



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 10:20 AM JST

PDB ID : 8IM3
Title : Crystal structure of human HPPD complexed with compound a10
Authors : Dong, J.; Lin, H.-Y.
Deposited on : 2023-03-05
Resolution : 2.78 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

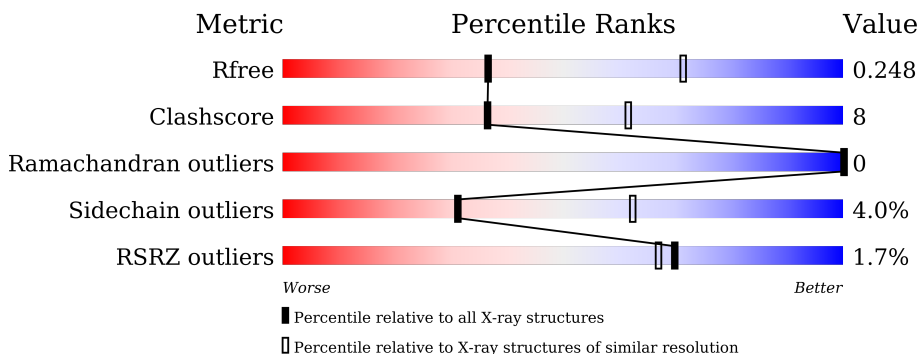
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	393	
1	B	393	
1	C	393	
1	D	393	
1	E	393	
1	F	393	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17896 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.

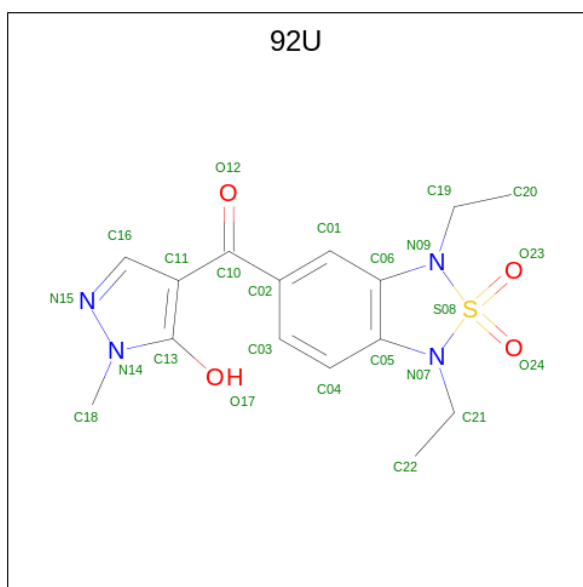
- Molecule 1 is a protein called 4-hydroxyphenylpyruvate dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	371	2968	1907	501	549	11	0	1	0
1	B	372	2955	1896	503	545	11	0	0	0
1	C	373	2946	1887	498	550	11	0	0	0
1	D	371	2958	1897	502	548	11	0	0	0
1	E	369	2920	1875	494	540	11	0	0	0
1	F	371	2850	1827	479	533	11	0	0	0

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

- Molecule 3 is [1,3-diethyl-2,2-bis(oxidanylidene)-2⁶,1,3-benzothiadiazol-5-yl]-(1-methyl-5-oxidanyl-pyrazol-4-yl)methanone (three-letter code: 92U) (formula: C₁₅H₁₈N₄O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	Total	C	N	O	S	0	0
			24	15	4	4	1		
3	B	1	Total	C	N	O	S	0	0
			24	15	4	4	1		
3	C	1	Total	C	N	O	S	0	0
			24	15	4	4	1		
3	D	1	Total	C	N	O	S	0	0
			24	15	4	4	1		
3	E	1	Total	C	N	O	S	0	0
			24	15	4	4	1		
3	F	1	Total	C	N	O	S	0	0
			24	15	4	4	1		

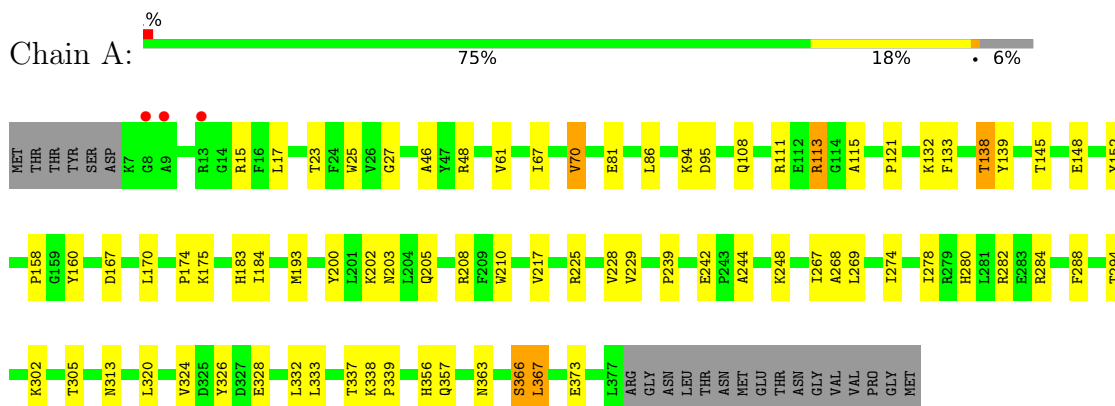
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	32	Total	O	0	0
			32	32		
4	C	32	Total	O	0	0
			32	32		
4	D	24	Total	O	0	0
			24	24		
4	E	15	Total	O	0	0
			15	15		
4	F	12	Total	O	0	0
			12	12		

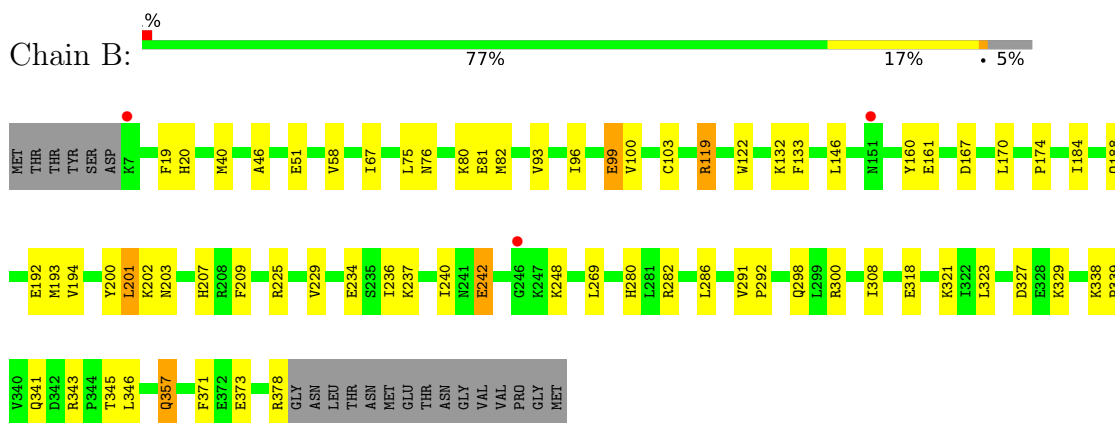
3 Residue-property plots [i](#)

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.

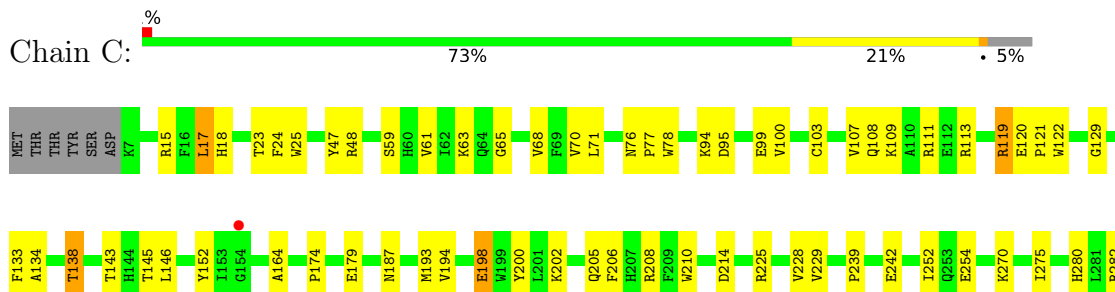
- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



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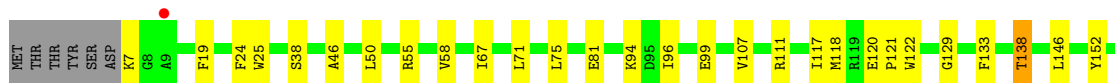
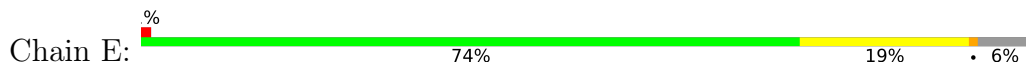




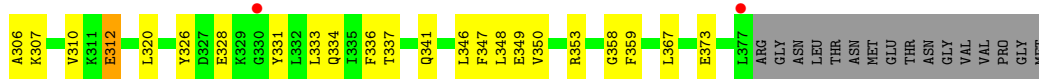
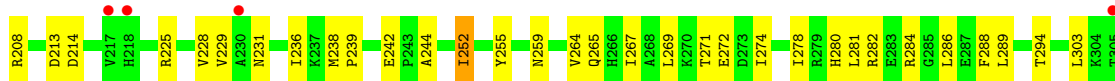
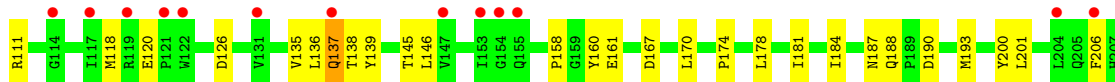
• Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



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• Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.03Å 88.89Å 94.28Å 97.27° 110.71° 110.29°	Depositor
Resolution (Å)	48.19 – 2.78 48.19 – 2.78	Depositor EDS
% Data completeness (in resolution range)	95.8 (48.19-2.78) 95.8 (48.19-2.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.77Å)	Xtrriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.217 , 0.247 0.217 , 0.248	Depositor DCC
R_{free} test set	2673 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtrriage
Anisotropy	0.322	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17896	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.62% 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: 92U, CO

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	0.26	0/3044	0.45	0/4118
1	B	0.28	0/3028	0.46	0/4100
1	C	0.26	0/3019	0.45	0/4092
1	D	0.26	0/3031	0.44	0/4103
1	E	0.26	0/2993	0.44	0/4055
1	F	0.29	0/2921	0.46	0/3974
All	All	0.27	0/18036	0.45	0/24442

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	2968	0	2887	44	0
1	B	2955	0	2861	41	0
1	C	2946	0	2819	45	0
1	D	2958	0	2867	39	0
1	E	2920	0	2814	45	0
1	F	2850	0	2661	64	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	24	0	0	0	0
3	B	24	0	0	0	0
3	C	24	0	0	0	0
3	D	24	0	0	0	0
3	E	24	0	0	0	0
3	F	24	0	0	0	0
4	A	34	0	0	1	0
4	B	32	0	0	2	0
4	C	32	0	0	1	0
4	D	24	0	0	0	0
4	E	15	0	0	1	0
4	F	12	0	0	0	0
All	All	17896	0	16909	273	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 8.

