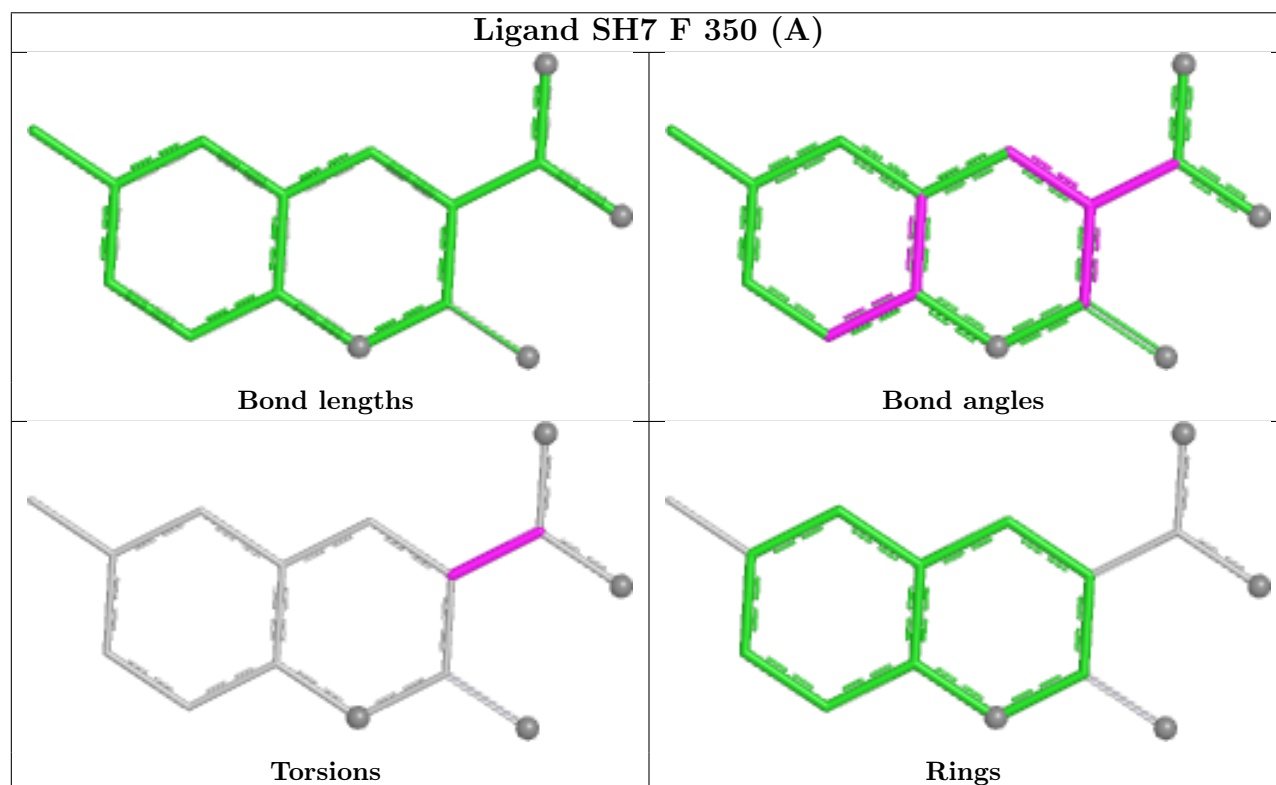
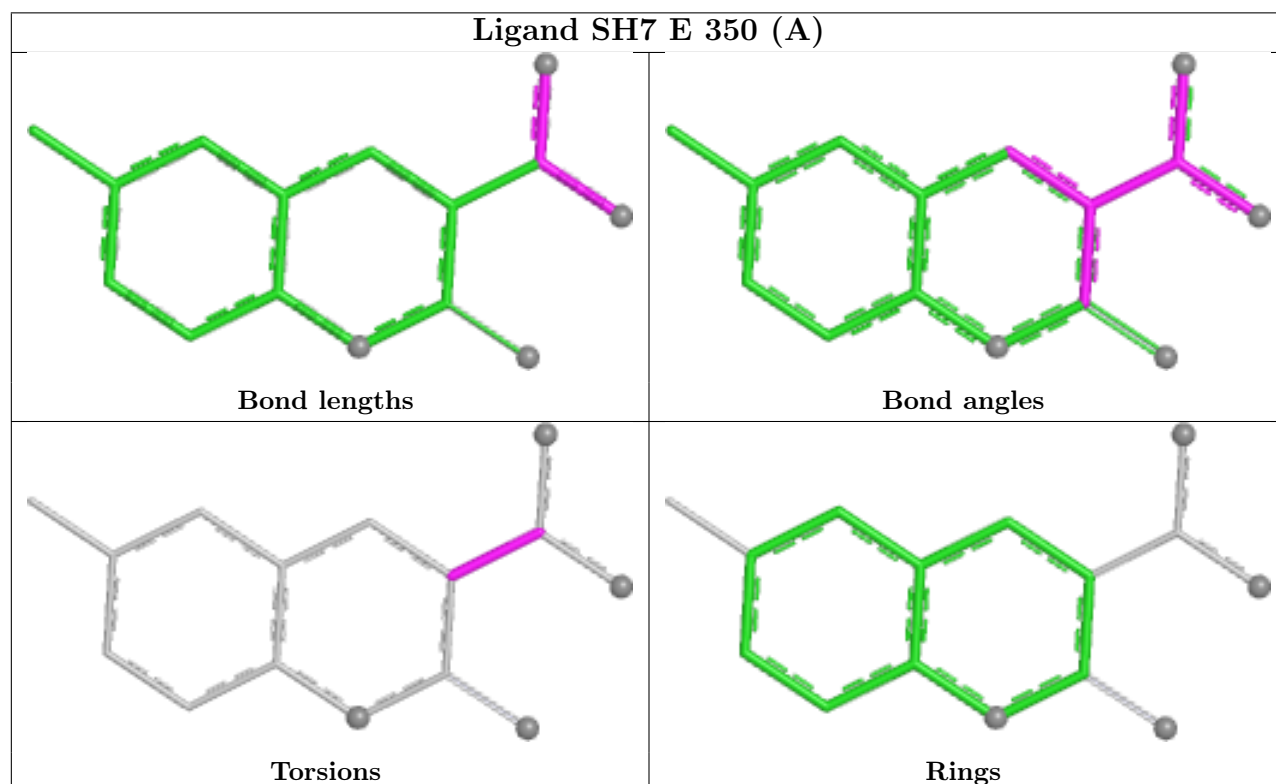
There are no ring outliers.

3 monomers are involved in 3 short contacts:

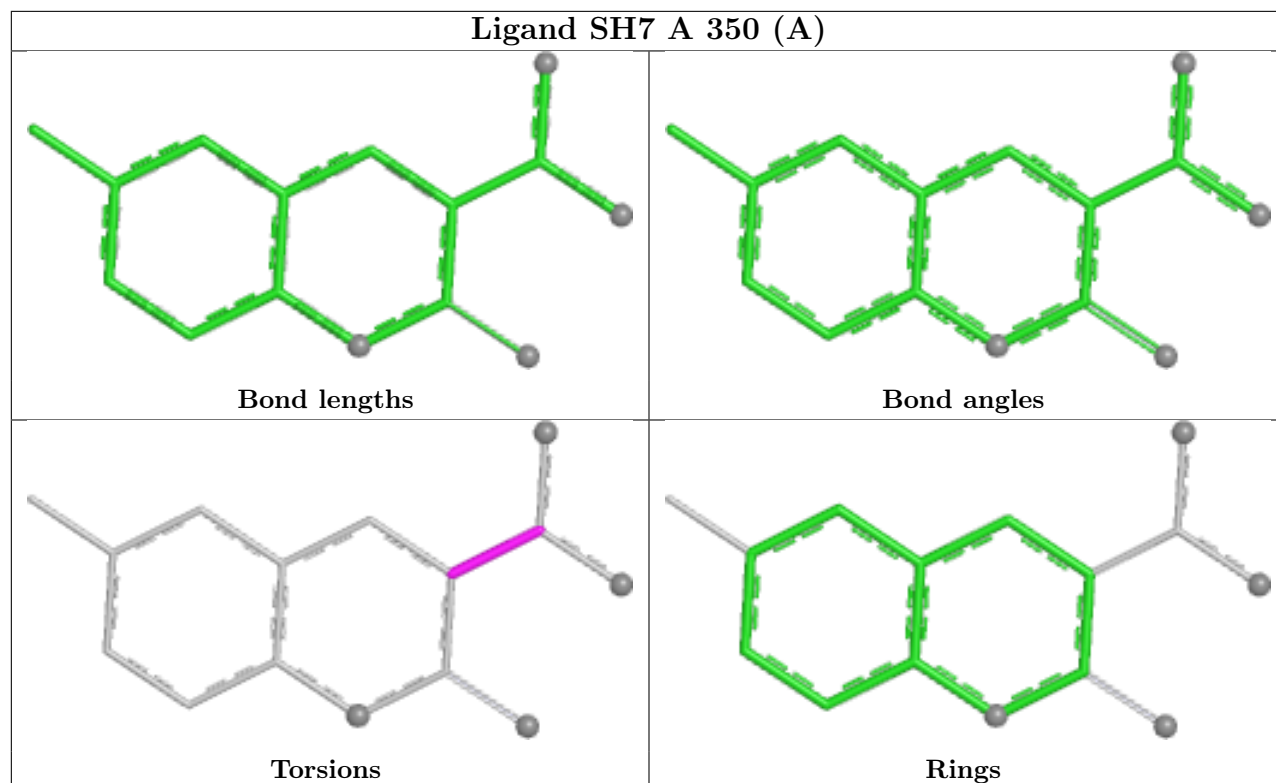
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	PGE	1	0
3	A	304	SO4	1	0
2	F	301	PGE	1	0

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.

