



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:00 PM UTC

PDB ID : 8IM3 / pdb_00008im3
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:

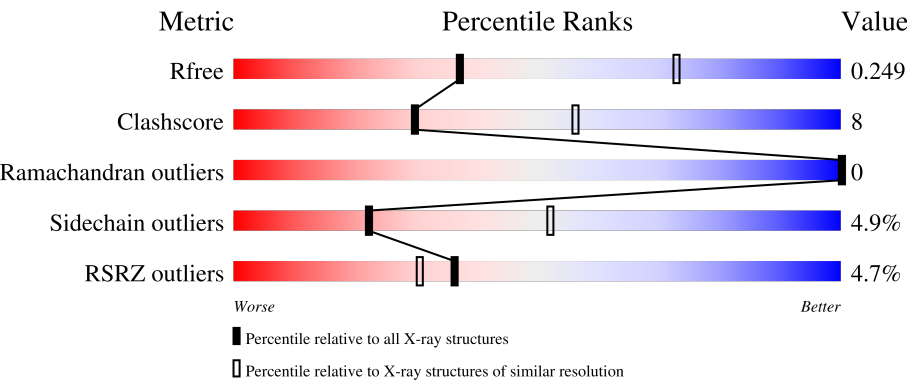
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

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}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (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	%73%20%• 6%
1	B	393	2%75%18%• 5%
1	C	393	2%72%21%• 5%
1	D	393	%75%19%6%
1	E	393	2%72%20%• 6%

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Mol	Chain	Length	Quality of chain
1	F	393	

2 Entry composition

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.

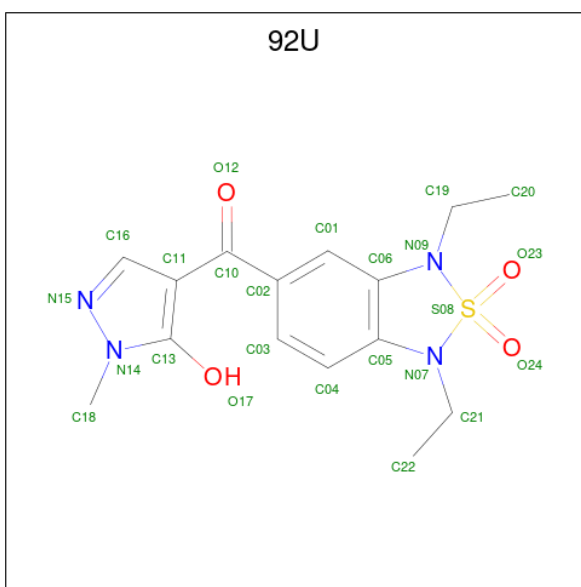
- Molecule 1 is a protein called 4-hydroxyphenylpyruvate dioxygenase.

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

- Molecule 2 is COBALT (II) ION (CCD ID: 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)-2 λ^6 ,1,3-benzothiadiazol-5-yl]-(1-methyl-5-oxidanyl-pyrazol-4-yl)methanone (CCD ID: 92U) (formula: C₁₅H₁₈N₄O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

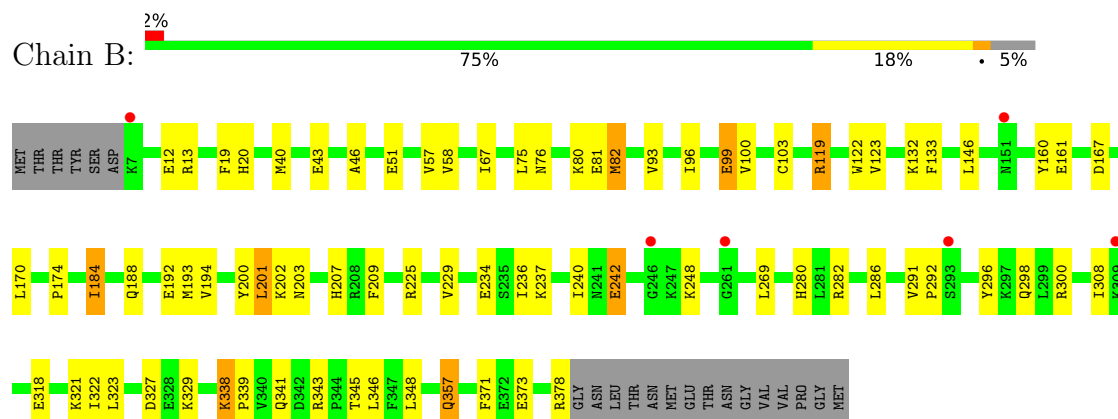
3 Residue-property plots

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.

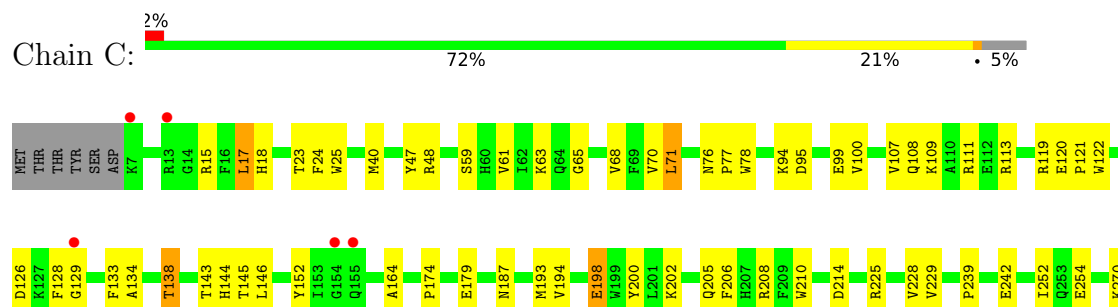
• Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