All (273) 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:341:GLN:HE22	1:F:346:LEU:HB3	1.33	0.94
1:E:193:MET:HB2	1:E:242:GLU:HB3	1.62	0.80
1:F:23:THR:HG22	1:F:95:ASP:HB3	1.63	0.79
1:F:126:ASP:HB3	1:F:158:PRO:HB3	1.67	0.75
1:F:312:GLU:HG3	1:F:333:LEU:HD11	1.68	0.75
1:B:291:VAL:HG11	1:B:323:LEU:HD21	1.69	0.74
1:C:100:VAL:HG11	1:C:146:LEU:HD23	1.73	0.70
1:E:46:ALA:HB1	1:E:160:TYR:HB3	1.75	0.69
1:F:174:PRO:O	1:F:284:ARG:NH1	2.26	0.69
1:D:193:MET:HB2	1:D:242:GLU:HB3	1.73	0.69
1:B:357:GLN:O	1:B:357:GLN:NE2	2.26	0.68
1:F:193:MET:HB2	1:F:242:GLU:HB3	1.77	0.67
1:B:298:GLN:NE2	1:B:373:GLU:OE2	2.28	0.66
1:B:225:ARG:NH1	1:B:242:GLU:OE2	2.28	0.66
1:A:282:ARG:NH2	4:A:501:HOH:O	2.28	0.66
1:F:228:VAL:HA	1:F:239:PRO:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:THR:HG21	1:A:373:GLU:HB3	1.78	0.65
1:C:353:ARG:NH2	1:C:358:GLY:O	2.29	0.65
1:C:337:THR:HG22	1:C:348:LEU:H	1.62	0.65
1:B:327:ASP:HB3	1:B:329:LYS:H	1.63	0.63
1:F:46:ALA:HB1	1:F:160:TYR:HB3	1.80	0.63
1:A:282:ARG:NH1	1:A:320:LEU:O	2.32	0.63
1:B:67:ILE:HD13	1:B:269:LEU:HD13	1.80	0.62
1:F:89:HIS:ND1	1:F:259:ASN:OD1	2.33	0.61
1:C:63:LYS:HB2	1:C:68:VAL:HG12	1.83	0.61
1:A:228:VAL:HA	1:A:239:PRO:HA	1.81	0.61
1:E:294:THR:HG21	1:E:373:GLU:HB3	1.83	0.60
1:D:113:ARG:O	1:D:202:LYS:NZ	2.34	0.60
1:F:167:ASP:HB3	1:F:170:LEU:HG	1.83	0.60
1:A:15:ARG:HH11	1:A:17:LEU:HD23	1.67	0.59
1:F:187:ASN:ND2	1:F:265:GLN:OE1	2.32	0.59
1:E:282:ARG:NH1	1:E:320:LEU:O	2.36	0.59
1:A:193:MET:HB2	1:A:242:GLU:HB3	1.84	0.59
1:B:234:GLU:O	1:B:237:LYS:NZ	2.36	0.58
1:B:209:PHE:HZ	1:B:357:GLN:HG3	1.67	0.58
1:D:64:GLN:HE21	1:D:178:LEU:H	1.50	0.58
1:A:67:ILE:HD13	1:A:269:LEU:HD22	1.83	0.58
1:F:118:MET:HB2	1:F:135:VAL:HG12	1.84	0.58
1:E:96:ILE:HD13	1:E:238:MET:HE1	1.85	0.58
1:B:300:ARG:NH1	4:B:505:HOH:O	2.36	0.58
1:F:135:VAL:HG22	1:F:145:THR:HG22	1.85	0.58
1:C:327:ASP:HB2	1:C:356:HIS:CD2	2.38	0.57
1:A:174:PRO:O	1:A:284:ARG:NH2	2.33	0.57
1:C:282:ARG:NH1	1:C:320:LEU:O	2.38	0.57
1:D:282:ARG:NH1	1:D:320:LEU:O	2.37	0.57
1:E:188:GLN:O	1:E:243:PRO:HD3	2.05	0.57
1:C:109:LYS:HG2	1:C:205:GLN:NE2	2.19	0.57
1:A:113:ARG:NE	1:A:202:LYS:O	2.36	0.57
1:E:167:ASP:HB3	1:E:170:LEU:HG	1.85	0.57
1:A:184:ILE:HG12	1:A:267:ILE:HG23	1.86	0.57
1:B:291:VAL:HG22	1:B:321:LYS:HD2	1.86	0.56
1:A:324:VAL:HG22	1:A:333:LEU:HD23	1.87	0.56
1:E:338:LYS:HG3	1:E:339:PRO:HD2	1.87	0.56
1:E:288:PHE:HA	1:E:337:THR:HA	1.87	0.56
1:A:363:ASN:HA	1:A:366:SER:HB2	1.87	0.56
1:C:108:GLN:OE1	1:C:111:ARG:NH1	2.39	0.56
1:E:7:LYS:N	4:E:502:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:288:PHE:HA	1:F:337:THR:HA	1.88	0.56
1:A:208:ARG:HG2	1:A:210:TRP:CZ2	2.41	0.55
1:C:228:VAL:HA	1:C:239:PRO:HA	1.87	0.55
1:E:107:VAL:HG13	1:E:117:ILE:HD12	1.87	0.55
1:F:44:PRO:HA	1:F:62:ILE:HG22	1.88	0.55
1:F:269:LEU:HD11	1:F:350:VAL:HG22	1.87	0.55
1:B:96:ILE:HD12	1:B:184:ILE:HD12	1.89	0.55
1:C:174:PRO:HB2	1:C:280:HIS:CG	2.41	0.55
1:F:353:ARG:NH2	1:F:358:GLY:O	2.32	0.55
1:A:225:ARG:HG3	1:A:244:ALA:HB2	1.87	0.54
1:A:167:ASP:HB3	1:A:170:LEU:HG	1.89	0.54
1:A:23:THR:HG23	1:A:70:VAL:HG22	1.89	0.54
1:D:312:GLU:OE2	1:D:331:TYR:OH	2.22	0.54
1:F:61:VAL:HG12	1:F:70:VAL:HG13	1.89	0.54
1:F:178:LEU:HB3	1:F:269:LEU:HD13	1.88	0.53
1:F:184:ILE:HG22	1:F:238:MET:HG2	1.90	0.53
1:F:341:GLN:NE2	1:F:346:LEU:HB3	2.13	0.53
1:B:202:LYS:HE2	1:B:203:ASN:OD1	2.09	0.53
1:A:121:PRO:HA	1:A:133:PHE:O	2.09	0.53
1:D:118:MET:HG2	1:D:137:GLN:HB2	1.89	0.53
1:C:275:ILE:HD11	1:C:312:GLU:HG2	1.90	0.53
1:E:67:ILE:HG12	1:E:181:ILE:HD12	1.90	0.53
1:C:310:VAL:HG21	1:C:314:ILE:HD11	1.90	0.53
1:D:202:LYS:NZ	1:D:203:ASN:OD1	2.38	0.52
1:A:132:LYS:HB3	1:A:148:GLU:HB3	1.89	0.52
1:E:190:ASP:HA	1:E:243:PRO:HD2	1.91	0.52
1:F:67:ILE:HG23	1:F:181:ILE:HD11	1.92	0.52
1:E:24:PHE:HB2	1:E:71:LEU:HD13	1.91	0.52
1:B:167:ASP:HB3	1:B:170:LEU:HG	1.92	0.52
1:D:206:PHE:HD2	1:D:229:VAL:HG12	1.75	0.52
1:B:40:MET:HG3	1:B:286:LEU:HD22	1.92	0.52
1:B:46:ALA:HB1	1:B:160:TYR:HB3	1.92	0.52
1:C:194:VAL:O	1:C:198:GLU:HB2	2.10	0.52
1:B:188:GLN:NE2	1:B:240:ILE:HG23	2.25	0.51
1:F:208:ARG:NH2	1:F:214:ASP:OD1	2.44	0.51
1:D:267:ILE:HB	1:D:348:LEU:HD23	1.92	0.51
1:A:27:GLY:HA2	1:A:86:LEU:HD21	1.93	0.51
1:D:96:ILE:HB	1:D:144:HIS:CE1	2.46	0.51
1:D:167:ASP:HB3	1:D:170:LEU:HG	1.93	0.51
1:E:133:PHE:HA	1:E:146:LEU:O	2.11	0.51
1:C:200:TYR:HB3	1:C:206:PHE:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:MET:HG2	1:F:286:LEU:HD22	1.93	0.51
1:F:282:ARG:NH1	1:F:320:LEU:O	2.44	0.51
1:F:58:VAL:HB	1:F:75:LEU:HD11	1.93	0.51
1:E:329:LYS:O	1:E:355:ASN:ND2	2.44	0.51
1:F:280:HIS:O	1:F:284:ARG:HG2	2.10	0.51
1:C:288:PHE:HA	1:C:337:THR:HA	1.92	0.50
1:A:152:TYR:CE1	1:A:158:PRO:HG3	2.47	0.50
1:C:326:TYR:HA	1:C:331:TYR:HA	1.93	0.50
1:E:200:TYR:CB	1:E:229:VAL:HG11	2.42	0.50
1:B:119:ARG:HD2	1:B:122:TRP:CE3	2.46	0.50
1:D:200:TYR:HB2	1:D:229:VAL:HG11	1.93	0.50
1:D:185:VAL:HG12	1:D:239:PRO:HB2	1.93	0.50
1:E:38:SER:O	1:E:284:ARG:HD3	2.12	0.50
1:F:42:PHE:HA	1:F:64:GLN:HB2	1.94	0.50
1:F:188:GLN:O	1:F:252:ILE:HD11	2.11	0.49
1:B:292:PRO:HD3	1:B:371:PHE:CE1	2.47	0.49
1:B:119:ARG:HD2	1:B:122:TRP:CZ3	2.47	0.49
1:B:282:ARG:NH2	4:B:504:HOH:O	2.33	0.49
1:E:278:ILE:O	1:E:282:ARG:HG3	2.12	0.49
1:B:200:TYR:HB2	1:B:229:VAL:HG11	1.95	0.49
1:C:113:ARG:HB3	1:C:202:LYS:HG2	1.95	0.49
1:B:343:ARG:O	1:B:345:THR:N	2.43	0.49
1:D:123:VAL:HG11	1:D:130:LYS:HE3	1.95	0.49
1:B:188:GLN:HE21	1:B:240:ILE:HG23	1.78	0.49
1:E:298:GLN:O	1:E:302:LYS:HG2	2.13	0.49
1:C:63:LYS:NZ	4:C:505:HOH:O	2.45	0.48
1:C:193:MET:HB2	1:C:242:GLU:HB3	1.95	0.48
1:D:185:VAL:HG23	1:D:265:GLN:HB3	1.94	0.48
1:D:335:ILE:HG22	1:D:350:VAL:HG13	1.95	0.48
1:E:206:PHE:HD1	1:E:229:VAL:HG12	1.79	0.48
1:F:336:PHE:CD1	1:F:349:GLU:HB3	2.48	0.48
1:C:95:ASP:OD1	1:C:143:THR:OG1	2.26	0.48
1:E:185:VAL:HG22	1:E:239:PRO:HB2	1.95	0.48
1:F:45:LEU:HB3	1:F:61:VAL:HG23	1.95	0.48
1:B:20:HIS:HD2	1:B:99:GLU:HG3	1.79	0.48
1:E:287:GLU:HG2	1:E:338:LYS:HB2	1.96	0.48
1:E:67:ILE:HD13	1:E:269:LEU:HD13	1.96	0.48
1:B:100:VAL:HG11	1:B:146:LEU:HD22	1.95	0.48
1:A:175:LYS:HB2	1:D:276:THR:HG21	1.95	0.47
1:C:225:ARG:NH1	1:C:242:GLU:OE2	2.47	0.47
1:F:138:THR:HG22	1:F:139:TYR:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:ASP:OD2	1:F:359:PHE:N	2.41	0.47
1:C:61:VAL:HG13	1:C:70:VAL:HG12	1.96	0.47
1:A:25:TRP:CE2	1:A:94:LYS:HG2	2.49	0.47
1:A:183:HIS:H	1:A:268:ALA:HB3	1.79	0.47