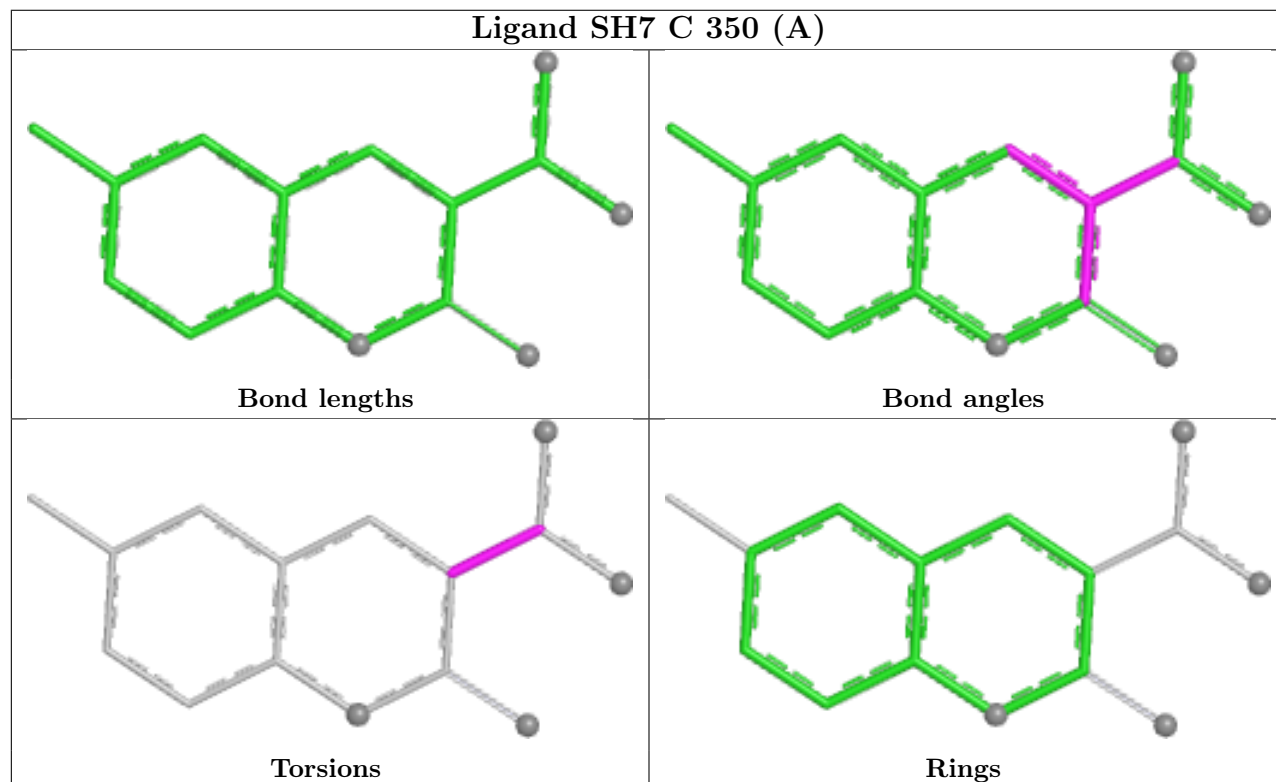
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



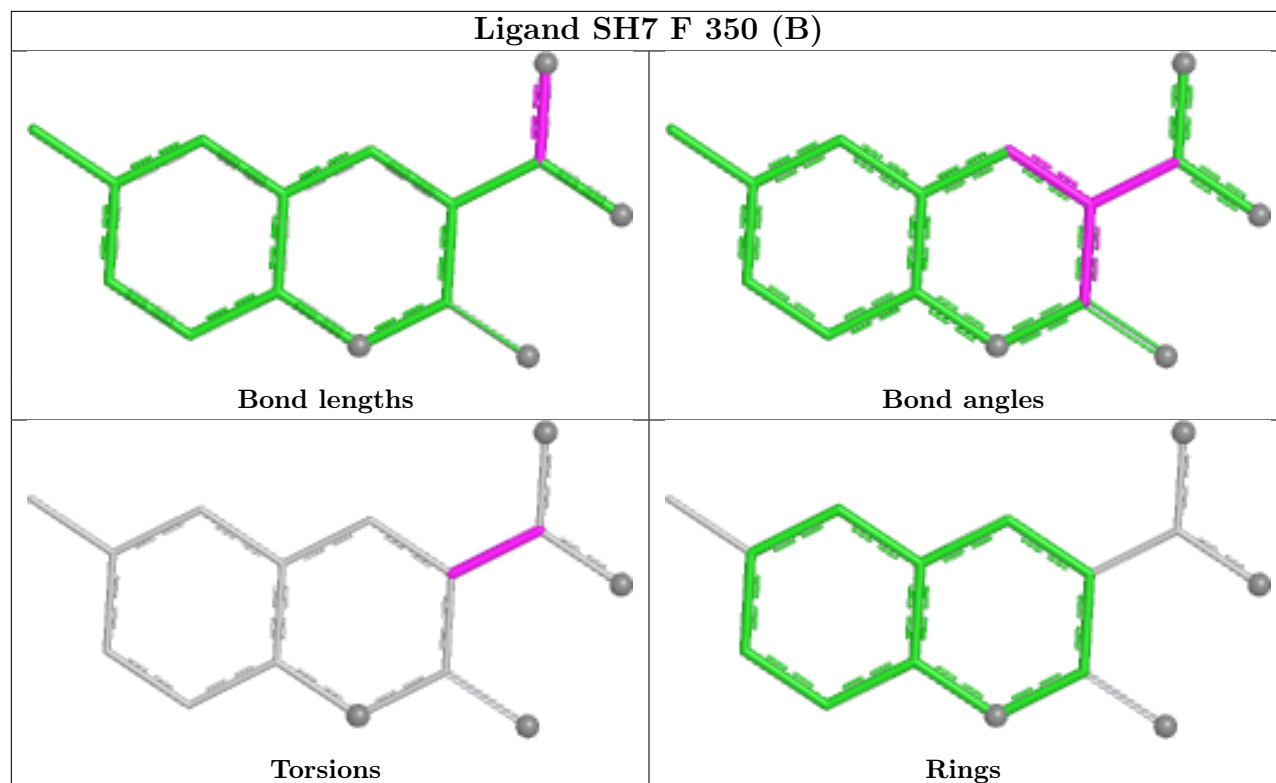
Ligand SH7 A 350 (A)



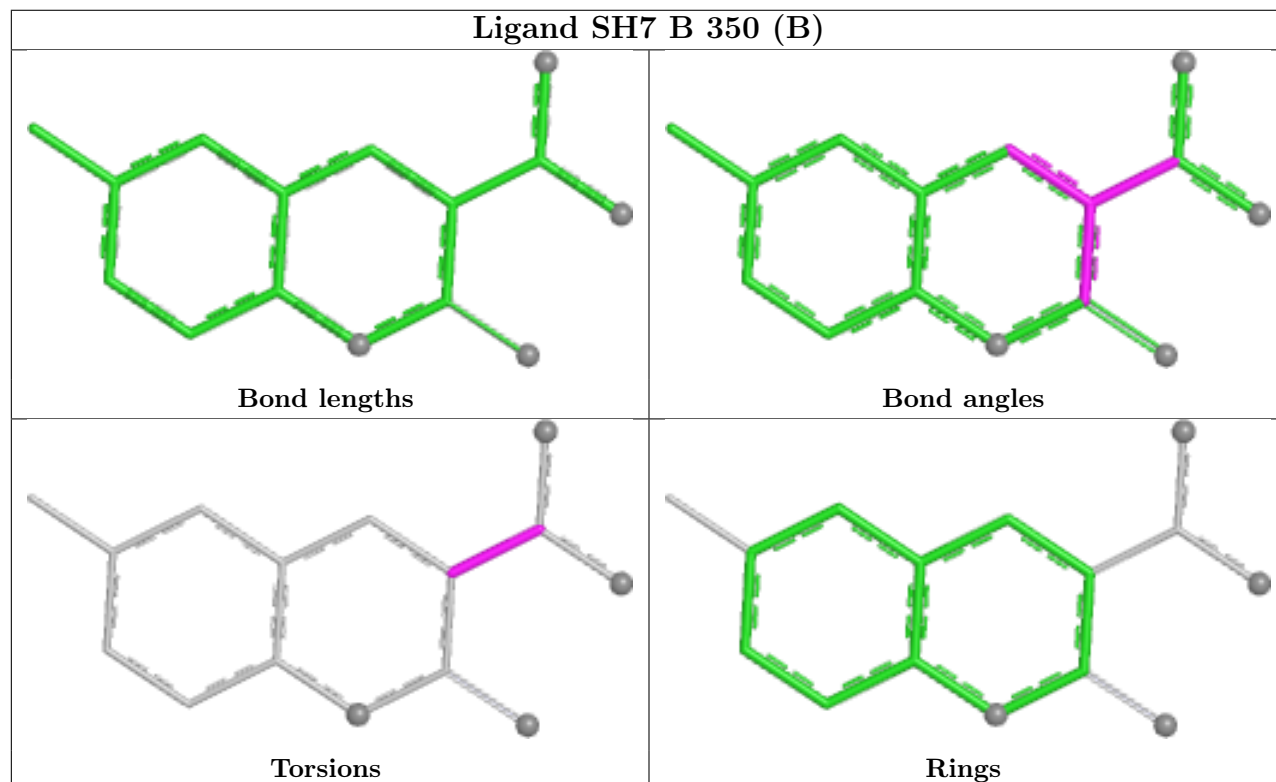
Ligand SH7 C 350 (A)



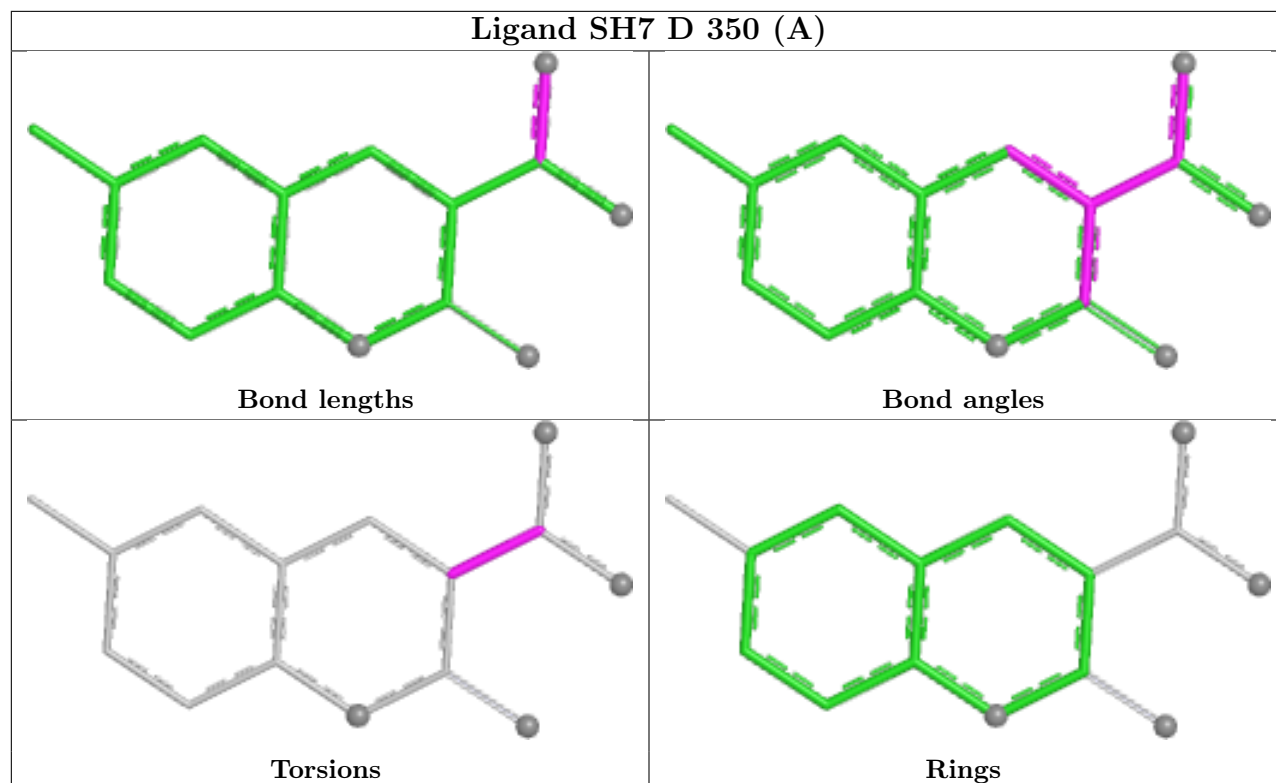
Ligand SH7 F 350 (B)



