



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 09:42 PM UTC

PDB ID : 9QMG / pdb_00009qmg
Title : Pseudomonas putida 4-hydroxyphenylpyruvate dioxygenase in complex with Tefuryltrione (Mn)
Authors : Alshref, F.M.; Dhingra, S.; Farcas, I.M.; Brewitz, L.; Allen, M.D.; Schofield, C.J.
Deposited on : 2025-03-23
Resolution : 2.70 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

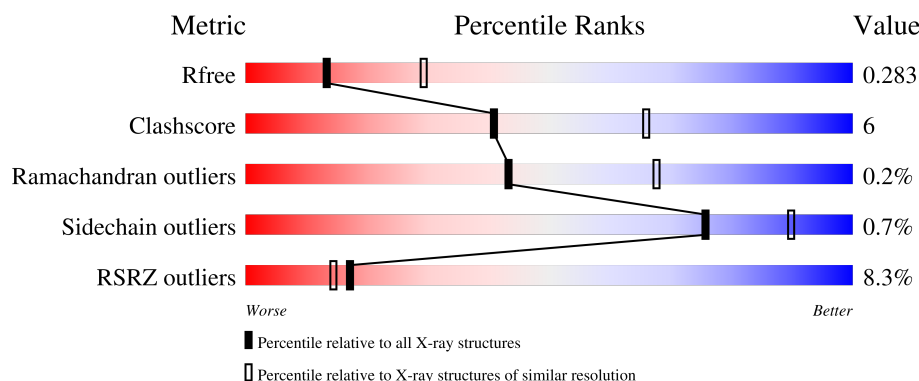
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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>13%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>8%</div> </div> </div>
1	B	361	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>8%</div> </div> </div>
1	C	361	<div> <div>11%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>8%</div> </div> </div>
1	D	361	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11039 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	333	Total	C	N	O	S	0	2	0
			2674	1713	458	490	13			
1	B	333	Total	C	N	O	S	0	1	0
			2663	1707	454	489	13			
1	C	333	Total	C	N	O	S	0	1	0
			2663	1707	454	489	13			
1	D	333	Total	C	N	O	S	0	0	0
			2652	1701	450	488	13			

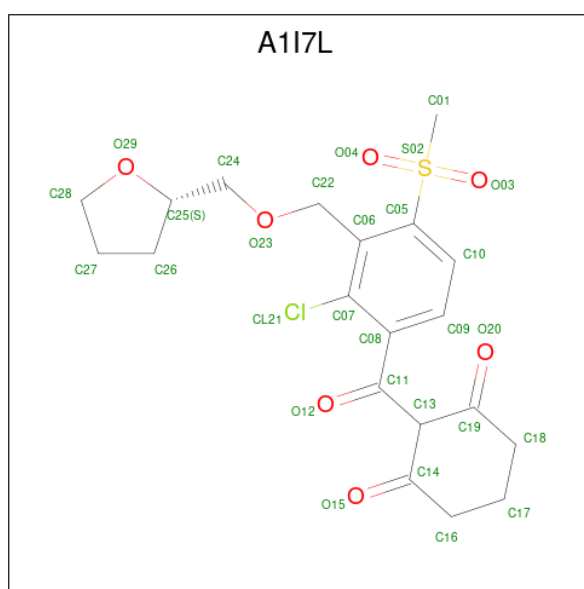
There are 16 discrepancies between the modelled and reference sequences:

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 Tefuryltrione (CCD ID: A1I7L) (formula: C₂₀H₂₃ClO₇S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Cl O S 29 20 1 7 1	0	0
3	B	1	Total C Cl O S 29 20 1 7 1	0	0
3	C	1	Total C Cl O S 29 20 1 7 1	0	0
3	D	1	Total C Cl O S 29 20 1 7 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	66	Total O 66 66	0	0

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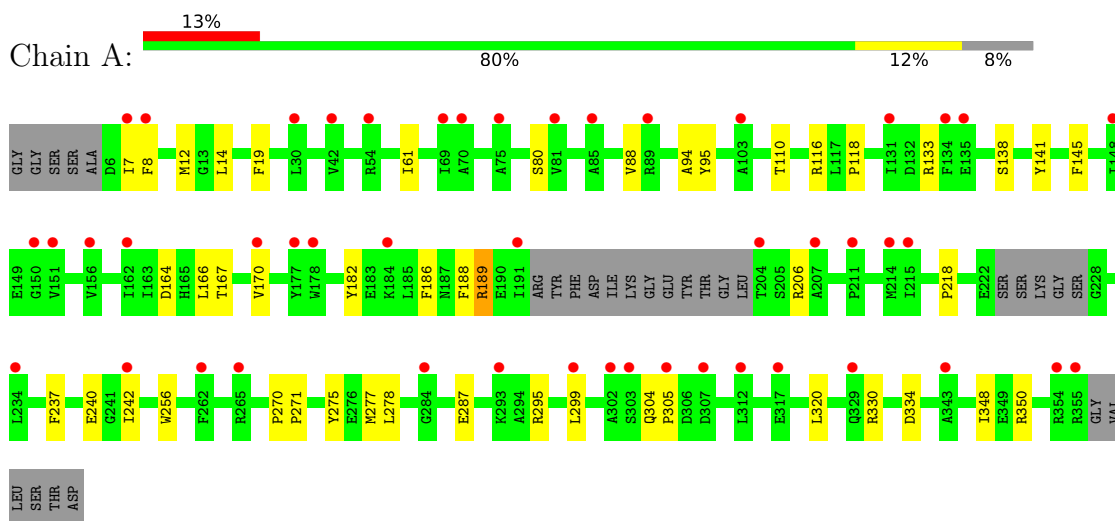
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	99	Total 99	O 99	0	0
4	C	38	Total 38	O 38	0	0
4	D	64	Total 64	O 64	0	0

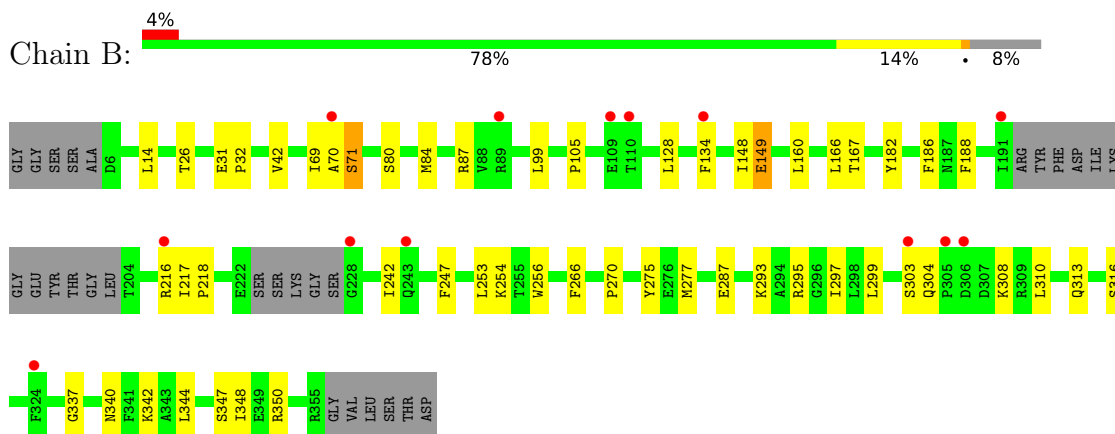
3 Residue-property plots [i](#)

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.