1:A:138:THR:HB	1:A:139:TYR:H	1.55	0.47
1:B:193:MET:HB2	1:B:242:GLU:HB3	1.97	0.47
1:F:265:GLN:O	1:F:346:LEU:HD12	2.14	0.47
1:B:93:VAL:HG23	1:B:346:LEU:HD11	1.95	0.47
1:E:200:TYR:HB2	1:E:229:VAL:HG11	1.96	0.47
1:F:200:TYR:HB2	1:F:229:VAL:HG11	1.97	0.47
1:F:307:LYS:HG3	1:F:328:GLU:HA	1.97	0.47
1:A:61:VAL:HG22	1:A:70:VAL:HB	1.95	0.47
1:A:200:TYR:HB2	1:A:229:VAL:HG21	1.96	0.47
1:F:100:VAL:HG11	1:F:146:LEU:HD13	1.97	0.47
1:E:111:ARG:NH2	1:E:120:GLU:OE1	2.48	0.47
1:A:108:GLN:OE1	1:A:111:ARG:NH1	2.47	0.47
1:C:24:PHE:HB2	1:C:71:LEU:HD13	1.97	0.47
1:E:182:ASP:OD2	1:E:270:LYS:NZ	2.48	0.47
1:E:297:LYS:NZ	1:E:373:GLU:OE1	2.48	0.47
1:E:121:PRO:HA	1:E:133:PHE:O	2.15	0.46
1:E:25:TRP:CE2	1:E:94:LYS:HG2	2.49	0.46
1:C:77:PRO:HB2	1:C:78:TRP:CD1	2.50	0.46
1:E:50:LEU:HG	1:E:75:LEU:HD13	1.98	0.46
1:A:95:ASP:OD2	1:A:145:THR:HG22	2.15	0.46
1:C:48:ARG:HG2	1:C:59:SER:HB2	1.97	0.46
1:F:310:VAL:HA	1:F:331:TYR:CZ	2.50	0.46
1:E:170:LEU:HB2	1:E:171:PRO:HD3	1.96	0.46
1:F:278:ILE:HD13	1:F:281:LEU:HD12	1.97	0.46
1:D:88:LYS:O	1:D:343:ARG:NH1	2.43	0.46
1:F:26:VAL:O	1:F:73:SER:HB3	2.16	0.46
1:C:134:ALA:O	1:C:145:THR:HA	2.16	0.45
1:F:206:PHE:CE2	1:F:236:ILE:HD11	2.50	0.45
1:F:334:GLN:NE2	1:F:359:PHE:O	2.46	0.45
1:A:48:ARG:HD2	1:A:160:TYR:CE2	2.51	0.45
1:F:347:PHE:O	1:F:348:LEU:HD12	2.16	0.45
1:B:174:PRO:HB2	1:B:280:HIS:CG	2.51	0.45
1:F:48:ARG:O	1:F:48:ARG:HG3	2.16	0.45
1:D:64:GLN:HE22	1:D:176:CYS:HB2	1.82	0.45
1:E:312:GLU:OE1	1:E:331:TYR:OH	2.25	0.45
1:C:23:THR:HB	1:C:95:ASP:HB3	1.98	0.45
1:C:138:THR:HG21	1:C:200:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:VAL:HG21	1:D:121:PRO:HG3	1.99	0.45
1:C:121:PRO:HA	1:C:133:PHE:O	2.17	0.45
1:F:41:GLY:HA2	1:F:284:ARG:NH2	2.32	0.45
1:B:19:PHE:CZ	1:B:236:ILE:HG23	2.51	0.45
1:F:21:SER:H	1:F:97:ALA:HB3	1.82	0.45
1:C:129:GLY:HA3	1:C:152:TYR:HA	1.98	0.44
1:F:271:THR:OG1	1:F:272:GLU:N	2.50	0.44
1:F:47:TYR:OH	1:F:51:GLU:OE1	2.23	0.44
1:B:194:VAL:HG11	1:C:214:ASP:O	2.17	0.44
1:C:208:ARG:HD3	1:C:210:TRP:CZ2	2.52	0.44
1:C:17:LEU:HD23	1:C:99:GLU:HG2	1.99	0.44
1:F:137:GLN:HG3	1:F:138:THR:H	1.83	0.44
1:C:187:ASN:HB3	1:C:252:ILE:HG23	2.00	0.44
1:D:338:LYS:HD2	1:D:339:PRO:HD2	1.99	0.44
1:E:186:GLY:HA2	1:E:264:VAL:HA	2.00	0.44
1:B:51:GLU:H	1:B:51:GLU:CD	2.20	0.44
1:D:318:GLU:O	1:D:321:LYS:NZ	2.47	0.44
1:E:67:ILE:HG23	1:E:181:ILE:HD11	2.00	0.44
1:F:267:ILE:HB	1:F:348:LEU:HG	1.99	0.44
1:E:122:TRP:CZ2	1:E:133:PHE:HB2	2.53	0.43
1:C:138:THR:HG21	1:C:200:TYR:CZ	2.53	0.43
1:D:50:LEU:HG	1:D:75:LEU:HD13	2.00	0.43
1:D:308:ILE:H	1:D:308:ILE:HG13	1.65	0.43
1:F:303:LEU:HA	1:F:306:ALA:HB2	1.99	0.43
1:A:115:ALA:HB2	1:A:203:ASN:ND2	2.33	0.43
1:A:174:PRO:HB2	1:A:280:HIS:CG	2.54	0.43
1:B:248:LYS:HB2	1:B:248:LYS:HE2	1.73	0.43
1:D:228:VAL:HA	1:D:239:PRO:HA	2.01	0.43
1:D:274:ILE:O	1:D:278:ILE:HG12	2.19	0.43
1:D:345:THR:OG1	1:D:346:LEU:N	2.51	0.43
1:F:326:TYR:HA	1:F:331:TYR:HA	2.00	0.43
1:A:367:LEU:HD23	1:A:367:LEU:HA	1.85	0.43
1:E:255:TYR:OH	1:E:264:VAL:O	2.25	0.43
1:A:302:LYS:HB3	1:A:326:TYR:OH	2.17	0.43
1:C:355:ASN:O	1:C:355:ASN:ND2	2.42	0.43
1:A:274:ILE:O	1:A:278:ILE:HG12	2.19	0.42
1:C:289:LEU:HD23	1:C:338:LYS:HG2	2.01	0.42
1:A:46:ALA:HB1	1:A:160:TYR:HB3	2.01	0.42
1:A:108:GLN:NE2	1:B:308:ILE:HG22	2.34	0.42
1:E:209:PHE:HB3	1:E:228:VAL:HG12	2.01	0.42
1:D:296:TYR:CE2	1:D:318:GLU:HA	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:289:LEU:HD23	1:F:289:LEU:HA	1.80	0.42
1:A:282:ARG:NH2	1:A:288:PHE:HB2	2.34	0.42
1:D:291:VAL:HG21	1:D:323:LEU:HD21	2.02	0.42
1:A:288:PHE:HA	1:A:337:THR:HA	2.01	0.42
1:B:103:CYS:HB3	1:B:132:LYS:HD2	2.00	0.42
1:C:107:VAL:HG21	1:C:121:PRO:HG3	2.01	0.42
1:C:317:LEU:HD22	1:C:322:ILE:HB	2.02	0.42
1:F:228:VAL:HG21	1:F:359:PHE:HE1	1.83	0.42
1:F:294:THR:HG21	1:F:373:GLU:HG2	2.01	0.42
1:E:129:GLY:HA3	1:E:152:TYR:HA	2.00	0.42
1:F:225:ARG:HG3	1:F:244:ALA:HB2	2.02	0.42
1:F:228:VAL:HG21	1:F:359:PHE:CE1	2.55	0.42
1:C:15:ARG:HE	1:C:17:LEU:CD1	2.33	0.42
1:B:188:GLN:HB3	1:B:192:GLU:HB2	2.02	0.42
1:A:248:LYS:HE2	1:A:248:LYS:HB3	1.83	0.41
1:B:201:LEU:HD21	1:B:207:HIS:HA	2.01	0.41
1:D:25:TRP:CE2	1:D:94:LYS:HG2	2.55	0.41
1:D:288:PHE:HA	1:D:337:THR:HA	2.02	0.41
1:D:68:VAL:HG11	1:D:156:PHE:CE1	2.55	0.41
1:A:332:LEU:HD23	1:A:356:HIS:ND1	2.34	0.41
1:D:111:ARG:NH1	1:D:117:ILE:HG13	2.36	0.41
1:E:274:ILE:O	1:E:278:ILE:HG12	2.20	0.41
1:A:313:ASN:HB2	1:D:172:LYS:HD3	2.00	0.41
1:B:58:VAL:HB	1:B:75:LEU:HD21	2.02	0.41
1:C:119:ARG:HB3	1:C:122:TRP:HZ3	1.84	0.41
1:E:19:PHE:CZ	1:E:236:ILE:HG23	2.55	0.41
1:D:138:THR:OG1	1:D:139:TYR:N	2.51	0.41
1:E:138:THR:HG21	1:E:200:TYR:OH	2.21	0.41
1:E:174:PRO:HB2	1:E:280:HIS:CG	2.56	0.41
1:E:271:THR:OG1	1:E:272:GLU:N	2.54	0.41
1:A:108:GLN:HG2	1:B:329:LYS:O	2.21	0.41
1:A:113:ARG:NH2	1:A:205:GLN:HG2	2.36	0.41
1:F:95:ASP:OD2	1:F:145:THR:OG1	2.34	0.41
1:B:338:LYS:HD3	1:B:339:PRO:HD2	2.03	0.41
1:D:248:LYS:HG2	1:D:249:LYS:H	1.86	0.41
1:C:47:TYR:CE1	1:C:164:ALA:HB2	2.56	0.41
1:F:23:THR:HA	1:F:70:VAL:O	2.20	0.41
1:B:300:ARG:NH2	1:B:318:GLU:OE2	2.47	0.40
1:D:268:ALA:HA	1:D:349:GLU:O	2.21	0.40
1:D:300:ARG:NH1	1:D:318:GLU:OE2	2.50	0.40
1:F:89:HIS:ND1	1:F:259:ASN:O	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LYS:HD3	1:A:339:PRO:HD2	2.02	0.40
1:C:25:TRP:CE2	1:C:94:LYS:HG2	2.56	0.40
1:C:65:GLY:HA3	1:C:179:GLU:HA	2.03	0.40
1:C:109:LYS:HG2	1:C:205:GLN:HE22	1.83	0.40
1:F:61:VAL:HB	1:F:70:VAL:HG22	2.03	0.40
1:F:252:ILE:O	1:F:255:TYR:HB3	2.20	0.40
1:B:122:TRP:CZ2	1:B:133:PHE:HB2	2.56	0.40
1:D:19:PHE:CZ	1:D:236:ILE:HG23	2.56	0.40
1:E:50:LEU:HD23	1:E:55:ARG:HA	2.02	0.40
1:F:206:PHE:CD1	1:F:231:ASN:HA	2.56	0.40
1:F:274:ILE:O	1:F:278:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	370/393 (94%)	353 (95%)	17 (5%)	0	100	100
1	B	370/393 (94%)	355 (96%)	15 (4%)	0	100	100
1	C	371/393 (94%)	351 (95%)	20 (5%)	0	100	100
1	D	369/393 (94%)	354 (96%)	15 (4%)	0	100	100
1	E	367/393 (93%)	346 (94%)	21 (6%)	0	100	100
1	F	369/393 (94%)	340 (92%)	29 (8%)	0	100	100
All	All	2216/2358 (94%)	2099 (95%)	117 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	313/343 (91%)	303 (97%)	10 (3%)	39	70
1	B	310/343 (90%)	298 (96%)	12 (4%)	32	63
1	C	307/343 (90%)	292 (95%)	15 (5%)	25	54
1	D	312/343 (91%)	304 (97%)	8 (3%)	46	76
1	E	305/343 (89%)	292 (96%)	13 (4%)	29	59
1	F	286/343 (83%)	270 (94%)	16 (6%)	21	48
All	All	1833/2058 (89%)	1759 (96%)	74 (4%)	31	62

