



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:49 PM UTC

PDB ID : 7XCM / pdb_00007xcm
Title : Crystal structure of sulfite MttB structure at 3.2 Å resolution
Authors : Li, J.; Chan, M.K.
Deposited on : 2022-03-24
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

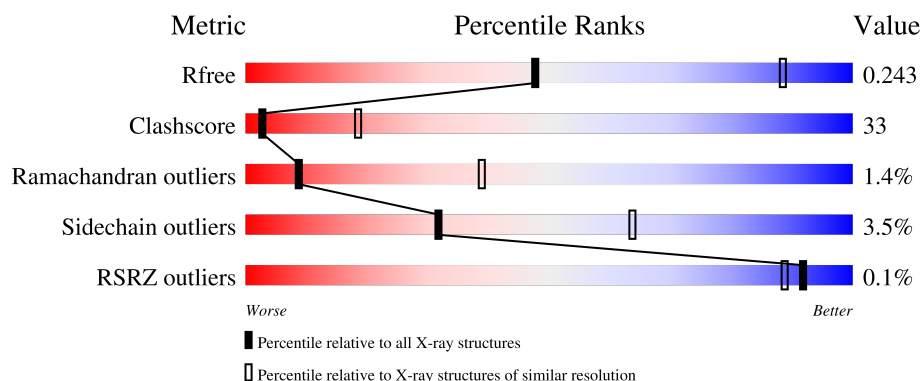
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

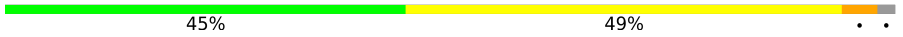
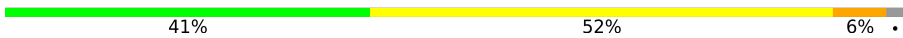
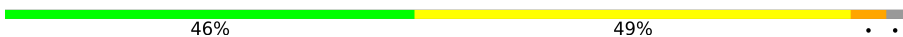
The reported resolution of this entry is 3.20 Å.

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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	503	
1	B	503	
1	C	503	
1	D	503	
1	E	503	

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Mol	Chain	Length	Quality of chain
1	F	503	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (41%), yellow (52%), and orange (5%). The segments are labeled with their respective percentages: 41%, 52%, and 5%.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	604	-	-	X	-
4	GOL	C	603	-	-	X	-
4	GOL	D	604	-	-	X	-
4	GOL	F	603	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22891 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 Trimethylamine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3765	2394	629	720	22			
1	B	494	Total	C	N	O	S	0	0	0
			3765	2394	629	720	22			
1	C	493	Total	C	N	O	S	0	0	0
			3757	2389	628	719	21			
1	D	494	Total	C	N	O	S	0	0	0
			3765	2394	629	720	22			
1	E	494	Total	C	N	O	S	0	0	0
			3765	2394	629	720	22			
1	F	494	Total	C	N	O	S	0	0	0
			3765	2394	629	720	22			

There are 54 discrepancies between the modelled and reference sequences:

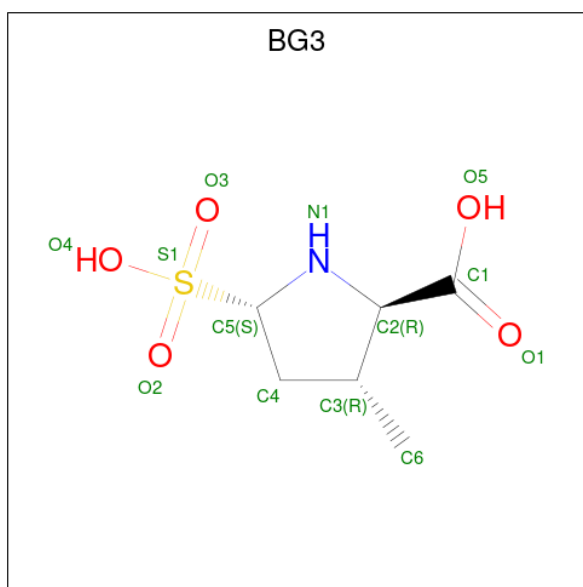
Chain	Residue	Modelled	Actual	Comment	Reference
A	334	LYS	PYL	conflict	UNP A0A0E3QRM4
A	496	GLY	-	expression tag	UNP A0A0E3QRM4
A	497	GLY	-	expression tag	UNP A0A0E3QRM4
A	498	HIS	-	expression tag	UNP A0A0E3QRM4
A	499	HIS	-	expression tag	UNP A0A0E3QRM4
A	500	HIS	-	expression tag	UNP A0A0E3QRM4
A	501	HIS	-	expression tag	UNP A0A0E3QRM4
A	502	HIS	-	expression tag	UNP A0A0E3QRM4
A	503	HIS	-	expression tag	UNP A0A0E3QRM4
B	334	LYS	PYL	conflict	UNP A0A0E3QRM4
B	496	GLY	-	expression tag	UNP A0A0E3QRM4
B	497	GLY	-	expression tag	UNP A0A0E3QRM4
B	498	HIS	-	expression tag	UNP A0A0E3QRM4
B	499	HIS	-	expression tag	UNP A0A0E3QRM4
B	500	HIS	-	expression tag	UNP A0A0E3QRM4
B	501	HIS	-	expression tag	UNP A0A0E3QRM4
B	502	HIS	-	expression tag	UNP A0A0E3QRM4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	503	HIS	-	expression tag	UNP A0A0E3QRM4
C	334	LYS	PYL	conflict	UNP A0A0E3QRM4
C	496	GLY	-	expression tag	UNP A0A0E3QRM4
C	497	GLY	-	expression tag	UNP A0A0E3QRM4
C	498	HIS	-	expression tag	UNP A0A0E3QRM4
C	499	HIS	-	expression tag	UNP A0A0E3QRM4
C	500	HIS	-	expression tag	UNP A0A0E3QRM4
C	501	HIS	-	expression tag	UNP A0A0E3QRM4
C	502	HIS	-	expression tag	UNP A0A0E3QRM4
C	503	HIS	-	expression tag	UNP A0A0E3QRM4
D	334	LYS	PYL	conflict	UNP A0A0E3QRM4
D	496	GLY	-	expression tag	UNP A0A0E3QRM4
D	497	GLY	-	expression tag	UNP A0A0E3QRM4
D	498	HIS	-	expression tag	UNP A0A0E3QRM4
D	499	HIS	-	expression tag	UNP A0A0E3QRM4
D	500	HIS	-	expression tag	UNP A0A0E3QRM4
D	501	HIS	-	expression tag	UNP A0A0E3QRM4
D	502	HIS	-	expression tag	UNP A0A0E3QRM4
D	503	HIS	-	expression tag	UNP A0A0E3QRM4
E	334	LYS	PYL	conflict	UNP A0A0E3QRM4
E	496	GLY	-	expression tag	UNP A0A0E3QRM4
E	497	GLY	-	expression tag	UNP A0A0E3QRM4
E	498	HIS	-	expression tag	UNP A0A0E3QRM4
E	499	HIS	-	expression tag	UNP A0A0E3QRM4
E	500	HIS	-	expression tag	UNP A0A0E3QRM4
E	501	HIS	-	expression tag	UNP A0A0E3QRM4
E	502	HIS	-	expression tag	UNP A0A0E3QRM4
E	503	HIS	-	expression tag	UNP A0A0E3QRM4
F	334	LYS	PYL	conflict	UNP A0A0E3QRM4
F	496	GLY	-	expression tag	UNP A0A0E3QRM4
F	497	GLY	-	expression tag	UNP A0A0E3QRM4
F	498	HIS	-	expression tag	UNP A0A0E3QRM4
F	499	HIS	-	expression tag	UNP A0A0E3QRM4
F	500	HIS	-	expression tag	UNP A0A0E3QRM4
F	501	HIS	-	expression tag	UNP A0A0E3QRM4
F	502	HIS	-	expression tag	UNP A0A0E3QRM4
F	503	HIS	-	expression tag	UNP A0A0E3QRM4

- Molecule 2 is 3-METHYL-5-SULFO-PYRROLIDINE-2-CARBOXYLIC ACID (CCD ID: BG3) (formula: C₆H₁₁NO₅S) (labeled as "Ligand of Interest" by depositor).