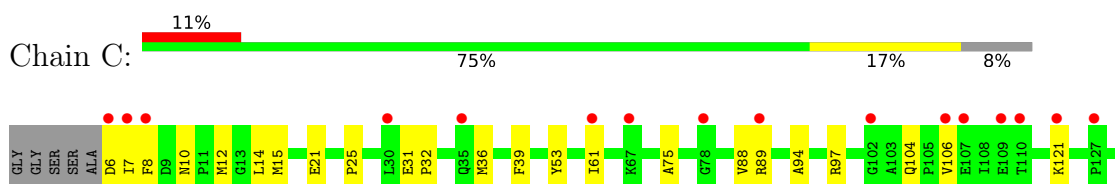
- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

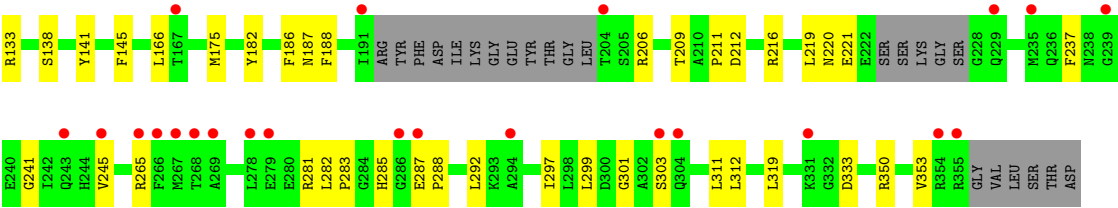


- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

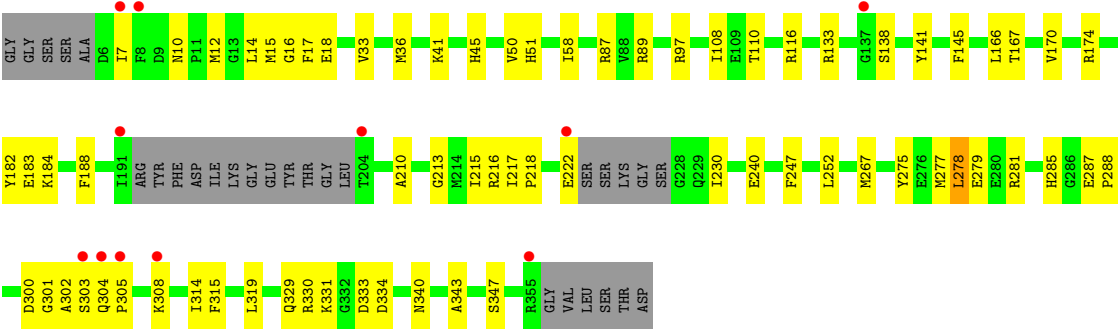


- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase





● 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	151.19Å 169.24Å 79.58Å 90.00° 91.88° 90.00°	Depositor
Resolution (Å)	45.46 – 2.70 45.46 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.8 (45.46-2.70) 96.4 (45.46-2.70)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.246 , 0.286 0.246 , 0.283	Depositor DCC
R_{free} test set	2493 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.188 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11039	wwPDB-VP
Average B, all atoms (Å ²)	60.0	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 56.07 % 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 2.8871e-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: A1I7L, MN

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	0.13	0/2737	0.29	0/3689
1	B	0.14	0/2726	0.33	0/3675
1	C	0.11	0/2726	0.27	0/3675
1	D	0.14	0/2715	0.32	0/3661
All	All	0.13	0/10904	0.30	0/14700

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	304	GLN	Peptide

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	2674	0	2616	26	0
1	B	2663	0	2604	32	0
1	C	2663	0	2604	39	0
1	D	2652	0	2592	42	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	29	0	0	0	0
3	B	29	0	0	0	0
3	C	29	0	0	0	0
3	D	29	0	0	0	0
4	A	66	0	0	0	0
4	B	99	0	0	2	0
4	C	38	0	0	0	0
4	D	64	0	0	1	0
All	All	11039	0	10416	137	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 6.