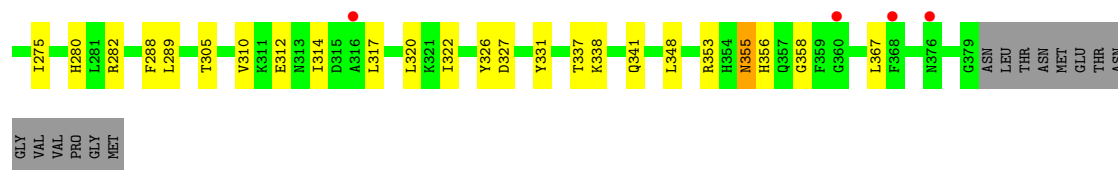


• Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

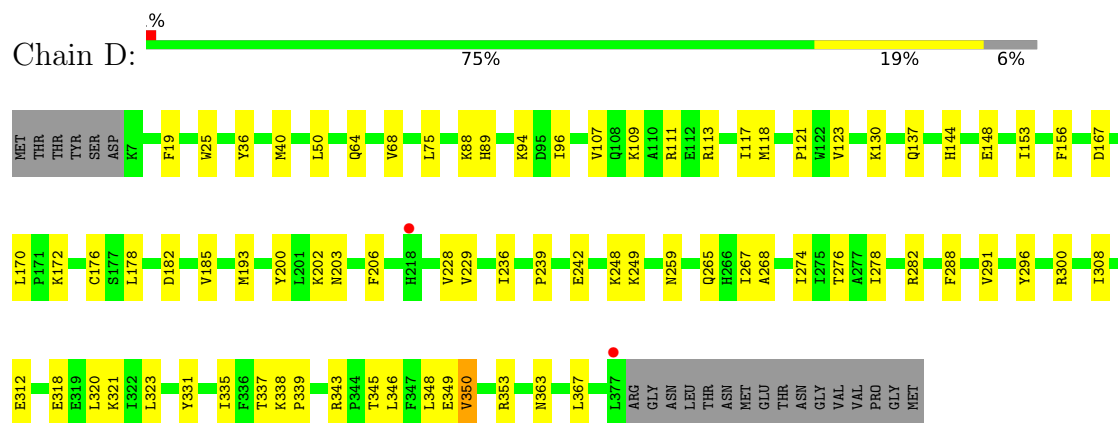


• Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

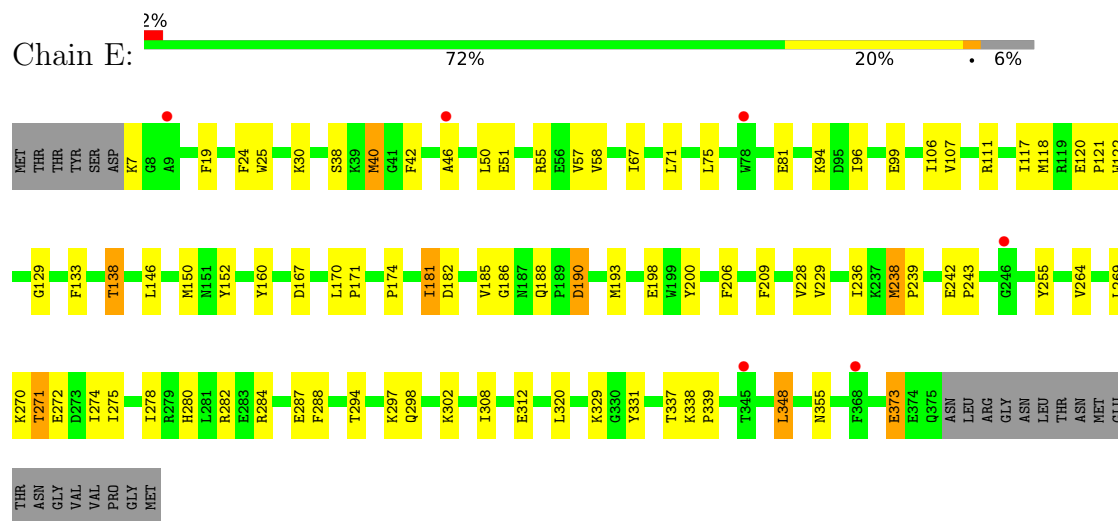




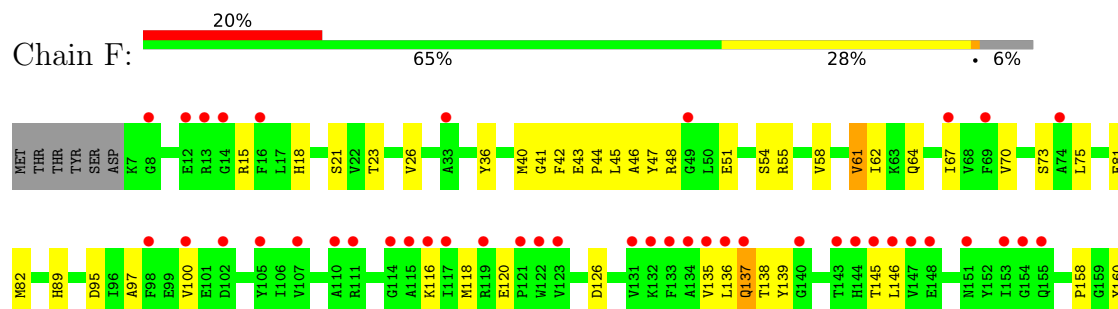
• Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

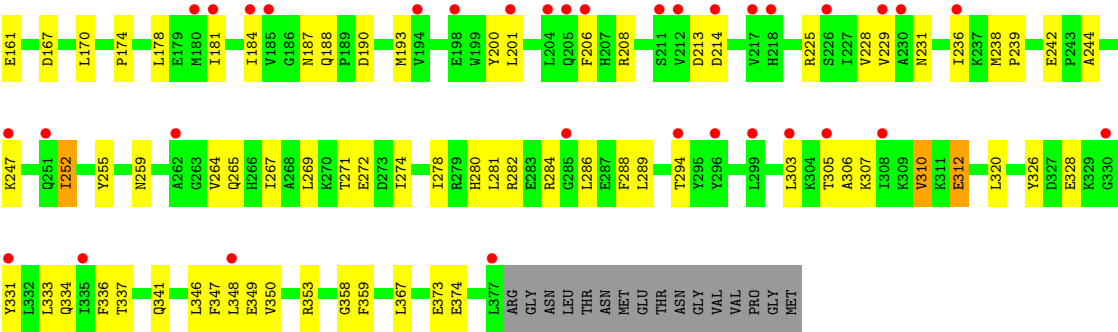


• Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



• 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) 96.0 (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)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.217 , 0.247 0.219 , 0.249	Depositor DCC
R_{free} test set	2673 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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	0.13	0/3044	0.35	0/4118
1	B	0.23	1/3028 (0.0%)	0.40	1/4100 (0.0%)
1	C	0.13	0/3019	0.35	0/4092
1	D	0.13	0/3031	0.35	0/4103
1	E	0.13	0/2993	0.34	0/4055
1	F	0.26	1/2921 (0.0%)	0.39	0/3974
All	All	0.18	2/18036 (0.0%)	0.36	1/24442 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	13	ARG	C-O	-6.33	1.16	1.23
1	F	81	GLU	CA-C	-5.14	1.46	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	12	GLU	N-CA-C	5.42	117.19	111.28

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	46	0
1	B	2955	0	2861	44	0
1	C	2946	0	2819	47	0
1	D	2958	0	2867	42	0
1	E	2920	0	2814	50	0
1	F	2850	0	2661	69	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
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	2	0
4	B	32	0	0	2	0
4	C	32	0	0	0	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	293	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 (293) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:96:ILE:HD13	1:E:238:MET:HE1	1.80	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:E:40:MET:HE1	1:E:348:LEU:HD22	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: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:F:40:MET:HE1	1:F:348:LEU:HD22	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:40:MET:HE1	1:A:348:LEU:HD13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:40:MET:HE1	1:C:348:LEU:HD22	1.95	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:D:36:TYR:HD1	1:D:40:MET:HE2	1.76	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:GLU:H	1:B:51:GLU:CD	2.20	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
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:F:36:TYR:HD1	1:F:40:MET:HE2	1.80	0.46
1:E:25:TRP:CE2	1:E:94:LYS:HG2	2.49	0.46
1:F:82:MET:HB3	1:F:82:MET:HE2	1.70	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:36:TYR:CD1	1:F:40:MET:HE2	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:TYR:CD1	1:D:40:MET:HE2	2.50	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:57:VAL:HG13	1:B:82:MET:HE1	1.97	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
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: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:F:95:ASP:OD2	1:F:145:THR:OG1	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:238:MET:HE2	1:F:238:MET:HB3	1.79	0.43
1:C:355:ASN:O	1:C:355:ASN:ND2	2.42	0.43
1:E:193:MET:HE2	1:E:193:MET:HB3	1.92	0.43
1:A:39:LYS:NZ	4:A:502:HOH:O	2.39	0.42
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:51:GLU:H	1:E:51:GLU:CD	2.26	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
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:E:40:MET:HE3	1:E:42:PHE:HE1	1.85	0.41
1:A:332:LEU:HD23	1:A:356:HIS:ND1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:40:MET:HE1	1:B:348:LEU:HD13	2.03	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: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:C:144:HIS:NE2	1:C:200:TYR:OH	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:E:40:MET:HE3	1:E:40:MET:HB3	1.85	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:89:HIS:HD1	1:D:259:ASN:CG	2.28	0.40
1:D:182:ASP:CG	1:D:353:ARG:HH21	2.29	0.40
1:D:268:ALA:HA	1:D:349:GLU:O	2.21	0.40
1:C:126:ASP:C	1:C:128:PHE:H	2.29	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
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:B:296:TYR:OH	1:B:322:ILE:O	2.34	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

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	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

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%)	299 (96%)	14 (4%)	24	55
1	B	310/343 (90%)	294 (95%)	16 (5%)	21	50
1	C	307/343 (90%)	293 (95%)	14 (5%)	24	55
1	D	312/343 (91%)	306 (98%)	6 (2%)	50	78
1	E	305/343 (89%)	286 (94%)	19 (6%)	16	42
1	F	286/343 (83%)	265 (93%)	21 (7%)	13	35
All	All	1833/2058 (89%)	1743 (95%)	90 (5%)	22	52