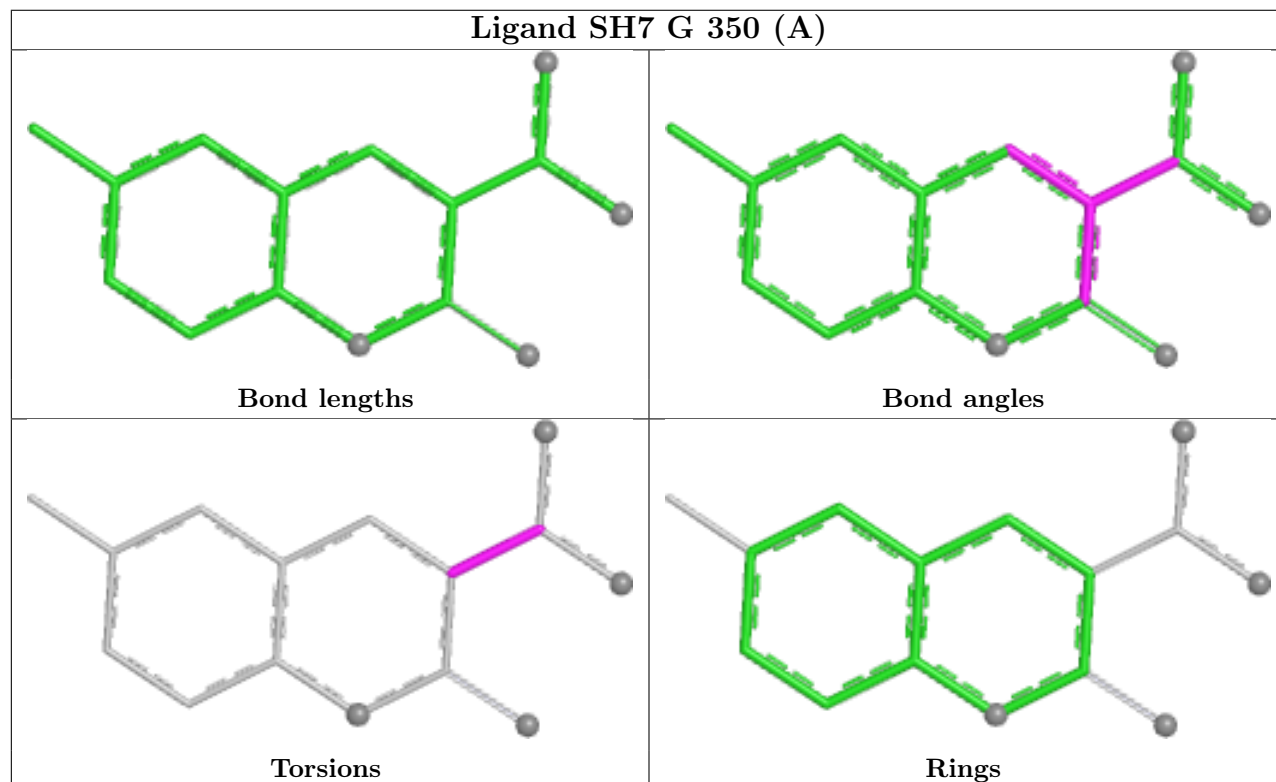
Ligand SH7 B 350 (B)



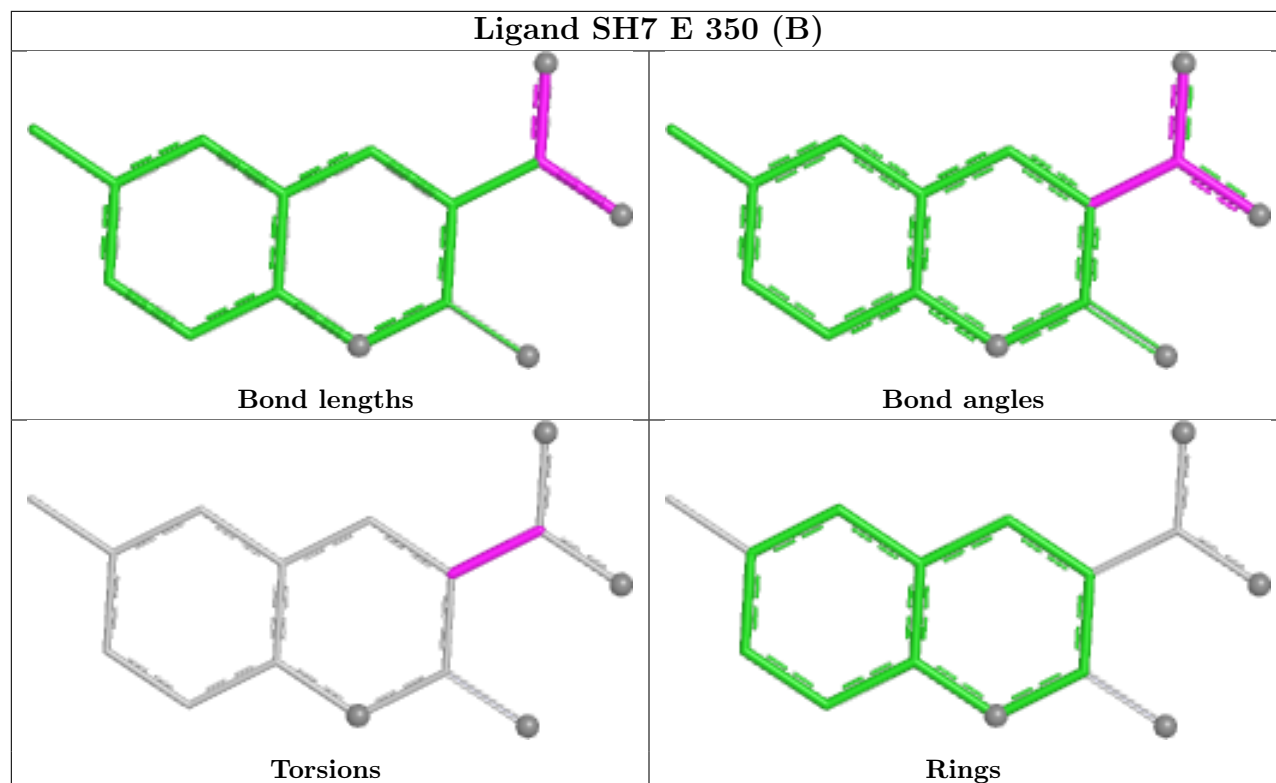
Ligand SH7 D 350 (A)



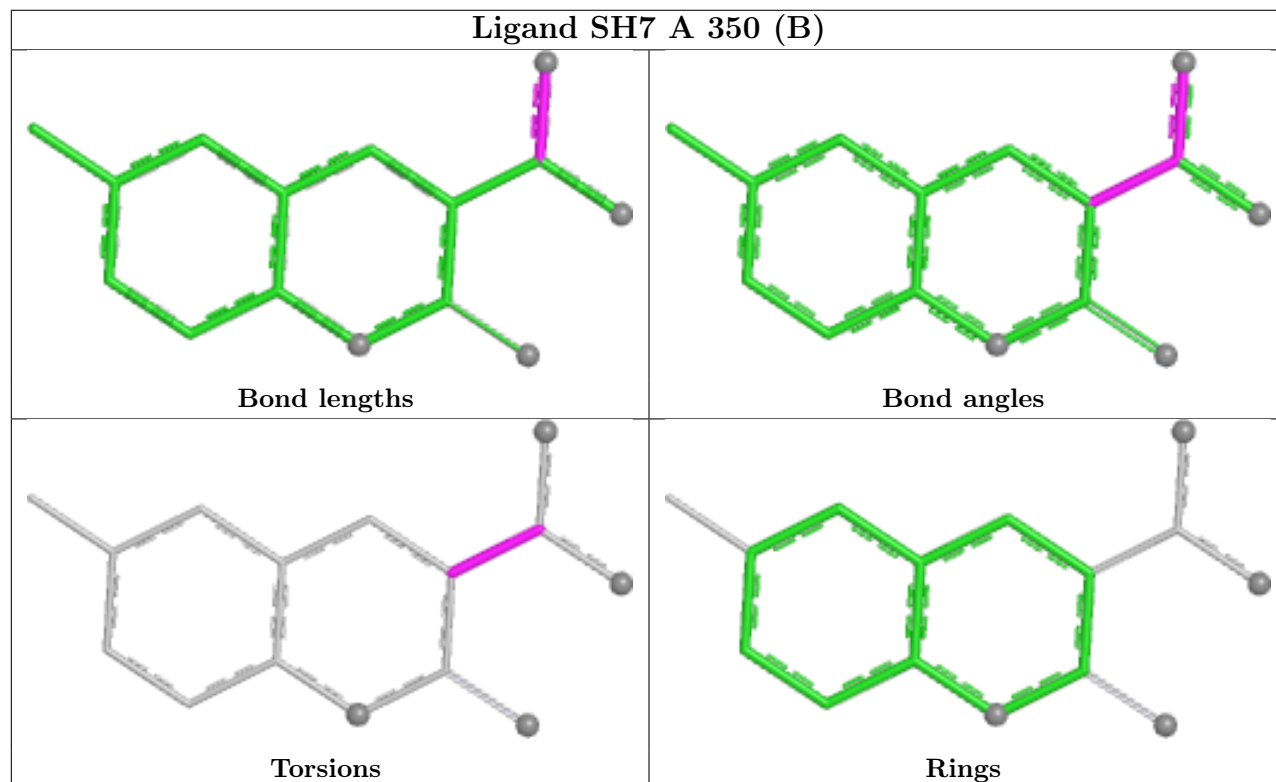
Ligand SH7 G 350 (A)