All (137) 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:D:222:GLU:HG2	1:D:230:ILE:HB	1.65	0.79
1:D:12:MET:HE3	1:D:97:ARG:HH11	1.56	0.69
1:C:12:MET:HE3	1:C:97:ARG:HH11	1.58	0.69
1:A:330:ARG:HH21	1:A:334:ASP:HA	1.63	0.63
1:D:267:MET:HG3	1:D:315:PHE:HB2	1.81	0.62
1:C:104:GLN:HB3	1:C:121:LYS:HG3	1.82	0.61
1:B:277:MET:HE1	1:B:347:SER:HA	1.82	0.60
1:C:166:LEU:HD12	1:C:245:VAL:HG13	1.84	0.60
1:C:209:THR:HG22	1:C:216:ARG:HG2	1.84	0.58
1:A:167:THR:HG22	1:A:218:PRO:HB2	1.86	0.56
1:B:313:GLN:HE21	1:B:340:ASN:HD22	1.53	0.56
1:D:33:VAL:HG13	1:D:319:LEU:HD13	1.88	0.56
1:D:300:ASP:HB2	1:D:340:ASN:HD21	1.70	0.56
1:A:166:LEU:HD13	1:A:242:ILE:HD13	1.88	0.55
1:B:14:LEU:HD11	1:B:186:PHE:HB3	1.87	0.55
1:B:344:LEU:O	1:B:348:ILE:HG12	2.08	0.54
1:D:275:TYR:HA	1:D:278:LEU:HD23	1.89	0.54
1:C:350:ARG:HA	1:C:353:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ARG:NH2	1:D:138:SER:HB2	2.24	0.53
1:C:106:VAL:HG22	1:C:121:LYS:HE2	1.90	0.52
1:C:283:PRO:HD2	1:C:303:SER:O	2.10	0.52
1:C:133:ARG:NH2	1:C:138:SER:HB2	2.26	0.51
1:D:216:ARG:HH12	1:D:330:ARG:NH2	2.08	0.51
1:D:330:ARG:HH21	1:D:334:ASP:HA	1.75	0.51
1:B:266:PHE:HA	1:B:316:SER:HA	1.92	0.51
1:A:189:ARG:HB2	1:A:189:ARG:HH11	1.75	0.51
1:A:287:GLU:HG3	1:A:299:LEU:HD21	1.93	0.51
1:C:104:GLN:HG2	1:C:121:LYS:HE3	1.90	0.51
1:C:12:MET:HG3	1:C:186:PHE:HA	1.93	0.51
1:D:110:THR:HG21	1:D:116:ARG:HA	1.93	0.50
1:A:14:LEU:HD11	1:A:186:PHE:HB3	1.93	0.50
1:A:182:TYR:HB3	1:A:188:PHE:CG	2.46	0.50
1:D:182:TYR:HB3	1:D:188:PHE:CG	2.47	0.50
1:B:270:PRO:HB3	1:B:344:LEU:HD21	1.94	0.49
1:D:166:LEU:O	1:D:217:ILE:HA	2.12	0.49
1:C:12:MET:HE3	1:C:97:ARG:HD3	1.94	0.49
1:D:300:ASP:HB2	1:D:340:ASN:ND2	2.27	0.49
1:A:133:ARG:NH2	1:A:138:SER:HB2	2.28	0.49
1:C:285:HIS:CD2	1:C:287:GLU:H	2.31	0.49
1:B:182:TYR:HB3	1:B:188:PHE:CG	2.49	0.48
1:D:170:VAL:HA	1:D:240:GLU:HG2	1.95	0.48
1:C:14:LEU:HD11	1:C:186:PHE:HB3	1.96	0.48
1:C:175:MET:HE3	1:C:221:GLU:HB3	1.95	0.48
1:C:175:MET:SD	1:C:206:ARG:HD3	2.54	0.48
1:D:340:ASN:HA	1:D:343:ALA:HB3	1.96	0.48
1:B:303:SER:HB2	1:B:310:LEU:HD21	1.96	0.48
1:B:80:SER:HB2	4:B:513:HOH:O	2.12	0.48
1:A:275:TYR:HA	1:A:278:LEU:HG	1.96	0.48
1:D:15:MET:HE3	1:D:89:ARG:HB2	1.96	0.48
1:B:275:TYR:CZ	1:B:293:LYS:HA	2.49	0.48
1:C:15:MET:SD	1:C:89[A]:ARG:HG2	2.54	0.48
1:C:182:TYR:HB3	1:C:188:PHE:CG	2.49	0.48
1:D:16:GLY:HA2	1:D:215:ILE:HG13	1.95	0.47
1:B:277:MET:HE2	1:B:350:ARG:HD2	1.96	0.47
1:A:256:TRP:CE2	1:A:295:ARG:HB3	2.49	0.47
1:A:271:PRO:HG3	1:A:348:ILE:HG13	1.95	0.47
1:B:254:LYS:HG3	4:B:520:HOH:O	2.14	0.47
1:D:45:HIS:HB2	1:D:50:VAL:HB	1.96	0.47
1:B:253:LEU:HD12	1:D:288:PRO:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:HIS:HD2	1:C:287:GLU:H	1.63	0.46
1:A:88:VAL:HG11	1:A:94:ALA:HB2	1.97	0.46
1:C:32:PRO:O	1:C:36:MET:HG3	2.15	0.46
1:C:311:LEU:HD23	1:C:333:ASP:HB3	1.97	0.46
1:C:39:PHE:HB3	1:C:53:TYR:HB3	1.96	0.46
1:B:70:ALA:O	1:B:71:SER:HB3	2.15	0.46
1:D:277:MET:HE1	1:D:347:SER:HA	1.98	0.46
1:D:174:ARG:HD3	1:D:240:GLU:OE2	2.15	0.46
1:C:6:ASP:OD2	1:C:212:ASP:HA	2.16	0.46
1:C:8:PHE:HE2	1:C:187:ASN:O	1.98	0.46
1:C:219:LEU:C	1:C:220:ASN:HD22	2.24	0.46
1:D:141:TYR:O	1:D:145:PHE:HB2	2.15	0.46
1:D:302:ALA:O	1:D:304:GLN:HG2	2.16	0.46
1:C:21:GLU:HG3	1:C:61:ILE:HG22	1.98	0.45
1:A:95:TYR:CD2	1:A:118:PRO:HB3	2.51	0.45
1:A:206:ARG:O	1:A:218:PRO:HA	2.17	0.45
1:D:108:ILE:HB	4:D:535:HOH:O	2.16	0.45
1:B:166:LEU:O	1:B:217:ILE:HA	2.17	0.45
1:C:299:LEU:HD13	1:C:312:LEU:HG	1.99	0.45
1:A:189:ARG:HB2	1:A:189:ARG:NH1	2.32	0.45
1:B:167:THR:HG22	1:B:218:PRO:HB2	1.97	0.45
1:D:12:MET:HB2	1:D:14:LEU:HD13	1.99	0.45
1:D:319:LEU:HD23	1:D:319:LEU:HA	1.80	0.45
1:B:308:LYS:NZ	1:D:308:LYS:HD2	2.32	0.45
1:D:14:LEU:HD23	1:D:210:ALA:HB1	1.99	0.45
1:D:252:LEU:HD21	1:D:314:ILE:HG22	1.98	0.45
1:A:170:VAL:HA	1:A:240:GLU:HG2	1.99	0.44
1:C:7:ILE:HB	1:C:8:PHE:CD1	2.52	0.44
1:D:41:LYS:HD2	1:D:51:HIS:HB3	2.00	0.44
1:A:110:THR:HG21	1:A:116:ARG:HA	2.00	0.44
1:C:31:GLU:H	1:C:31:GLU:CD	2.25	0.44
1:B:160:LEU:HD22	1:B:247:PHE:HB2	2.00	0.44
1:B:84:MET:HE3	1:B:128:LEU:HD13	2.00	0.43
1:D:36:MET:HE1	1:D:319:LEU:HD21	2.00	0.43
1:A:141:TYR:O	1:A:145:PHE:HB2	2.18	0.43
1:C:265:ARG:HH21	1:C:319:LEU:HD12	1.83	0.43
1:C:237:PHE:CE2	1:C:241:GLY:HA3	2.54	0.43
1:A:270:PRO:HG2	1:A:275:TYR:CE2	2.54	0.43
1:B:84:MET:HE2	1:B:84:MET:HB3	1.81	0.43
1:C:301:GLY:HA2	1:C:333:ASP:OD2	2.19	0.43
1:D:167:THR:HG22	1:D:218:PRO:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:GLU:HG2	1:D:188:PHE:O	2.19	0.43
1:D:301:GLY:HA2	1:D:333:ASP:OD2	2.19	0.43
1:A:12:MET:HG3	1:A:186:PHE:HA	1.99	0.43
1:C:281:ARG:HG2	1:C:282:LEU:HG	2.00	0.42
1:A:80:SER:HB2	1:A:237:PHE:HE1	1.85	0.42
1:C:88:VAL:HG11	1:C:94:ALA:HB2	2.01	0.42
1:B:295:ARG:HB2	1:B:297:ILE:HG12	2.01	0.42
1:C:141:TYR:O	1:C:145:PHE:HB2	2.20	0.42
1:B:149:GLU:O	1:B:149:GLU:HG3	2.19	0.42
1:D:184:LYS:HB3	1:D:184:LYS:HE3	1.84	0.42
1:A:304:GLN:O	1:A:305:PRO:C	2.61	0.42
1:B:342:LYS:HD3	1:B:342:LYS:HA	1.86	0.41
1:C:297:ILE:H	1:C:297:ILE:HG12	1.71	0.41
1:A:164:ASP:OD2	1:A:330:ARG:HD2	2.20	0.41
1:B:99:LEU:HD22	1:B:105:PRO:HG3	2.02	0.41
1:B:69:ILE:H	1:B:69:ILE:HD12	1.86	0.41
1:C:25:PRO:HB3	1:C:75:ALA:HA	2.02	0.41
1:A:277:MET:HE3	1:A:350:ARG:CZ	2.51	0.41
1:C:10:ASN:HD21	1:C:14:LEU:H	1.69	0.41
1:C:288:PRO:O	1:C:292:LEU:HG	2.21	0.41
1:B:287:GLU:HG3	1:B:299:LEU:HD21	2.03	0.41
1:B:167:THR:O	1:B:242:ILE:HA	2.21	0.41
1:B:256:TRP:CE2	1:B:295:ARG:HB3	2.56	0.41
1:D:285:HIS:HD2	1:D:287:GLU:H	1.69	0.41
1:B:313:GLN:NE2	1:B:337:GLY:HA3	2.36	0.41
1:D:17:PHE:CE2	1:D:215:ILE:HG23	2.55	0.41
1:B:87:ARG:HH21	1:B:134:PHE:HB2	1.85	0.41
1:D:58:ILE:HD13	1:D:247:PHE:CD1	2.56	0.41
1:D:329:GLN:NE2	1:D:331:LYS:HE3	2.35	0.41
1:A:19:PHE:CE1	1:A:61:ILE:HD12	2.56	0.40
1:B:42:VAL:O	1:B:148:ILE:HG13	2.20	0.40
1:D:10:ASN:ND2	1:D:14:LEU:H	2.20	0.40
1:A:7:ILE:HG22	1:A:8:PHE:CE2	2.57	0.40
1:C:10:ASN:ND2	1:C:211:PRO:HG2	2.36	0.40
1:D:18:GLU:OE1	1:D:87:ARG:HG2	2.21	0.40
1:D:7:ILE:HD11	1:D:213:GLY:HA2	2.03	0.40
1:B:31:GLU:HB2	1:B:32:PRO:HD3	2.02	0.40

There are no symmetry-related clashes.