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	VAL
1	A	81	GLU
1	A	113	ARG
1	A	138	THR
1	A	217	VAL
1	A	305	THR
1	A	328	GLU
1	A	357	GLN
1	A	366	SER
1	A	367	LEU
1	B	76	ASN
1	B	80	LYS
1	B	81	GLU
1	B	82	MET
1	B	99	GLU
1	B	119	ARG
1	B	161	GLU
1	B	201	LEU
1	B	242	GLU
1	B	341	GLN
1	B	357	GLN
1	B	378	ARG

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Mol	Chain	Res	Type
1	C	17	LEU
1	C	18	HIS
1	C	76	ASN
1	C	103	CYS
1	C	119	ARG
1	C	120	GLU
1	C	138	THR
1	C	198	GLU
1	C	229	VAL
1	C	254	GLU
1	C	270	LYS
1	C	305	THR
1	C	341	GLN
1	C	355	ASN
1	C	367	LEU
1	D	113	ARG
1	D	148	GLU
1	D	315	ASP
1	D	321	LYS
1	D	350	VAL
1	D	354	HIS
1	D	363	ASN
1	D	367	LEU
1	E	58	VAL
1	E	81	GLU
1	E	99	GLU
1	E	118	MET
1	E	138	THR
1	E	161	GLU
1	E	190	ASP
1	E	198	GLU
1	E	238	MET
1	E	271	THR
1	E	275	ILE
1	E	348	LEU
1	E	373	GLU
1	F	15	ARG
1	F	18	HIS
1	F	48	ARG
1	F	55	ARG
1	F	61	VAL
1	F	111	ARG

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Mol	Chain	Res	Type
1	F	120	GLU
1	F	136	LEU
1	F	137	GLN
1	F	161	GLU
1	F	190	ASP
1	F	201	LEU
1	F	252	ILE
1	F	264	VAL
1	F	312	GLU
1	F	367	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	357	GLN
1	C	205	GLN
1	D	64	GLN
1	D	125	GLN
1	D	183	HIS
1	F	64	GLN
1	F	137	GLN
1	F	341	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 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	92U	A	402	2	20,26,26	4.04	10 (50%)	29,40,40	2.05	7 (24%)
3	92U	C	402	2	20,26,26	4.07	10 (50%)	29,40,40	2.09	7 (24%)
3	92U	E	402	2	20,26,26	4.04	12 (60%)	29,40,40	2.15	6 (20%)
3	92U	F	402	2	20,26,26	4.07	12 (60%)	29,40,40	2.08	6 (20%)
3	92U	D	402	2	20,26,26	4.13	11 (55%)	29,40,40	2.25	7 (24%)
3	92U	B	402	2	20,26,26	4.14	11 (55%)	29,40,40	2.10	7 (24%)

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	92U	A	402	2	-	5/6/32/32	0/3/3/3
3	92U	C	402	2	-	4/6/32/32	0/3/3/3
3	92U	E	402	2	-	1/6/32/32	0/3/3/3
3	92U	F	402	2	-	1/6/32/32	0/3/3/3
3	92U	D	402	2	-	4/6/32/32	0/3/3/3
3	92U	B	402	2	-	5/6/32/32	0/3/3/3

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	92U	C06-C05	9.01	1.59	1.40
3	B	402	92U	C06-N09	9.01	1.52	1.43
3	D	402	92U	C06-C05	9.01	1.59	1.40
3	F	402	92U	C06-C05	8.98	1.59	1.40
3	A	402	92U	C06-C05	8.95	1.59	1.40
3	B	402	92U	C06-C05	8.93	1.59	1.40
3	E	402	92U	C06-C05	8.93	1.59	1.40
3	D	402	92U	C06-N09	8.90	1.52	1.43
3	C	402	92U	C06-N09	8.90	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	92U	C05-N07	8.73	1.52	1.43
3	E	402	92U	C06-N09	8.57	1.52	1.43
3	F	402	92U	C06-N09	8.54	1.52	1.43
3	A	402	92U	C06-N09	8.53	1.52	1.43
3	A	402	92U	C05-N07	8.47	1.52	1.43
3	D	402	92U	C05-N07	8.45	1.52	1.43
3	F	402	92U	C05-N07	8.43	1.52	1.43
3	C	402	92U	C05-N07	8.21	1.51	1.43
3	E	402	92U	C05-N07	8.13	1.51	1.43
3	D	402	92U	C03-C02	6.66	1.50	1.39
3	F	402	92U	C03-C02	6.60	1.50	1.39
3	B	402	92U	C03-C02	6.51	1.50	1.39
3	C	402	92U	C03-C02	6.45	1.50	1.39
3	E	402	92U	C03-C02	6.45	1.50	1.39
3	A	402	92U	C03-C02	6.36	1.50	1.39
3	B	402	92U	C01-C02	3.62	1.44	1.39
3	E	402	92U	C01-C02	3.61	1.44	1.39
3	C	402	92U	C01-C02	3.61	1.44	1.39
3	D	402	92U	C01-C02	3.60	1.44	1.39
3	A	402	92U	C01-C02	3.55	1.44	1.39
3	F	402	92U	C01-C02	3.46	1.44	1.39
3	B	402	92U	C04-C03	3.25	1.44	1.38
3	F	402	92U	C04-C03	3.25	1.44	1.38
3	D	402	92U	C04-C03	3.24	1.44	1.38
3	C	402	92U	C04-C03	3.14	1.44	1.38
3	E	402	92U	C04-C03	3.10	1.44	1.38
3	A	402	92U	C04-C03	3.08	1.44	1.38
3	D	402	92U	O17-C13	2.64	1.40	1.32
3	A	402	92U	O17-C13	2.58	1.40	1.32
3	F	402	92U	O17-C13	2.54	1.40	1.32
3	C	402	92U	O17-C13	2.47	1.39	1.32
3	B	402	92U	O17-C13	2.47	1.39	1.32
3	E	402	92U	O17-C13	2.41	1.39	1.32
3	B	402	92U	O24-S08	2.34	1.47	1.42
3	E	402	92U	O24-S08	2.26	1.47	1.42
3	C	402	92U	O24-S08	2.25	1.47	1.42
3	E	402	92U	C02-C10	2.25	1.53	1.49
3	D	402	92U	O12-C10	-2.24	1.18	1.22
3	D	402	92U	O23-S08	2.24	1.47	1.42
3	A	402	92U	O12-C10	-2.23	1.18	1.22
3	D	402	92U	O24-S08	2.22	1.47	1.42
3	A	402	92U	O23-S08	2.21	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	402	92U	O24-S08	2.21	1.47	1.42
3	E	402	92U	O12-C10	-2.20	1.18	1.22
3	F	402	92U	O12-C10	-2.20	1.18	1.22
3	F	402	92U	O23-S08	2.19	1.47	1.42
3	A	402	92U	O24-S08	2.17	1.46	1.42
3	C	402	92U	O23-S08	2.17	1.46	1.42
3	B	402	92U	O12-C10	-2.16	1.18	1.22
3	C	402	92U	O12-C10	-2.16	1.18	1.22
3	B	402	92U	O23-S08	2.15	1.46	1.42
3	E	402	92U	O23-S08	2.15	1.46	1.42
3	F	402	92U	C01-C06	-2.11	1.36	1.39
3	B	402	92U	C02-C10	2.11	1.53	1.49
3	F	402	92U	C02-C10	2.06	1.53	1.49
3	E	402	92U	C04-C05	-2.06	1.36	1.39
3	D	402	92U	C01-C06	-2.03	1.36	1.39

