



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 10:37 PM UTC

PDB ID : 9QMF / pdb_00009qmf
Title : Pseudomonas putida 4-hydroxyphenylpyruvate dioxygenase in complex with Tembotrione (Mn)
Authors : Alshref, F.M.; Dhingra, S.; Farcas, I.M.; Brewitz, L.; Allen, M.D.; Schofield, C.J.
Deposited on : 2025-03-23
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

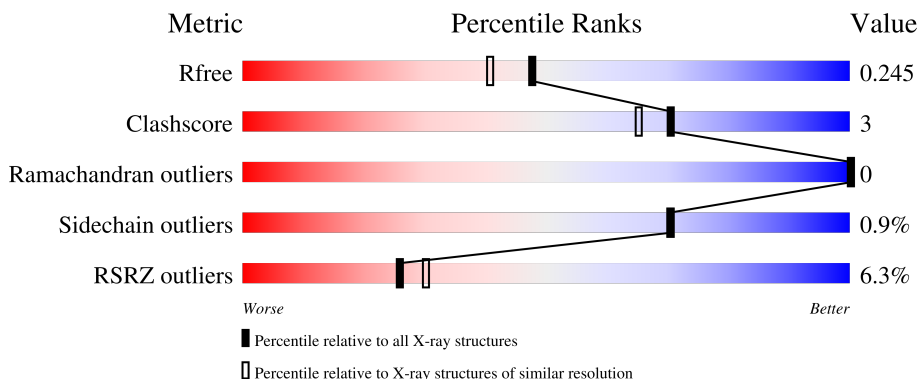
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	361	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>8%</div> </div> </div>
1	B	361	<div> <div>8%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>9%</div> </div> </div>
1	C	361	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>7%</div> </div> </div>
1	D	361	<div> <div>7%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>7%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12055 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 4-hydroxyphenylpyruvate dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	3	0
			2666	1708	454	491	13			
1	B	330	Total	C	N	O	S	0	3	0
			2656	1705	453	485	13			
1	C	337	Total	C	N	O	S	0	5	0
			2719	1738	465	503	13			
1	D	336	Total	C	N	O	S	0	2	0
			2688	1723	458	494	13			

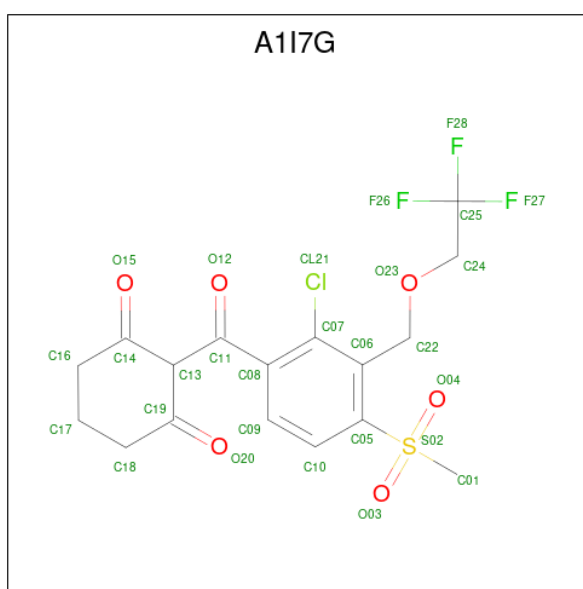
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A1L5PRA6
A	2	GLY	-	expression tag	UNP A0A1L5PRA6
A	3	SER	-	expression tag	UNP A0A1L5PRA6
A	4	SER	-	expression tag	UNP A0A1L5PRA6
B	1	GLY	-	expression tag	UNP A0A1L5PRA6
B	2	GLY	-	expression tag	UNP A0A1L5PRA6
B	3	SER	-	expression tag	UNP A0A1L5PRA6
B	4	SER	-	expression tag	UNP A0A1L5PRA6
C	1	GLY	-	expression tag	UNP A0A1L5PRA6
C	2	GLY	-	expression tag	UNP A0A1L5PRA6
C	3	SER	-	expression tag	UNP A0A1L5PRA6
C	4	SER	-	expression tag	UNP A0A1L5PRA6
D	1	GLY	-	expression tag	UNP A0A1L5PRA6
D	2	GLY	-	expression tag	UNP A0A1L5PRA6
D	3	SER	-	expression tag	UNP A0A1L5PRA6
D	4	SER	-	expression tag	UNP A0A1L5PRA6

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0

- Molecule 3 is Tembotrione (CCD ID: A1I7G) (formula: C₁₇H₁₆ClF₃O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 28	C 17	Cl 1	F 3	O 6	S 1	0	0
3	B	1	Total 56	C 34	Cl 2	F 6	O 12	S 2	0	1
3	C	1	Total 56	C 34	Cl 2	F 6	O 12	S 2	0	1
3	D	1	Total 28	C 17	Cl 1	F 3	O 6	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	307	Total O 307 307	0	0

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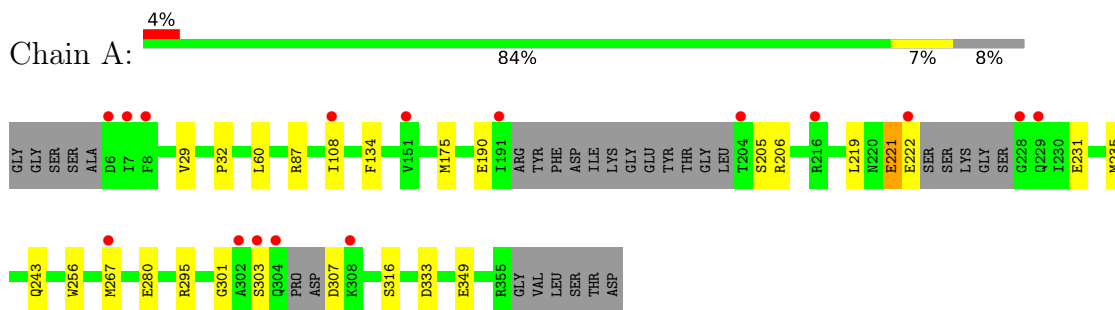
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	215	Total 215	O 215	0	0
4	C	343	Total 343	O 343	0	0
4	D	289	Total 289	O 289	0	0

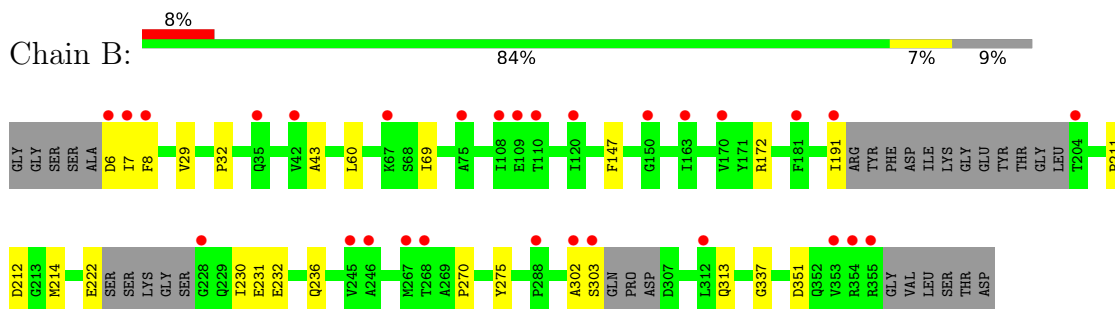
3 Residue-property plots

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.