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	329/361 (91%)	320 (97%)	9 (3%)	0	100	100
1	B	328/361 (91%)	318 (97%)	9 (3%)	1 (0%)	36	60
1	C	328/361 (91%)	324 (99%)	4 (1%)	0	100	100
1	D	327/361 (91%)	320 (98%)	5 (2%)	2 (1%)	21	44
All	All	1312/1444 (91%)	1282 (98%)	27 (2%)	3 (0%)	43	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	71	SER
1	D	305	PRO
1	D	303	SER

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	279/298 (94%)	277 (99%)	2 (1%)	76	90
1	B	278/298 (93%)	275 (99%)	3 (1%)	65	85
1	C	278/298 (93%)	278 (100%)	0	100	100
1	D	277/298 (93%)	274 (99%)	3 (1%)	65	85
All	All	1112/1192 (93%)	1104 (99%)	8 (1%)	76	90

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	ARG
1	A	320	LEU
1	B	26	THR
1	B	149	GLU
1	B	216	ARG
1	D	278	LEU
1	D	279	GLU
1	D	281	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	ASN
1	B	51	HIS
1	B	90	ASN
1	B	313	GLN
1	C	92	HIS
1	C	220	ASN
1	D	10	ASN
1	D	238	ASN
1	D	243	GLN
1	D	340	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	A1I7L	A	402	2	29,31,31	2.44	12 (41%)	35,45,45	2.14	7 (20%)
3	A1I7L	B	402	2	29,31,31	2.50	13 (44%)	35,45,45	2.29	6 (17%)
3	A1I7L	D	402	2	29,31,31	2.50	13 (44%)	35,45,45	2.20	7 (20%)
3	A1I7L	C	402	2	29,31,31	2.39	12 (41%)	35,45,45	2.37	7 (20%)

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	A1I7L	A	402	2	-	8/20/41/41	0/3/3/3
3	A1I7L	B	402	2	-	14/20/41/41	0/3/3/3
3	A1I7L	D	402	2	-	9/20/41/41	0/3/3/3
3	A1I7L	C	402	2	-	10/20/41/41	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	A1I7L	C05-S02	6.10	1.86	1.78
3	D	402	A1I7L	C05-S02	5.89	1.85	1.78
3	A	402	A1I7L	C05-S02	5.69	1.85	1.78
3	C	402	A1I7L	C05-S02	5.44	1.85	1.78
3	B	402	A1I7L	C22-C06	5.16	1.61	1.51
3	D	402	A1I7L	C22-C06	5.09	1.60	1.51
3	A	402	A1I7L	C22-C06	5.01	1.60	1.51
3	C	402	A1I7L	C22-C06	4.80	1.60	1.51
3	D	402	A1I7L	C10-C05	4.25	1.44	1.39
3	B	402	A1I7L	C10-C05	4.16	1.44	1.39
3	A	402	A1I7L	C10-C05	3.96	1.43	1.39
3	C	402	A1I7L	C10-C05	3.94	1.43	1.39
3	A	402	A1I7L	O29-C28	3.79	1.53	1.43
3	C	402	A1I7L	O29-C28	3.77	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	A1I7L	O29-C28	3.76	1.53	1.43
3	B	402	A1I7L	O29-C28	3.71	1.53	1.43
3	C	402	A1I7L	C26-C25	-3.67	1.33	1.52
3	A	402	A1I7L	C26-C25	-3.67	1.33	1.52
3	D	402	A1I7L	C26-C25	-3.60	1.34	1.52
3	D	402	A1I7L	C13-C11	3.58	1.60	1.53
3	B	402	A1I7L	C26-C25	-3.57	1.34	1.52
3	A	402	A1I7L	C13-C11	3.53	1.60	1.53
3	C	402	A1I7L	C13-C11	3.53	1.60	1.53
3	B	402	A1I7L	C13-C11	3.44	1.59	1.53
3	D	402	A1I7L	C08-C11	3.20	1.54	1.49
3	B	402	A1I7L	C08-C11	3.11	1.54	1.49
3	A	402	A1I7L	C08-C11	3.04	1.54	1.49
3	D	402	A1I7L	C09-C08	2.89	1.44	1.39
3	C	402	A1I7L	C08-C11	2.86	1.53	1.49
3	A	402	A1I7L	C09-C08	2.79	1.44	1.39
3	B	402	A1I7L	C09-C08	2.69	1.44	1.39
3	C	402	A1I7L	C09-C08	2.62	1.43	1.39
3	B	402	A1I7L	C01-S02	2.48	1.83	1.75
3	A	402	A1I7L	C01-S02	2.45	1.83	1.75
3	D	402	A1I7L	C01-S02	2.43	1.83	1.75
3	C	402	A1I7L	C01-S02	2.38	1.83	1.75
3	B	402	A1I7L	O29-C25	2.28	1.53	1.42
3	D	402	A1I7L	O29-C25	2.24	1.52	1.42
3	B	402	A1I7L	C24-C25	2.21	1.57	1.50
3	C	402	A1I7L	C07-CL21	2.20	1.77	1.72
3	A	402	A1I7L	O29-C25	2.19	1.52	1.42
3	C	402	A1I7L	O29-C25	2.19	1.52	1.42
3	D	402	A1I7L	C24-C25	2.19	1.57	1.50
3	D	402	A1I7L	C07-CL21	2.17	1.77	1.72
3	B	402	A1I7L	C07-C06	2.10	1.44	1.39
3	A	402	A1I7L	C24-C25	2.07	1.57	1.50
3	A	402	A1I7L	C07-CL21	2.06	1.77	1.72
3	C	402	A1I7L	C24-C25	2.05	1.57	1.50
3	B	402	A1I7L	C07-CL21	2.03	1.77	1.72
3	D	402	A1I7L	C07-C06	2.01	1.44	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	A1I7L	O04-S02-O03	-9.63	101.66	117.99
3	D	402	A1I7L	O04-S02-O03	-9.57	101.75	117.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	A1I7L	O04-S02-O03	-9.28	102.25	117.99
3	C	402	A1I7L	O04-S02-O03	-9.19	102.41	117.99
3	C	402	A1I7L	O04-S02-C05	6.50	115.79	108.24
3	B	402	A1I7L	O04-S02-C05	5.95	115.15	108.24
3	C	402	A1I7L	O03-S02-C05	4.30	113.24	108.24
3	A	402	A1I7L	O03-S02-C05	3.81	112.67	108.24
3	D	402	A1I7L	O03-S02-C05	3.70	112.54	108.24
3	A	402	A1I7L	O04-S02-C05	3.42	112.21	108.24
3	D	402	A1I7L	O04-S02-C05	3.40	112.19	108.24
3	D	402	A1I7L	C01-S02-C05	3.15	109.63	105.09
3	D	402	A1I7L	C07-C06-C05	2.87	119.95	115.86
3	A	402	A1I7L	C07-C06-C05	2.84	119.90	115.86
3	C	402	A1I7L	C09-C08-C07	2.75	120.87	118.60
3	B	402	A1I7L	O03-S02-C05	2.75	111.43	108.24
3	B	402	A1I7L	C07-C06-C05	2.51	119.43	115.86
3	C	402	A1I7L	C07-C06-C05	2.48	119.40	115.86
3	A	402	A1I7L	O04-S02-C01	2.48	112.11	108.47
3	C	402	A1I7L	O12-C11-C13	2.48	122.75	119.58
3	C	402	A1I7L	C08-C07-C06	-2.37	119.84	122.92
3	A	402	A1I7L	C08-C07-C06	-2.33	119.89	122.92
3	D	402	A1I7L	C08-C07-C06	-2.29	119.95	122.92
3	D	402	A1I7L	O04-S02-C01	2.28	111.81	108.47
3	A	402	A1I7L	C01-S02-C05	2.23	108.31	105.09
3	B	402	A1I7L	C01-S02-C05	2.08	108.09	105.09
3	B	402	A1I7L	O20-C19-C18	-2.06	118.45	122.13

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	A1I7L	C06-C05-S02-C01
3	A	402	A1I7L	C10-C05-S02-C01
3	A	402	A1I7L	C08-C11-C13-C19
3	A	402	A1I7L	O12-C11-C13-C19
3	B	402	A1I7L	C08-C11-C13-C19
3	B	402	A1I7L	O12-C11-C13-C19
3	B	402	A1I7L	O23-C24-C25-O29
3	C	402	A1I7L	C08-C11-C13-C19
3	C	402	A1I7L	O12-C11-C13-C19
3	D	402	A1I7L	C06-C05-S02-C01
3	D	402	A1I7L	C10-C05-S02-C01
3	D	402	A1I7L	C08-C11-C13-C19