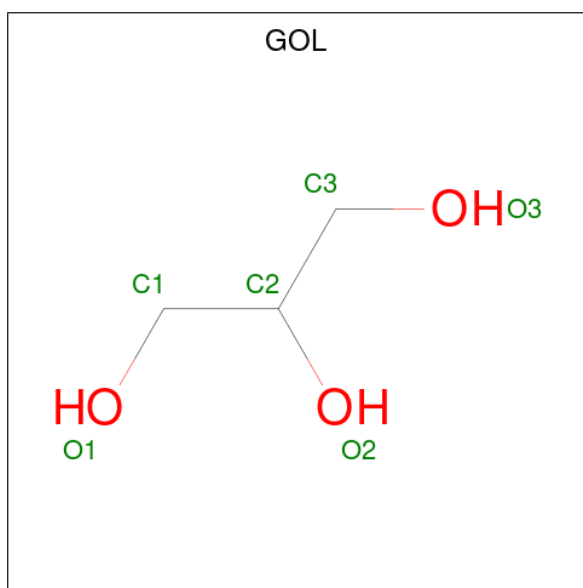


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		
3	F	1	Total	Na	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

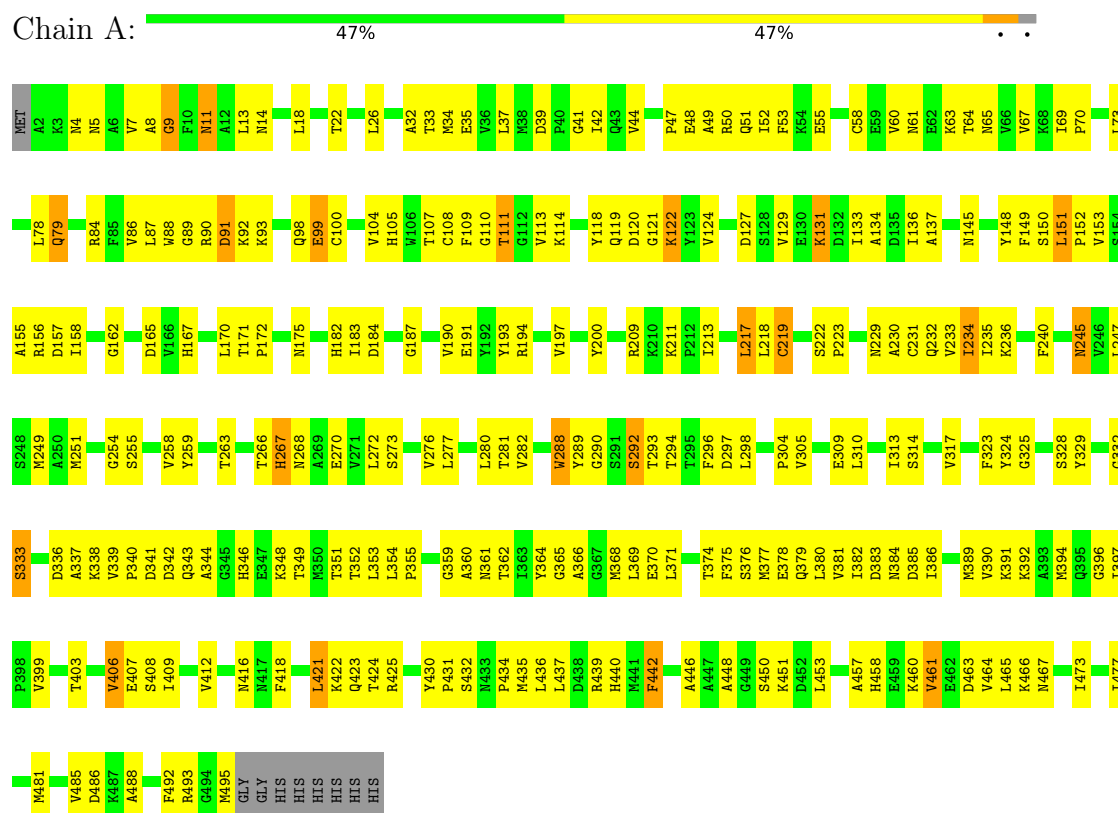
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total 30	O 30	0	0
5	B	28	Total 28	O 28	0	0
5	C	23	Total 23	O 23	0	0
5	D	29	Total 29	O 29	0	0
5	E	25	Total 25	O 25	0	0
5	F	30	Total 30	O 30	0	0

3 Residue-property plots

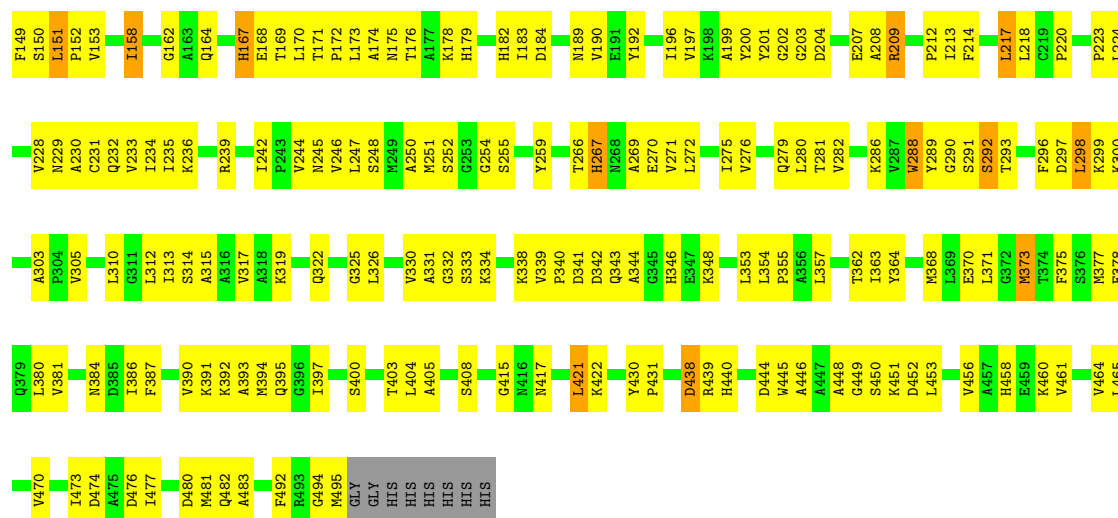
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Trimethylamine methyltransferase