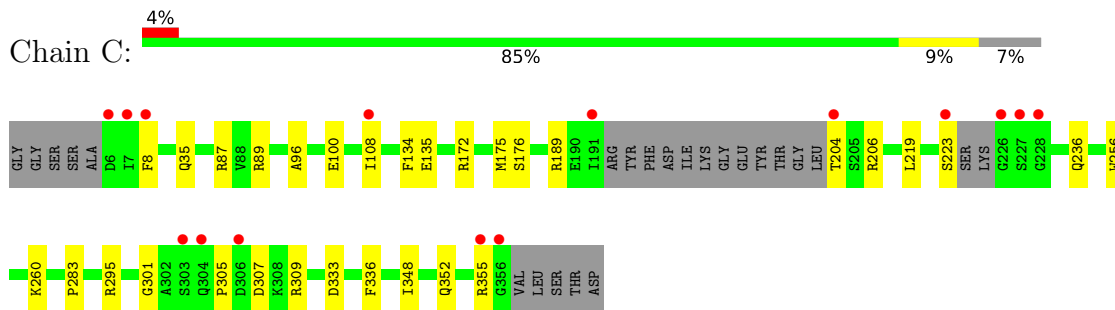
- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



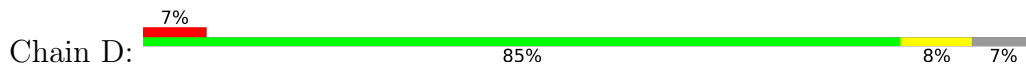
- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

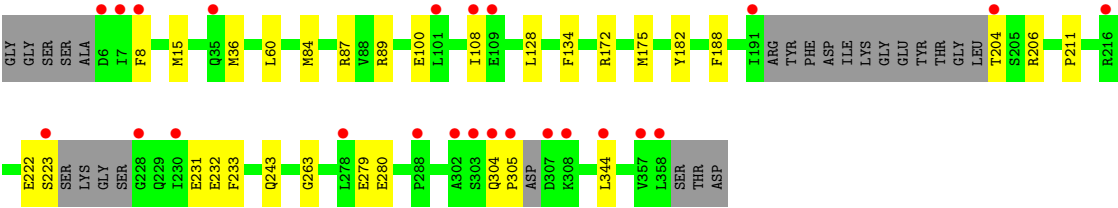


- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.01Å 168.36Å 81.81Å 90.00° 91.98° 90.00°	Depositor
Resolution (Å)	52.64 – 1.95 52.64 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.8 (52.64-1.95) 99.2 (52.64-1.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.210 , 0.245 0.211 , 0.245	Depositor DCC
R_{free} test set	7332 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.219 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12055	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.8595e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MN, A1I7G

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	0.63	0/2727	0.73	0/3673
1	B	0.46	0/2717	0.60	0/3659
1	C	0.70	0/2782	0.73	0/3749
1	D	0.54	0/2750	0.62	0/3706
All	All	0.59	0/10976	0.68	0/14787

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2666	0	2602	17	0
1	B	2656	0	2606	18	0
1	C	2719	0	2650	21	0
1	D	2688	0	2630	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	56	0	0	0	0
3	C	56	0	0	1	0
3	D	28	0	0	0	0
4	A	307	0	0	3	2
4	B	215	0	0	7	1
4	C	343	0	0	7	4
4	D	289	0	0	7	1
All	All	12055	0	10488	73	5

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 3.

All (73) 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:A:280:GLU:HG3	4:A:514:HOH:O	1.73	0.87
1:C:35:GLN:HG2	4:C:520:HOH:O	1.80	0.81
1:B:222:GLU:HG2	1:B:230:ILE:HB	1.64	0.80
1:D:280:GLU:HG3	4:D:513:HOH:O	1.85	0.77
1:B:69:ILE:HD12	4:B:511:HOH:O	1.84	0.76
1:A:243:GLN:OE1	4:A:501:HOH:O	2.04	0.75
1:C:236:GLN:OE1	4:C:501:HOH:O	2.08	0.72
1:D:279:GLU:HG2	4:D:565:HOH:O	1.92	0.70
1:D:304:GLN:HB2	1:D:305:PRO:HD3	1.76	0.67
1:B:6:ASP:N	4:B:501:HOH:O	2.29	0.65
1:B:191:ILE:HG12	4:B:503:HOH:O	1.96	0.64
1:D:175:MET:HG2	1:D:206:ARG:HD3	1.78	0.64
1:B:172:ARG:HH21	1:D:231:GLU:CD	2.06	0.63
1:A:175:MET:HE3	1:A:221:GLU:HB2	1.80	0.62
1:D:222:GLU:HB3	4:D:526:HOH:O	1.98	0.62
1:A:175:MET:SD	1:A:206:ARG:HG3	2.41	0.61
1:B:7:ILE:HD13	4:B:695:HOH:O	2.01	0.61
1:A:256:TRP:CE2	1:A:295:ARG:HB3	2.38	0.58
1:C:135:GLU:HG3	4:C:564:HOH:O	2.06	0.56
1:C:260:LYS:HD2	4:C:582:HOH:O	2.06	0.55
1:C:309:ARG:NH2	4:C:510:HOH:O	2.40	0.55
1:C:301:GLY:HA2	1:C:333:ASP:OD2	2.07	0.55
1:C:8:PHE:CE1	1:C:189:ARG:HG3	2.42	0.54
1:C:307:ASP:OD1	1:C:309:ARG:HD3	2.07	0.54
1:B:302:ALA:C	4:B:506:HOH:O	2.50	0.53
1:B:303:SER:N	4:B:506:HOH:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:ILE:O	1:C:352:GLN:HG3	2.09	0.53
1:D:36:MET:HE3	1:D:263:GLY:O	2.09	0.52
1:B:270:PRO:HG2	1:B:275:TYR:CE2	2.45	0.52
1:C:204:THR:OG1	4:C:502:HOH:O	2.19	0.52
1:D:243:GLN:HG3	4:D:506:HOH:O	2.10	0.51
1:D:100:GLU:HG3	4:D:515:HOH:O	2.10	0.51
1:D:15:MET:HB2	1:D:87:ARG:HG2	1.94	0.50
1:B:313:GLN:OE1	1:B:337:GLY:HA3	2.12	0.49
1:D:204:THR:N	1:D:223:SER:HG	2.10	0.49
1:C:175:MET:SD	1:C:206:ARG:HG3	2.53	0.49
1:A:190:GLU:OE2	1:A:206:ARG:HD3	2.12	0.49
1:C:87:ARG:HG3	1:C:134:PHE:CD2	2.48	0.49
1:B:232:GLU:HG3	1:B:236:GLN:HE21	1.78	0.49
1:B:232:GLU:HG3	1:B:236:GLN:NE2	2.28	0.48
1:C:204:THR:HG23	1:C:223:SER:HB2	1.94	0.48
1:A:267:MET:HE2	1:A:316:SER:O	2.13	0.48
1:A:87:ARG:HG3	1:A:134:PHE:CD2	2.49	0.48
1:A:175:MET:HE2	1:A:219:LEU:C	2.39	0.47
1:C:283:PRO:HG2	1:C:305:PRO:HG3	1.96	0.47
1:C:96:ALA:O	1:C:100:GLU:HG3	2.15	0.47
1:A:303:SER:HA	1:A:307:ASP:O	2.14	0.47
1:A:231:GLU:CD	1:C:172:ARG:HH21	2.22	0.47
1:B:231:GLU:HG2	1:D:172:ARG:NH1	2.30	0.47
1:C:256:TRP:CE2	1:C:295:ARG:HB3	2.49	0.46
1:C:175:MET:HE2	1:C:219:LEU:C	2.41	0.45
1:C:89:ARG:NE	4:C:506:HOH:O	2.34	0.45
1:D:232:GLU:OE2	4:D:501:HOH:O	2.21	0.45
1:B:212:ASP:HB2	1:B:214:MET:HE3	1.98	0.45
1:B:29:VAL:O	1:B:32:PRO:HD2	2.18	0.44
1:D:89:ARG:HG2	4:D:597:HOH:O	2.17	0.44
1:D:84:MET:O	1:D:128:LEU:HA	2.18	0.43
1:A:108:ILE:HD13	1:A:108:ILE:HA	1.89	0.43
1:A:235:MET:HE2	1:A:235:MET:HB3	1.58	0.43
1:A:29:VAL:O	1:A:32:PRO:HD2	2.18	0.43
1:A:301:GLY:HA2	1:A:333:ASP:OD2	2.18	0.42
1:D:87:ARG:HG3	1:D:134:PHE:CD2	2.54	0.42
1:D:8:PHE:CD2	1:D:211:PRO:HB3	2.55	0.42
1:B:8:PHE:CD1	1:B:211:PRO:HB3	2.55	0.41
1:C:336:PHE:HB3	3:C:402[B]:A1I7G:C14	2.51	0.41
1:A:235:MET:HG3	4:A:650:HOH:O	2.20	0.41
1:D:182:TYR:HB3	1:D:188:PHE:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ALA:HB2	1:B:147:PHE:HA	2.03	0.41
1:A:205:SER:HA	1:A:219:LEU:O	2.21	0.40
1:B:7:ILE:HG21	4:B:695:HOH:O	2.20	0.40
1:D:344:LEU:HD23	1:D:344:LEU:HA	1.76	0.40
1:C:352:GLN:HG2	1:C:355:ARG:NH2	2.36	0.40
1:D:233:PHE:CE2	1:D:243:GLN:HA	2.57	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:706:HOH:O	4:C:793:HOH:O[2_556]	1.81	0.39
4:A:562:HOH:O	4:C:775:HOH:O[4_546]	1.90	0.30
4:A:705:HOH:O	4:C:795:HOH:O[4_546]	2.11	0.09
4:C:603:HOH:O	4:C:769:HOH:O[2_556]	2.15	0.05
4:B:675:HOH:O	4:D:533:HOH:O[4_545]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	326/361 (90%)	318 (98%)	8 (2%)	0	100	100
1	B	325/361 (90%)	320 (98%)	5 (2%)	0	100	100
1	C	336/361 (93%)	330 (98%)	6 (2%)	0	100	100
1	D	330/361 (91%)	324 (98%)	6 (2%)	0	100	100
All	All	1317/1444 (91%)	1292 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/298 (93%)	274 (99%)	4 (1%)	59	56
1	B	277/298 (93%)	275 (99%)	2 (1%)	76	76
1	C	284/298 (95%)	282 (99%)	2 (1%)	76	76
1	D	281/298 (94%)	279 (99%)	2 (1%)	76	76
All	All	1120/1192 (94%)	1110 (99%)	10 (1%)	70	70

