



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 08:29 PM EDT

PDB ID : 6N4I
Title : Structural basis of Nav1.7 inhibition by a gating-modifier spider toxin
Authors : Xu, H.; Koth, C.M.; Payandeh, J.
Deposited on : 2018-11-19
Resolution : 3.54 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:

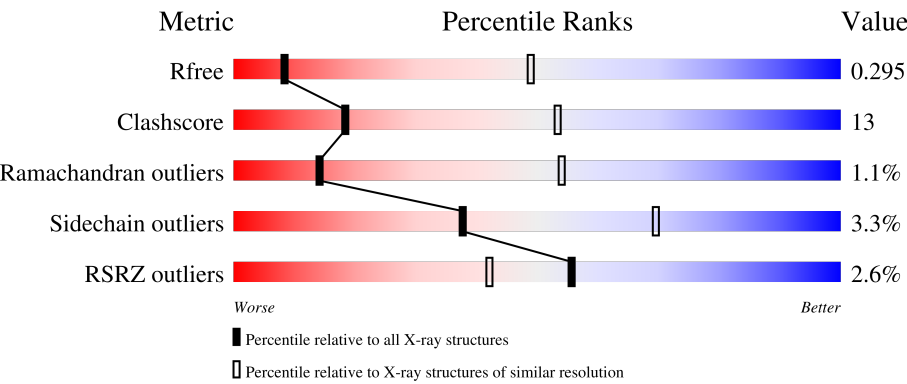
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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 3.54 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	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)

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	288	<div><div>%</div><div><div></div><div>51%</div><div>25%</div><div>•</div><div>22%</div></div></div>
1	B	288	<div><div></div><div>52%</div><div>25%</div><div>•</div><div>22%</div></div>
1	C	288	<div><div></div><div>61%</div><div>16%</div><div>•</div><div>22%</div></div>
1	D	288	<div><div>%</div><div><div></div><div>56%</div><div>20%</div><div>•</div><div>22%</div></div></div>
2	E	30	<div><div>13%</div><div><div></div><div>67%</div><div>33%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	30	
2	G	30	
2	H	30	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	6OU	D	1005	-	-	-	X
3	6OU	E	101	-	-	-	X
3	6OU	G	101	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8629 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.

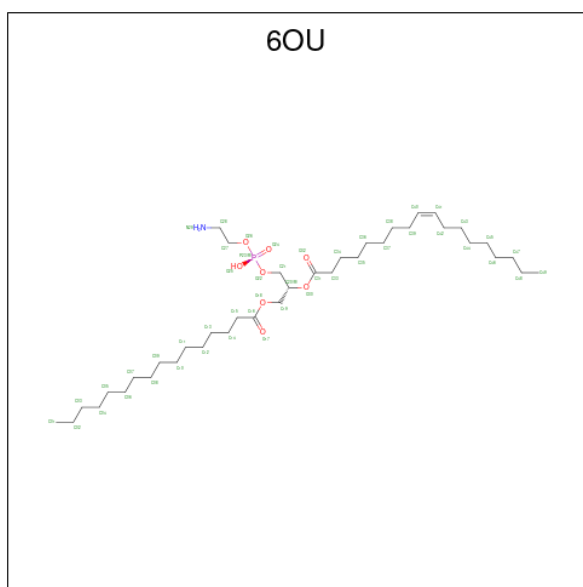
- Molecule 1 is a protein called Nav1.7 VSD2-NavAb channel chimera protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1823	1238	273	299	13			
1	B	225	Total	C	N	O	S	0	0	0
			1819	1235	272	299	13			
1	C	226	Total	C	N	O	S	0	0	0
			1818	1235	270	300	13			
1	D	225	Total	C	N	O	S	0	0	0
			1808	1229	269	297	13			

- Molecule 2 is a protein called Beta/omega-theraphotoxin-Tp2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	30	Total	C	N	O	S	0	0	0
			262	168	46	40	8			
2	F	30	Total	C	N	O	S	0	0	0
			262	168	46	40	8			
2	G	30	Total	C	N	O	S	0	0	0
			258	165	45	40	8			
2	H	30	Total	C	N	O	S	0	0	0
			262	168	46	40	8			