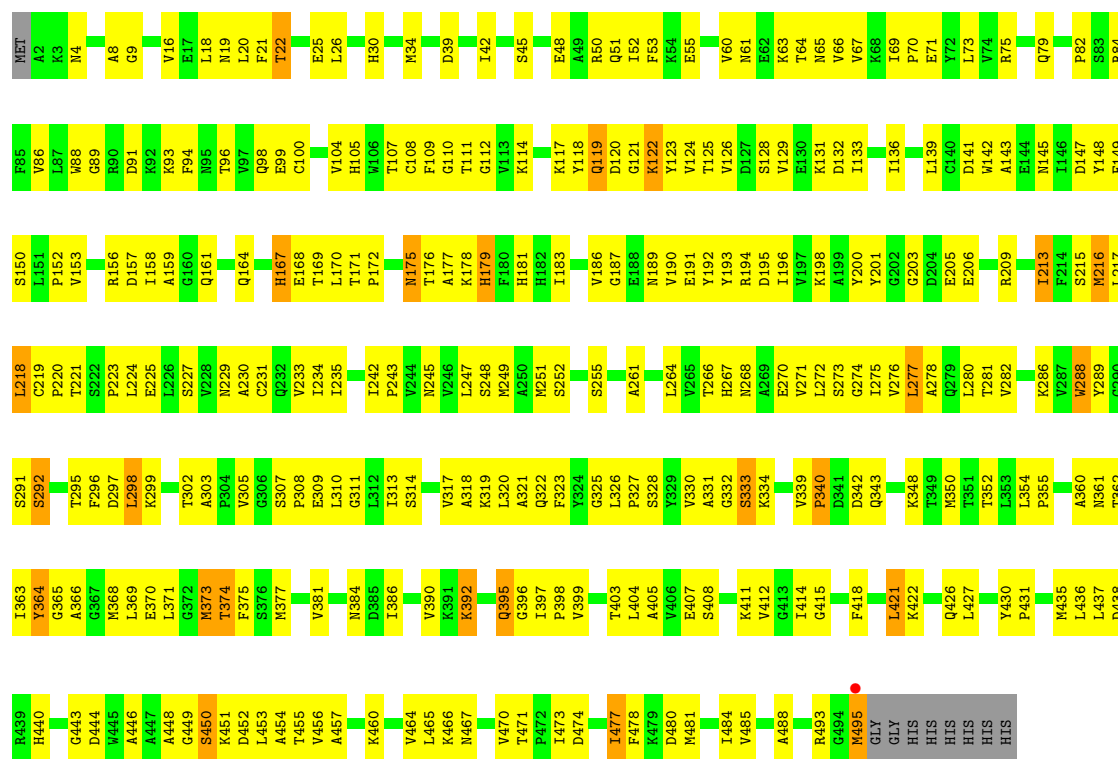


• Molecule 1: Trimethylamine methyltransferase





- Molecule 1: Trimethylamine methyltransferase



- Molecule 1: Trimethylamine methyltransferase



H458	L380	V305	G306	S307	P308	E309	L310	G311	V317	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379	
E459	V381	G306	S307	P308	E309	L310	G311	V317	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379		
K460	I382	C231	Q232	V233	I234	I235	K236	G241	I242	N245	V246	L247	S248	M249	A250	M251	S252	Y259	L260	A261	H267	N268	V271	L272	S273	G274	I275	A278	Q279	L280	T281	V282	P283	G284	A285	K286	V287	W288	Y289	G290	S291	S292	T293	T294	T295	F296	D297	L298	K299	K300	G301	T302	A303	F304		
V461	D383	D232	V233	I234	V166	H167	E168	T169	L170	T171	P172	L173	A174	N175	T176	A177	K178	H179	F180	H181	D184	P185	V186	G187	E188	N189	V190	G121	K122	Y123	V124	T125	V126	D127	S128	V129	E130	K131	D132	A133	I133	D135	I136	D141	W142	N145	I146	D147	Y148	F149	S150	I151	P152	V153	R156	D157
E462	N384	Q232	V233	I234	V166	H167	E168	T169	L170	T171	P172	L173	A174	N175	T176	A177	K178	H179	F180	H181	D184	P185	V186	G187	E188	N189	V190	G121	K122	Y123	V124	T125	V126	D127	S128	V129	E130	K131	D132	A133	I133	D135	I136	D141	W142	N145	I146	D147	Y148	F149	S150	I151	P152	V153	R156	D157
D463	D385	G311	V317	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379							
V464	I386	G311	V317	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379							
L465	F387	V317	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379								
N466	V390	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
N467	K391	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
H468	K392	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
T471	Q395	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
F472	T403	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
D474	L404	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
A475	A405	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
D476	S408	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
F478	G415	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
K479	M416	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
D480	N417	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
M481	Q482	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
A483	F418	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
I484	L419	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
V485	A420	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
D486	L421	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
K487	K422	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
A488	Q423	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
D489	T424	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
K490	R425	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
A491	Q426	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
F492	L427	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	K360	M361	T362	I363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379									
M495	W428	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359																									

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.84Å 174.84Å 300.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.20 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	84.5 (20.00-3.20) 84.1 (20.00-3.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.22Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.167 , 0.243 0.167 , 0.243	Depositor DCC
R_{free} test set	7479 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 77.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22891	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: NA, GOL, BG3

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	0.42	0/3840	0.97	13/5209 (0.2%)
1	B	0.44	0/3840	1.00	14/5209 (0.3%)
1	C	0.41	0/3832	0.98	16/5199 (0.3%)
1	D	0.42	0/3840	1.00	15/5209 (0.3%)
1	E	0.42	0/3840	0.96	14/5209 (0.3%)
1	F	0.43	0/3840	0.99	19/5209 (0.4%)
All	All	0.42	0/23032	0.98	91/31244 (0.3%)

There are no bond length outliers.

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	69	ILE	N-CA-C	8.58	115.36	107.56
1	C	69	ILE	N-CA-C	8.31	117.08	107.77
1	E	69	ILE	N-CA-C	7.89	115.73	107.76
1	E	22	THR	N-CA-C	-7.88	99.16	110.59
1	C	149	PHE	N-CA-C	7.88	121.48	108.96

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	3765	0	3762	268	0
1	B	3765	0	3762	238	0
1	C	3757	0	3753	284	0
1	D	3765	0	3762	259	0
1	E	3765	0	3762	268	0
1	F	3765	0	3762	303	0
2	A	12	0	10	3	0
2	B	12	0	9	2	0
2	C	12	0	10	1	0
2	D	12	0	10	0	0
2	E	12	0	10	0	0
2	F	12	0	10	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	12	0	16	4	0
4	B	12	0	16	2	0
4	C	6	0	8	5	0
4	D	18	0	24	9	0
4	E	12	0	16	1	0
4	F	6	0	8	7	0
5	A	30	0	0	3	0
5	B	28	0	0	1	0
5	C	23	0	0	3	0
5	D	29	0	0	4	0
5	E	25	0	0	3	0
5	F	30	0	0	3	0
All	All	22891	0	22710	1504	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 33.