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	221	GLU
1	A	222	GLU
1	A	349	GLU
1	B	60	LEU
1	B	351	ASP
1	C	108	ILE
1	C	176	SER
1	D	60	LEU
1	D	108	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	243	GLN
1	A	272	GLN
1	B	92	HIS
1	B	104	GLN
1	B	236	GLN
1	B	243	GLN
1	C	35	GLN
1	C	272	GLN

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Mol	Chain	Res	Type
1	C	304	GLN
1	D	169	ASN
1	D	229	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\# Z > 2$
3	A1I7G	B	402[B]	2	27,29,29	1.54	4 (14%)	35,44,44	2.87	9 (25%)
3	A1I7G	C	402[A]	2	27,29,29	1.42	3 (11%)	35,44,44	3.41	10 (28%)
3	A1I7G	A	402	2	27,29,29	1.52	5 (18%)	35,44,44	4.44	12 (34%)
3	A1I7G	B	402[A]	2	27,29,29	1.50	4 (14%)	35,44,44	3.10	10 (28%)
3	A1I7G	D	402	2	27,29,29	1.62	5 (18%)	35,44,44	3.40	11 (31%)
3	A1I7G	C	402[B]	2	27,29,29	1.34	3 (11%)	35,44,44	3.19	12 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1I7G	B	402[B]	2	-	9/21/35/35	0/2/2/2
3	A1I7G	C	402[A]	2	-	12/21/35/35	0/2/2/2
3	A1I7G	A	402	2	-	11/21/35/35	0/2/2/2
3	A1I7G	B	402[A]	2	-	10/21/35/35	0/2/2/2
3	A1I7G	D	402	2	-	13/21/35/35	0/2/2/2
3	A1I7G	C	402[B]	2	-	8/21/35/35	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402[A]	A1I7G	C05-S02	3.63	1.82	1.78
3	D	402	A1I7G	O12-C11	-3.44	1.17	1.22
3	B	402[B]	A1I7G	O12-C11	-3.29	1.17	1.22
3	D	402	A1I7G	C07-CL21	3.23	1.79	1.72
3	B	402[A]	A1I7G	C07-CL21	3.23	1.79	1.72
3	B	402[B]	A1I7G	C05-S02	3.20	1.82	1.78
3	B	402[B]	A1I7G	C07-CL21	3.02	1.79	1.72
3	B	402[A]	A1I7G	C05-S02	2.96	1.81	1.78
3	C	402[B]	A1I7G	C08-C11	2.91	1.54	1.49
3	B	402[A]	A1I7G	O12-C11	-2.91	1.18	1.22
3	A	402	A1I7G	O03-S02	2.86	1.51	1.44
3	C	402[A]	A1I7G	C07-CL21	2.80	1.78	1.72
3	A	402	A1I7G	C07-C06	-2.60	1.34	1.39
3	D	402	A1I7G	C05-S02	2.57	1.81	1.78
3	A	402	A1I7G	C08-C07	-2.51	1.37	1.39
3	B	402[B]	A1I7G	C08-C11	2.44	1.53	1.49
3	A	402	A1I7G	C08-C11	2.42	1.53	1.49
3	C	402[B]	A1I7G	O20-C19	-2.40	1.17	1.21
3	D	402	A1I7G	C08-C11	2.36	1.53	1.49
3	C	402[B]	A1I7G	C07-CL21	2.34	1.77	1.72
3	D	402	A1I7G	C08-C07	-2.32	1.37	1.39
3	C	402[A]	A1I7G	C08-C07	-2.25	1.37	1.39
3	A	402	A1I7G	C07-CL21	2.15	1.77	1.72
3	B	402[A]	A1I7G	C01-S02	2.00	1.82	1.75