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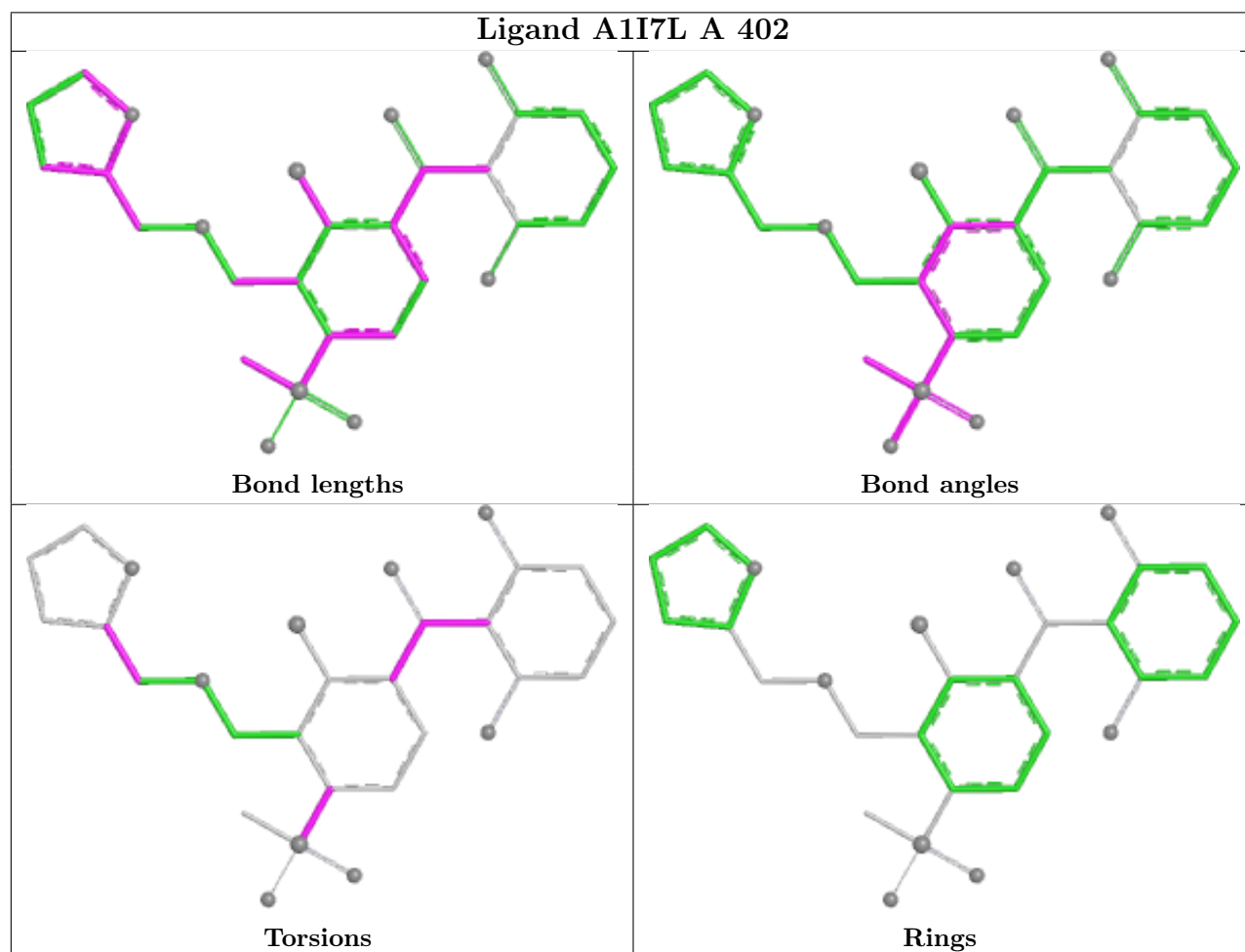
Mol	Chain	Res	Type	Atoms
3	D	402	A1I7L	O12-C11-C13-C19
3	D	402	A1I7L	O23-C24-C25-O29
3	B	402	A1I7L	C10-C05-S02-O03
3	C	402	A1I7L	C10-C05-S02-O03
3	B	402	A1I7L	C09-C08-C11-O12
3	B	402	A1I7L	C09-C08-C11-C13
3	D	402	A1I7L	O23-C24-C25-C26
3	B	402	A1I7L	C10-C05-S02-C01
3	B	402	A1I7L	C10-C05-S02-O04
3	C	402	A1I7L	C10-C05-S02-C01
3	A	402	A1I7L	O12-C11-C13-C14
3	C	402	A1I7L	C08-C11-C13-C14
3	C	402	A1I7L	O12-C11-C13-C14
3	D	402	A1I7L	C08-C11-C13-C14
3	D	402	A1I7L	O12-C11-C13-C14
3	B	402	A1I7L	C06-C05-S02-C01
3	C	402	A1I7L	C06-C05-S02-C01
3	B	402	A1I7L	C07-C08-C11-O12
3	B	402	A1I7L	C06-C05-S02-O03
3	C	402	A1I7L	C06-C05-S02-O03
3	C	402	A1I7L	C10-C05-S02-O04
3	B	402	A1I7L	C25-C24-O23-C22
3	B	402	A1I7L	C06-C22-O23-C24
3	C	402	A1I7L	C09-C08-C11-C13
3	D	402	A1I7L	C09-C08-C11-C13
3	A	402	A1I7L	C08-C11-C13-C14
3	A	402	A1I7L	O23-C24-C25-C26
3	B	402	A1I7L	O23-C24-C25-C26
3	A	402	A1I7L	C09-C08-C11-C13

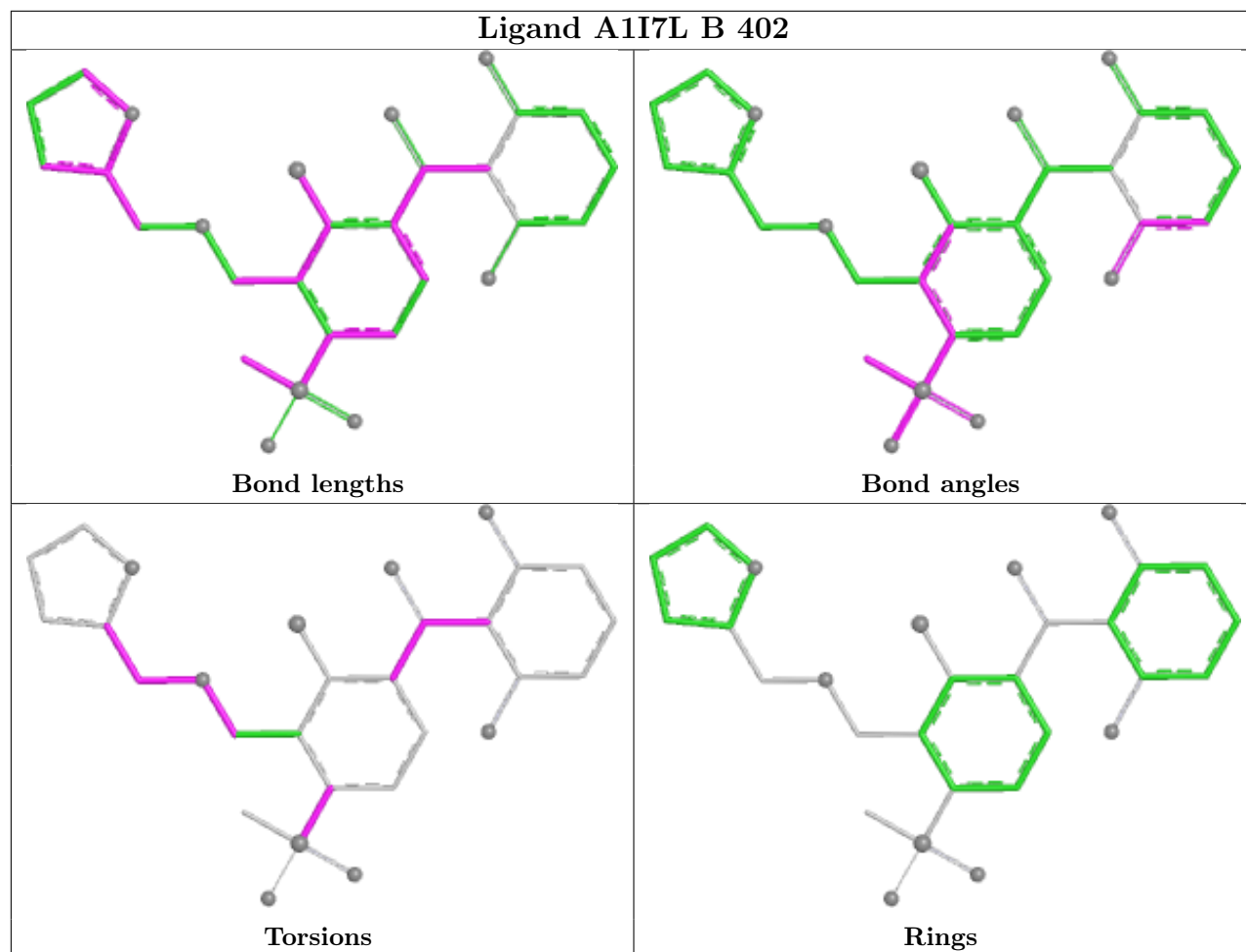
There are no ring outliers.