The worst 5 of 1504 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:F:251:MET:HE3	1:F:303:ALA:HB2	1.27	1.16
1:C:368:MET:HG2	1:C:369:LEU:H	1.22	1.05
1:F:209:ARG:HH12	1:F:241:GLY:HA3	1.21	1.05
1:D:118:TYR:H	4:D:604:GOL:H12	1.23	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:473:ILE:HD13	1:E:481:MET:HE1	1.45	0.98

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	492/503 (98%)	434 (88%)	55 (11%)	3 (1%)	21	56
1	B	492/503 (98%)	435 (88%)	52 (11%)	5 (1%)	12	45
1	C	491/503 (98%)	424 (86%)	57 (12%)	10 (2%)	6	31
1	D	492/503 (98%)	424 (86%)	63 (13%)	5 (1%)	12	45
1	E	492/503 (98%)	417 (85%)	64 (13%)	11 (2%)	5	29
1	F	492/503 (98%)	433 (88%)	51 (10%)	8 (2%)	7	36
All	All	2951/3018 (98%)	2567 (87%)	342 (12%)	42 (1%)	9	39

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	371	LEU
1	E	421	LEU
1	F	62	GLU
1	C	421	LEU
1	D	202	GLY

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	405/412 (98%)	386 (95%)	19 (5%)	23	57
1	B	405/412 (98%)	389 (96%)	16 (4%)	28	61
1	C	404/412 (98%)	388 (96%)	16 (4%)	28	61
1	D	405/412 (98%)	393 (97%)	12 (3%)	36	66
1	E	405/412 (98%)	392 (97%)	13 (3%)	34	65
1	F	405/412 (98%)	395 (98%)	10 (2%)	42	69
All	All	2429/2472 (98%)	2343 (96%)	86 (4%)	32	64

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	209	ARG
1	E	364	TYR
1	D	267	HIS
1	E	120	ASP
1	E	495	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	232	GLN
1	E	189	ASN
1	D	268	ASN
1	D	458	HIS
1	E	384	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 6 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	$\# Z > 2$
2	BG3	A	601	1	8,12,13	1.21	1 (12%)	12,18,20	1.44	3 (25%)
2	BG3	C	601	1	8,12,13	1.20	0	12,18,20	1.33	2 (16%)
4	GOL	D	605	-	5,5,5	0.35	0	5,5,5	0.52	0
4	GOL	A	603	-	5,5,5	0.35	0	5,5,5	0.35	0
2	BG3	D	601	1	8,12,13	0.99	0	12,18,20	1.44	3 (25%)
4	GOL	D	604	-	5,5,5	0.31	0	5,5,5	0.84	0
4	GOL	D	603	-	5,5,5	0.30	0	5,5,5	0.52	0
4	GOL	E	603	-	5,5,5	0.34	0	5,5,5	0.51	0
2	BG3	B	601	1	8,12,13	1.28	0	12,18,20	1.38	3 (25%)
4	GOL	A	604	-	5,5,5	0.29	0	5,5,5	0.51	0
4	GOL	E	604	-	5,5,5	0.35	0	5,5,5	1.00	0
4	GOL	F	603	-	5,5,5	0.31	0	5,5,5	1.37	1 (20%)
4	GOL	B	603	-	5,5,5	0.28	0	5,5,5	0.85	0
4	GOL	B	604	-	5,5,5	0.38	0	5,5,5	0.75	0
2	BG3	E	601	1	8,12,13	1.11	0	12,18,20	1.37	3 (25%)
2	BG3	F	601	1	8,12,13	1.04	0	12,18,20	1.30	3 (25%)
4	GOL	C	603	-	5,5,5	0.32	0	5,5,5	0.85	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
2	BG3	A	601	1	-	1/1/20/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BG3	C	601	1	-	0/1/20/22	0/1/1/1
4	GOL	D	605	-	-	4/4/4/4	-
4	GOL	A	603	-	-	4/4/4/4	-
2	BG3	D	601	1	-	1/1/20/22	0/1/1/1
4	GOL	D	604	-	-	1/4/4/4	-
4	GOL	D	603	-	-	2/4/4/4	-
4	GOL	E	603	-	-	2/4/4/4	-
2	BG3	B	601	1	-	1/1/20/22	0/1/1/1
4	GOL	A	604	-	-	4/4/4/4	-
4	GOL	E	604	-	-	0/4/4/4	-
4	GOL	F	603	-	-	1/4/4/4	-
4	GOL	B	603	-	-	3/4/4/4	-
4	GOL	B	604	-	-	4/4/4/4	-
2	BG3	E	601	1	-	1/1/20/22	0/1/1/1
2	BG3	F	601	1	-	1/1/20/22	0/1/1/1
4	GOL	C	603	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	BG3	C4-C3	-2.07	1.50	1.54

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	BG3	C6-C3-C4	-2.72	108.21	113.09
2	F	601	BG3	C2-N1-C5	-2.71	97.98	106.47
2	A	601	BG3	C2-N1-C5	-2.57	98.42	106.47
2	C	601	BG3	C2-N1-C5	-2.55	98.47	106.47
2	A	601	BG3	C6-C3-C4	-2.52	108.56	113.09

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

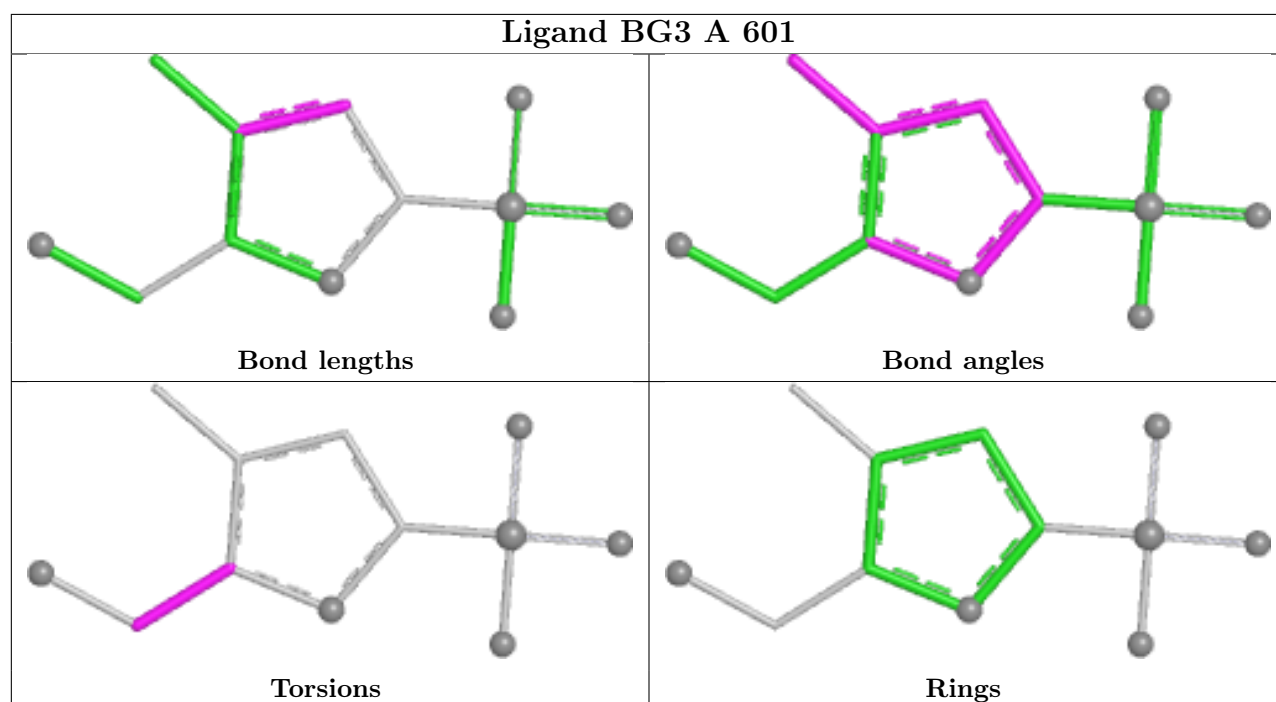
Mol	Chain	Res	Type	Atoms
2	A	601	BG3	O1-C1-C2-C3
2	D	601	BG3	O1-C1-C2-C3
2	E	601	BG3	O1-C1-C2-C3
4	A	603	GOL	O1-C1-C2-C3
4	A	603	GOL	C1-C2-C3-O3