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	THR
1	A	70	VAL
1	A	81	GLU
1	A	113	ARG
1	A	138	THR
1	A	148	GLU
1	A	153	ILE
1	A	217	VAL
1	A	305	THR
1	A	314	ILE
1	A	328	GLU
1	A	357	GLN
1	A	366	SER
1	A	367	LEU
1	B	43	GLU
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	123	VAL
1	B	161	GLU
1	B	184	ILE
1	B	201	LEU
1	B	242	GLU
1	B	338	LYS
1	B	341	GLN
1	B	357	GLN
1	B	378	ARG
1	C	17	LEU
1	C	18	HIS
1	C	71	LEU
1	C	76	ASN
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

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Mol	Chain	Res	Type
1	C	355	ASN
1	C	367	LEU
1	D	109	LYS
1	D	148	GLU
1	D	153	ILE
1	D	350	VAL
1	D	363	ASN
1	D	367	LEU
1	E	30	LYS
1	E	40	MET
1	E	57	VAL
1	E	58	VAL
1	E	81	GLU
1	E	99	GLU
1	E	106	ILE
1	E	118	MET
1	E	138	THR
1	E	150	MET
1	E	181	ILE
1	E	190	ASP
1	E	198	GLU
1	E	238	MET
1	E	271	THR
1	E	275	ILE
1	E	308	ILE
1	E	348	LEU
1	E	373	GLU
1	F	15	ARG
1	F	18	HIS
1	F	43	GLU
1	F	54	SER
1	F	55	ARG
1	F	61	VAL
1	F	116	LYS
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	247	LYS
1	F	252	ILE

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Mol	Chain	Res	Type
1	F	264	VAL
1	F	305	THR
1	F	310	VAL
1	F	312	GLU
1	F	367	LEU
1	F	374	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	GLN
1	A	313	ASN
1	A	341	GLN
1	B	253	GLN
1	B	266	HIS
1	B	298	GLN
1	B	341	GLN
1	B	357	GLN
1	B	376	ASN
1	C	253	GLN
1	D	64	GLN
1	D	85	HIS
1	D	125	GLN
1	D	137	GLN
1	D	183	HIS
1	D	205	GLN
1	F	64	GLN
1	F	341	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 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	E	402	2	22,26,26	4.09	13 (59%)	33,40,40	2.19	8 (24%)
3	92U	F	402	2	22,26,26	4.13	12 (54%)	33,40,40	2.17	8 (24%)
3	92U	A	402	2	22,26,26	4.09	10 (45%)	33,40,40	2.18	9 (27%)
3	92U	D	402	2	22,26,26	4.18	11 (50%)	33,40,40	2.35	9 (27%)
3	92U	B	402	2	22,26,26	4.20	12 (54%)	33,40,40	2.18	9 (27%)
3	92U	C	402	2	22,26,26	4.13	12 (54%)	33,40,40	2.18	8 (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	E	402	2	-	1/10/32/32	0/3/3/3
3	92U	F	402	2	-	1/10/32/32	0/3/3/3
3	92U	A	402	2	-	5/10/32/32	0/3/3/3
3	92U	D	402	2	-	4/10/32/32	0/3/3/3
3	92U	B	402	2	-	3/10/32/32	0/3/3/3
3	92U	C	402	2	-	4/10/32/32	0/3/3/3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	92U	C06-N09	9.62	1.52	1.43
3	D	402	92U	C06-N09	9.50	1.52	1.43
3	C	402	92U	C06-N09	9.50	1.52	1.43
3	B	402	92U	C05-N07	9.32	1.52	1.43
3	E	402	92U	C06-N09	9.15	1.52	1.43
3	F	402	92U	C06-N09	9.11	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	92U	C06-N09	9.11	1.52	1.43
3	C	402	92U	C06-C05	9.09	1.59	1.40
3	D	402	92U	C06-C05	9.09	1.59	1.40
3	F	402	92U	C06-C05	9.06	1.59	1.40
3	A	402	92U	C05-N07	9.05	1.52	1.43
3	A	402	92U	C06-C05	9.04	1.59	1.40
3	D	402	92U	C05-N07	9.03	1.52	1.43
3	B	402	92U	C06-C05	9.02	1.59	1.40
3	E	402	92U	C06-C05	9.01	1.59	1.40
3	F	402	92U	C05-N07	9.01	1.52	1.43
3	C	402	92U	C05-N07	8.77	1.51	1.43
3	E	402	92U	C05-N07	8.69	1.51	1.43
3	D	402	92U	C03-C02	7.45	1.50	1.39
3	F	402	92U	C03-C02	7.39	1.50	1.39
3	B	402	92U	C03-C02	7.28	1.50	1.39
3	C	402	92U	C03-C02	7.22	1.50	1.39
3	E	402	92U	C03-C02	7.21	1.50	1.39
3	A	402	92U	C03-C02	7.11	1.50	1.39
3	B	402	92U	C04-C03	3.63	1.44	1.38
3	F	402	92U	C04-C03	3.62	1.44	1.38
3	D	402	92U	C04-C03	3.61	1.44	1.38
3	B	402	92U	C01-C02	3.53	1.44	1.39
3	E	402	92U	C01-C02	3.52	1.44	1.39
3	C	402	92U	C01-C02	3.51	1.44	1.39
3	D	402	92U	C01-C02	3.51	1.44	1.39
3	C	402	92U	C04-C03	3.50	1.44	1.38
3	A	402	92U	C01-C02	3.46	1.44	1.39
3	E	402	92U	C04-C03	3.45	1.44	1.38
3	A	402	92U	C04-C03	3.43	1.44	1.38
3	F	402	92U	C01-C02	3.37	1.44	1.39
3	D	402	92U	O17-C13	3.12	1.40	1.31
3	A	402	92U	O17-C13	3.06	1.40	1.31
3	F	402	92U	O17-C13	3.02	1.40	1.31
3	C	402	92U	O17-C13	2.96	1.39	1.31
3	B	402	92U	O17-C13	2.95	1.39	1.31
3	E	402	92U	O17-C13	2.90	1.39	1.31
3	B	402	92U	O24-S08	2.50	1.47	1.42
3	E	402	92U	O24-S08	2.41	1.47	1.42
3	C	402	92U	O24-S08	2.41	1.47	1.42
3	D	402	92U	O23-S08	2.39	1.47	1.42
3	D	402	92U	O24-S08	2.37	1.47	1.42
3	A	402	92U	O23-S08	2.36	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	402	92U	O24-S08	2.36	1.47	1.42
3	F	402	92U	O23-S08	2.34	1.47	1.42
3	A	402	92U	O24-S08	2.32	1.46	1.42
3	C	402	92U	O23-S08	2.31	1.46	1.42
3	B	402	92U	O23-S08	2.30	1.46	1.42
3	E	402	92U	O23-S08	2.29	1.46	1.42
3	E	402	92U	N14-N15	-2.28	1.32	1.36
3	E	402	92U	C04-C05	-2.18	1.36	1.39
3	D	402	92U	O12-C10	-2.17	1.18	1.23
3	A	402	92U	O12-C10	-2.16	1.18	1.23
3	E	402	92U	O12-C10	-2.13	1.18	1.23
3	F	402	92U	O12-C10	-2.13	1.18	1.23
3	E	402	92U	C02-C10	2.12	1.53	1.49
3	F	402	92U	C01-C06	-2.12	1.36	1.39
3	C	402	92U	N14-N15	-2.12	1.33	1.36
3	F	402	92U	N14-N15	-2.11	1.33	1.36
3	B	402	92U	O12-C10	-2.10	1.18	1.23
3	C	402	92U	O12-C10	-2.10	1.18	1.23
3	B	402	92U	N14-N15	-2.08	1.33	1.36
3	C	402	92U	C04-C05	-2.04	1.36	1.39
3	D	402	92U	C01-C06	-2.04	1.36	1.39
3	B	402	92U	C02-C10	2.00	1.53	1.49