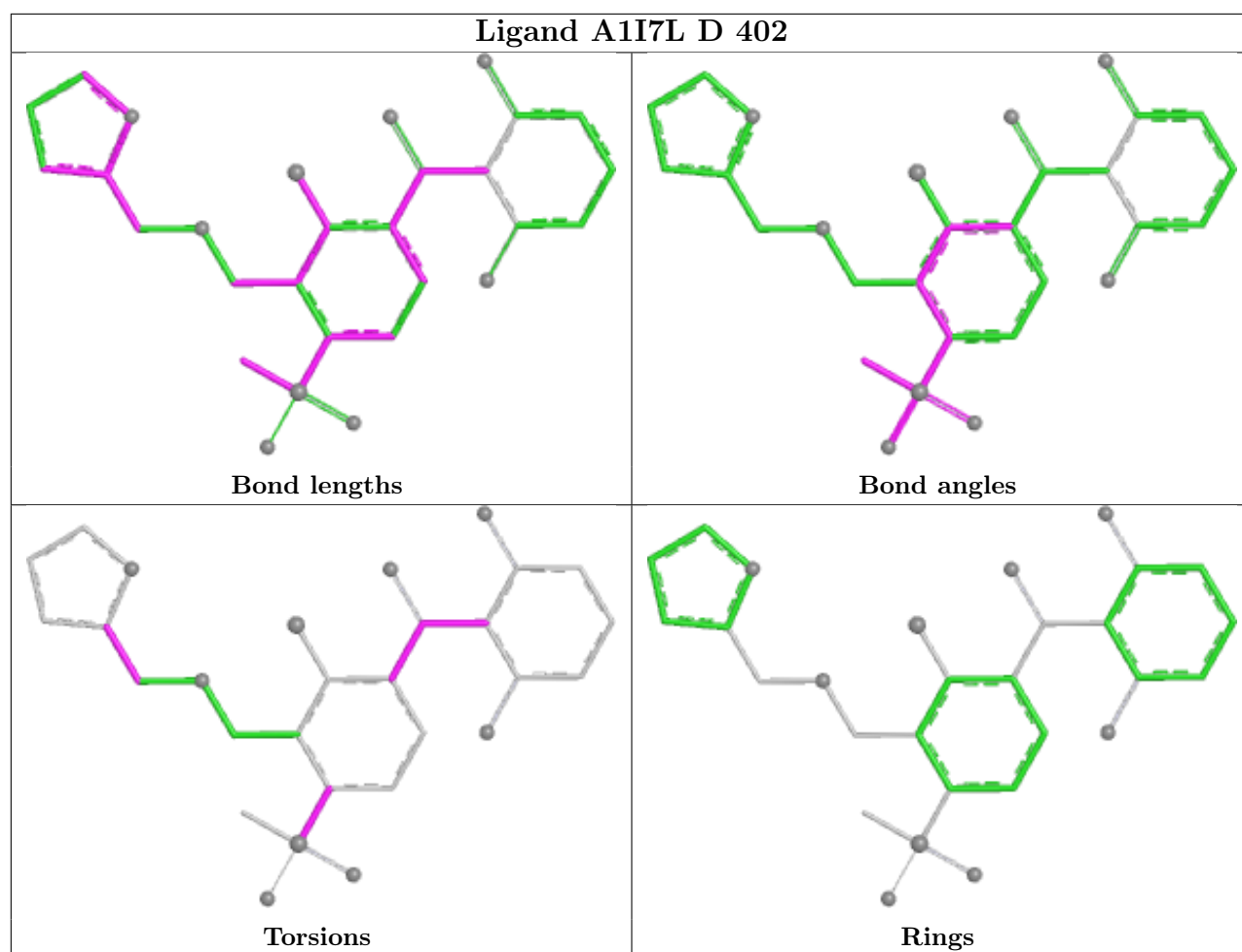
No monomer is involved in short contacts.