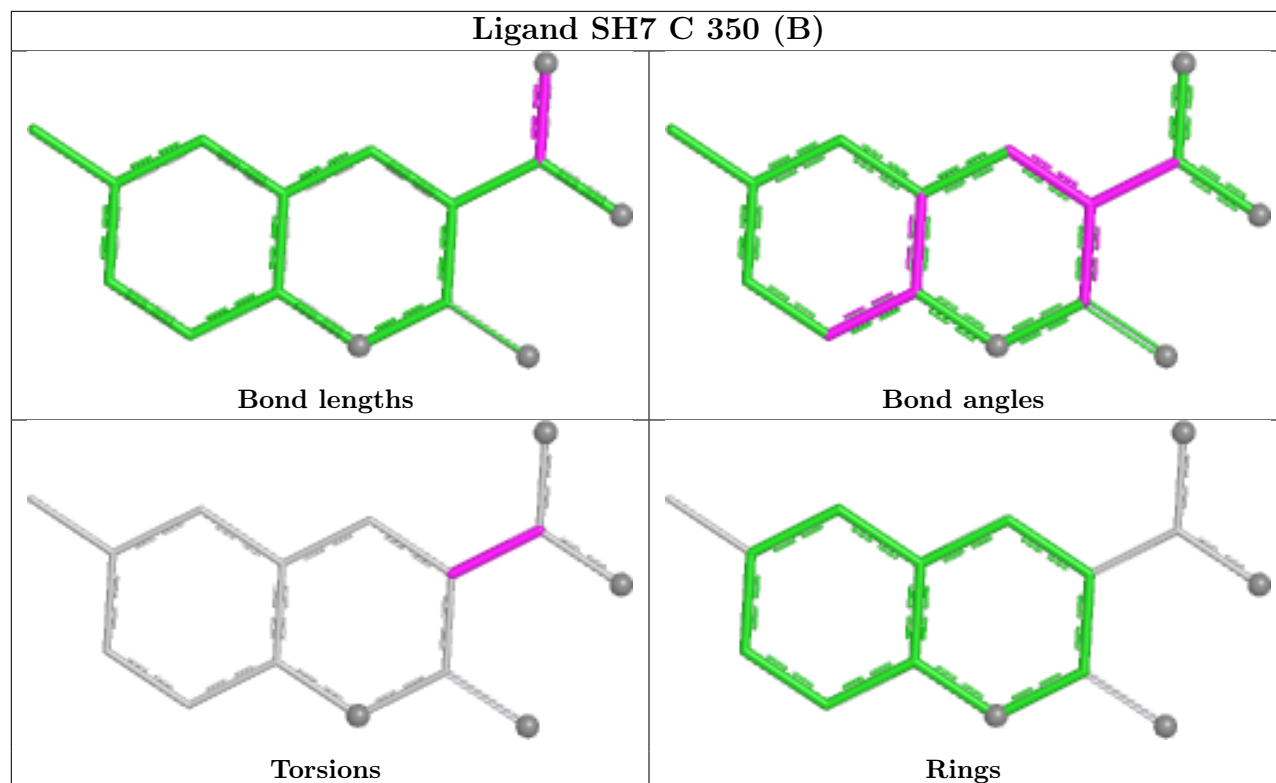
Ligand SH7 E 350 (B)



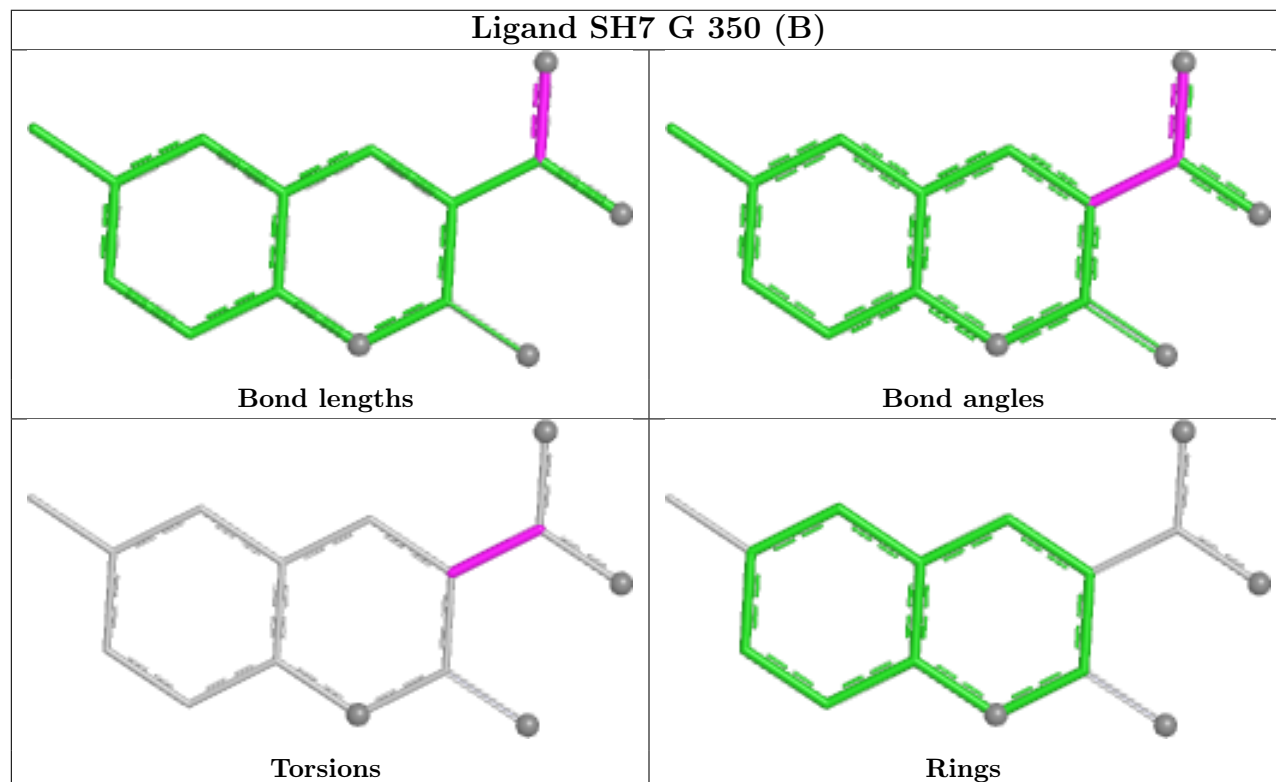
Ligand SH7 A 350 (B)



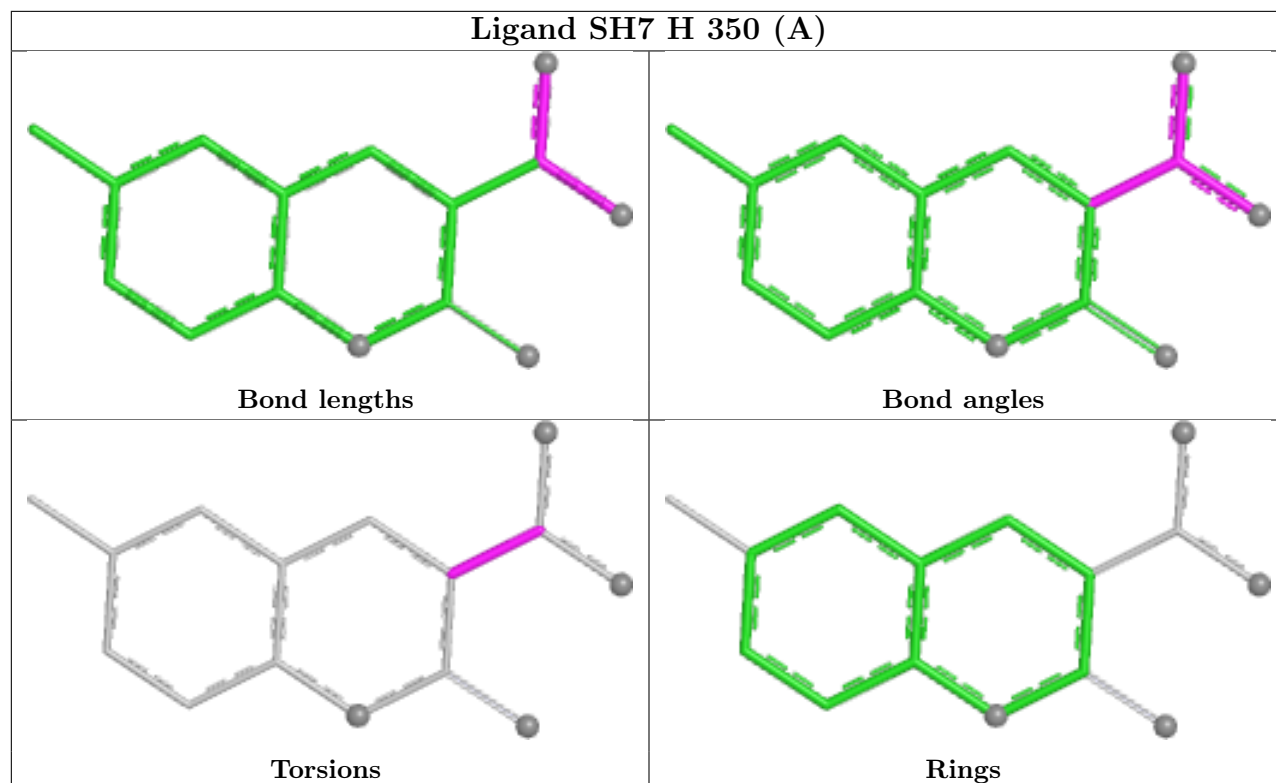
Ligand SH7 C 350 (B)