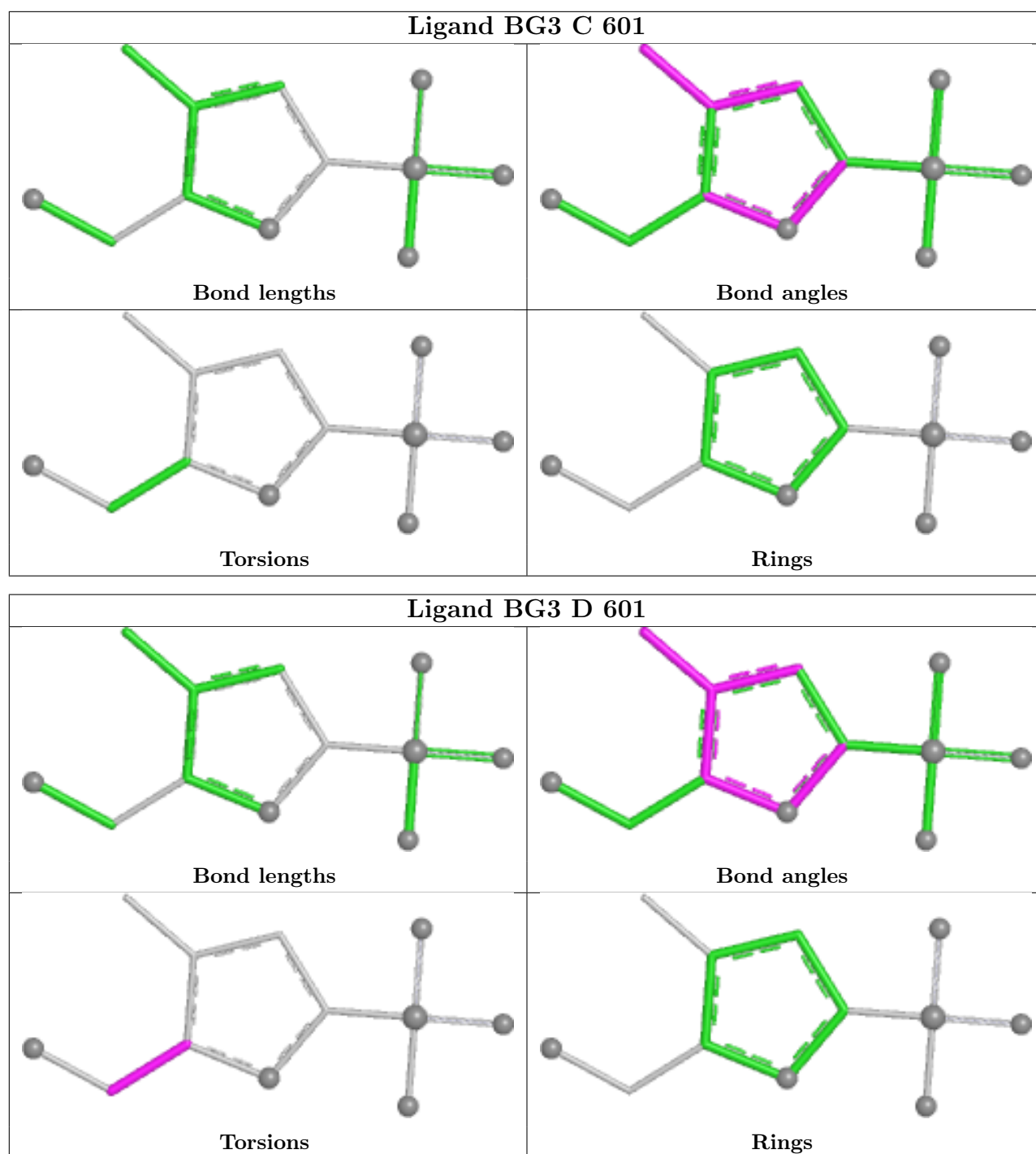
There are no ring outliers.