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	A1I7G	O23-C24-C25	16.52	121.25	107.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402[A]	A1I7G	O04-S02-O03	-11.94	97.74	117.99
3	A	402	A1I7G	O04-S02-O03	-11.20	99.00	117.99
3	C	402[B]	A1I7G	O04-S02-O03	-10.96	99.40	117.99
3	B	402[A]	A1I7G	O04-S02-O03	-10.02	101.00	117.99
3	C	402[A]	A1I7G	C01-S02-C05	9.88	119.35	105.09
3	B	402[B]	A1I7G	O04-S02-O03	-9.41	102.03	117.99
3	A	402	A1I7G	C01-S02-C05	9.26	118.45	105.09
3	A	402	A1I7G	C08-C11-C13	9.08	130.43	118.89
3	D	402	A1I7G	C01-S02-C05	8.81	117.81	105.09
3	D	402	A1I7G	O04-S02-O03	-8.79	103.08	117.99
3	D	402	A1I7G	C08-C11-C13	8.40	129.57	118.89
3	D	402	A1I7G	O12-C11-C08	-7.74	108.89	120.75
3	B	402[A]	A1I7G	C01-S02-C05	7.59	116.05	105.09
3	B	402[B]	A1I7G	C08-C11-C13	7.51	128.43	118.89
3	B	402[A]	A1I7G	C08-C11-C13	7.49	128.41	118.89
3	C	402[B]	A1I7G	C08-C11-C13	7.08	127.88	118.89
3	C	402[A]	A1I7G	C08-C11-C13	7.03	127.83	118.89
3	B	402[B]	A1I7G	C01-S02-C05	6.66	114.71	105.09
3	C	402[B]	A1I7G	O23-C24-C25	6.15	112.87	107.89
3	B	402[A]	A1I7G	O12-C11-C08	-5.94	111.65	120.75
3	C	402[B]	A1I7G	O03-S02-C05	5.87	115.05	108.24
3	B	402[B]	A1I7G	O12-C11-C08	-5.34	112.56	120.75
3	A	402	A1I7G	O12-C11-C08	-5.34	112.58	120.75
3	D	402	A1I7G	O03-S02-C01	4.92	115.68	108.47
3	C	402[A]	A1I7G	O12-C11-C08	-4.79	113.41	120.75
3	C	402[B]	A1I7G	O04-S02-C01	4.42	114.96	108.47
3	C	402[A]	A1I7G	C07-C08-C11	-4.40	115.25	123.75
3	D	402	A1I7G	O04-S02-C05	-4.24	103.32	108.24
3	A	402	A1I7G	O23-C22-C06	4.21	120.27	108.98
3	B	402[B]	A1I7G	O23-C24-C25	4.10	111.21	107.89
3	D	402	A1I7G	C07-C08-C11	-3.96	116.11	123.75
3	C	402[B]	A1I7G	C22-O23-C24	3.92	119.55	112.25
3	A	402	A1I7G	C07-C08-C11	-3.74	116.53	123.75
3	B	402[A]	A1I7G	C07-C08-C11	-3.53	116.94	123.75
3	C	402[B]	A1I7G	C06-C07-CL21	-3.51	114.91	120.01
3	C	402[B]	A1I7G	O12-C11-C08	-3.45	115.47	120.75
3	A	402	A1I7G	C09-C08-C07	3.34	121.35	118.60
3	C	402[A]	A1I7G	C09-C08-C07	3.32	121.33	118.60
3	B	402[A]	A1I7G	C07-C06-C05	3.31	120.57	115.86
3	A	402	A1I7G	O04-S02-C05	-3.13	104.61	108.24
3	D	402	A1I7G	C07-C06-C05	3.09	120.26	115.86
3	A	402	A1I7G	O03-S02-C05	2.99	111.72	108.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402[A]	A1I7G	O03-S02-C05	2.84	111.54	108.24
3	B	402[A]	A1I7G	C22-O23-C24	-2.83	106.98	112.25
3	C	402[B]	A1I7G	O04-S02-C05	2.79	111.49	108.24
3	C	402[B]	A1I7G	C08-C07-CL21	2.76	124.05	120.11
3	B	402[B]	A1I7G	O03-S02-C01	2.76	112.52	108.47
3	D	402	A1I7G	C09-C08-C07	2.76	120.87	118.60
3	C	402[A]	A1I7G	C07-C06-C05	2.73	119.75	115.86
3	B	402[A]	A1I7G	C09-C08-C07	2.63	120.77	118.60
3	B	402[B]	A1I7G	O23-C22-C06	2.43	115.50	108.98
3	B	402[A]	A1I7G	C08-C07-C06	-2.42	119.78	122.92
3	C	402[A]	A1I7G	F26-C25-C24	-2.37	103.32	111.90
3	C	402[B]	A1I7G	O12-C11-C13	-2.34	116.60	119.58
3	A	402	A1I7G	O12-C11-C13	-2.28	116.67	119.58
3	A	402	A1I7G	C10-C09-C08	-2.26	117.13	120.86
3	B	402[A]	A1I7G	O03-S02-C01	2.24	111.75	108.47
3	B	402[B]	A1I7G	O20-C19-C18	-2.24	118.14	122.13
3	D	402	A1I7G	C08-C07-C06	-2.24	120.02	122.92
3	C	402[A]	A1I7G	C10-C05-C06	-2.20	119.34	121.41
3	B	402[B]	A1I7G	C22-C06-C07	-2.11	114.96	121.89
3	C	402[B]	A1I7G	O15-C14-C16	-2.10	118.39	122.13
3	D	402	A1I7G	C17-C16-C14	2.07	116.36	111.62

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	A1I7G	C06-C05-S02-O03
3	A	402	A1I7G	C08-C11-C13-C19
3	A	402	A1I7G	O12-C11-C13-C19
3	A	402	A1I7G	O23-C24-C25-F27
3	A	402	A1I7G	C25-C24-O23-C22
3	B	402[A]	A1I7G	C06-C05-S02-O03
3	B	402[A]	A1I7G	C08-C11-C13-C19
3	B	402[A]	A1I7G	O12-C11-C13-C19
3	B	402[A]	A1I7G	O23-C24-C25-F26
3	B	402[B]	A1I7G	C06-C05-S02-O03
3	B	402[B]	A1I7G	C07-C06-C22-O23
3	B	402[B]	A1I7G	C07-C08-C11-O12
3	B	402[B]	A1I7G	C08-C11-C13-C19
3	B	402[B]	A1I7G	O12-C11-C13-C19
3	C	402[A]	A1I7G	C06-C05-S02-C01
3	C	402[A]	A1I7G	C06-C05-S02-O03

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Mol	Chain	Res	Type	Atoms
3	C	402[A]	A1I7G	C10-C05-S02-O03
3	C	402[A]	A1I7G	C08-C11-C13-C19
3	C	402[A]	A1I7G	O12-C11-C13-C19
3	C	402[B]	A1I7G	C08-C11-C13-C19
3	C	402[B]	A1I7G	O12-C11-C13-C19
3	D	402	A1I7G	C06-C05-S02-O03
3	D	402	A1I7G	C08-C11-C13-C19
3	D	402	A1I7G	O12-C11-C13-C19
3	D	402	A1I7G	O23-C24-C25-F27
3	D	402	A1I7G	O23-C24-C25-F28
3	A	402	A1I7G	O23-C24-C25-F26
3	B	402[A]	A1I7G	O23-C24-C25-F27
3	B	402[A]	A1I7G	O23-C24-C25-F28
3	D	402	A1I7G	O23-C24-C25-F26
3	B	402[B]	A1I7G	C05-C06-C22-O23
3	A	402	A1I7G	O23-C24-C25-F28
3	C	402[A]	A1I7G	C09-C08-C11-O12
3	A	402	A1I7G	C09-C08-C11-C13
3	C	402[B]	A1I7G	C09-C08-C11-C13
3	D	402	A1I7G	C10-C05-S02-O03
3	A	402	A1I7G	C09-C08-C11-O12
3	B	402[A]	A1I7G	C09-C08-C11-O12
3	C	402[B]	A1I7G	C09-C08-C11-O12
3	D	402	A1I7G	C09-C08-C11-O12
3	C	402[B]	A1I7G	C06-C22-O23-C24
3	B	402[A]	A1I7G	C09-C08-C11-C13
3	C	402[A]	A1I7G	C09-C08-C11-C13
3	D	402	A1I7G	C09-C08-C11-C13
3	C	402[A]	A1I7G	C06-C22-O23-C24
3	C	402[A]	A1I7G	C10-C05-S02-C01
3	B	402[B]	A1I7G	C25-C24-O23-C22
3	C	402[A]	A1I7G	C25-C24-O23-C22
3	D	402	A1I7G	C06-C22-O23-C24
3	D	402	A1I7G	C06-C05-S02-C01
3	A	402	A1I7G	C07-C08-C11-O12
3	B	402[A]	A1I7G	C07-C08-C11-O12
3	C	402[A]	A1I7G	C07-C08-C11-O12
3	C	402[B]	A1I7G	C07-C08-C11-O12
3	D	402	A1I7G	C07-C08-C11-O12
3	B	402[B]	A1I7G	C10-C05-S02-O03
3	A	402	A1I7G	C07-C08-C11-C13
3	C	402[B]	A1I7G	C07-C08-C11-C13