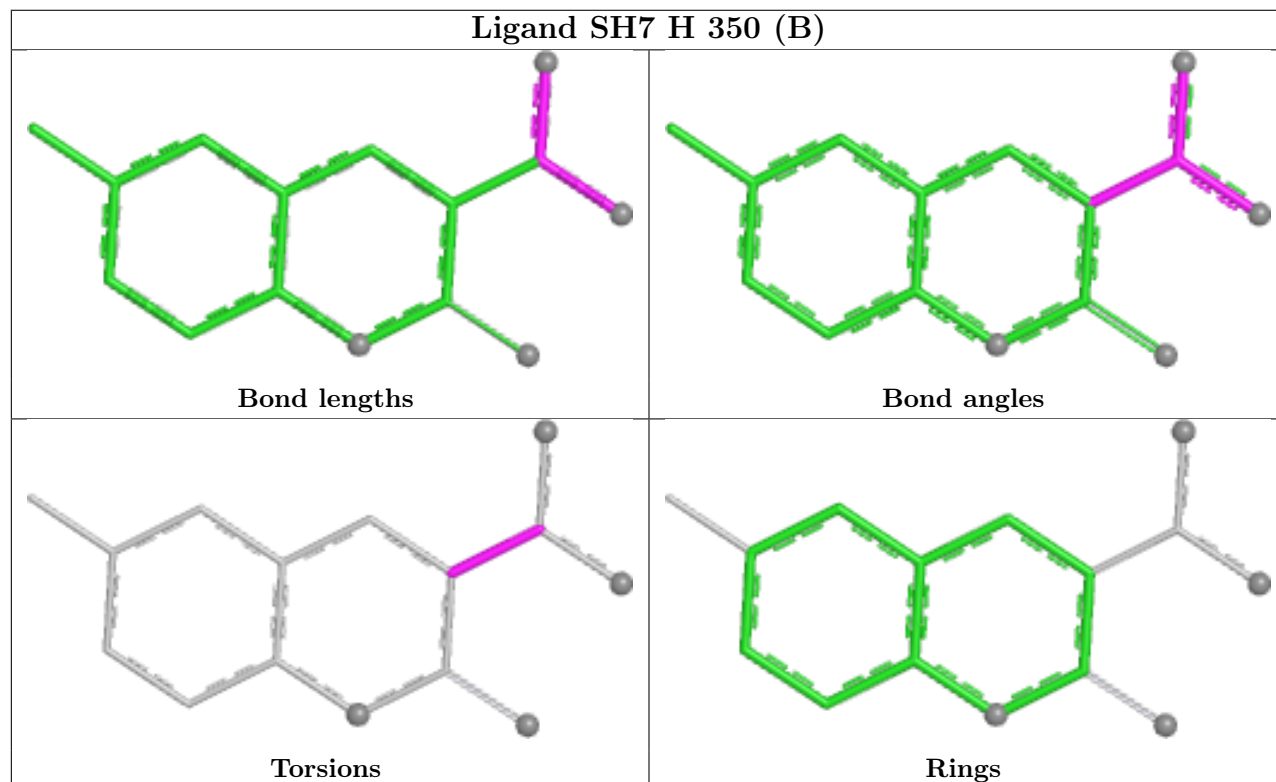
Ligand SH7 G 350 (B)

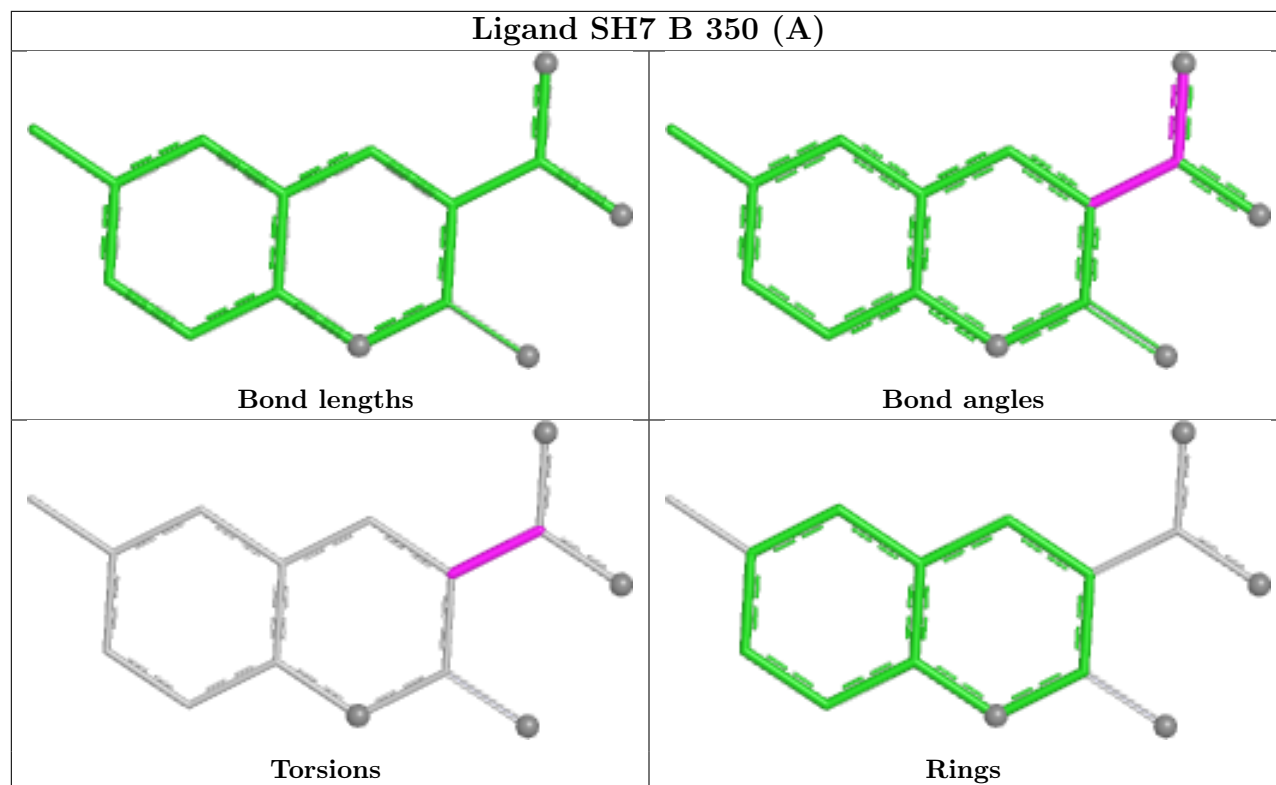


Ligand SH7 H 350 (A)



Ligand SH7 H 350 (B)





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	224/224 (100%)	-0.00	1 (0%) 88 88	17, 35, 53, 89	4 (1%)
1	B	224/224 (100%)	-0.01	1 (0%) 88 88	18, 34, 53, 86	4 (1%)
1	C	224/224 (100%)	-0.03	2 (0%) 81 80	20, 35, 54, 70	2 (0%)
1	D	224/224 (100%)	0.16	2 (0%) 81 80	18, 38, 58, 75	2 (0%)
1	E	224/224 (100%)	0.07	5 (2%) 62 61	16, 36, 54, 79	3 (1%)
1	F	224/224 (100%)	0.03	0 100 100	19, 35, 54, 81	2 (0%)
1	G	224/224 (100%)	0.39	4 (1%) 67 67	22, 47, 67, 86	1 (0%)
1	H	224/224 (100%)	0.48	3 (1%) 75 74	23, 49, 66, 91	1 (0%)
All	All	1792/1792 (100%)	0.14	18 (1%) 79 79	16, 38, 60, 91	19 (1%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	61	ASN	3.0
1	D	175	LEU	2.6
1	H	168	CYS	2.5
1	E	157	CYS	2.4
1	E	246	ARG	2.3
1	G	157	CYS	2.2
1	C	99[A]	HIS	2.2
1	E	99	HIS	2.2
1	H	98	THR	2.2
1	G	61	ASN	2.1
1	H	99	HIS	2.1
1	C	151	PHE	2.1
1	E	192	ASN	2.1
1	G	148	ASP	2.1
1	A	151	PHE	2.1
1	G	99	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	99[A]	HIS	2.0
1	D	99	HIS	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(Å ²)	Q<0.9
3	SO4	G	308	5/5	0.57	0.14	138,139,139,139	0
3	SO4	D	310	5/5	0.61	0.14	116,118,118,119	0
3	SO4	G	304	5/5	0.65	0.14	126,127,127,128	0
3	SO4	C	307	5/5	0.66	0.16	147,147,147,148	0
3	SO4	B	311	5/5	0.67	0.12	132,132,133,133	0
3	SO4	A	305	5/5	0.70	0.16	96,97,98,99	0
3	SO4	E	306	5/5	0.70	0.16	132,132,133,133	0
3	SO4	G	309	5/5	0.70	0.12	112,112,113,113	0
3	SO4	H	306	5/5	0.71	0.13	110,110,111,112	0
3	SO4	E	309	5/5	0.72	0.17	80,82,84,87	0
3	SO4	H	305	5/5	0.73	0.14	83,84,85,87	0
3	SO4	E	304	5/5	0.74	0.14	82,82,84,86	0
3	SO4	B	313	5/5	0.74	0.17	88,91,93,94	0
3	SO4	E	308	5/5	0.74	0.19	110,111,112,112	0
3	SO4	H	311	5/5	0.74	0.11	98,99,99,99	0
3	SO4	A	310	5/5	0.75	0.17	88,91,97,97	0
3	SO4	B	308	5/5	0.75	0.16	119,119,119,120	0
3	SO4	H	312	5/5	0.75	0.11	105,106,108,108	0
2	PGE	A	301	10/10	0.76	0.14	44,48,51,53	0
3	SO4	G	306	5/5	0.76	0.13	123,124,124,125	0
4	SH7	E	350[A]	15/22	0.76	0.23	33,38,43,45	15

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SH7	E	350[B]	15/22	0.76	0.23	40,49,51,52	15
3	SO4	A	309	5/5	0.77	0.12	96,97,97,97	0
3	SO4	C	305	5/5	0.77	0.10	88,88,89,90	0
3	SO4	G	310	5/5	0.77	0.10	127,127,128,128	0
3	SO4	H	310	5/5	0.78	0.11	105,107,107,108	0
3	SO4	C	311	5/5	0.78	0.17	88,88,90,92	0
3	SO4	C	309	5/5	0.78	0.14	93,94,94,95	0
3	SO4	G	307	5/5	0.78	0.12	136,137,137,137	0
3	SO4	F	311	5/5	0.78	0.12	104,105,106,106	0
5	EPE	G	301	15/15	0.78	0.20	101,105,115,116	0
5	EPE	H	301	15/15	0.78	0.23	95,97,101,102	0
3	SO4	B	307	5/5	0.79	0.10	94,94,95,96	0
2	PGE	F	301	10/10	0.79	0.13	41,47,52,53	0
3	SO4	F	309	5/5	0.79	0.11	112,113,114,115	0
3	SO4	F	310	5/5	0.79	0.18	170,170,170,171	0
3	SO4	B	309	5/5	0.79	0.10	104,105,105,106	0
3	SO4	B	306	5/5	0.79	0.13	103,104,104,105	0
3	SO4	G	305	5/5	0.79	0.13	95,95,96,98	0
4	SH7	C	350[A]	15/22	0.80	0.27	44,45,48,49	15
4	SH7	C	350[B]	15/22	0.80	0.27	57,62,65,65	15
3	SO4	B	310	5/5	0.80	0.14	110,110,111,114	0
3	SO4	E	305	5/5	0.81	0.11	109,110,110,111	0
3	SO4	D	308	5/5	0.81	0.12	95,95,97,98	0
3	SO4	F	305	5/5	0.81	0.12	87,89,90,91	0
4	SH7	A	350[A]	15/22	0.82	0.24	32,38,44,45	15
4	SH7	A	350[B]	15/22	0.82	0.24	45,51,54,54	15
3	SO4	D	311	5/5	0.82	0.10	99,99,100,101	0
3	SO4	F	308	5/5	0.82	0.10	78,80,82,83	0
4	SH7	D	350[A]	15/22	0.82	0.23	38,41,46,48	15
4	SH7	D	350[B]	15/22	0.82	0.23	36,48,51,52	15
3	SO4	E	307	5/5	0.82	0.10	97,98,98,98	0
3	SO4	A	308	5/5	0.82	0.12	90,90,93,94	0
2	PGE	E	301	10/10	0.82	0.13	46,50,54,54	0
3	SO4	G	303	5/5	0.82	0.11	93,94,95,96	0
4	SH7	F	350[B]	15/22	0.83	0.23	46,54,58,59	15
3	SO4	F	306	5/5	0.83	0.12	76,79,81,83	0
4	SH7	F	350[A]	15/22	0.83	0.23	33,35,39,43	15
4	SH7	B	350[A]	15/22	0.84	0.26	44,48,49,50	15
4	SH7	G	350[A]	15/22	0.84	0.28	50,51,52,52	15
4	SH7	G	350[B]	15/22	0.84	0.28	47,50,55,56	15
4	SH7	B	350[B]	15/22	0.84	0.26	48,53,55,56	15
3	SO4	D	309	5/5	0.84	0.11	97,99,100,101	0