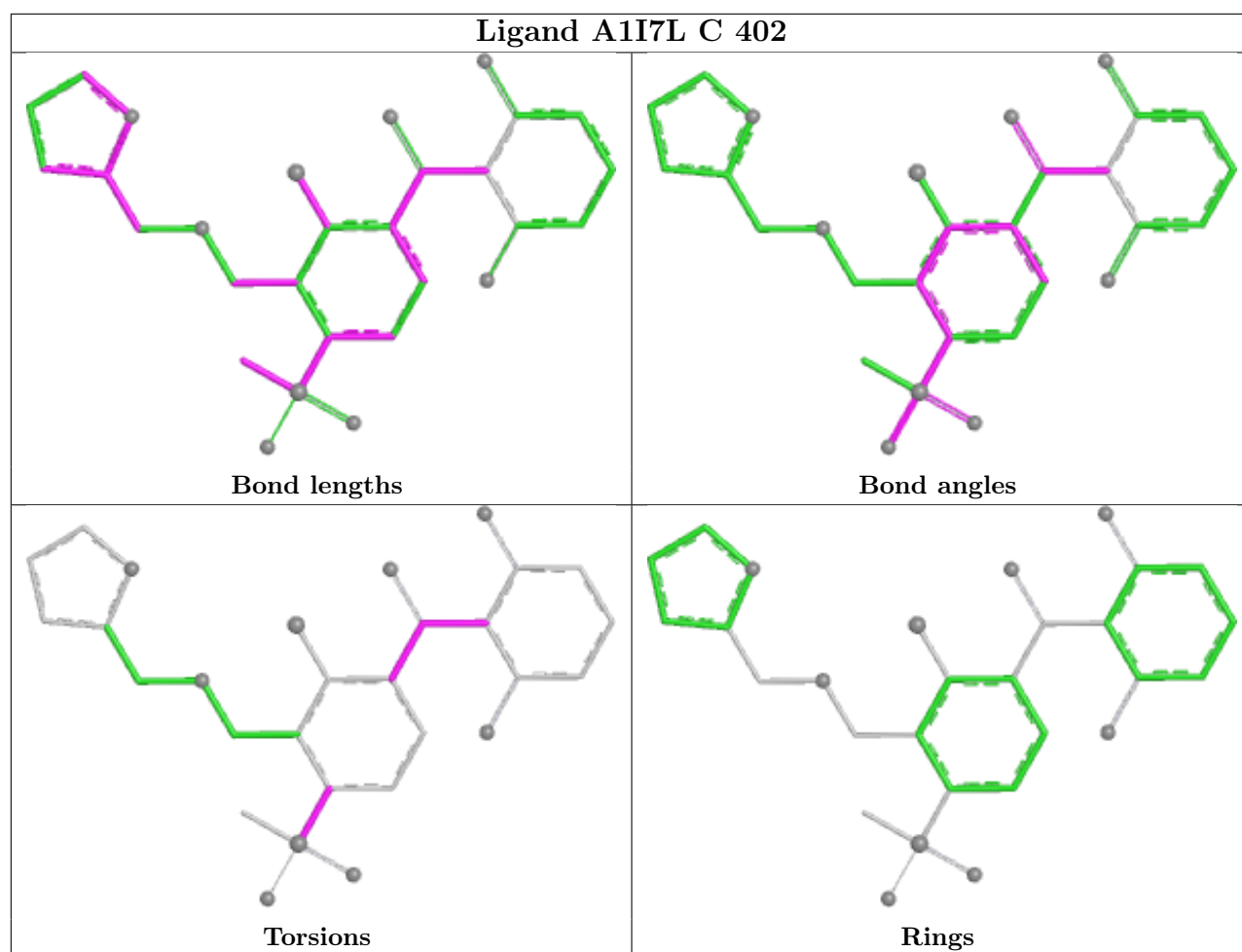
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	333/361 (92%)	1.17	47 (14%) 6 5	31, 68, 84, 108	2 (0%)
1	B	333/361 (92%)	0.27	13 (3%) 43 39	24, 45, 72, 114	1 (0%)
1	C	333/361 (92%)	1.08	39 (11%) 9 7	36, 71, 87, 107	1 (0%)
1	D	333/361 (92%)	0.35	11 (3%) 49 45	39, 50, 80, 110	0
All	All	1332/1444 (92%)	0.72	110 (8%) 17 14	24, 64, 82, 114	4 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	SER	5.7
1	A	8	PHE	4.5
1	C	7	ILE	4.5
1	A	7	ILE	4.1
1	C	78	GLY	3.9
1	C	304	GLN	3.9
1	D	308	LYS	3.9
1	D	191	ILE	3.8
1	C	303	SER	3.7
1	D	355	ARG	3.7
1	C	109	GLU	3.6
1	B	228	GLY	3.6
1	D	222	GLU	3.4
1	D	303	SER	3.4
1	A	191	ILE	3.3
1	C	89[A]	ARG	3.2
1	C	6	ASP	3.2
1	C	8	PHE	3.1
1	D	7	ILE	3.1
1	C	191	ILE	3.1
1	A	305	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	229	GLN	3.0
1	A	89[A]	ARG	3.0
1	A	148	ILE	3.0
1	B	243	GLN	3.0
1	C	204	THR	2.9
1	B	89[A]	ARG	2.9
1	C	35	GLN	2.8
1	D	305	PRO	2.8
1	A	265[A]	ARG	2.8
1	C	110	THR	2.8
1	A	150	GLY	2.8
1	A	299	LEU	2.7
1	A	134	PHE	2.7
1	C	354	ARG	2.7
1	A	184	LYS	2.7
1	A	355	ARG	2.7
1	C	331	LYS	2.7
1	C	243	GLN	2.6
1	A	234	LEU	2.6
1	B	70	ALA	2.6
1	A	69	ILE	2.6
1	C	267	MET	2.6
1	A	135	GLU	2.6
1	A	103	ALA	2.6
1	B	303	SER	2.6
1	A	214	MET	2.6
1	A	177	TYR	2.6
1	A	30	LEU	2.5
1	C	294	ALA	2.5
1	B	306	ASP	2.5
1	C	265	ARG	2.5
1	C	106	VAL	2.5
1	A	70	ALA	2.5
1	C	121	LYS	2.4
1	A	312	LEU	2.4
1	C	127	PRO	2.4
1	B	191	ILE	2.4
1	A	54	ARG	2.4
1	A	207	ALA	2.4
1	A	262	PHE	2.4
1	C	279	GLU	2.4
1	C	30	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	61	ILE	2.3
1	A	204	THR	2.3
1	A	329	GLN	2.3
1	D	204	THR	2.3
1	A	81	VAL	2.3
1	C	245	VAL	2.3
1	A	307	ASP	2.2
1	A	302	ALA	2.2
1	A	211	PRO	2.2
1	C	286	GLY	2.2
1	A	75	ALA	2.2
1	C	269	ALA	2.2
1	D	304	GLN	2.2
1	C	67	LYS	2.2
1	C	235	MET	2.2
1	C	266	PHE	2.2
1	C	107	GLU	2.2
1	A	293	LYS	2.2
1	A	42	VAL	2.2
1	A	215	ILE	2.2
1	C	268	THR	2.1
1	C	355	ARG	2.1
1	C	278	LEU	2.1
1	C	287	GLU	2.1
1	B	110	THR	2.1
1	A	170	VAL	2.1
1	C	102	GLY	2.1
1	A	85	ALA	2.1
1	A	178	TRP	2.1
1	C	167	THR	2.1
1	A	162	ILE	2.1
1	A	151	VAL	2.1
1	A	156	VAL	2.1
1	D	8	PHE	2.1
1	B	109	GLU	2.0
1	B	305	PRO	2.0
1	A	242	ILE	2.0
1	C	239	GLY	2.0
1	A	317	GLU	2.0
1	B	134	PHE	2.0
1	B	324	PHE	2.0
1	A	343	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	131	ILE	2.0
1	A	284	GLY	2.0
1	D	137	GLY	2.0
1	A	354	ARG	2.0
1	B	216	ARG	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](#)

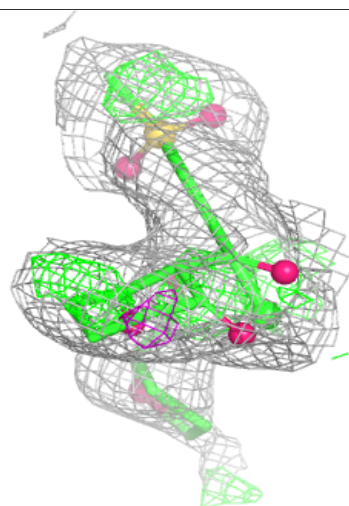
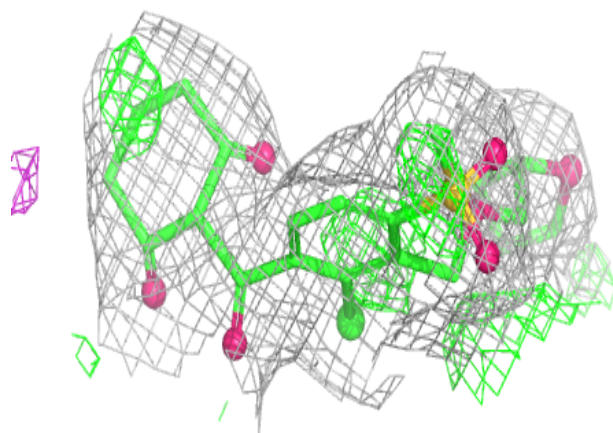
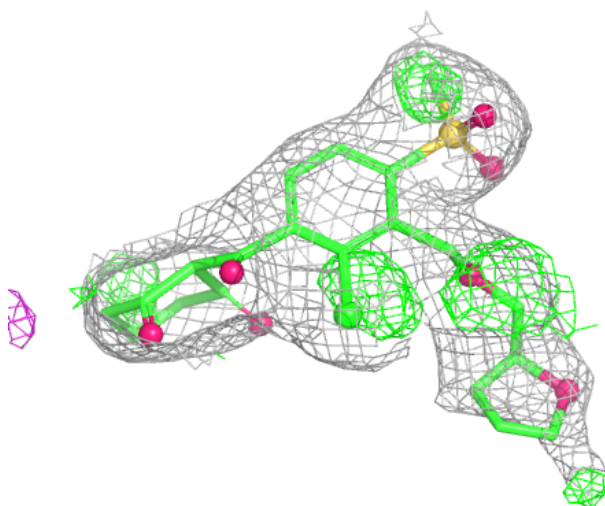
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A1I7L	A	402	29/29	0.88	0.19	72,74,88,103	0
3	A1I7L	B	402	29/29	0.91	0.14	43,49,75,80	0
3	A1I7L	C	402	29/29	0.92	0.13	56,58,80,88	0
3	A1I7L	D	402	29/29	0.92	0.14	50,54,83,100	0
2	MN	C	401	1/1	0.99	0.05	64,64,64,64	0
2	MN	D	401	1/1	0.99	0.09	52,52,52,52	0
2	MN	B	401	1/1	0.99	0.02	42,42,42,42	0
2	MN	A	401	1/1	1.00	0.06	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.