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	402	92U	C21-N07-S08	5.64	127.57	120.77
3	A	402	92U	C18-N14-C13	-5.51	124.06	127.79
3	D	402	92U	C18-N14-C13	-5.44	124.11	127.79
3	C	402	92U	C16-N15-N14	5.31	110.12	105.06
3	E	402	92U	C16-N15-N14	5.25	110.07	105.06
3	B	402	92U	C16-N15-N14	5.23	110.04	105.06
3	F	402	92U	C19-N09-S08	5.20	127.03	120.77
3	D	402	92U	C16-N15-N14	5.18	110.00	105.06
3	F	402	92U	C16-N15-N14	5.17	109.99	105.06
3	E	402	92U	C19-N09-S08	5.12	126.93	120.77
3	D	402	92U	C21-N07-S08	4.99	126.78	120.77
3	A	402	92U	C16-N15-N14	4.99	109.81	105.06
3	B	402	92U	C19-N09-S08	4.95	126.73	120.77
3	D	402	92U	C19-N09-S08	4.89	126.66	120.77
3	C	402	92U	C21-N07-S08	4.82	126.58	120.77
3	A	402	92U	C19-N09-S08	4.77	126.52	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	92U	C21-N07-S08	4.74	126.48	120.77
3	F	402	92U	C18-N14-C13	-4.72	124.60	127.79
3	C	402	92U	C19-N09-S08	4.68	126.41	120.77
3	D	402	92U	C01-C06-N09	4.57	132.97	128.29
3	C	402	92U	C18-N14-C13	-4.45	124.77	127.79
3	F	402	92U	C21-N07-S08	4.40	126.07	120.77
3	D	402	92U	C11-C16-N15	-4.37	107.03	112.45
3	C	402	92U	C11-C16-N15	-4.30	107.11	112.45
3	B	402	92U	C18-N14-C13	-4.29	124.89	127.79
3	F	402	92U	C11-C16-N15	-4.17	107.28	112.45
3	A	402	92U	C11-C16-N15	-4.07	107.39	112.45
3	B	402	92U	C11-C16-N15	-4.02	107.45	112.45
3	A	402	92U	C21-N07-S08	4.02	125.62	120.77
3	B	402	92U	C01-C06-N09	3.96	132.34	128.29
3	E	402	92U	C01-C06-N09	3.93	132.31	128.29
3	E	402	92U	C18-N14-C13	-3.87	125.17	127.79
3	E	402	92U	C11-C16-N15	-3.85	107.67	112.45
3	C	402	92U	C01-C06-N09	3.83	132.20	128.29
3	A	402	92U	C01-C06-N09	3.63	132.00	128.29
3	F	402	92U	C01-C06-N09	3.41	131.78	128.29
3	D	402	92U	C18-N14-N15	2.95	125.10	119.22
3	A	402	92U	C18-N14-N15	2.92	125.03	119.22
3	D	402	92U	C04-C05-N07	2.80	132.46	128.21
3	B	402	92U	C18-N14-N15	2.74	124.69	119.22
3	F	402	92U	C18-N14-N15	2.74	124.68	119.22
3	C	402	92U	C18-N14-N15	2.70	124.60	119.22
3	E	402	92U	C18-N14-N15	2.66	124.51	119.22
3	B	402	92U	O24-S08-O23	-2.47	112.22	116.89
3	F	402	92U	C04-C05-N07	2.36	131.79	128.21
3	A	402	92U	O24-S08-O23	-2.25	112.64	116.89
3	B	402	92U	C04-C05-N07	2.22	131.58	128.21
3	D	402	92U	O24-S08-O23	-2.15	112.82	116.89
3	C	402	92U	O24-S08-O23	-2.10	112.92	116.89
3	A	402	92U	C04-C05-N07	2.05	131.32	128.21
3	E	402	92U	O24-S08-O23	-2.04	113.02	116.89

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402	92U	C03-C02-C10-O12
3	C	402	92U	C01-C02-C10-O12

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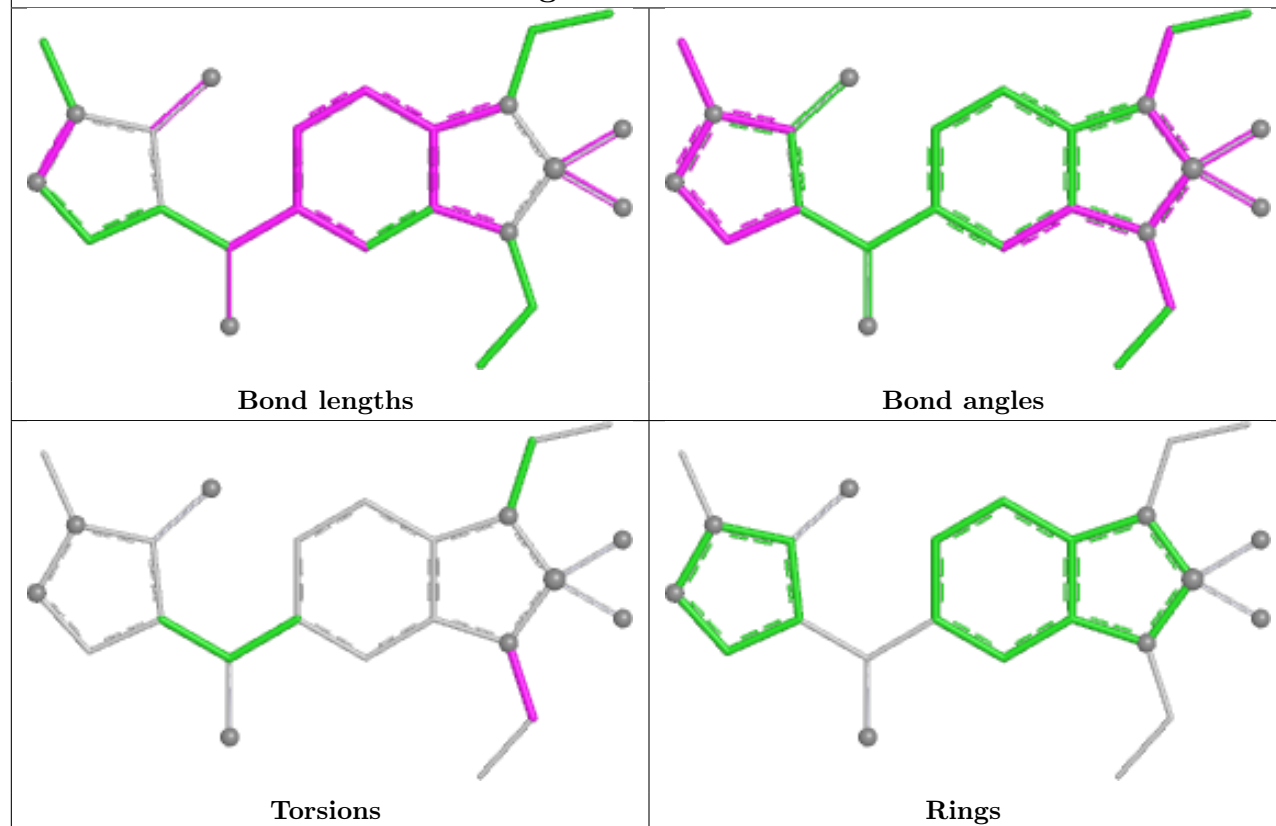
Mol	Chain	Res	Type	Atoms
3	A	402	92U	C01-C02-C10-O12
3	A	402	92U	C03-C02-C10-O12
3	C	402	92U	C03-C02-C10-C11
3	C	402	92U	C01-C02-C10-C11
3	A	402	92U	C01-C02-C10-C11
3	A	402	92U	C03-C02-C10-C11
3	B	402	92U	C20-C19-N09-C06
3	F	402	92U	C20-C19-N09-C06
3	D	402	92U	C01-C02-C10-O12
3	A	402	92U	C20-C19-N09-C06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

There are no ring outliers.