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	402	92U	C21-N07-S08	5.76	127.57	120.71
3	C	402	92U	C16-N15-N14	5.66	110.12	104.23
3	E	402	92U	C16-N15-N14	5.61	110.07	104.23
3	B	402	92U	C16-N15-N14	5.58	110.04	104.23
3	D	402	92U	C16-N15-N14	5.54	110.00	104.23
3	F	402	92U	C16-N15-N14	5.53	109.99	104.23
3	A	402	92U	C16-N15-N14	5.36	109.81	104.23
3	F	402	92U	C19-N09-S08	5.31	127.03	120.71
3	E	402	92U	C19-N09-S08	5.23	126.93	120.71
3	D	402	92U	C21-N07-S08	5.10	126.78	120.71
3	B	402	92U	C19-N09-S08	5.06	126.73	120.71
3	D	402	92U	C19-N09-S08	5.00	126.66	120.71
3	C	402	92U	C21-N07-S08	4.93	126.58	120.71
3	A	402	92U	C19-N09-S08	4.88	126.52	120.71
3	B	402	92U	C21-N07-S08	4.85	126.48	120.71
3	C	402	92U	C19-N09-S08	4.79	126.41	120.71
3	F	402	92U	C21-N07-S08	4.50	126.07	120.71
3	D	402	92U	C01-C06-N09	4.28	132.97	127.93
3	A	402	92U	C21-N07-S08	4.12	125.62	120.71
3	D	402	92U	C04-C05-N07	4.03	132.46	127.66
3	A	402	92U	C18-N14-C13	-3.87	124.06	128.85
3	D	402	92U	C18-N14-C13	-3.83	124.11	128.85
3	B	402	92U	C01-C06-N09	3.75	132.34	127.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	402	92U	C01-C06-N09	3.72	132.31	127.93
3	C	402	92U	C01-C06-N09	3.63	132.20	127.93
3	F	402	92U	C04-C05-N07	3.46	131.79	127.66
3	A	402	92U	C01-C06-N09	3.46	132.00	127.93
3	F	402	92U	C18-N14-C13	-3.43	124.60	128.85
3	B	402	92U	C04-C05-N07	3.29	131.58	127.66
3	C	402	92U	C18-N14-C13	-3.29	124.77	128.85
3	F	402	92U	C01-C06-N09	3.27	131.78	127.93
3	B	402	92U	C18-N14-C13	-3.20	124.89	128.85
3	A	402	92U	C04-C05-N07	3.07	131.32	127.66
3	E	402	92U	C18-N14-C13	-2.97	125.17	128.85
3	E	402	92U	C04-C05-N07	2.95	131.18	127.66
3	C	402	92U	C04-C05-N07	2.83	131.04	127.66
3	B	402	92U	O24-S08-O23	-2.38	112.22	116.82
3	A	402	92U	O24-S08-O23	-2.17	112.64	116.82
3	D	402	92U	O24-S08-O23	-2.07	112.82	116.82
3	C	402	92U	O24-S08-O23	-2.02	112.92	116.82

There are no chirality outliers.

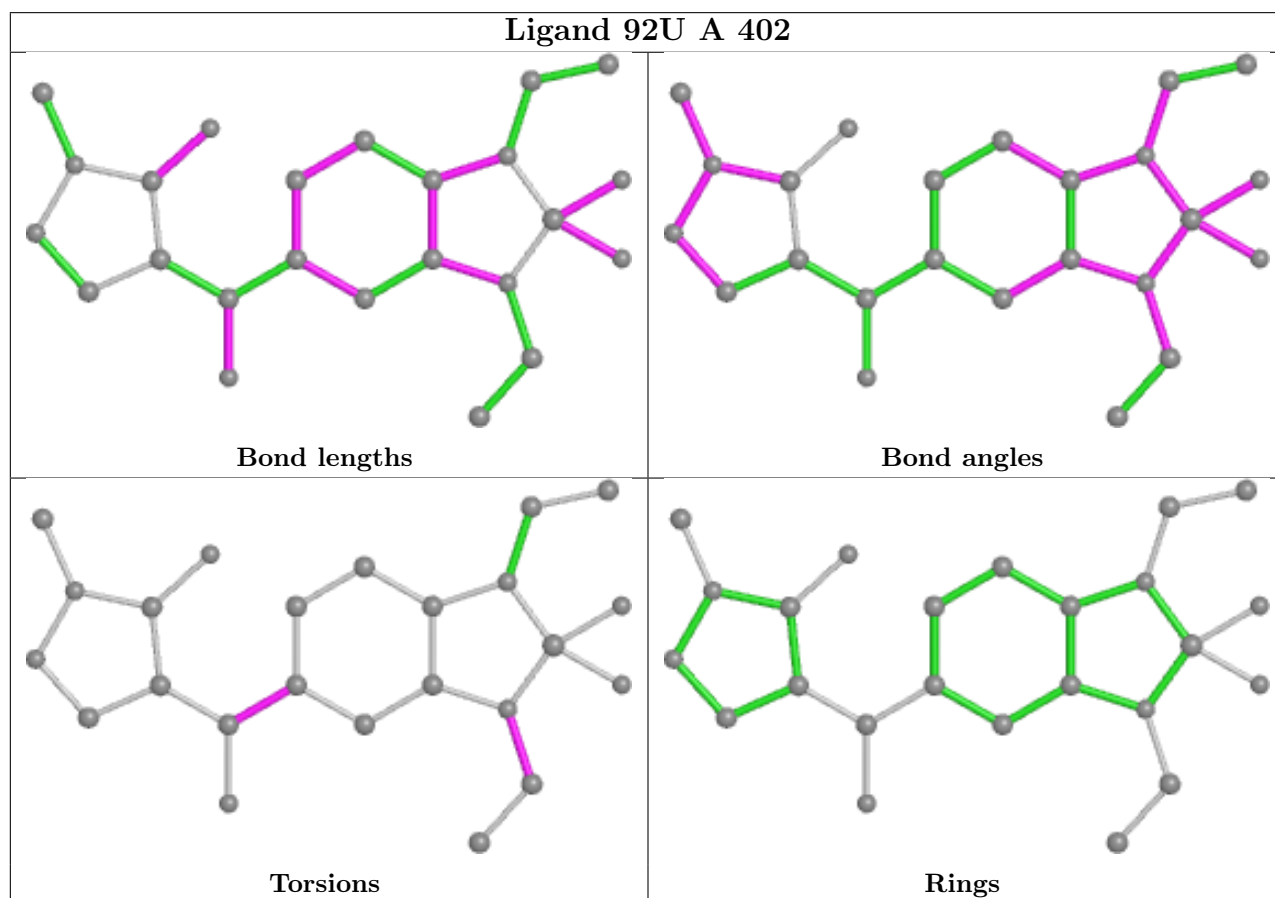
All (20) torsion outliers are listed below:

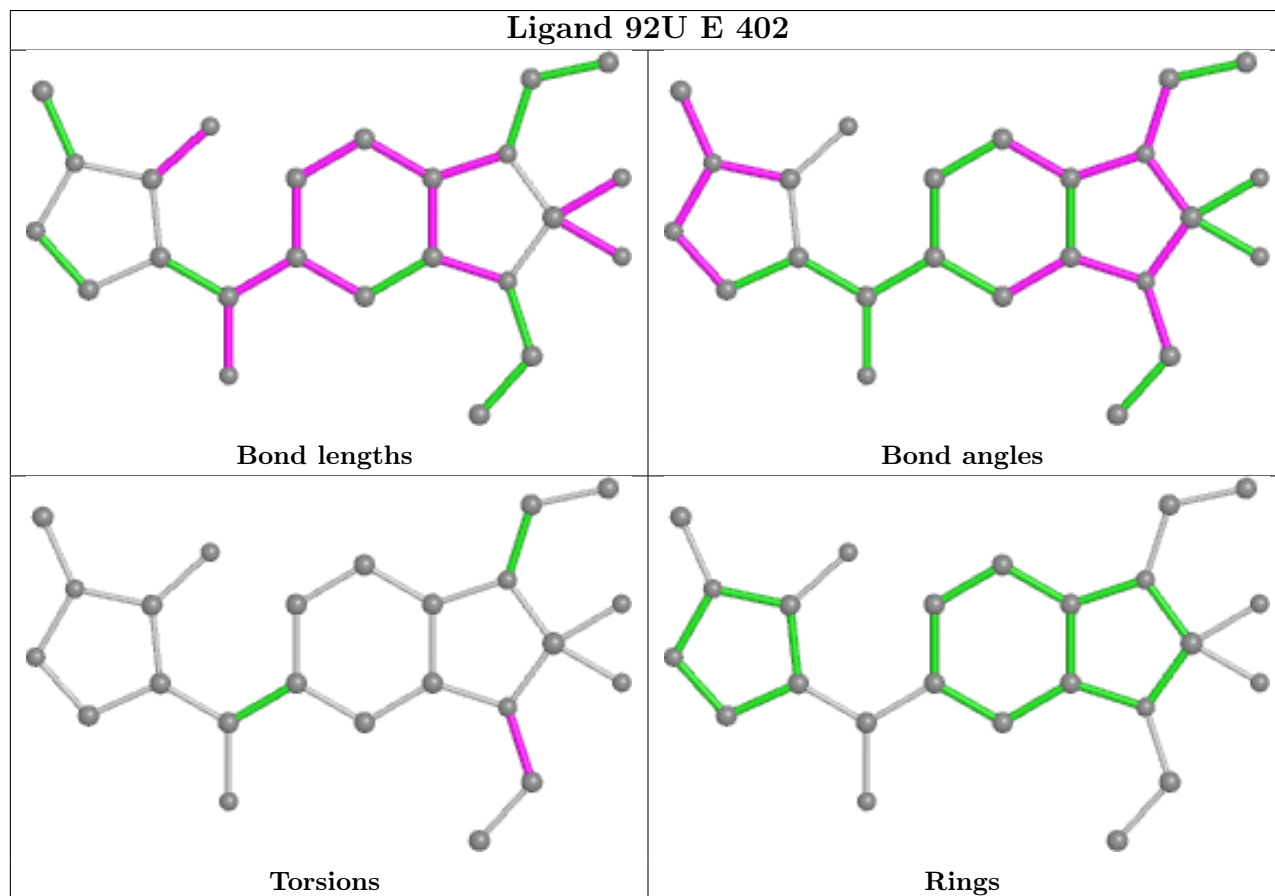
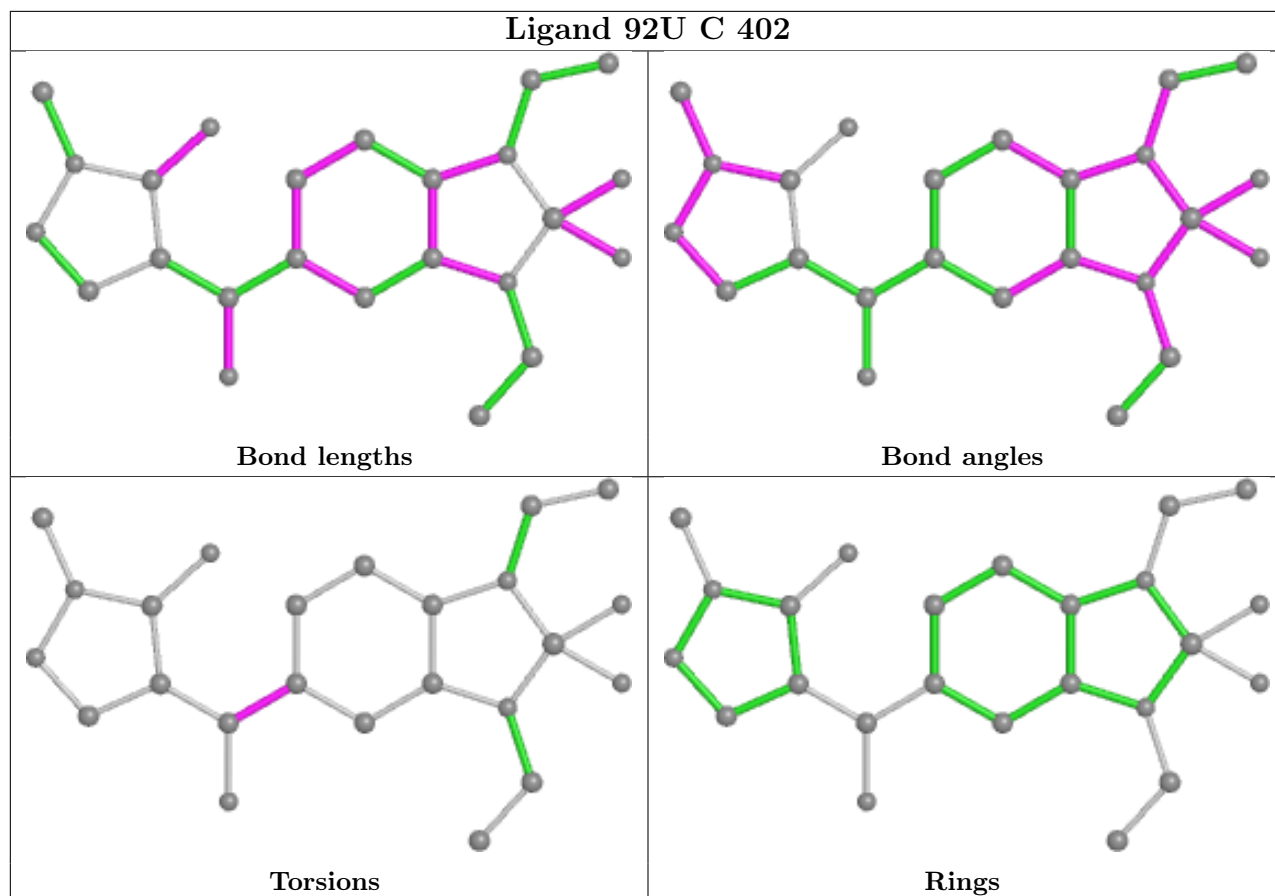
Mol	Chain	Res	Type	Atoms
3	C	402	92U	C01-C02-C10-O12
3	C	402	92U	C03-C02-C10-O12
3	C	402	92U	C01-C02-C10-C11
3	C	402	92U	C03-C02-C10-C11
3	A	402	92U	C01-C02-C10-O12
3	A	402	92U	C01-C02-C10-C11
3	A	402	92U	C03-C02-C10-C11
3	A	402	92U	C03-C02-C10-O12
3	D	402	92U	C01-C02-C10-O12
3	D	402	92U	C01-C02-C10-C11
3	B	402	92U	C20-C19-N09-C06
3	F	402	92U	C20-C19-N09-C06
3	D	402	92U	C03-C02-C10-O12
3	B	402	92U	C01-C02-C10-C11
3	D	402	92U	C03-C02-C10-C11
3	B	402	92U	C01-C02-C10-O12
3	A	402	92U	C20-C19-N09-C06
3	B	402	92U	C03-C02-C10-C11
3	B	402	92U	C03-C02-C10-O12
3	E	402	92U	C20-C19-N09-C06

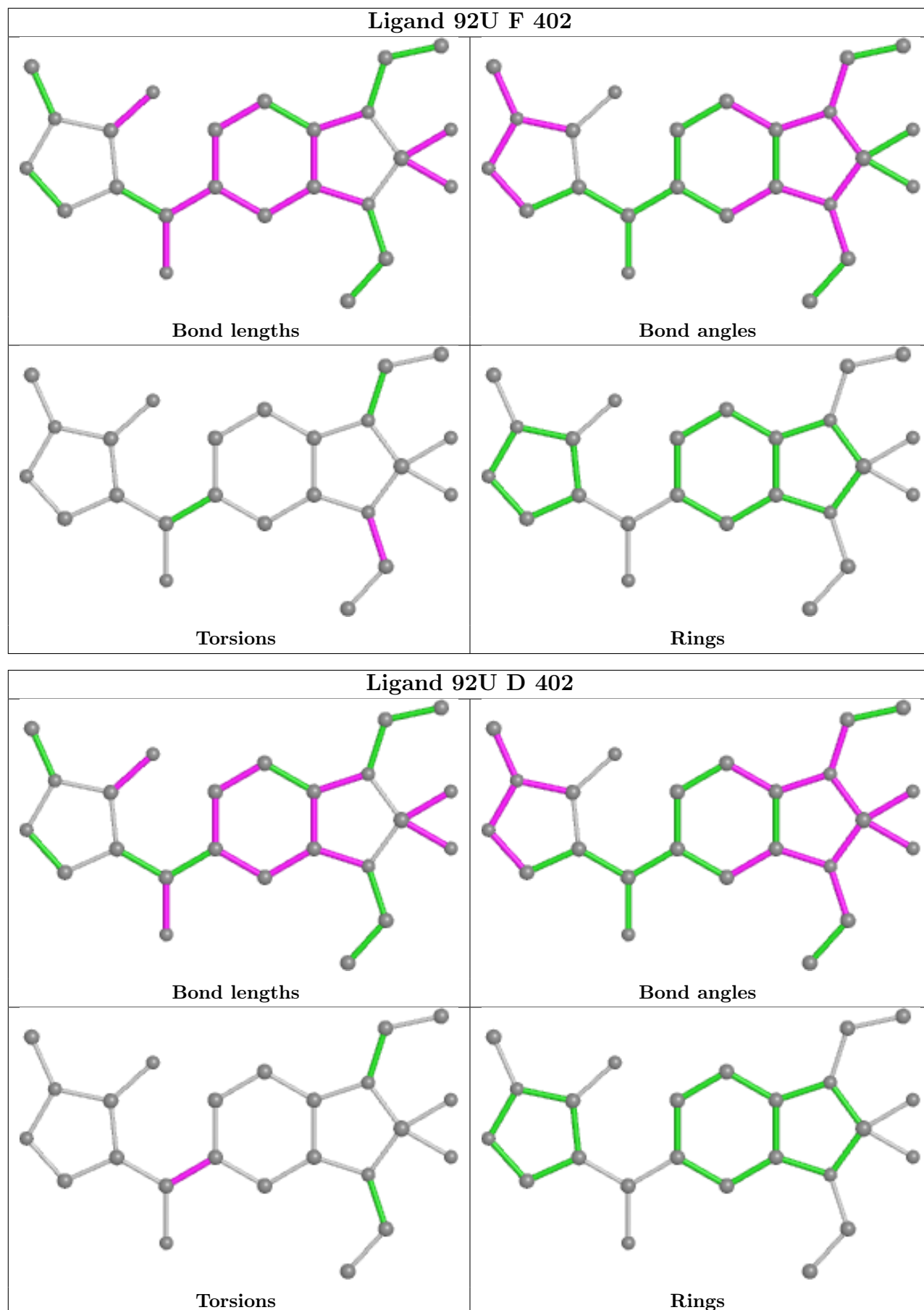
There are no ring outliers.