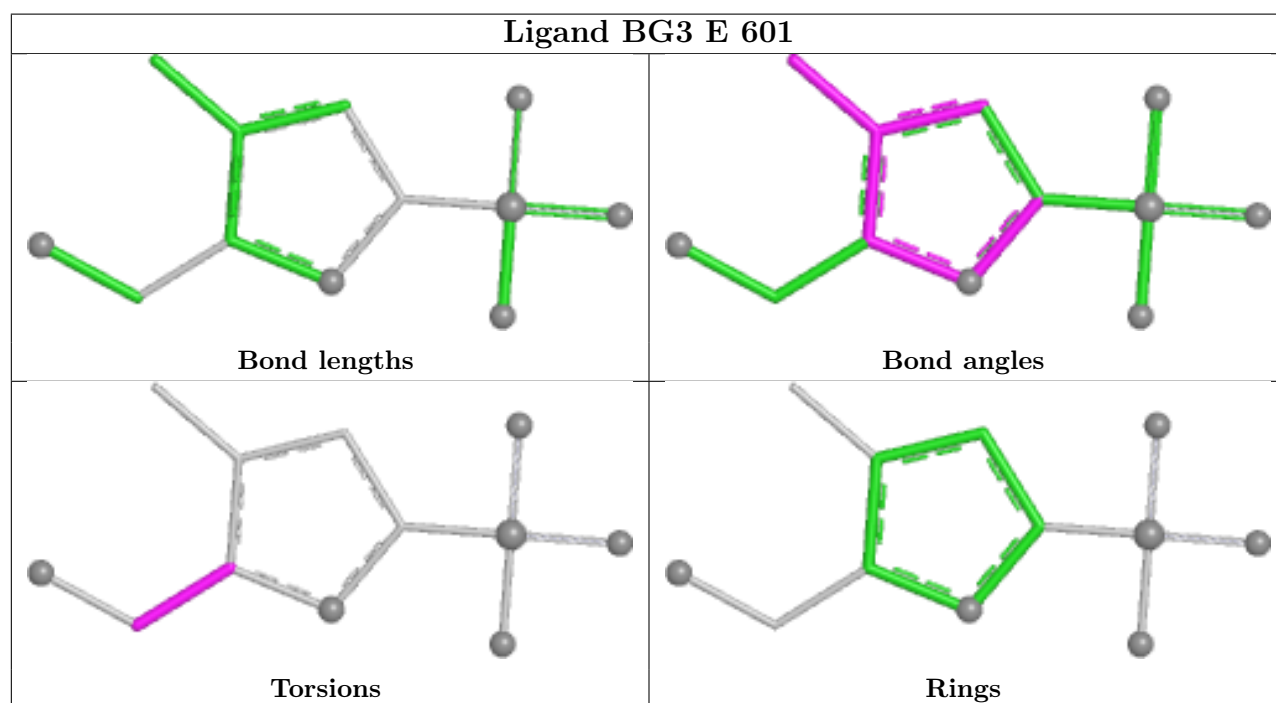
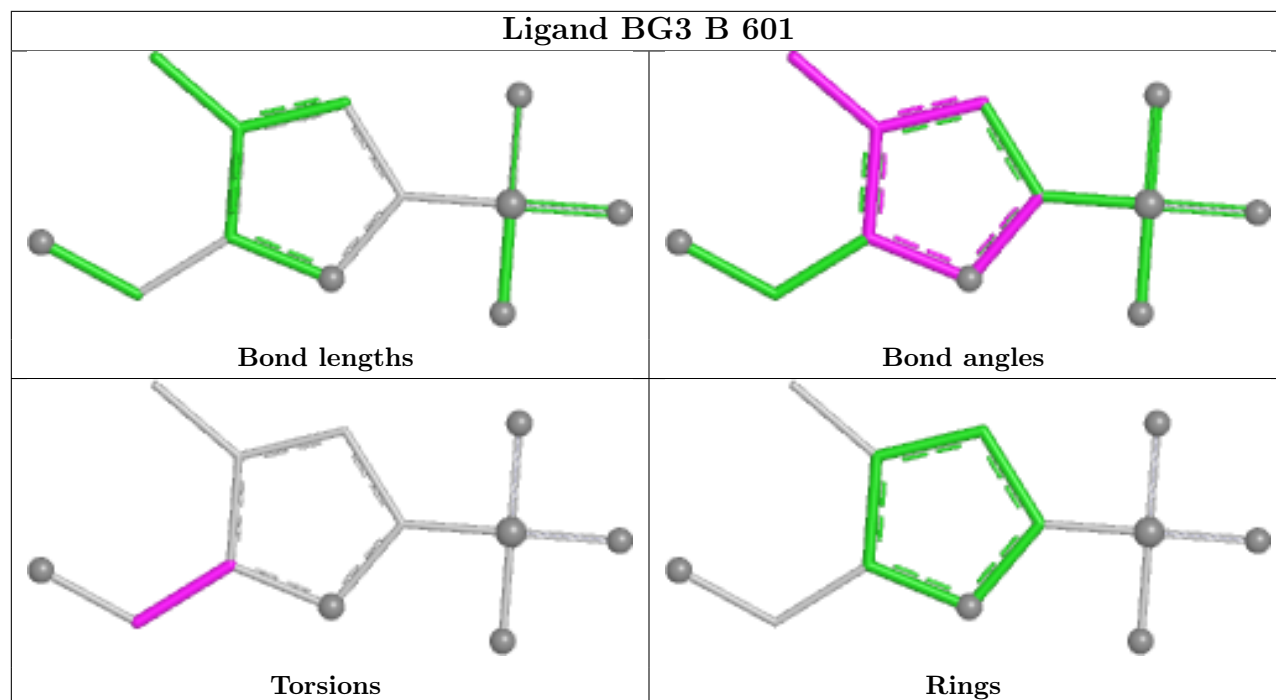
9 monomers are involved in 34 short contacts:

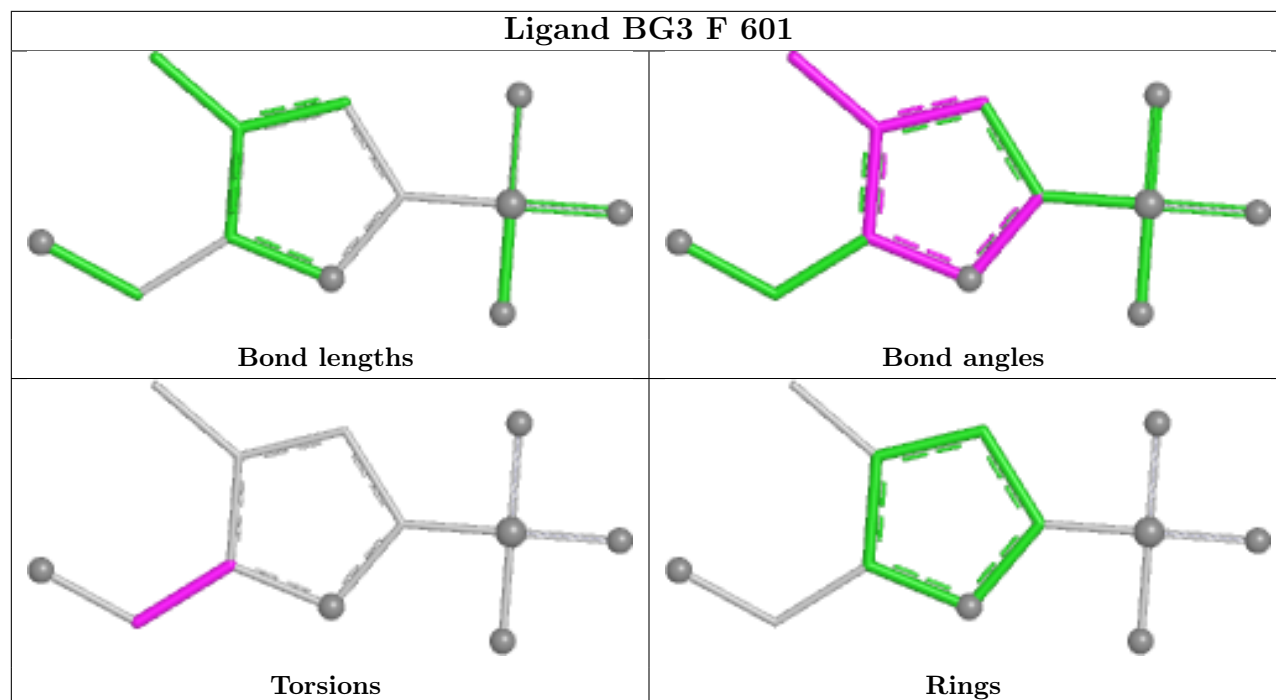
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	BG3	3	0
2	C	601	BG3	1	0
4	D	604	GOL	9	0
2	B	601	BG3	2	0
4	A	604	GOL	4	0
4	E	604	GOL	1	0
4	F	603	GOL	7	0
4	B	603	GOL	2	0
4	C	603	GOL	5	0

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	494/503 (98%)	-0.76	0 100 100	22, 47, 74, 132	0
1	B	494/503 (98%)	-0.84	0 100 100	19, 44, 70, 132	0
1	C	493/503 (98%)	-0.50	2 (0%) 88 79	27, 61, 96, 134	0
1	D	494/503 (98%)	-0.70	0 100 100	19, 50, 80, 123	0
1	E	494/503 (98%)	-0.73	1 (0%) 91 85	18, 48, 80, 132	0
1	F	494/503 (98%)	-0.64	0 100 100	22, 52, 87, 115	0
All	All	2963/3018 (98%)	-0.69	3 (0%) 92 89	18, 50, 85, 134	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	494	GLY	3.2
1	E	495	MET	2.4
1	C	298	LEU	2.3