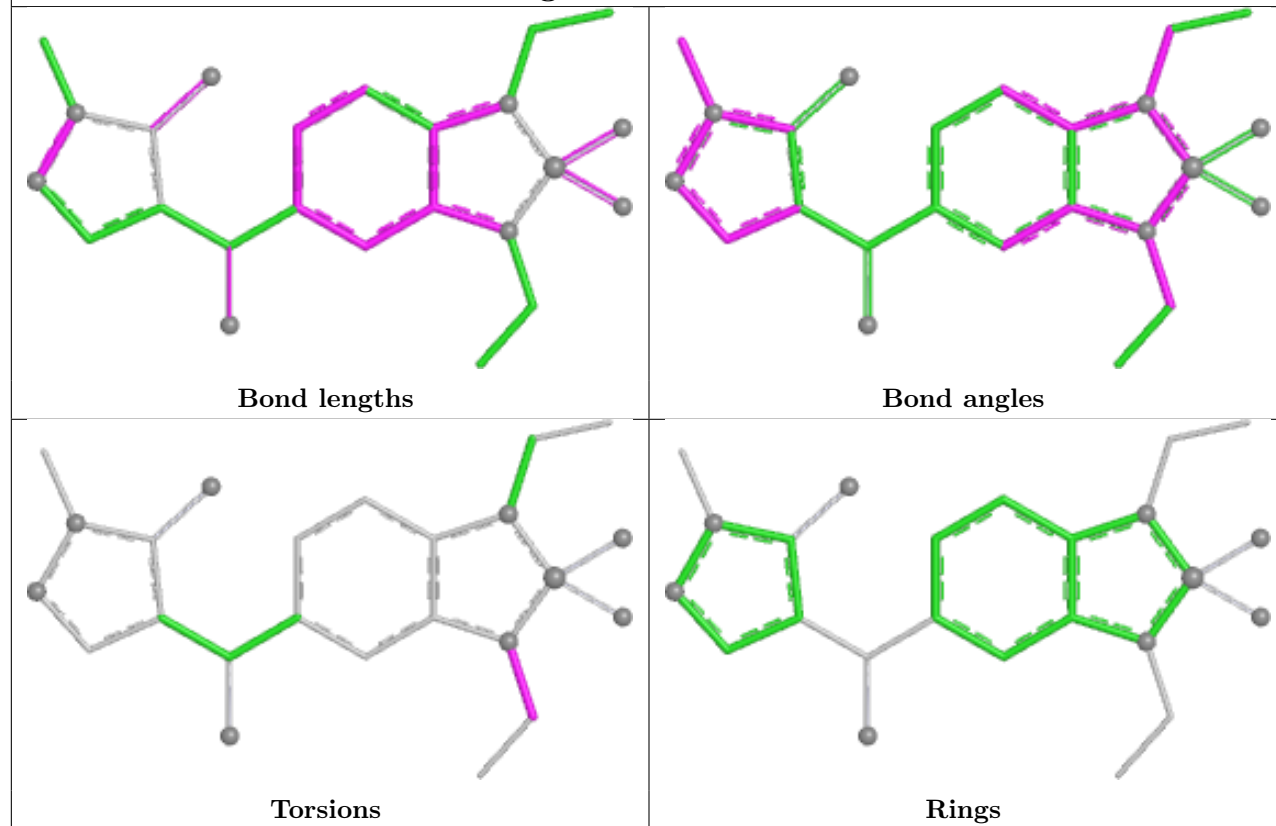
No monomer is involved in short contacts.

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.