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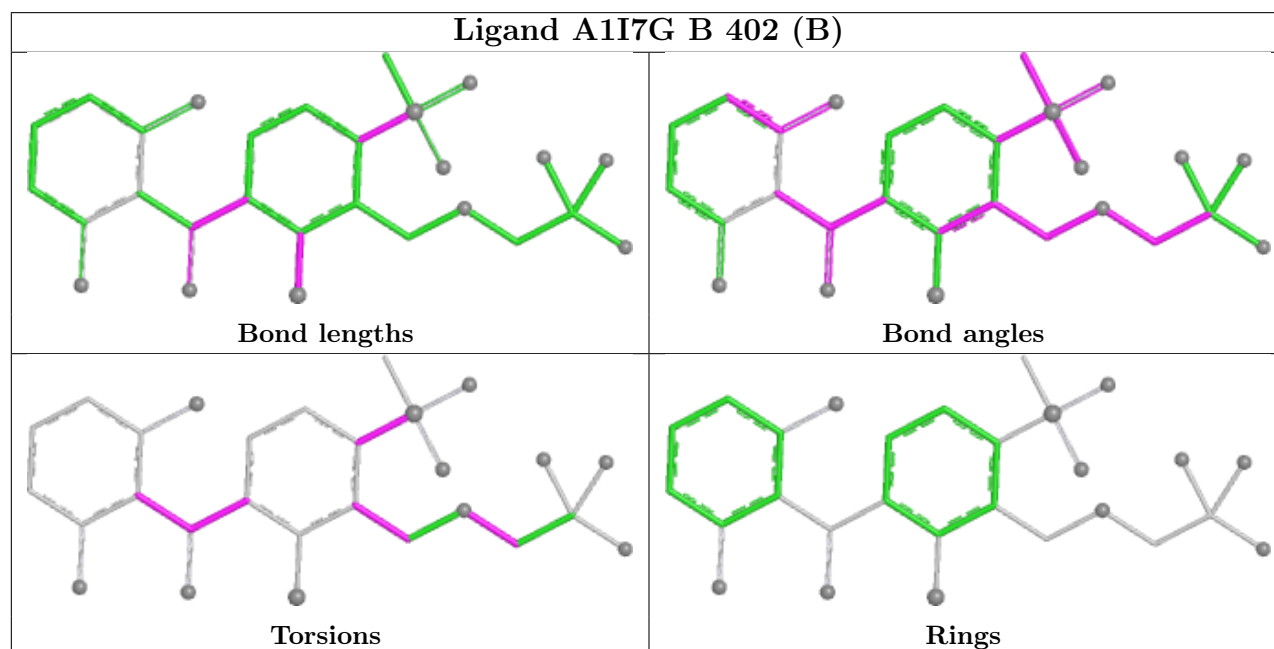
Mol	Chain	Res	Type	Atoms
3	B	402[A]	A1I7G	C10-C05-S02-O03
3	C	402[B]	A1I7G	C25-C24-O23-C22
3	D	402	A1I7G	C25-C24-O23-C22
3	B	402[B]	A1I7G	C09-C08-C11-O12
3	C	402[A]	A1I7G	C08-C11-C13-C14

There are no ring outliers.

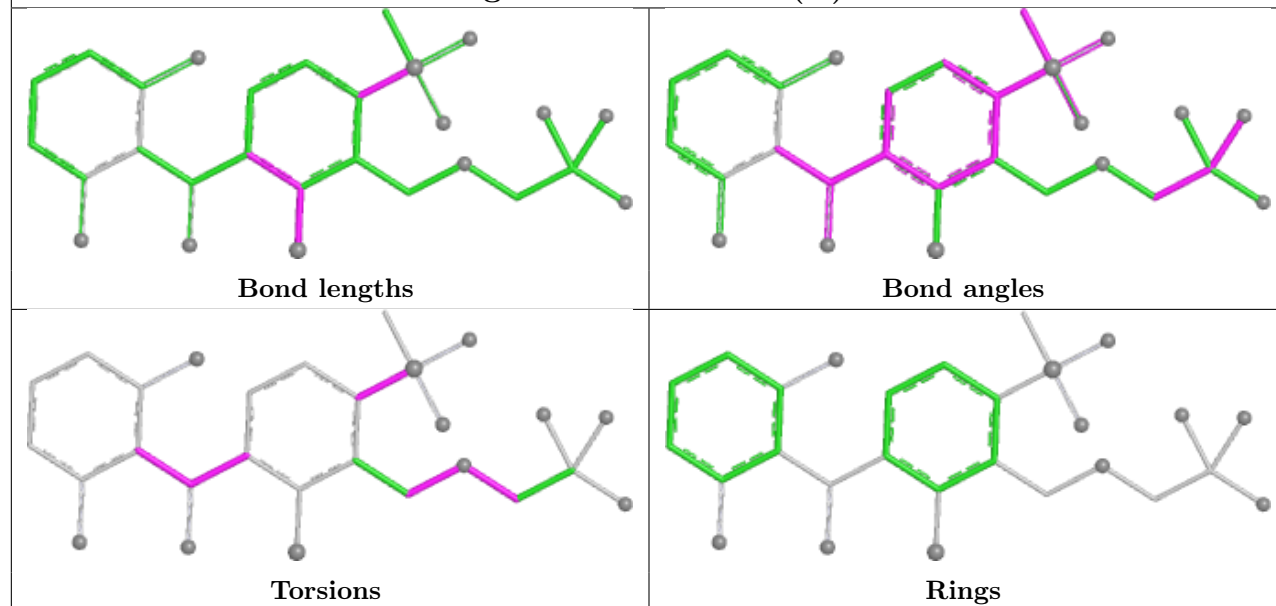
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402[B]	A1I7G	1	0

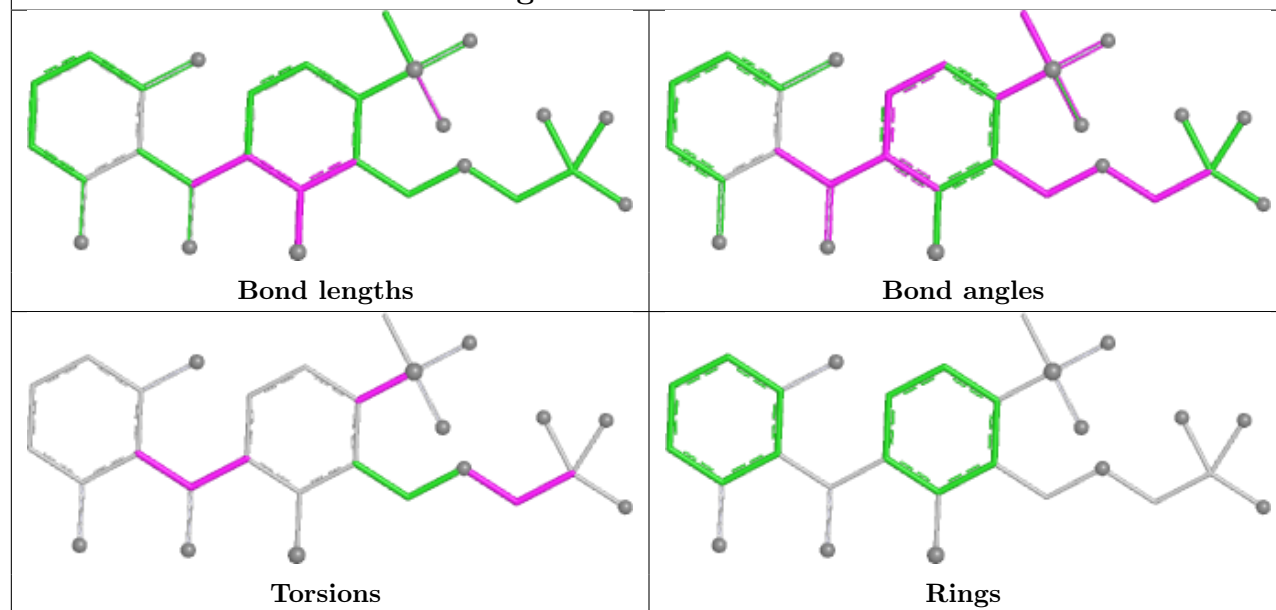
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