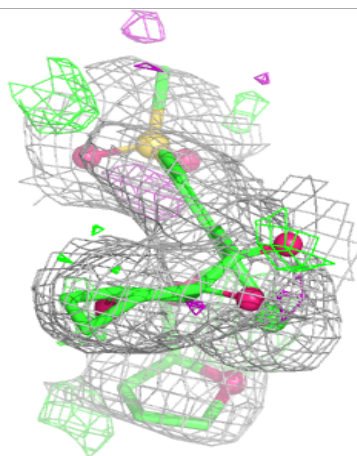
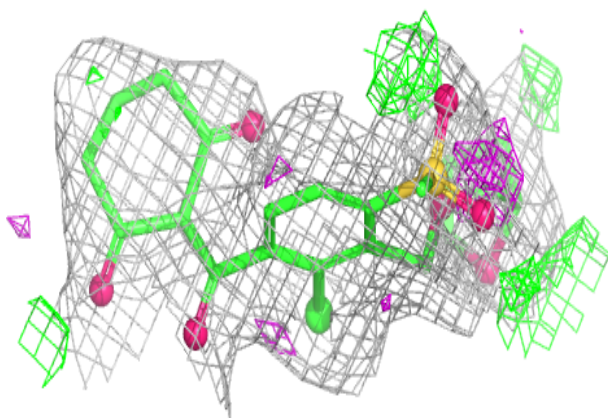
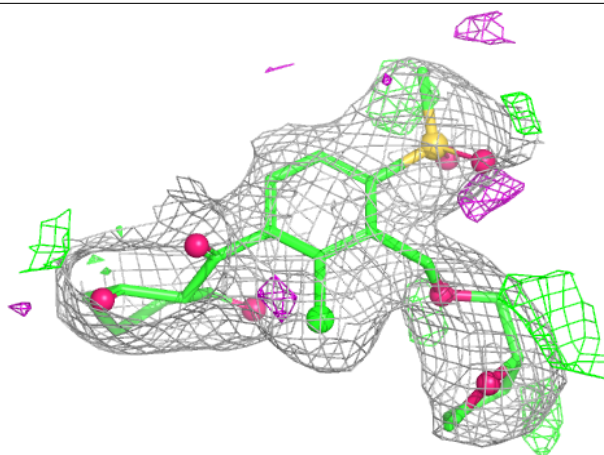
Electron density around A1I7L A 402:

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



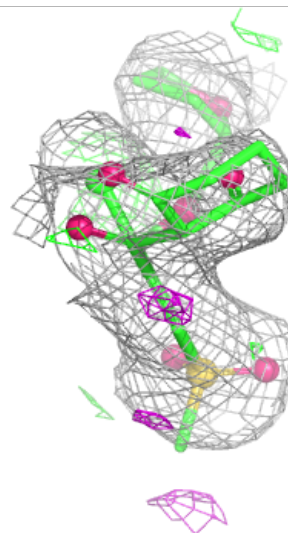
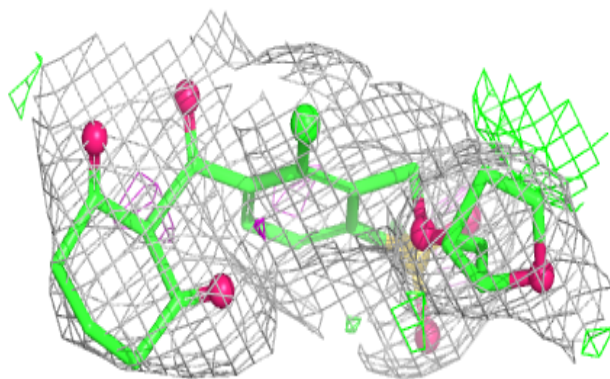
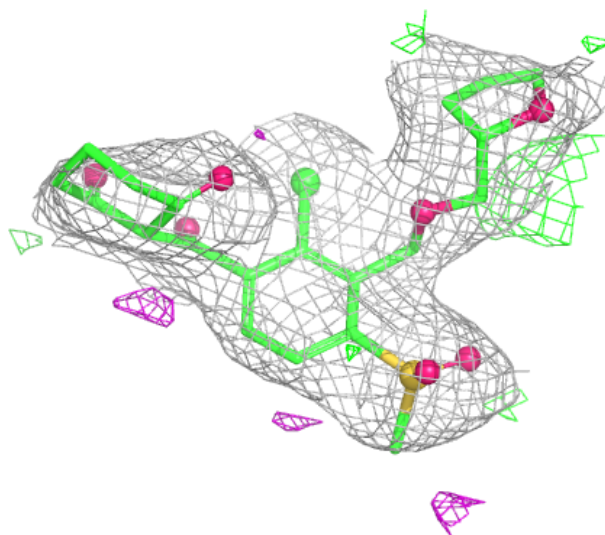
Electron density around A1I7L B 402:

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



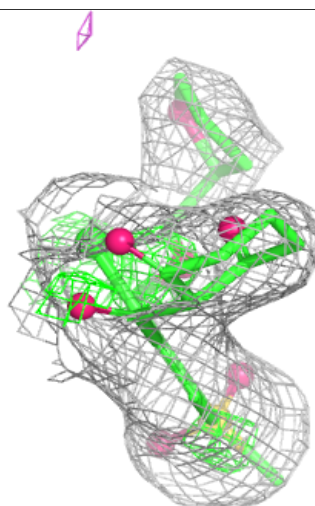
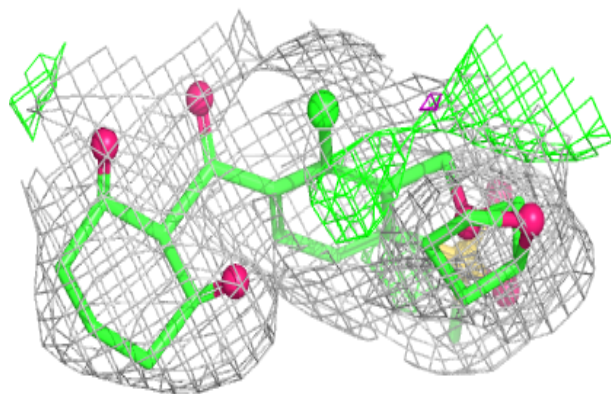
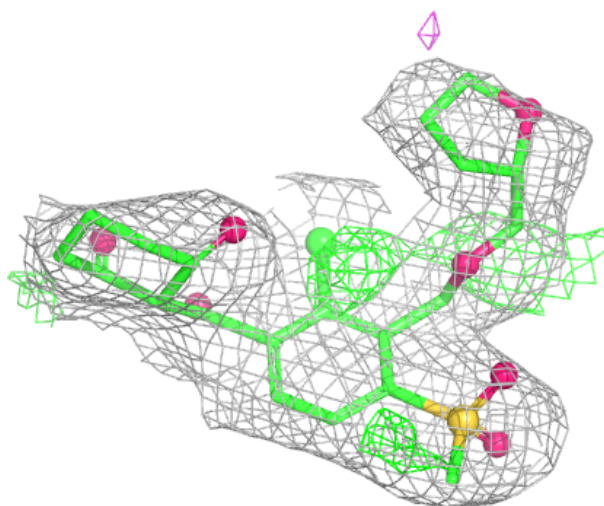
Electron density around A1I7L C 402:

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



Electron density around A1I7L 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.