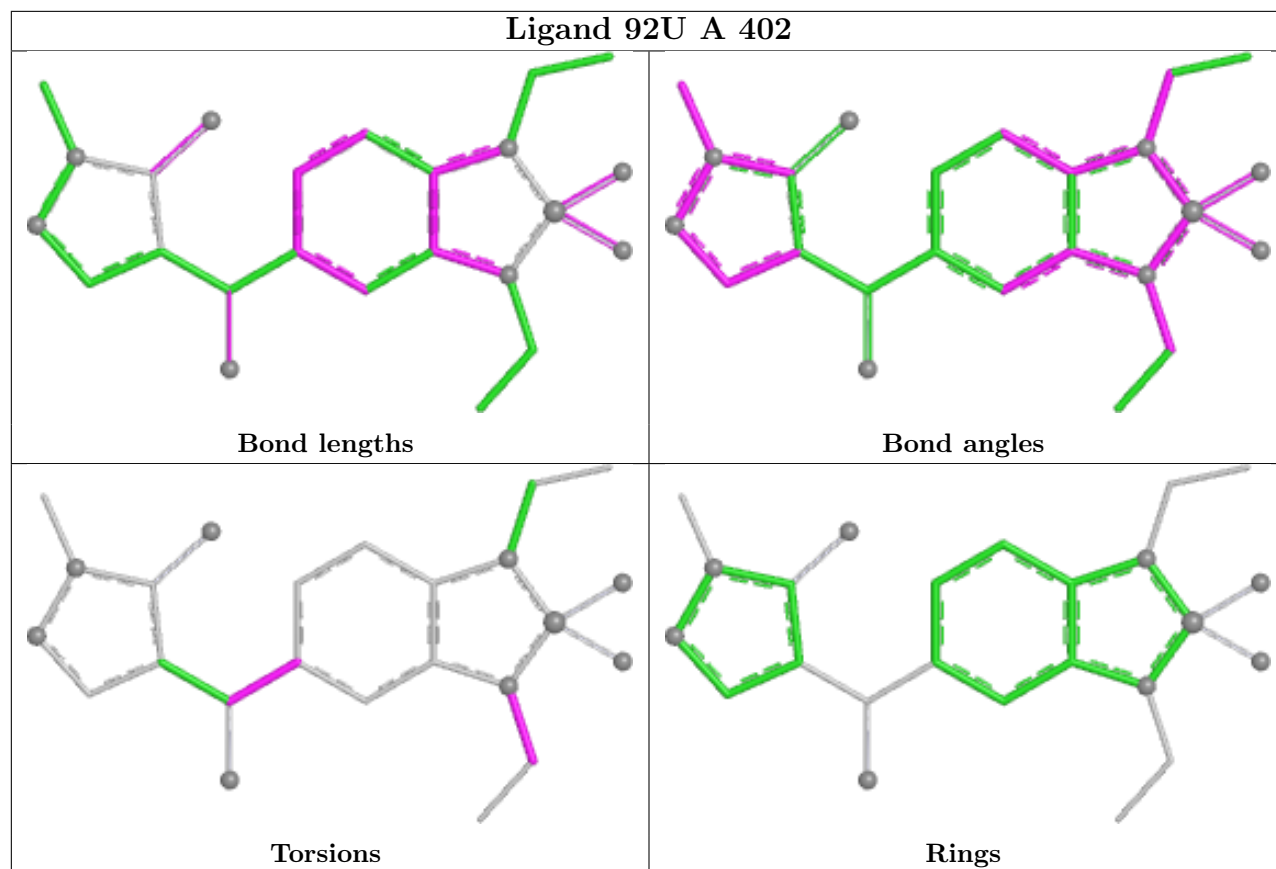
Ligand 92U E 402



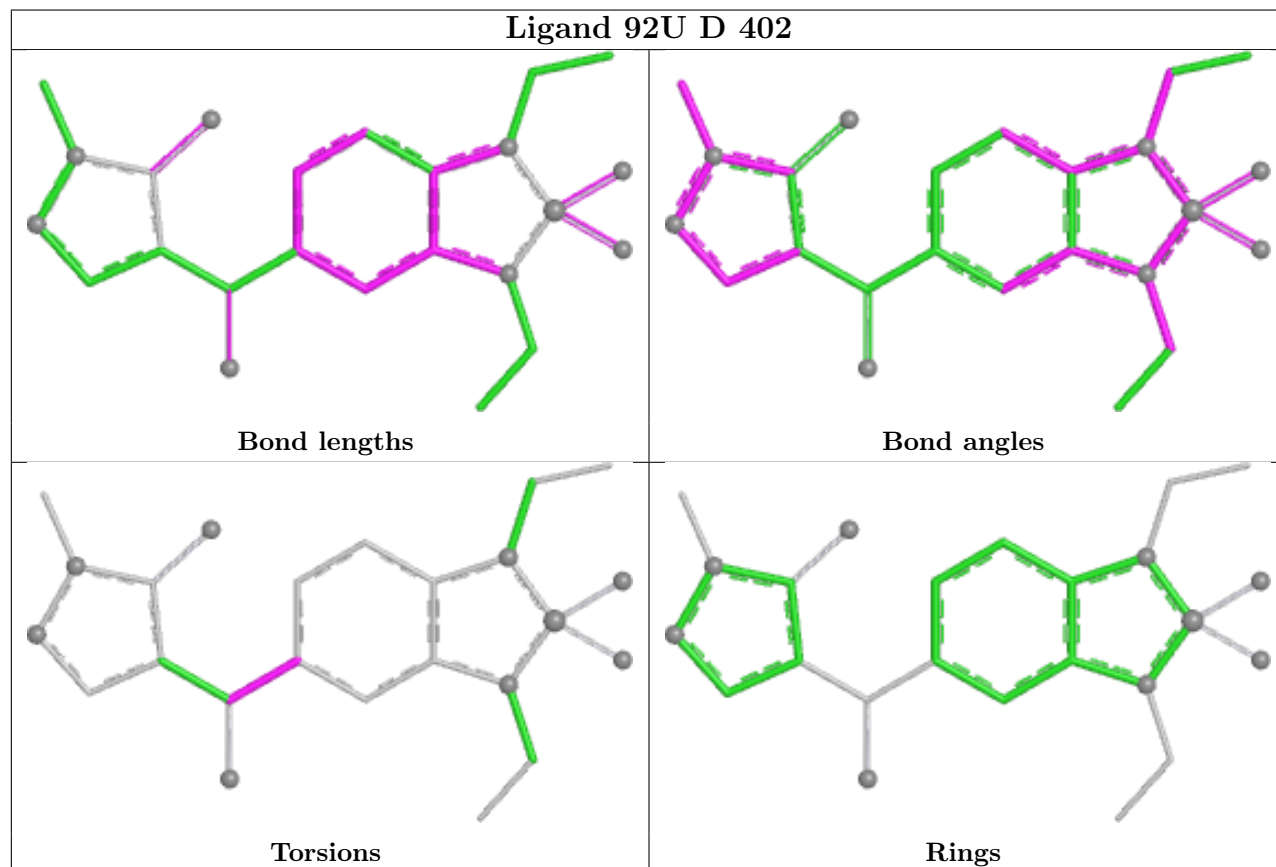
Ligand 92U F 402



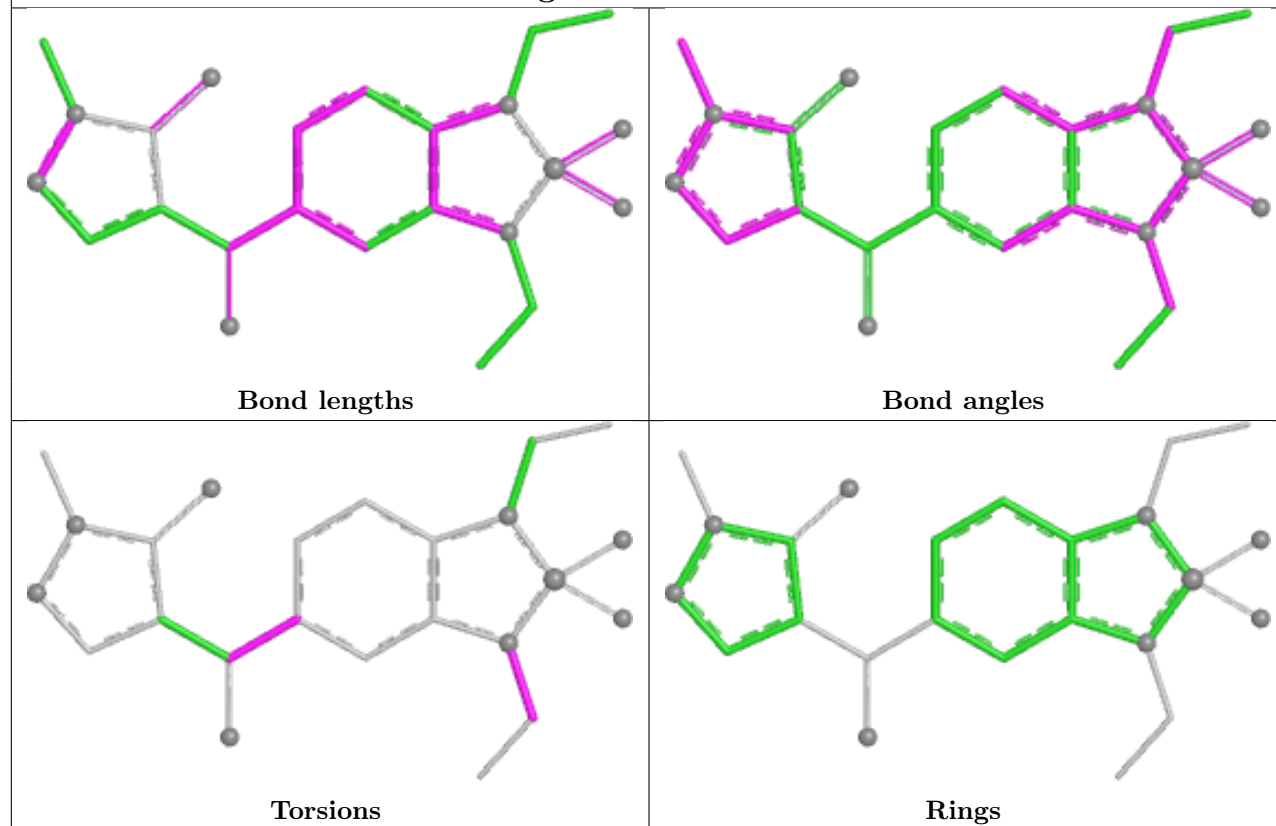
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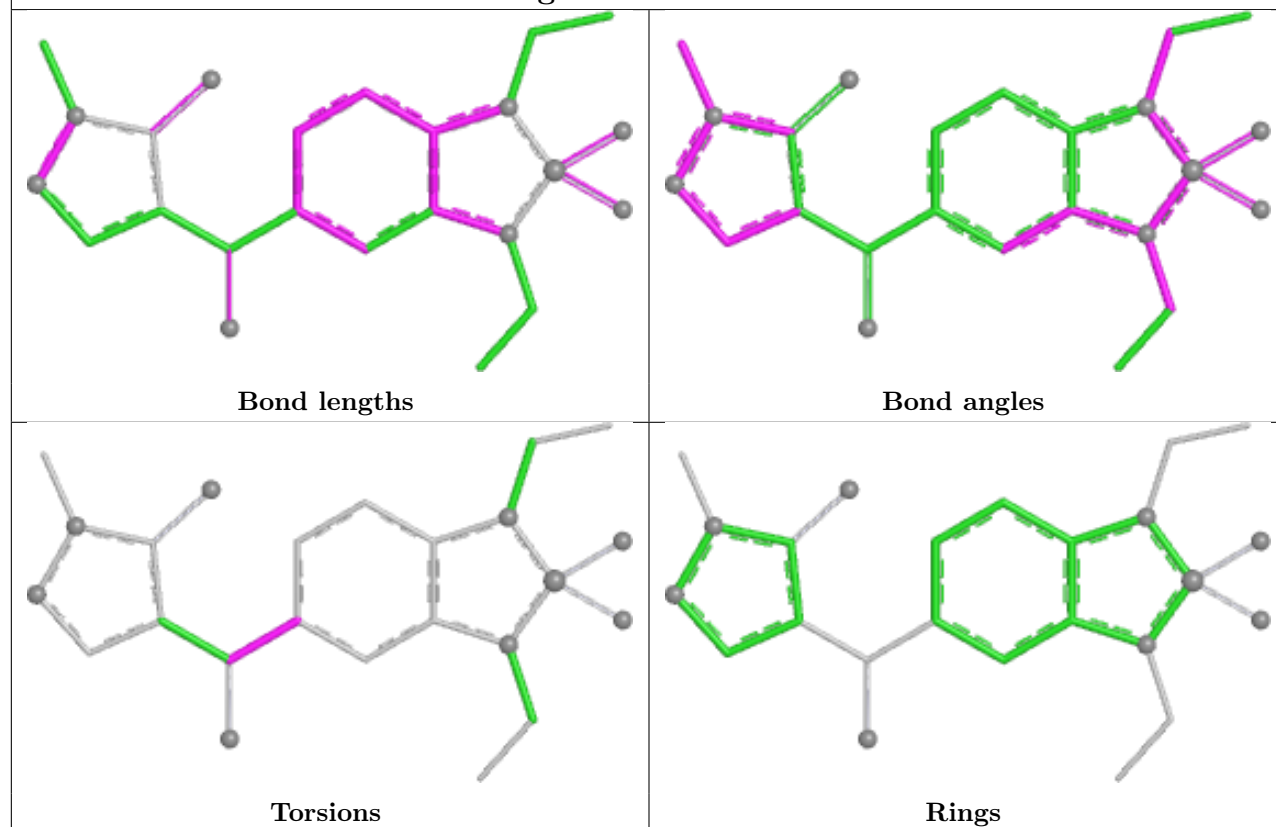
Ligand 92U D 402