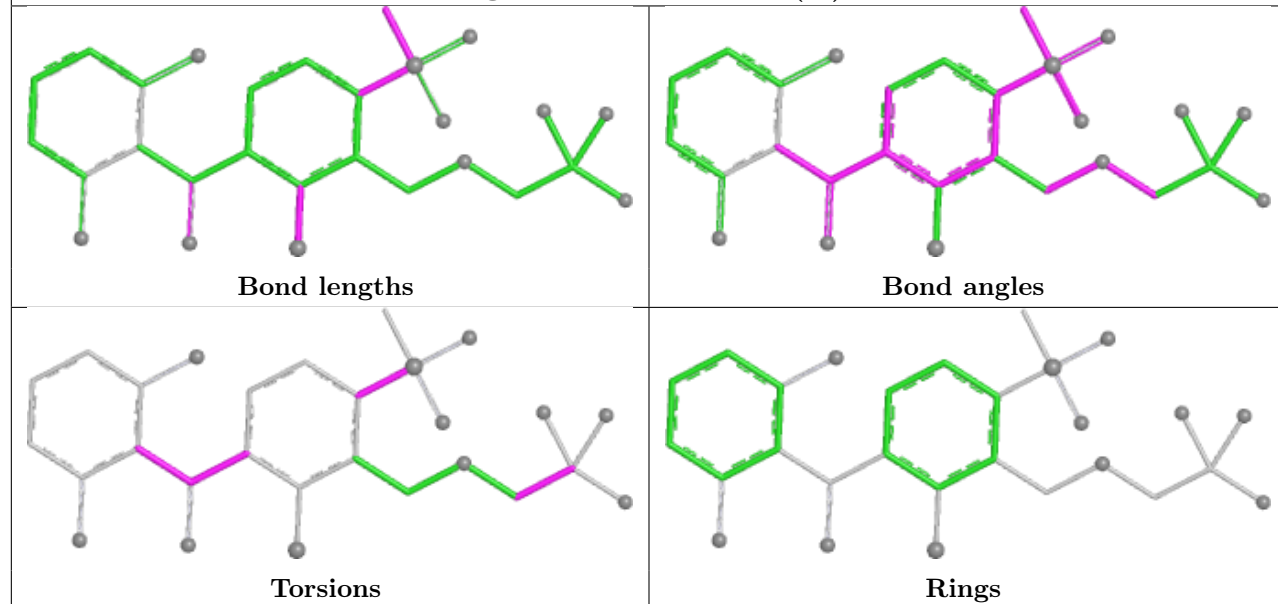
Ligand A1I7G C 402 (A)



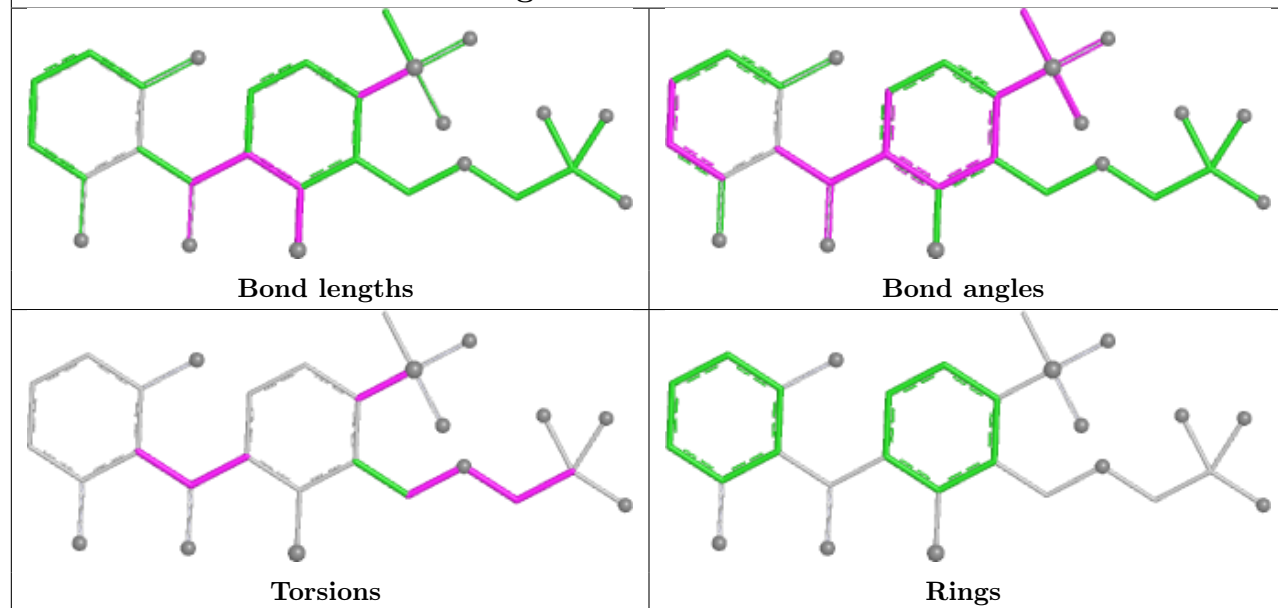
Ligand A1I7G A 402

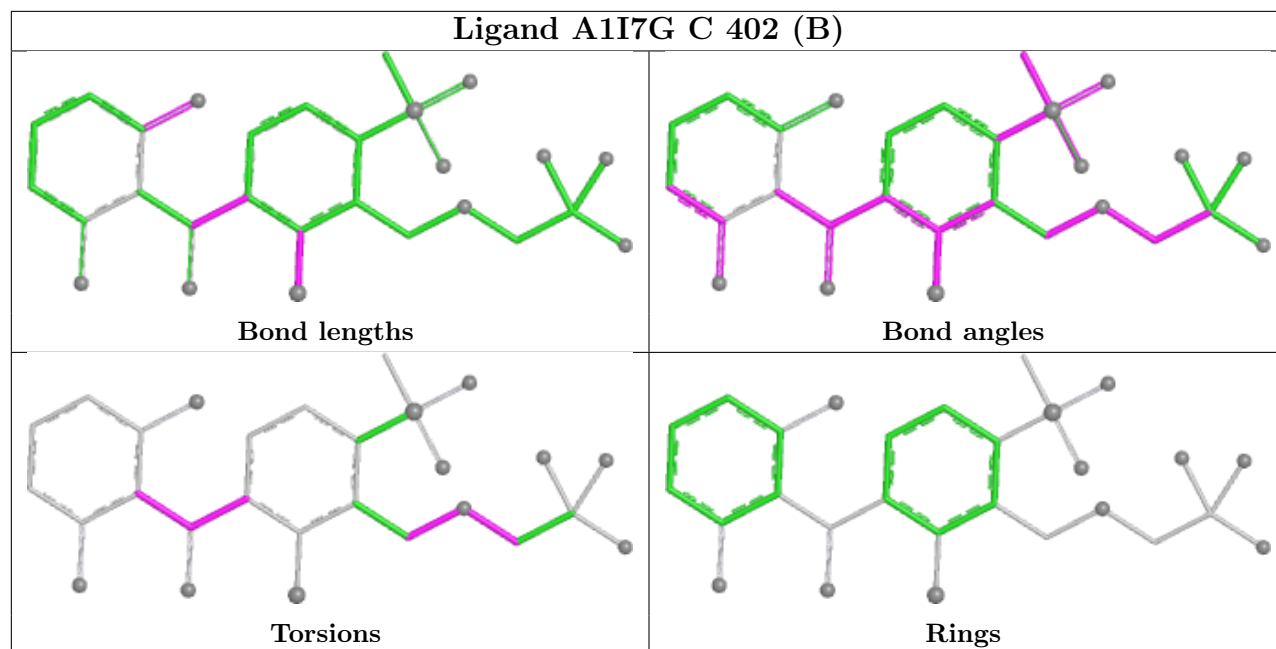


Ligand A1I7G B 402 (A)