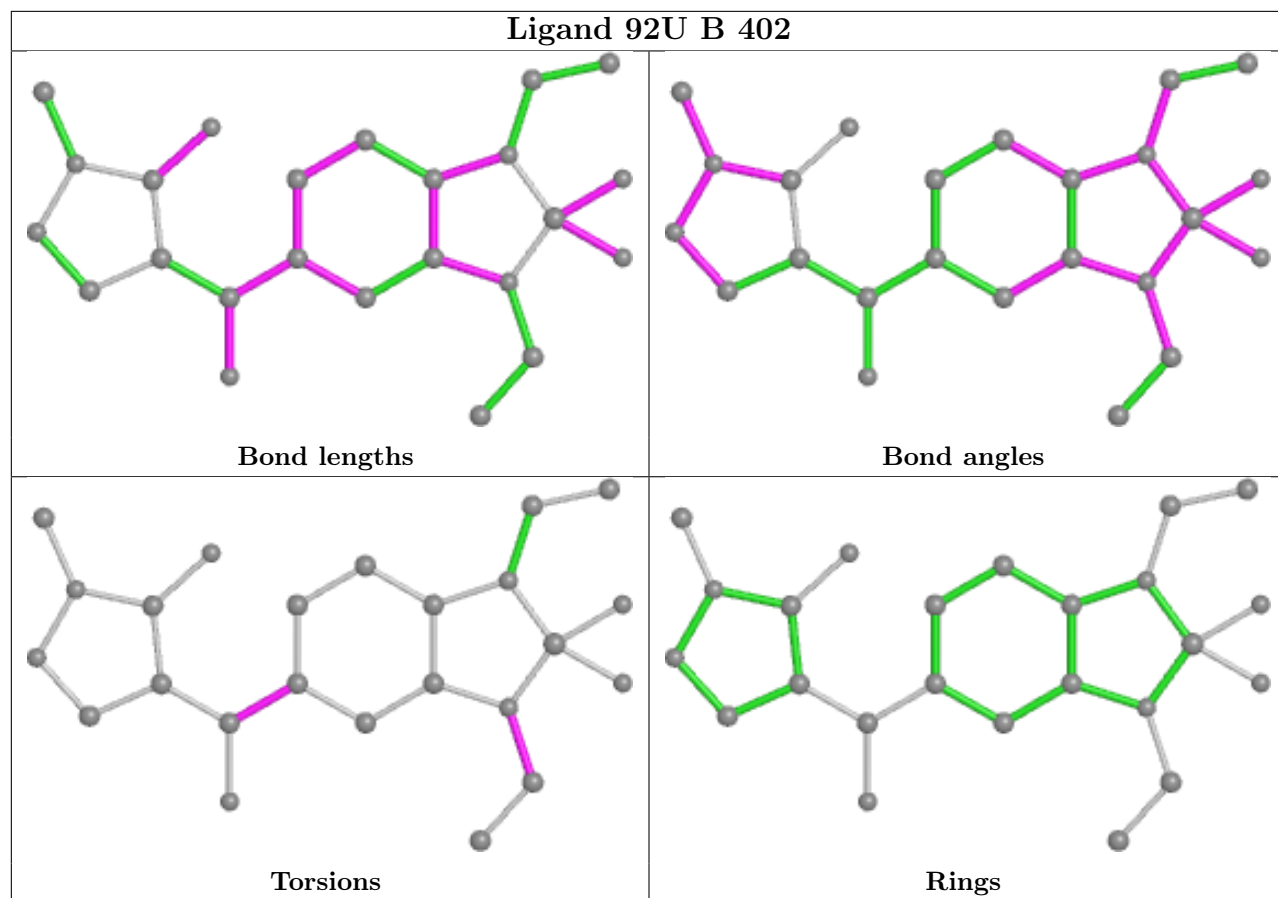
No monomer is involved in short contacts.

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

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	371/393 (94%)	-0.35	3 (0%) 86 84	20, 33, 57, 73	0
1	B	372/393 (94%)	-0.27	3 (0%) 86 84	22, 37, 60, 77	0
1	C	373/393 (94%)	-0.18	3 (0%) 86 84	21, 41, 61, 71	0
1	D	371/393 (94%)	-0.33	0 100 100	24, 36, 55, 68	0
1	E	369/393 (93%)	-0.19	3 (0%) 86 84	23, 40, 58, 73	0
1	F	371/393 (94%)	0.44	25 (6%) 17 13	30, 56, 78, 109	0
All	All	2227/2358 (94%)	-0.15	37 (1%) 70 67	20, 40, 66, 109	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	154	GLY	8.0
1	F	12	GLU	5.9
1	F	147	VAL	5.6
1	F	13	ARG	5.4
1	F	217	VAL	5.4
1	F	330	GLY	4.5
1	C	154	GLY	3.7
1	E	246	GLY	3.2
1	F	100	VAL	3.2
1	F	230	ALA	3.2
1	A	8	GLY	3.2
1	F	206	PHE	3.1
1	E	9	ALA	2.9
1	C	379	GLY	2.9
1	F	218	HIS	2.8
1	B	7	LYS	2.8
1	E	368	PHE	2.7
1	F	153	ILE	2.7
1	F	137	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	11	PRO	2.6
1	F	114	GLY	2.6
1	F	131	VAL	2.5
1	F	14	GLY	2.3
1	C	376	ASN	2.3
1	B	151	ASN	2.3
1	F	119	ARG	2.3
1	A	9	ALA	2.3
1	F	305	THR	2.3
1	F	204	LEU	2.3
1	F	122	TRP	2.2
1	F	121	PRO	2.2
1	F	117	ILE	2.2
1	B	246	GLY	2.1
1	F	377	LEU	2.1
1	F	155	GLN	2.0
1	A	13	ARG	2.0
1	F	101	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.

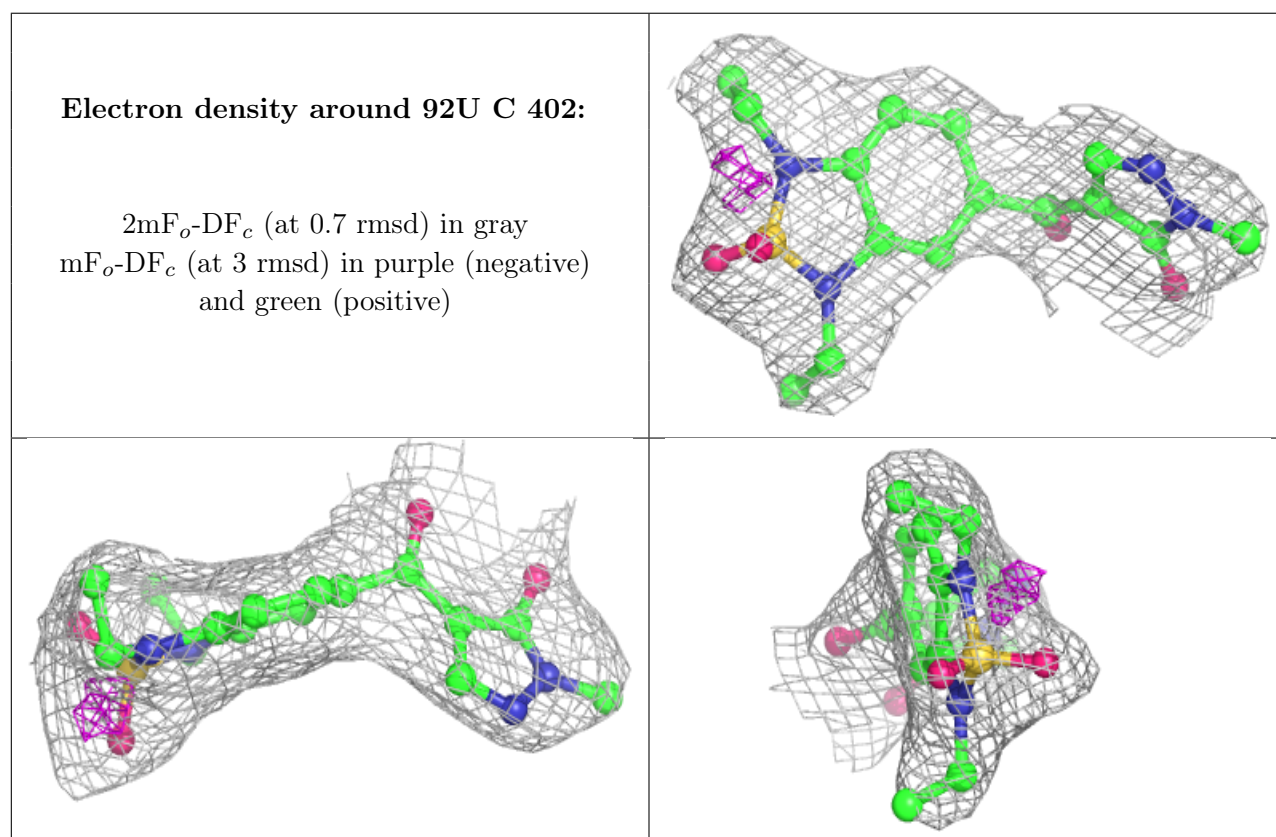
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CO	E	401	1/1	0.77	0.07	68,68,68,68	0
2	CO	A	401	1/1	0.87	0.05	59,59,59,59	0
2	CO	C	401	1/1	0.92	0.06	59,59,59,59	0
3	92U	C	402	24/24	0.94	0.14	27,39,46,50	0
3	92U	F	402	24/24	0.94	0.20	38,57,67,70	0

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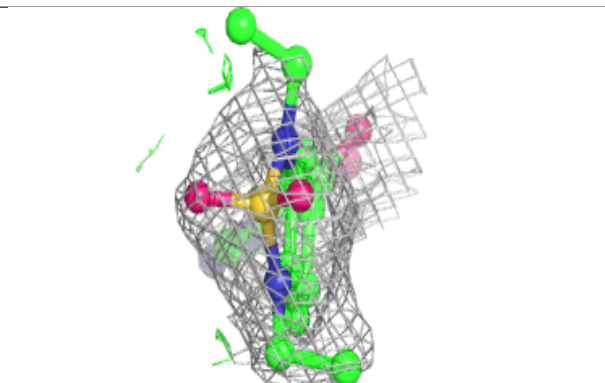
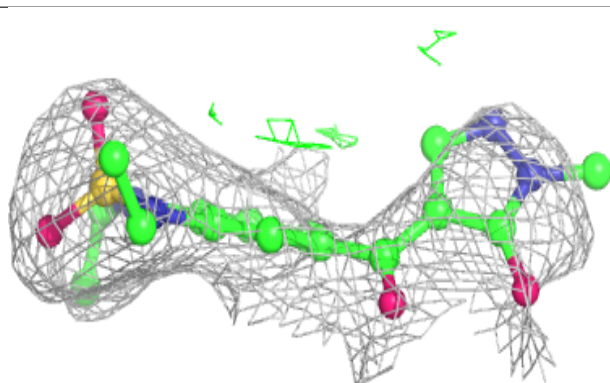
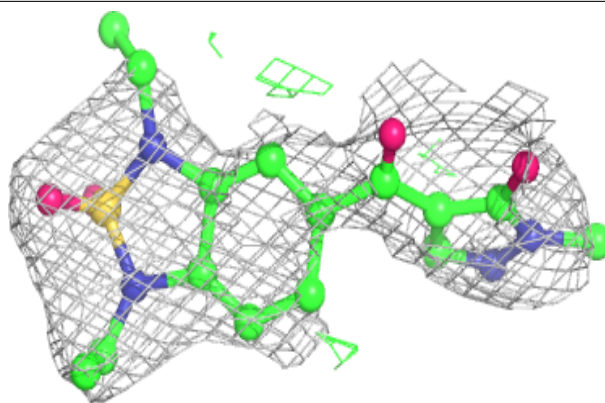
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	92U	D	402	24/24	0.95	0.17	33,39,45,52	0
3	92U	B	402	24/24	0.96	0.14	32,39,43,49	0
2	CO	D	401	1/1	0.96	0.06	66,66,66,66	0
2	CO	F	401	1/1	0.96	0.06	64,64,64,64	0
3	92U	E	402	24/24	0.96	0.13	28,40,45,46	0
3	92U	A	402	24/24	0.96	0.14	16,24,30,31	0
2	CO	B	401	1/1	0.98	0.08	49,49,49,49	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.