Ligand 92U B 402



Ligand 92U C 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	371/393 (94%)	0.32	4 (1%)	78 72	20, 33, 57, 73	1 (0%)
1	B	372/393 (94%)	0.30	6 (1%)	70 63	22, 37, 60, 77	0
1	C	373/393 (94%)	0.53	9 (2%)	59 52	21, 41, 61, 71	0
1	D	371/393 (94%)	0.27	2 (0%)	87 83	24, 36, 55, 68	0
1	E	369/393 (93%)	0.44	6 (1%)	70 63	23, 40, 58, 73	0
1	F	371/393 (94%)	1.26	77 (20%)	2 2	30, 56, 78, 109	0
All	All	2227/2358 (94%)	0.52	104 (4%)	36 31	20, 40, 66, 109	1 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	230	ALA	4.2
1	F	151	ASN	4.2
1	C	154	GLY	3.9
1	F	217	VAL	3.8
1	F	206	PHE	3.6
1	F	377	LEU	3.6
1	F	147	VAL	3.5
1	F	212	VAL	3.5
1	F	154	GLY	3.4
1	F	131	VAL	3.3
1	F	145	THR	3.3
1	F	115	ALA	3.3
1	D	377	LEU	3.2
1	F	226	SER	3.2
1	F	153	ILE	3.1
1	F	330	GLY	3.1
1	E	246	GLY	3.0
1	F	135	VAL	3.0
1	F	114	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	185	VAL	3.0
1	C	155	GLN	3.0
1	C	129	GLY	2.9
1	F	12	GLU	2.8
1	F	137	GLN	2.8
1	C	376	ASN	2.8
1	F	117	ILE	2.8
1	A	8	GLY	2.8
1	F	201	LEU	2.8
1	F	119	ARG	2.8
1	E	368	PHE	2.8
1	F	229	VAL	2.8
1	F	296	TYR	2.8
1	F	123	VAL	2.7
1	F	204	LEU	2.7
1	F	107	VAL	2.7
1	C	7	LYS	2.7
1	F	247	LYS	2.7
1	A	9	ALA	2.6
1	F	74	ALA	2.6
1	F	140	GLY	2.6
1	F	251	GLN	2.6
1	F	49	GLY	2.6
1	F	122	TRP	2.5
1	F	180	MET	2.5
1	E	9	ALA	2.5
1	F	348	LEU	2.5
1	A	120	GLU	2.5
1	C	13	ARG	2.5
1	C	360	GLY	2.5
1	C	368	PHE	2.4
1	F	111	ARG	2.4
1	F	335	ILE	2.4
1	F	102	ASP	2.4
1	F	33	ALA	2.4
1	F	136	LEU	2.4
1	F	121	PRO	2.4
1	F	110	ALA	2.4
1	F	105	TYR	2.3
1	F	67	ILE	2.3
1	F	308	ILE	2.3
1	B	309	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	13	ARG	2.3
1	B	293	SER	2.3
1	F	14	GLY	2.3
1	E	345	THR	2.3
1	F	69	PHE	2.3
1	F	155	GLN	2.3
1	B	246	GLY	2.3
1	B	7	LYS	2.2
1	F	133	PHE	2.2
1	B	151	ASN	2.2
1	F	100	VAL	2.2
1	F	116	LYS	2.2
1	F	211	SER	2.2
1	F	214	ASP	2.2
1	F	303	LEU	2.2
1	E	78	TRP	2.2
1	F	16	PHE	2.2
1	F	144	HIS	2.2
1	F	181	ILE	2.2
1	F	134	ALA	2.2
1	D	218	HIS	2.2
1	F	194	VAL	2.2
1	F	8	GLY	2.1
1	F	98	PHE	2.1
1	F	205	GLN	2.1
1	B	261	GLY	2.1
1	E	46	ALA	2.1
1	F	148	GLU	2.1
1	F	146	LEU	2.1
1	F	236	ILE	2.1
1	C	316	ALA	2.1
1	F	143	THR	2.1
1	F	294	THR	2.1
1	F	305	THR	2.1
1	A	375	GLN	2.1
1	F	218	HIS	2.1
1	F	132	LYS	2.0
1	F	184	ILE	2.0
1	F	285	GLY	2.0
1	F	198	GLU	2.0
1	F	262	ALA	2.0
1	F	299	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	331	TYR	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](#)

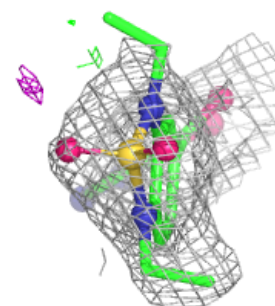
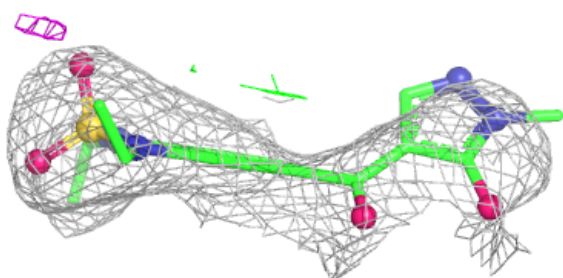
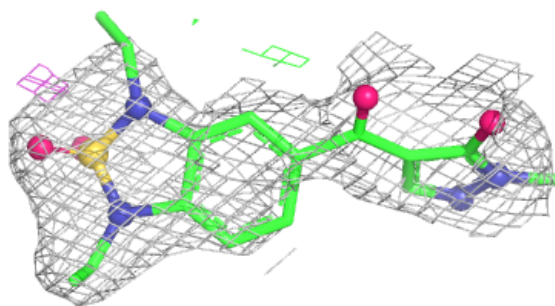
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CO	E	401	1/1	0.85	0.10	68,68,68,68	0
3	92U	F	402	24/24	0.88	0.14	38,57,67,70	0
3	92U	C	402	24/24	0.92	0.11	27,39,46,50	0
3	92U	D	402	24/24	0.93	0.11	33,39,45,52	0
2	CO	A	401	1/1	0.93	0.06	59,59,59,59	0
3	92U	E	402	24/24	0.94	0.09	28,40,45,46	0
3	92U	B	402	24/24	0.94	0.09	32,39,43,49	0
3	92U	A	402	24/24	0.95	0.09	16,24,30,31	0
2	CO	C	401	1/1	0.95	0.07	59,59,59,59	0
2	CO	D	401	1/1	0.96	0.05	66,66,66,66	0
2	CO	B	401	1/1	0.99	0.02	49,49,49,49	0
2	CO	F	401	1/1	0.99	0.03	64,64,64,64	0