Ligand A1I7G D 402





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	331/361 (91%)	0.30	16 (4%)	35 41	16, 34, 58, 73	3 (0%)
1	B	330/361 (91%)	1.01	29 (8%)	15 18	24, 48, 65, 88	3 (0%)
1	C	337/361 (93%)	0.22	15 (4%)	38 44	15, 32, 58, 79	5 (1%)
1	D	336/361 (93%)	0.90	24 (7%)	22 25	21, 44, 62, 89	2 (0%)
All	All	1334/1444 (92%)	0.60	84 (6%)	26 30	15, 42, 62, 89	13 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	191	ILE	5.4
1	D	305	PRO	5.4
1	C	303	SER	4.9
1	D	228	GLY	4.4
1	A	302	ALA	4.4
1	D	7	ILE	4.3
1	C	356	GLY	4.2
1	B	7	ILE	4.0
1	D	358	LEU	4.0
1	D	191	ILE	3.9
1	B	191	ILE	3.9
1	D	8	PHE	3.9
1	D	216[A]	ARG	3.8
1	A	228	GLY	3.8
1	C	304	GLN	3.7
1	B	228	GLY	3.6
1	C	226	GLY	3.6
1	B	355	ARG	3.5
1	D	357	VAL	3.5
1	A	191	ILE	3.4
1	B	8	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	108	ILE	3.3
1	A	108	ILE	3.2
1	D	35	GLN	3.1
1	D	303	SER	3.1
1	A	204	THR	3.1
1	A	303	SER	3.0
1	C	108	ILE	3.0
1	B	6	ASP	3.0
1	B	67[A]	LYS	3.0
1	C	355	ARG	3.0
1	D	302	ALA	3.0
1	B	108	ILE	3.0
1	A	304	GLN	2.9
1	D	204	THR	2.9
1	A	8	PHE	2.8
1	D	6	ASP	2.8
1	A	7	ILE	2.8
1	B	245	VAL	2.8
1	B	303	SER	2.7
1	A	222	GLU	2.6
1	C	223	SER	2.6
1	B	75	ALA	2.6
1	D	307	ASP	2.6
1	B	312	LEU	2.5
1	C	306	ASP	2.5
1	A	308	LYS	2.5
1	B	354	ARG	2.5
1	A	6	ASP	2.5
1	C	228	GLY	2.5
1	B	163	ILE	2.4
1	B	204	THR	2.4
1	C	7	ILE	2.4
1	A	229	GLN	2.4
1	D	344	LEU	2.3
1	C	8	PHE	2.3
1	B	288	PRO	2.3
1	B	267	MET	2.3
1	C	227	SER	2.3
1	D	223	SER	2.3
1	B	268	THR	2.3
1	D	308	LYS	2.3
1	B	35	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	110	THR	2.3
1	C	204	THR	2.3
1	C	6	ASP	2.2
1	B	109	GLU	2.2
1	B	302	ALA	2.2
1	B	120	ILE	2.2
1	D	278	LEU	2.2
1	B	246	ALA	2.2
1	B	181	PHE	2.1
1	D	230	ILE	2.1
1	B	42	VAL	2.1
1	D	109	GLU	2.1
1	A	216[A]	ARG	2.1
1	A	267	MET	2.1
1	D	304	GLN	2.1
1	B	353	VAL	2.1
1	D	288	PRO	2.1
1	B	170	VAL	2.0
1	D	101	LEU	2.0
1	B	150	GLY	2.0
1	A	151	VAL	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(\AA^2)	Q<0.9
3	A1I7G	B	402[A]	28/28	0.91	0.19	60,63,74,77	28
3	A1I7G	B	402[B]	28/28	0.91	0.19	60,64,72,75	28

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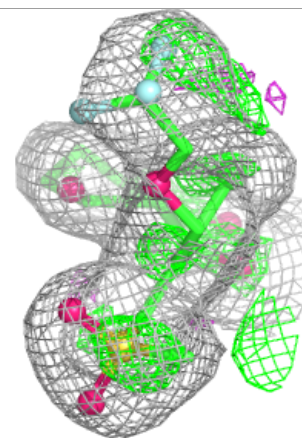
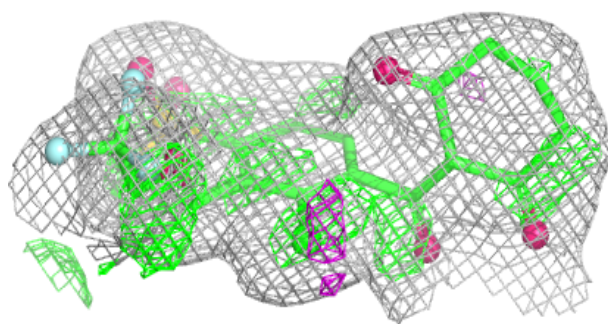
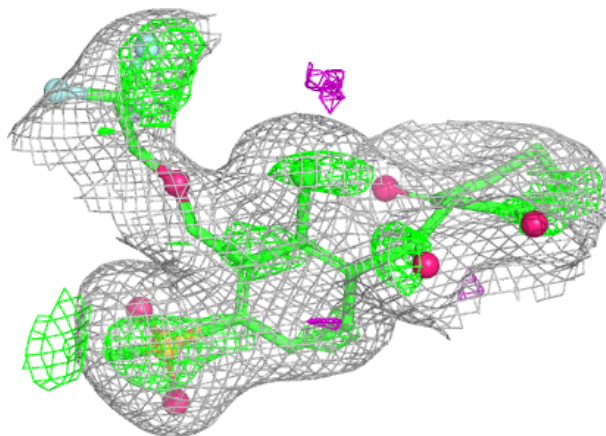
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	A1I7G	A	402	28/28	0.93	0.12	38,42,76,82	0
3	A1I7G	D	402	28/28	0.93	0.12	45,51,66,70	0
3	A1I7G	C	402[B]	28/28	0.95	0.10	26,30,37,45	28
3	A1I7G	C	402[A]	28/28	0.95	0.10	27,31,42,46	28
2	MN	B	401	1/1	0.99	0.04	44,44,44,44	0
2	MN	A	401	1/1	1.00	0.02	28,28,28,28	0
2	MN	C	401	1/1	1.00	0.03	27,27,27,27	0
2	MN	D	401	1/1	1.00	0.04	38,38,38,38	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.

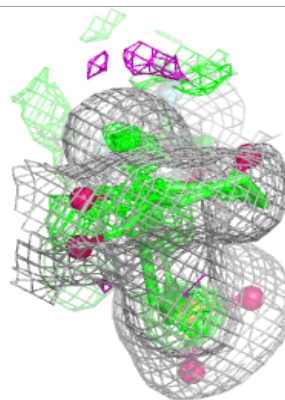
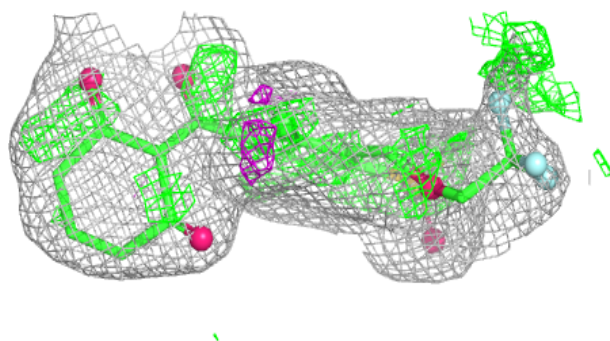
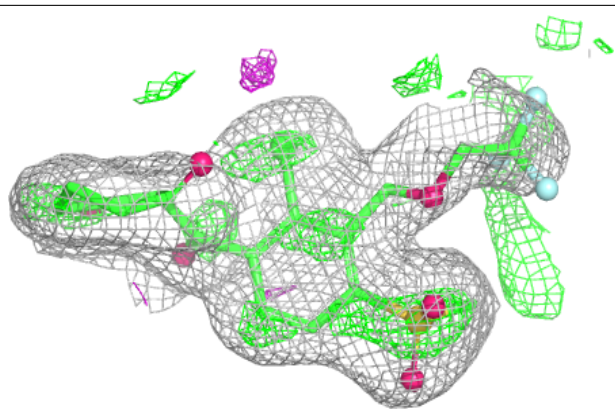
Electron density around A1I7G B 402 (A):