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,

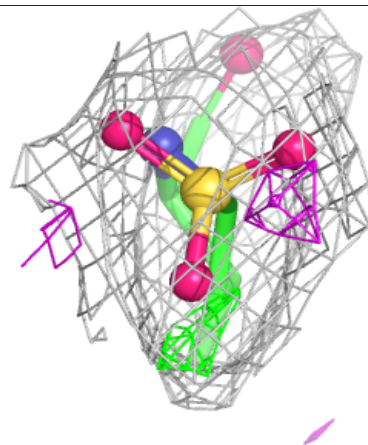
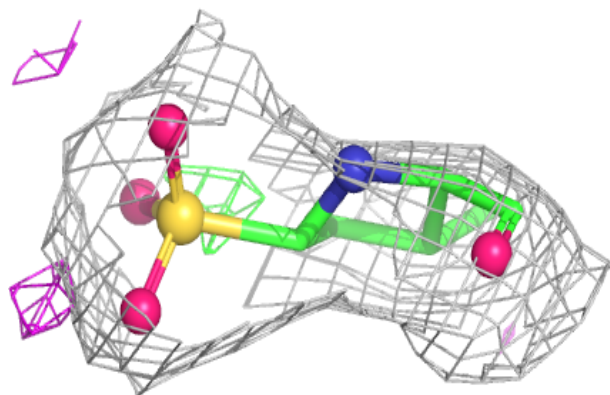
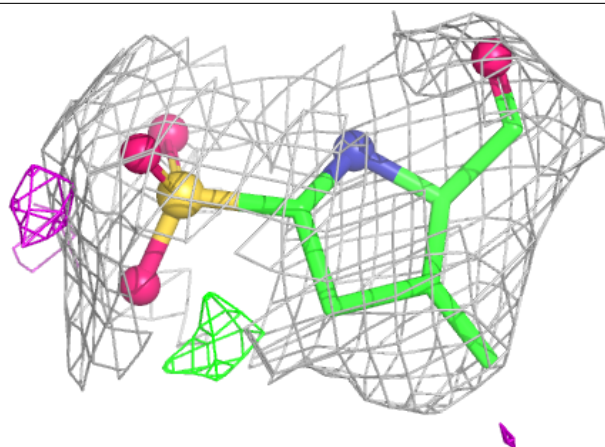
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	D	605	6/6	0.88	0.15	53,76,80,86	0
4	GOL	D	604	6/6	0.90	0.12	43,63,69,70	0
4	GOL	A	604	6/6	0.91	0.08	42,64,72,80	0
2	BG3	F	601	12/13	0.92	0.10	48,72,80,82	0
4	GOL	C	603	6/6	0.92	0.14	63,67,74,76	0
4	GOL	E	603	6/6	0.92	0.11	43,51,59,66	0
4	GOL	F	603	6/6	0.92	0.10	46,53,64,65	0
4	GOL	B	603	6/6	0.93	0.09	30,60,65,72	0
4	GOL	E	604	6/6	0.93	0.09	50,62,71,73	0
4	GOL	A	603	6/6	0.93	0.12	38,68,70,71	0
2	BG3	C	601	12/13	0.94	0.11	68,99,106,108	0
4	GOL	B	604	6/6	0.94	0.09	28,57,64,65	0
4	GOL	D	603	6/6	0.95	0.11	29,74,81,92	0
2	BG3	A	601	12/13	0.95	0.11	58,75,85,91	0
2	BG3	D	601	12/13	0.96	0.09	37,70,83,91	0
3	NA	D	602	1/1	0.97	0.08	73,73,73,73	0
2	BG3	B	601	12/13	0.97	0.09	32,65,72,85	0
3	NA	B	602	1/1	0.97	0.07	44,44,44,44	0
2	BG3	E	601	12/13	0.98	0.08	44,69,77,80	0
3	NA	C	602	1/1	0.98	0.05	56,56,56,56	0
3	NA	F	602	1/1	0.99	0.03	50,50,50,50	0
3	NA	A	602	1/1	0.99	0.04	63,63,63,63	0
3	NA	E	602	1/1	0.99	0.03	62,62,62,62	0

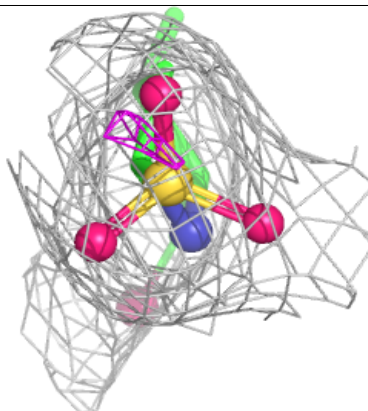
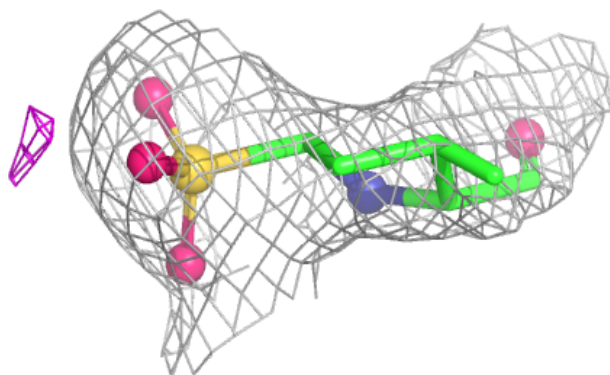
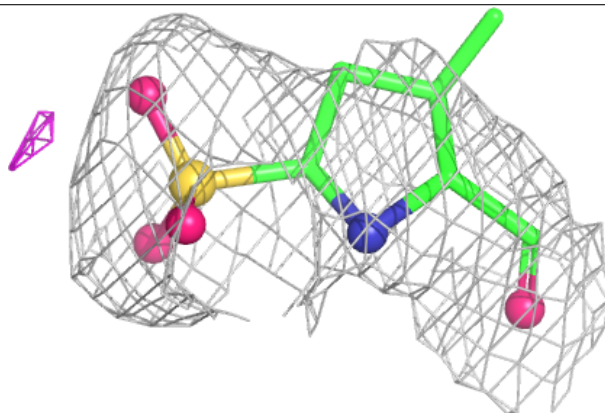
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BG3 F 601:

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

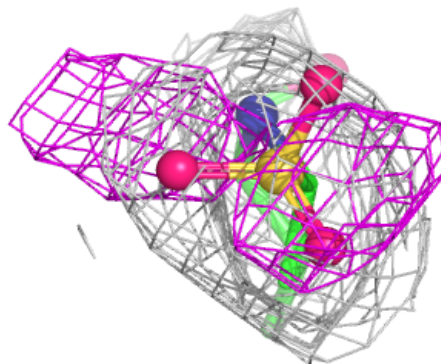
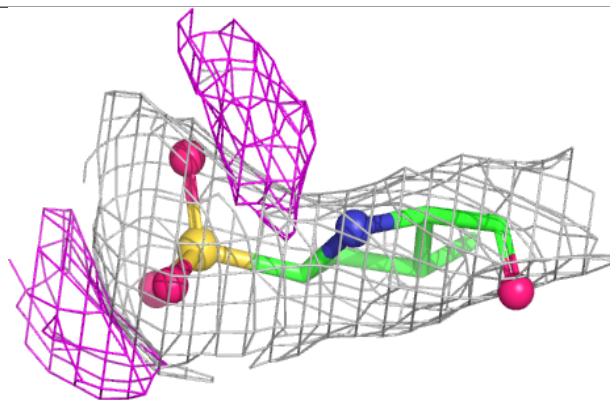
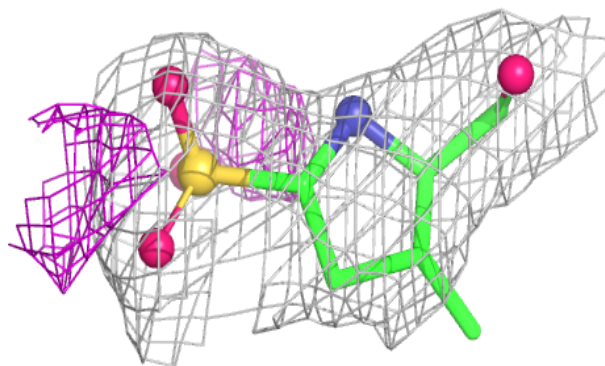
**Electron density around BG3 C 601:**