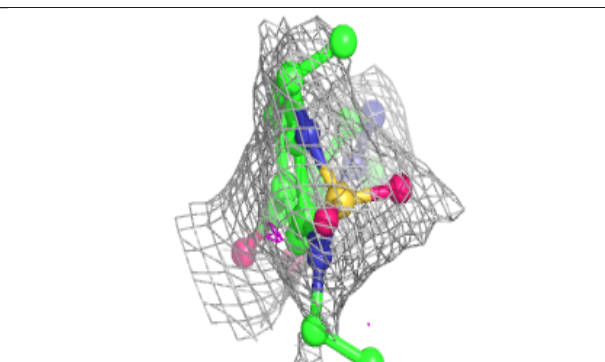
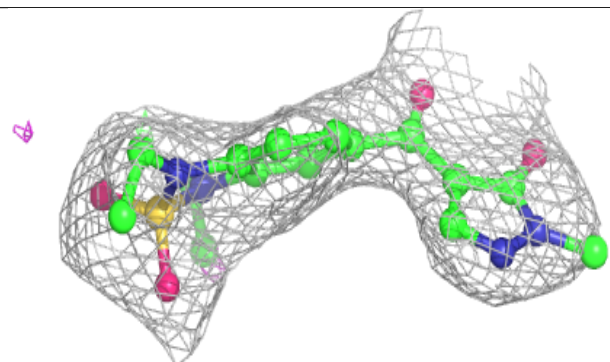
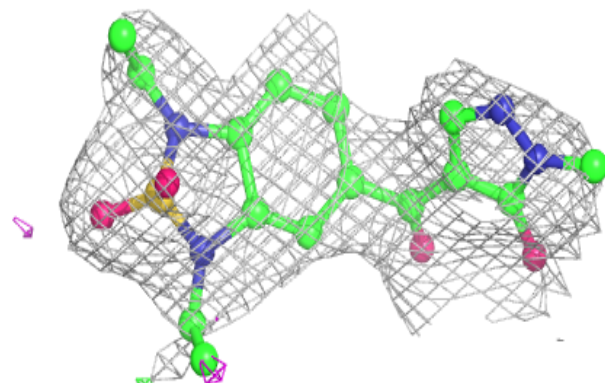


Electron density around 92U F 402:

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

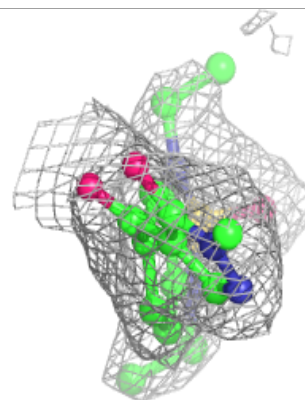
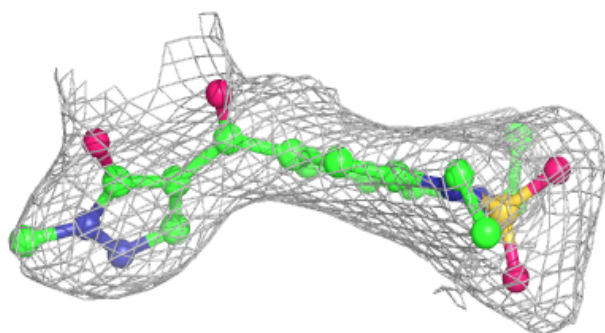
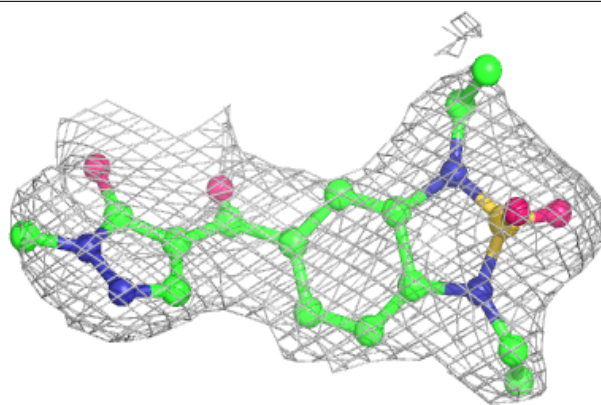
**Electron density around 92U D 402:**

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

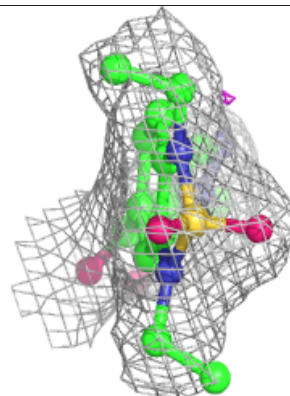
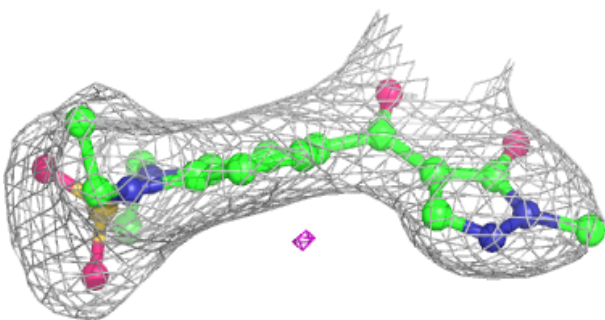
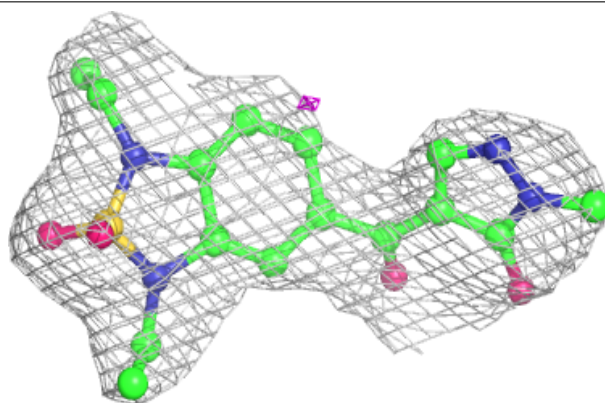


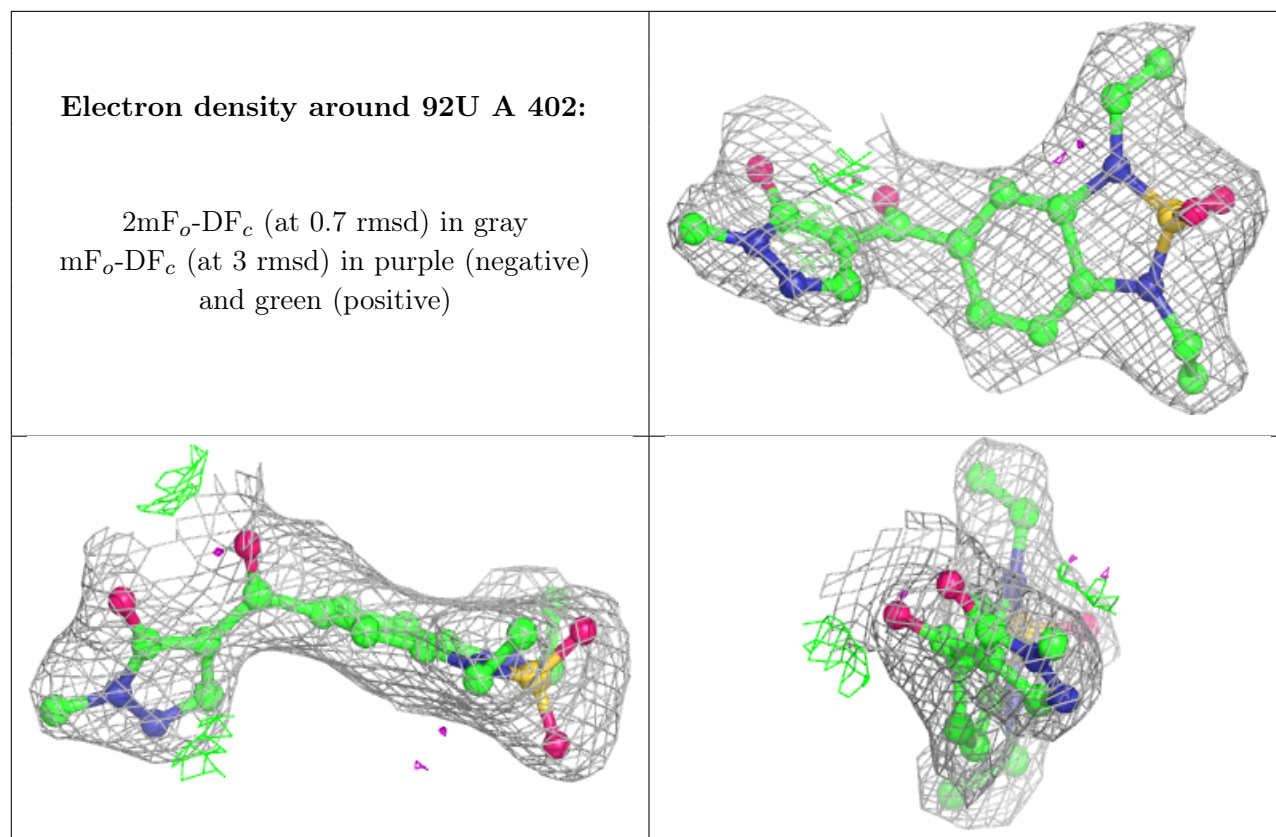
Electron density around 92U B 402:

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

**Electron density around 92U E 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.