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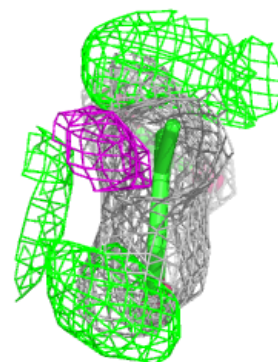
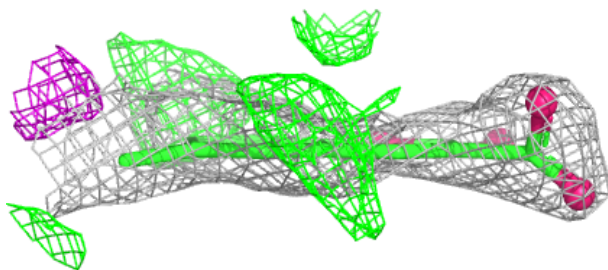
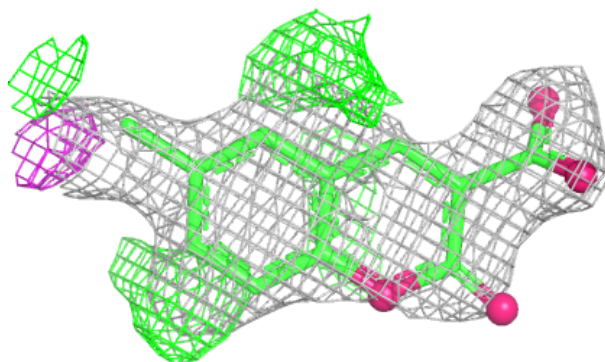
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	H	307	5/5	0.85	0.10	106,107,108,110	0
3	SO4	A	306	5/5	0.85	0.09	93,94,95,96	0
4	SH7	H	350[A]	15/22	0.85	0.27	41,50,53,54	15
4	SH7	H	350[B]	15/22	0.85	0.27	53,55,57,59	15
3	SO4	C	308	5/5	0.85	0.11	81,82,83,84	0
2	PGE	D	301	10/10	0.85	0.11	47,49,52,52	0
3	SO4	H	309	5/5	0.86	0.11	105,106,106,108	0
3	SO4	C	312	5/5	0.86	0.12	94,94,95,99	0
3	SO4	H	308	5/5	0.87	0.09	100,101,101,102	0
3	SO4	D	307	5/5	0.88	0.09	88,88,89,91	0
3	SO4	C	310	5/5	0.88	0.14	90,90,92,94	0
3	SO4	D	303	5/5	0.88	0.10	83,84,84,85	0
3	SO4	B	304	5/5	0.89	0.09	72,72,74,74	0
3	SO4	B	305	5/5	0.89	0.10	86,86,88,88	0
3	SO4	D	306	5/5	0.89	0.09	75,78,80,80	0
3	SO4	H	304	5/5	0.89	0.09	84,87,87,88	0
3	SO4	C	306	5/5	0.89	0.11	81,82,83,85	0
3	SO4	B	312	5/5	0.89	0.12	96,97,97,98	0
3	SO4	F	307	5/5	0.90	0.09	61,64,66,68	0
3	SO4	A	304	5/5	0.90	0.10	79,80,81,82	0
3	SO4	C	313	5/5	0.91	0.11	77,78,79,85	0
3	SO4	A	307	5/5	0.91	0.10	72,75,76,76	0
3	SO4	F	304	5/5	0.91	0.09	76,76,77,77	0
3	SO4	F	303	5/5	0.92	0.08	67,69,70,70	0
3	SO4	B	303	5/5	0.92	0.10	78,79,79,82	0
3	SO4	C	304	5/5	0.92	0.10	74,76,77,79	0
3	SO4	D	305	5/5	0.92	0.07	72,75,76,78	0
3	SO4	A	303	5/5	0.93	0.09	63,64,65,66	0
3	SO4	C	303	5/5	0.94	0.09	63,63,65,72	0
3	SO4	D	304	5/5	0.95	0.07	60,61,63,63	0
3	SO4	H	303	5/5	0.96	0.07	58,59,62,62	0
3	SO4	E	303	5/5	0.96	0.07	63,63,66,69	0
3	SO4	E	302	5/5	0.96	0.08	48,49,52,53	0
3	SO4	H	302	5/5	0.96	0.07	53,53,56,57	0
3	SO4	B	302	5/5	0.97	0.08	52,55,56,59	0
3	SO4	A	302	5/5	0.97	0.08	48,48,51,51	0
3	SO4	C	301	5/5	0.97	0.07	48,48,50,51	0
3	SO4	C	302	5/5	0.97	0.08	45,47,49,50	0
3	SO4	G	302	5/5	0.97	0.06	53,54,59,60	0
3	SO4	F	302	5/5	0.97	0.08	49,51,53,54	0
3	SO4	D	302	5/5	0.98	0.06	40,45,50,52	0
3	SO4	B	301	5/5	0.98	0.06	47,47,49,51	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.

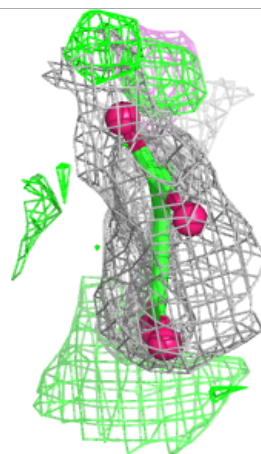
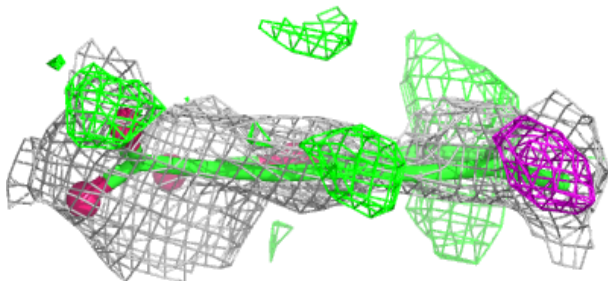
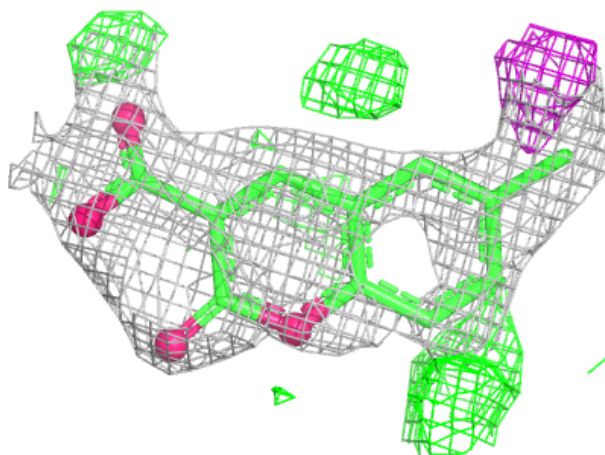
Electron density around SH7 E 350 (A):

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



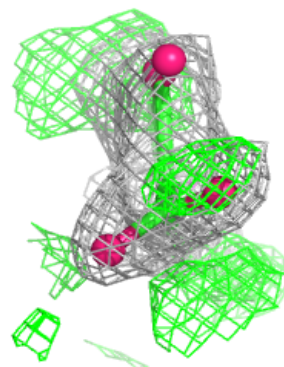
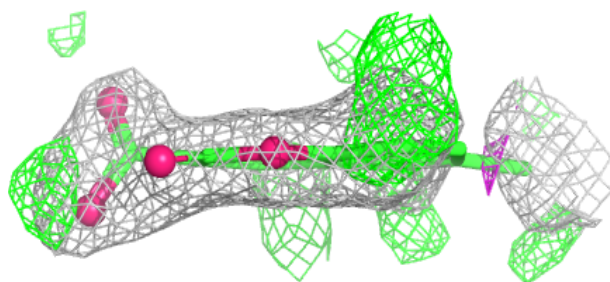
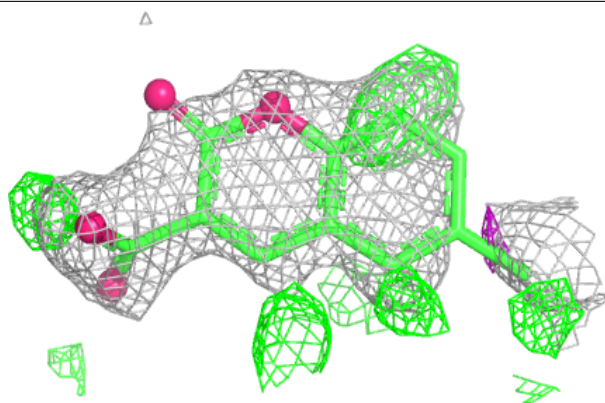
Electron density around SH7 E 350 (B):