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

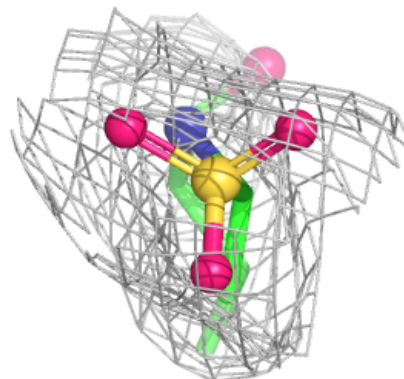
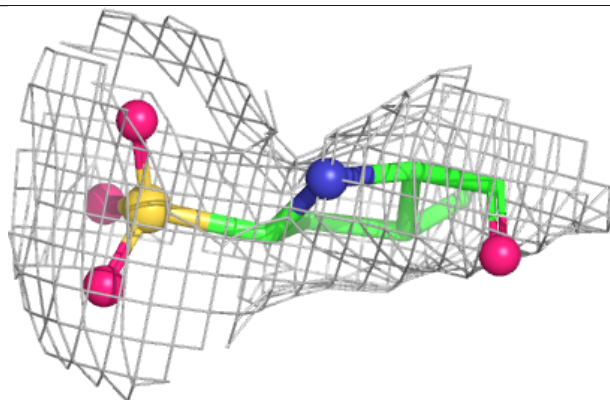
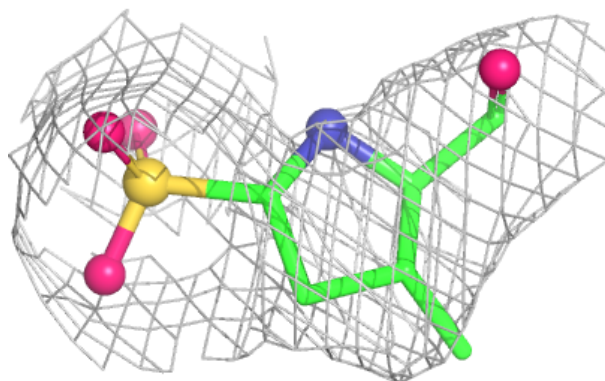


Electron density around BG3 A 601:

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

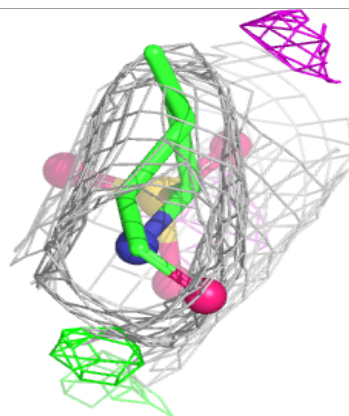
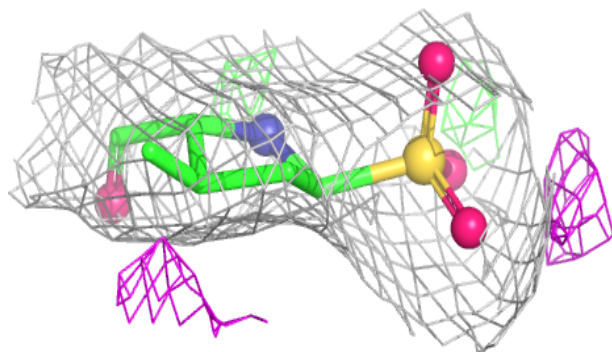
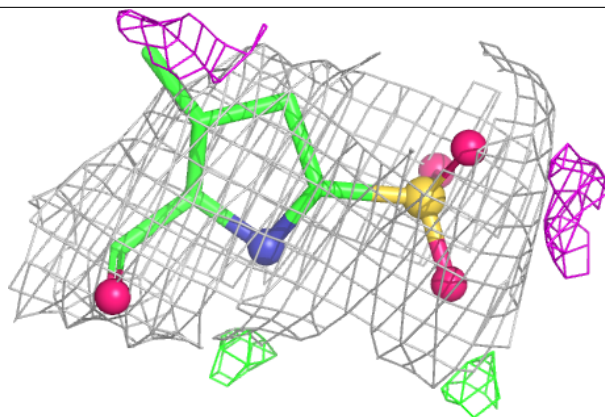
**Electron density around BG3 D 601:**

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

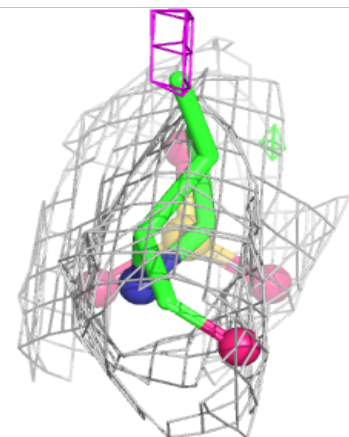
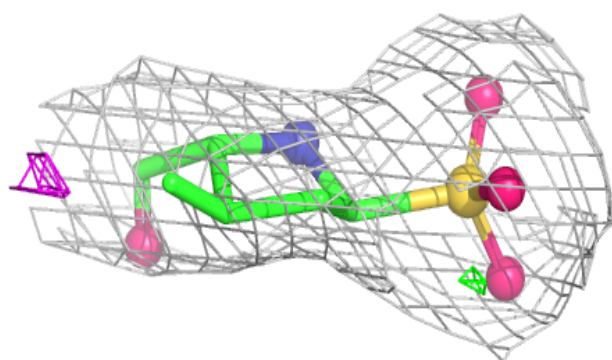
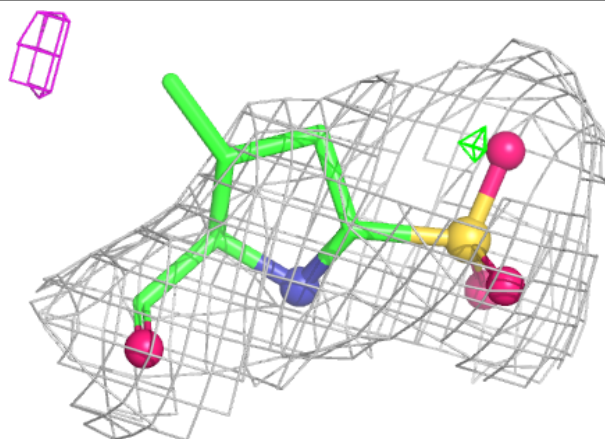


Electron density around BG3 B 601:

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

**Electron density around BG3 E 601:**

$2mF_o-DF_c$ (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.