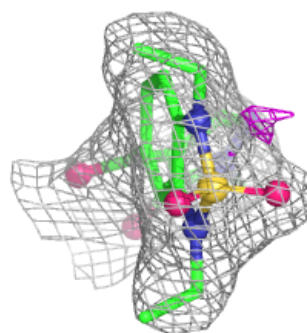
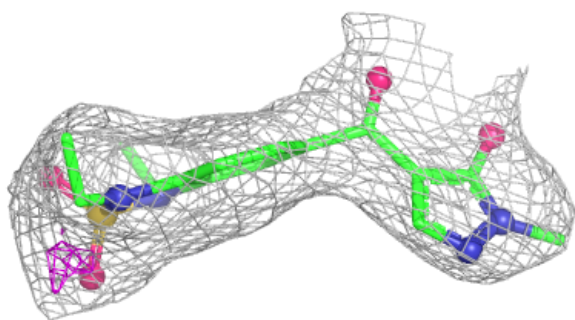
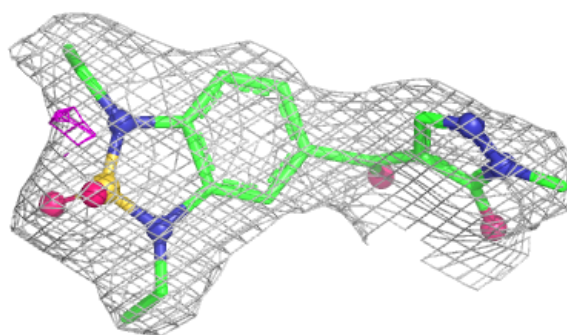
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

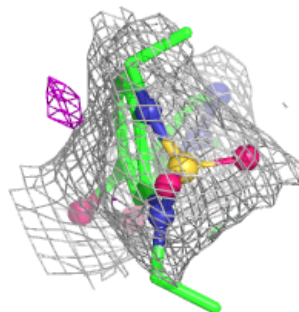
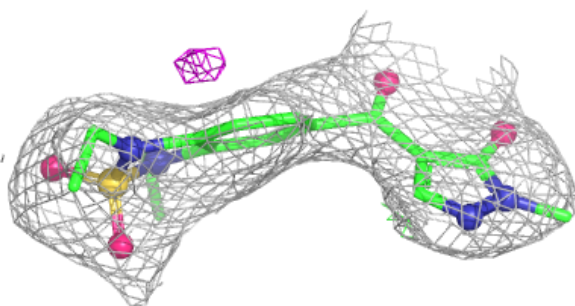
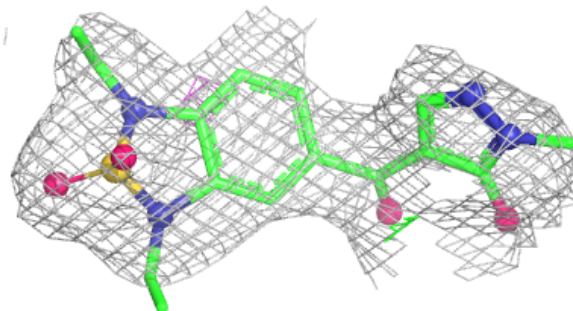
**Electron density around 92U C 402:**

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

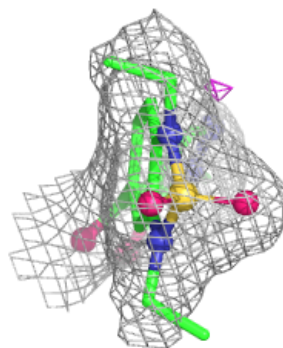
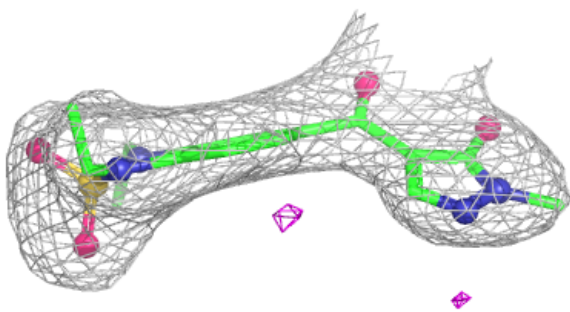
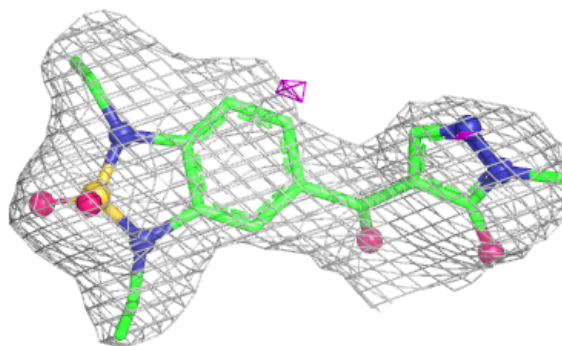


Electron density around 92U D 402:

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

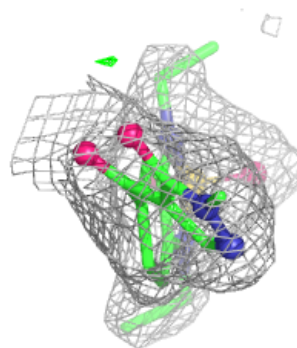
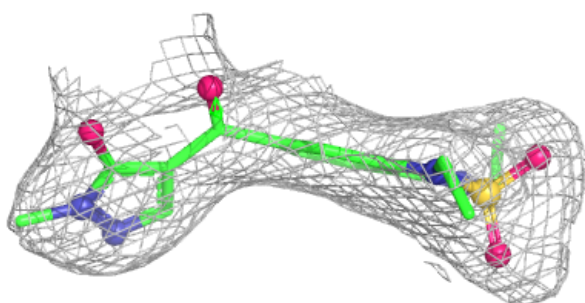
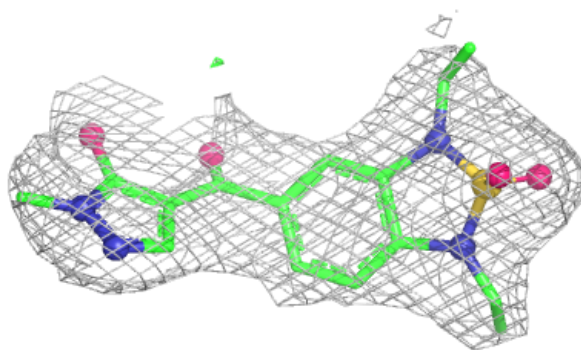
**Electron density around 92U E 402:**

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

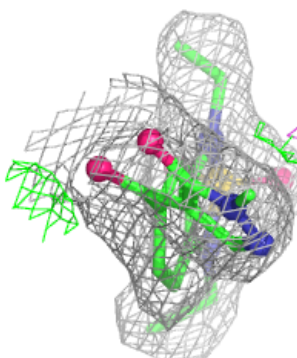
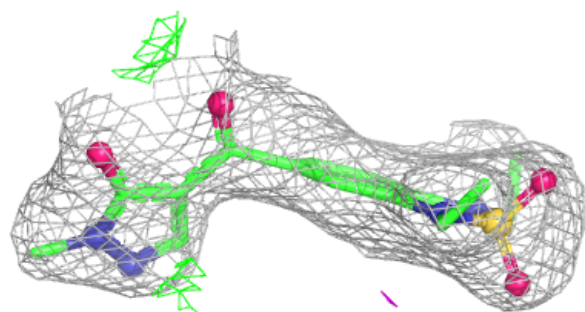
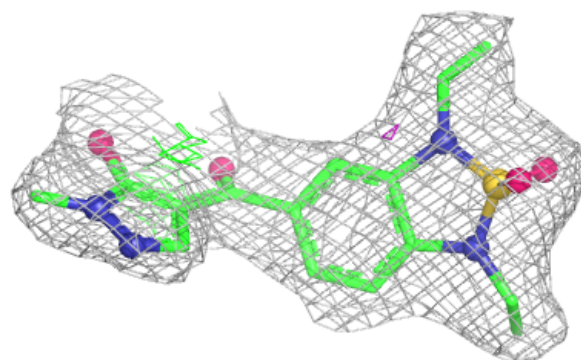


Electron density around 92U B 402:

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

**Electron density around 92U 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.