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

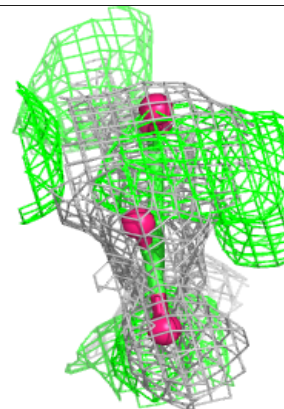
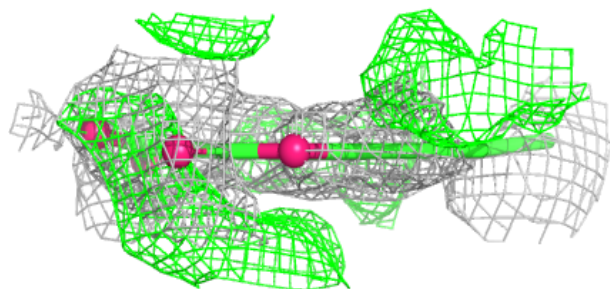
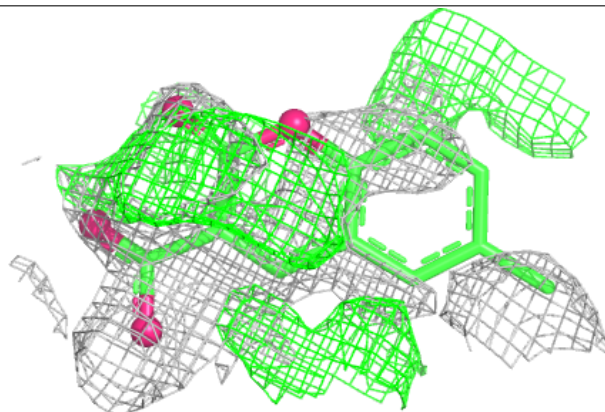


Electron density around SH7 C 350 (A):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

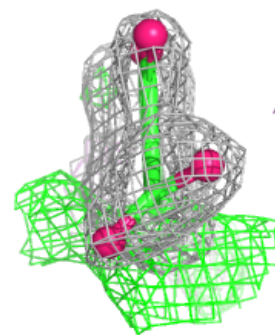
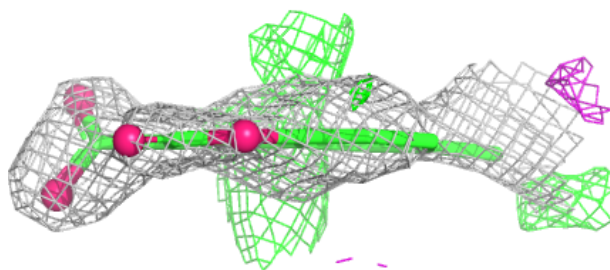
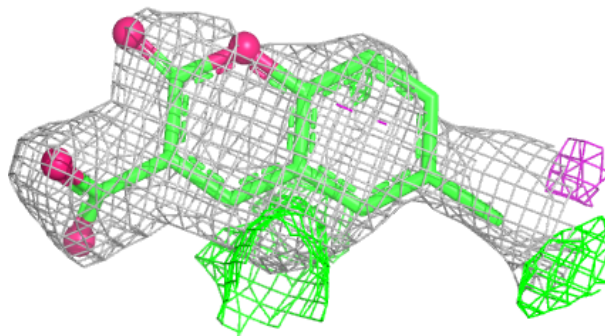
**Electron density around SH7 C 350 (B):**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

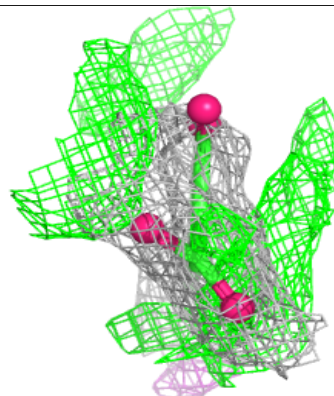
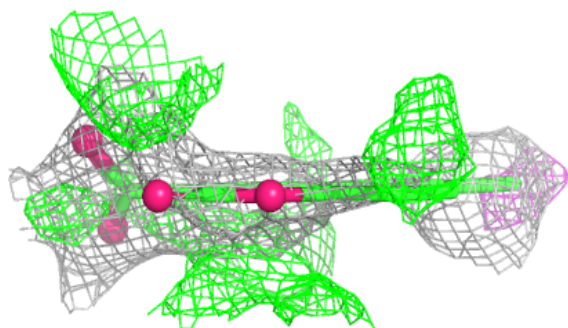
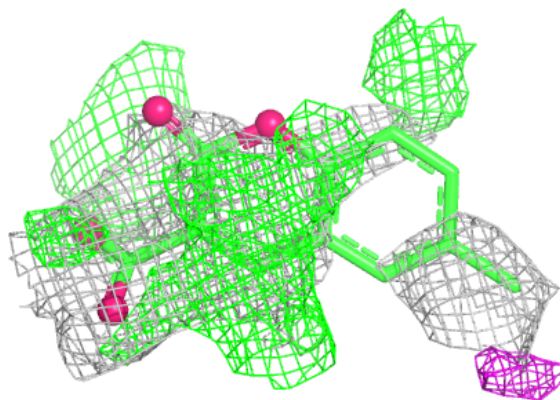


Electron density around SH7 A 350 (A):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

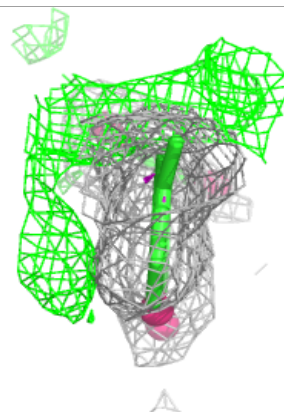
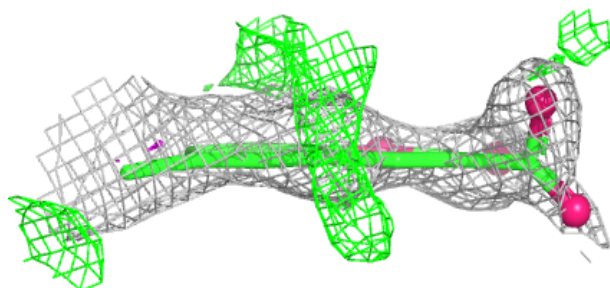
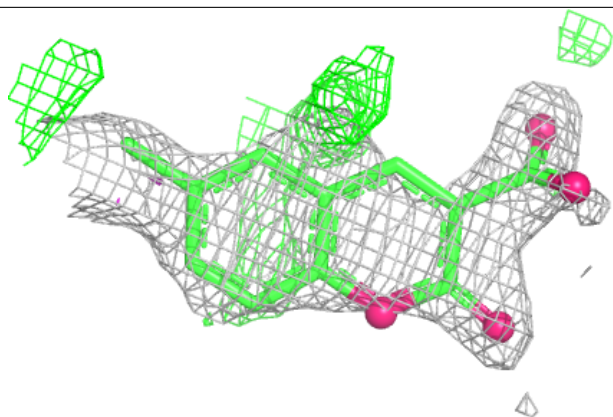
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and green (positive)

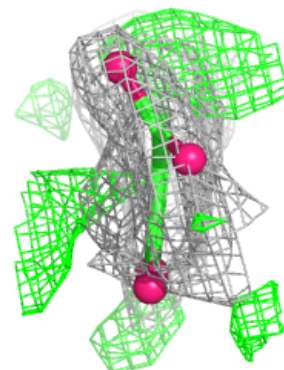
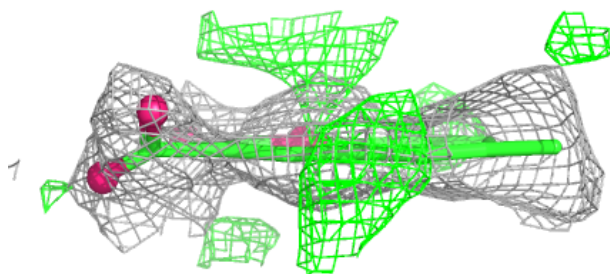
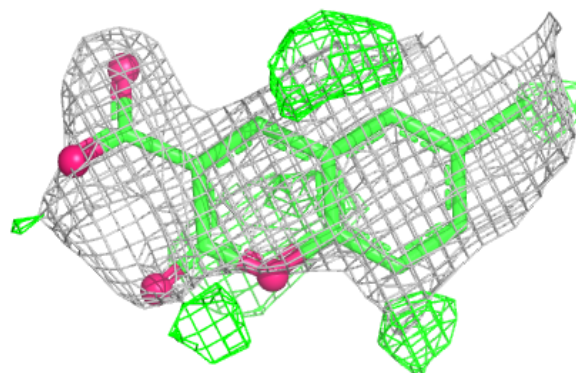


Electron density around SH7 D 350 (A):

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and green (positive)

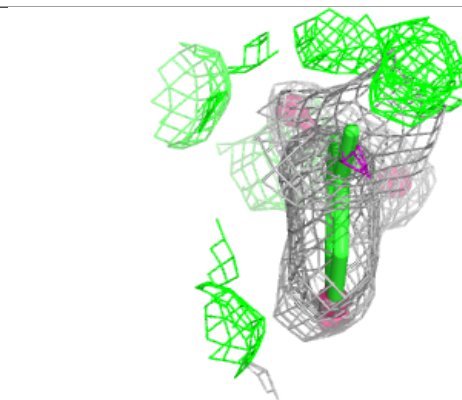
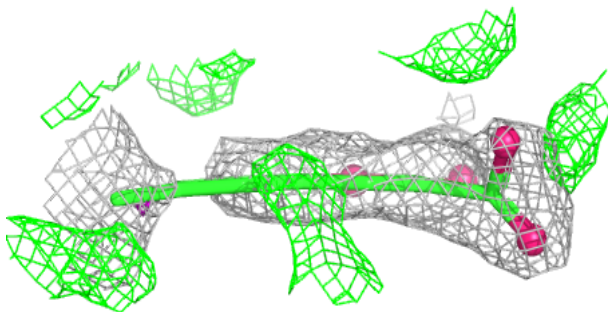
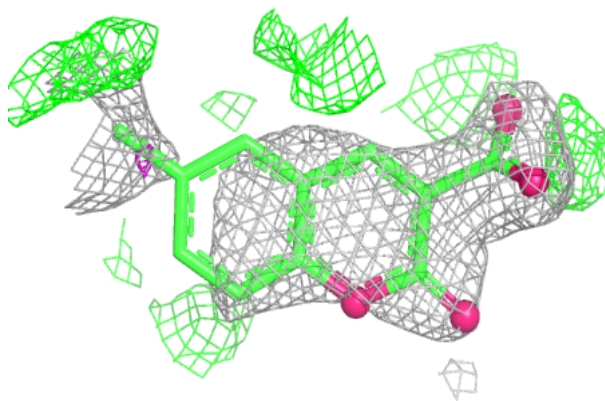
**Electron density around SH7 F 350 (B):**