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



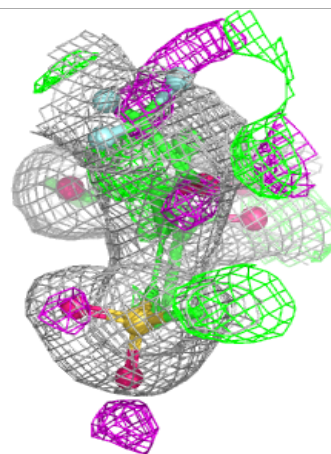
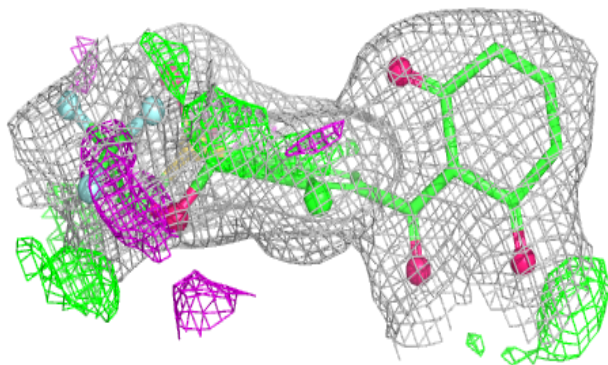
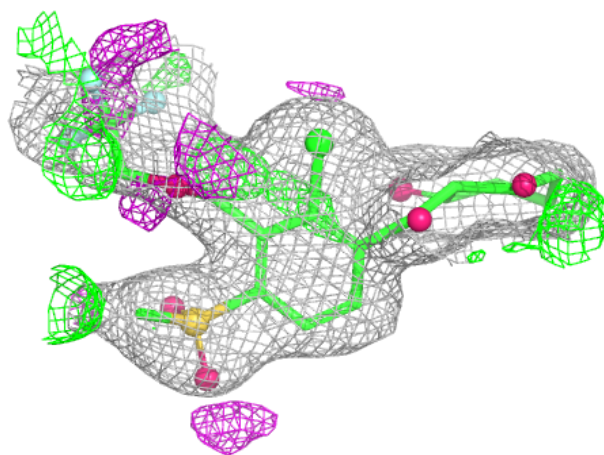
Electron density around A1I7G B 402 (B):

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



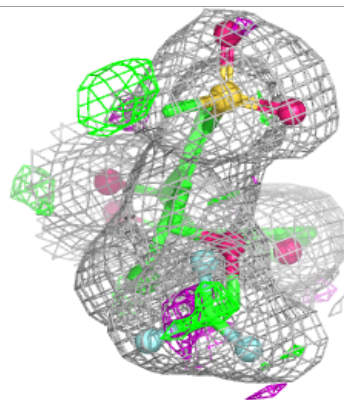
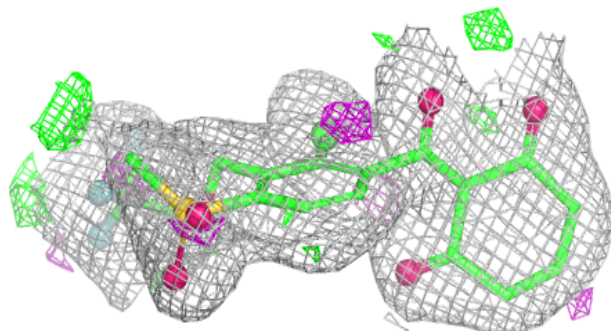
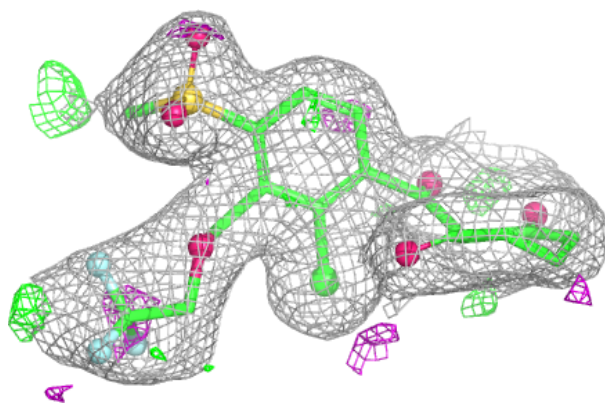
Electron density around A1I7G A 402:

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

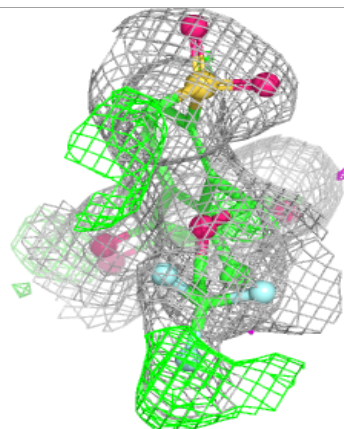
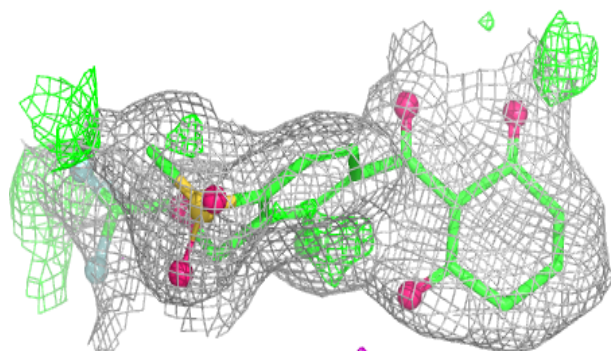
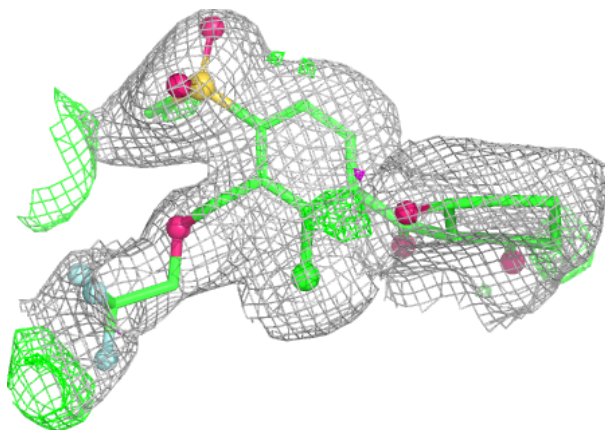


Electron density around A1I7G D 402:

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

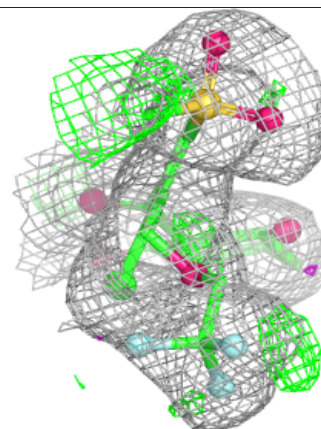
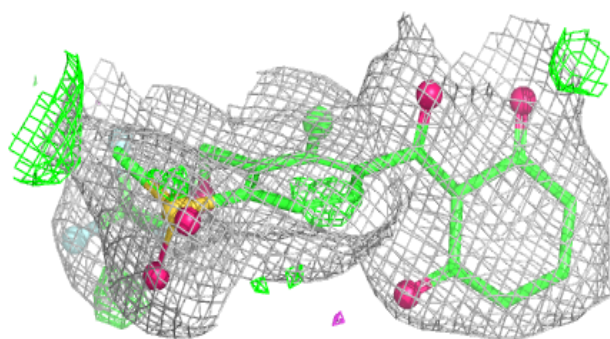
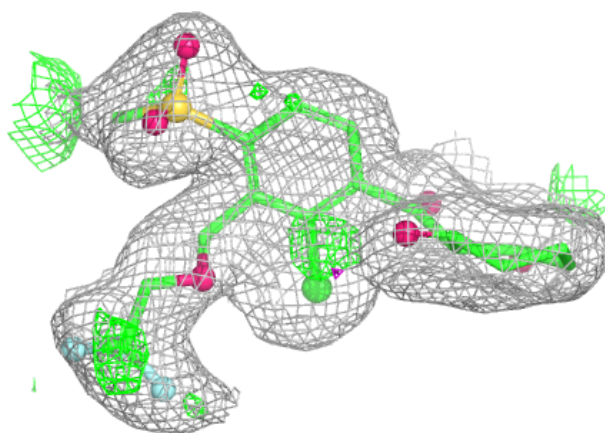
**Electron density around A1I7G C 402 (B):**

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



Electron density around A1I7G C 402 (A):

$2mF_o-DF_c$ (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.