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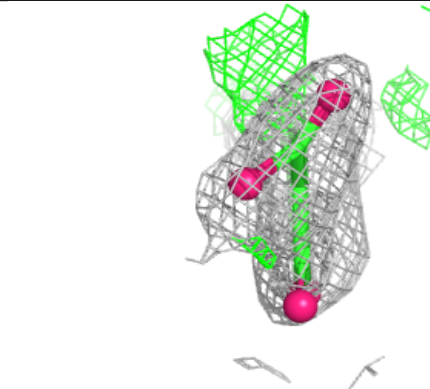
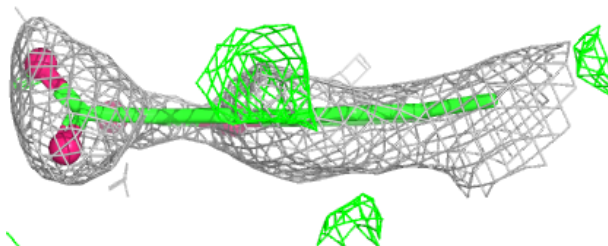
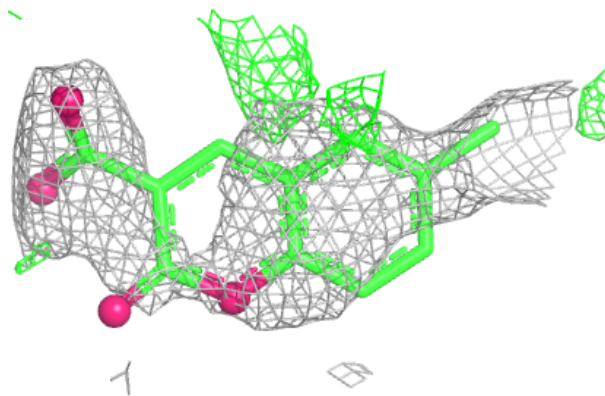


Electron density around SH7 F 350 (A):

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and green (positive)

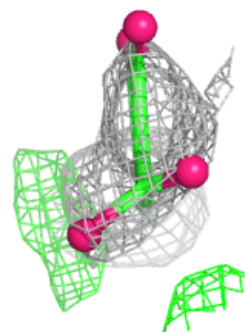
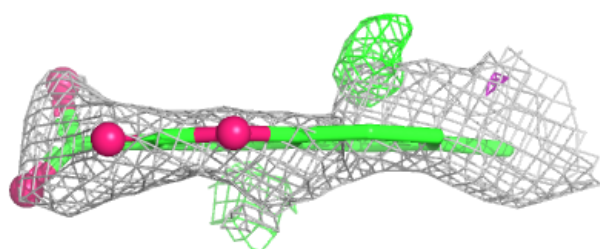
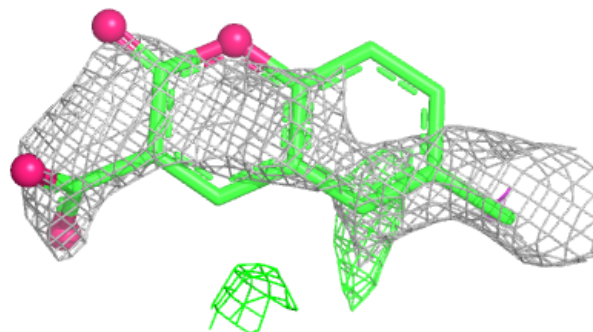
**Electron density around SH7 B 350 (A):**

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and green (positive)



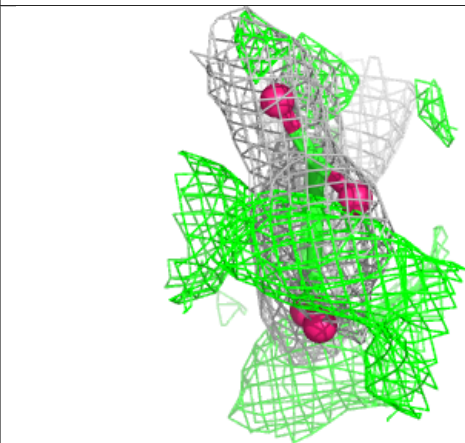
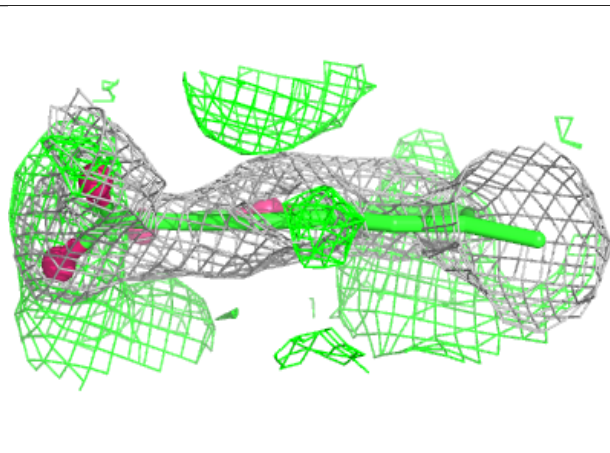
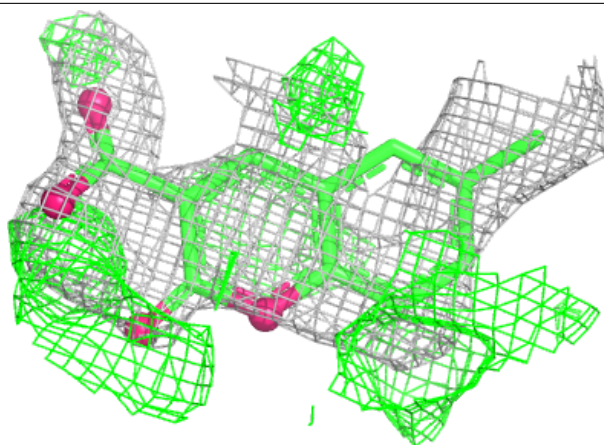
Electron density around SH7 G 350 (A):

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and green (positive)



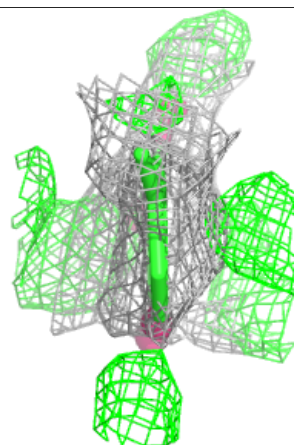
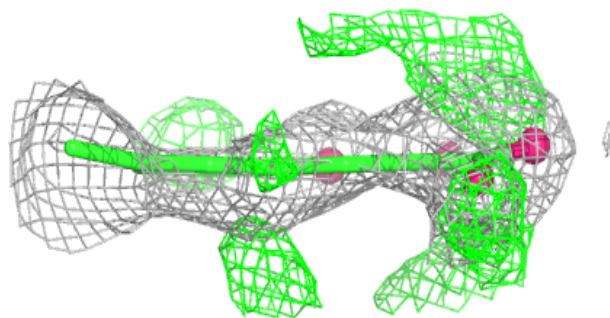
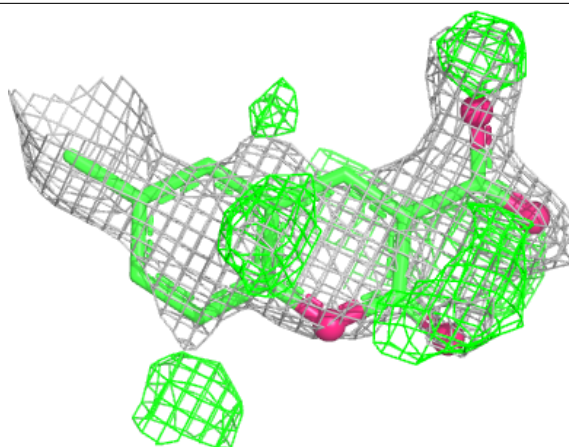
Electron density around SH7 G 350 (B):

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and green (positive)



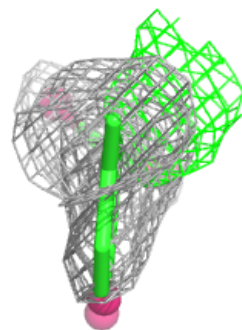
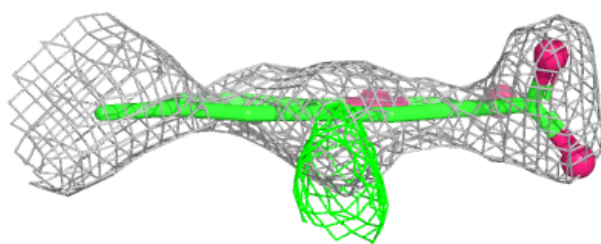
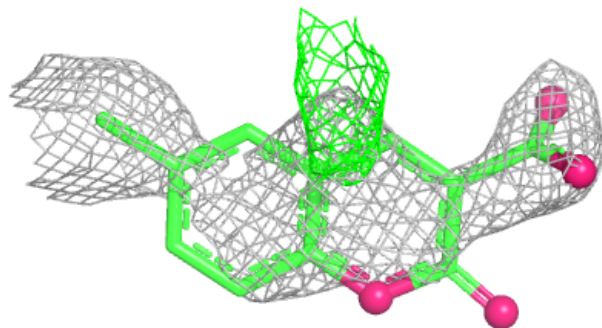
Electron density around SH7 B 350 (B):

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

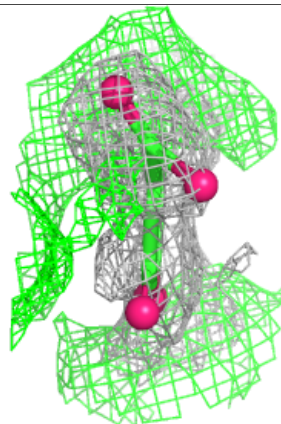
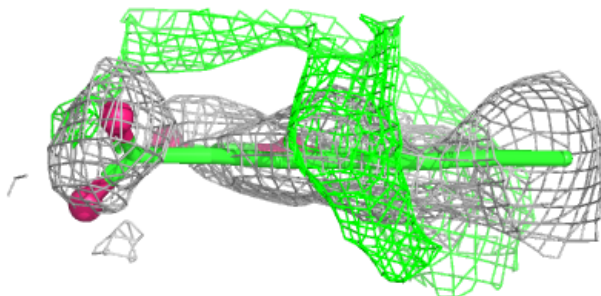
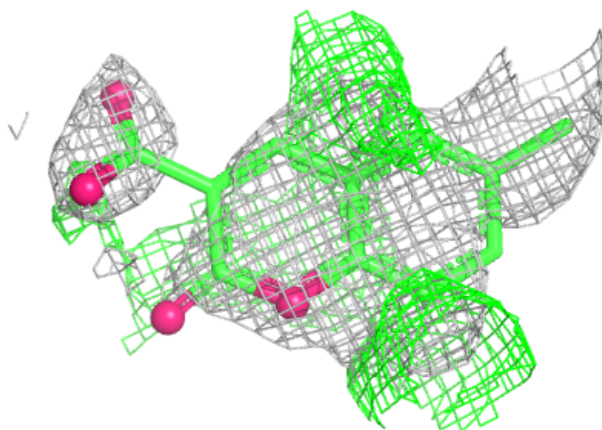


Electron density around SH7 H 350 (A):

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

**Electron density around SH7 H 350 (B):**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.