- Molecule 3 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ({Z})-octadec-9-enoate (three-letter code: 6OU) (formula: C₃₉H₇₆NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 24	C 15	O 8	P 1	0	0	
3	A	1	Total 27	C 17	N 1	O 8	P 1	0	0
3	A	1	Total 16	C 7	N 1	O 7	P 1	0	0
3	B	1	Total 24	C 15	O 8	P 1	0	0	
3	B	1	Total 27	C 17	N 1	O 8	P 1	0	0
3	B	1	Total 18	C 9	N 1	O 7	P 1	0	0
3	C	1	Total 24	C 15	O 8	P 1	0	0	
3	C	1	Total 27	C 17	N 1	O 8	P 1	0	0
3	D	1	Total 24	C 15	O 8	P 1	0	0	
3	D	1	Total 27	C 17	N 1	O 8	P 1	0	0
3	D	1	Total 14	C 6	N 1	O 6	P 1	0	0
3	D	1	Total 17	C 8	N 1	O 7	P 1	0	0
3	D	1	Total 11	C 5	N 1	O 4	P 1	0	0
3	E	1	Total 13	C 6	O 6	P 1	0	0	

Continued on next page...

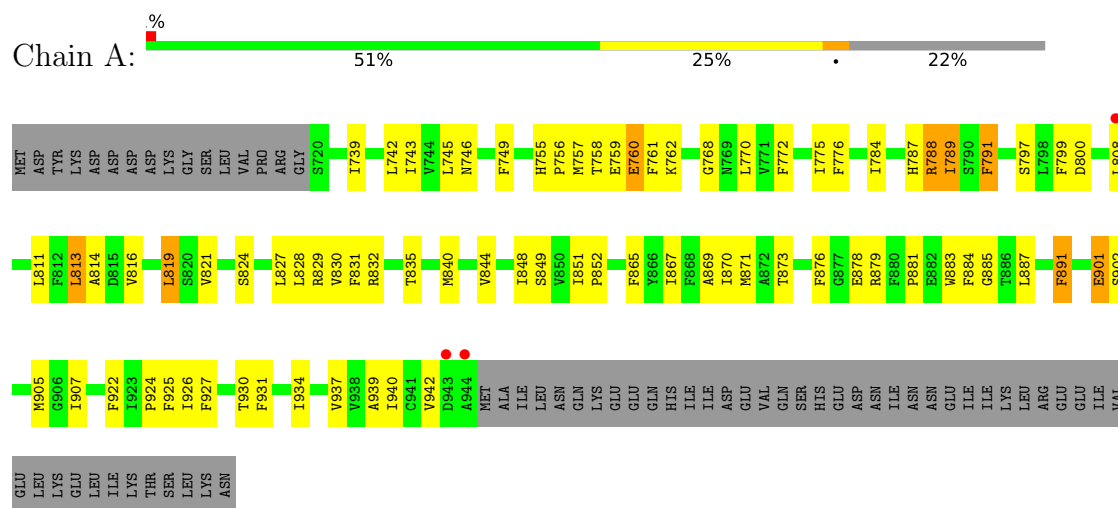
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			9	3	1	4	1		
3	G	1	Total	C	N	O	P	0	0
			15	7	1	6	1		

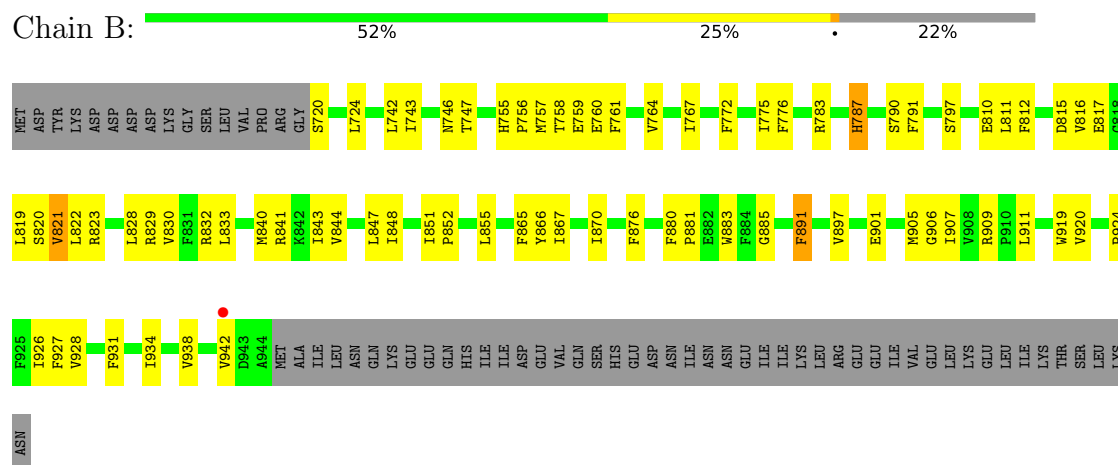
3 Residue-property plots

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: Nav1.7 VSD2-NavAb channel chimera protein

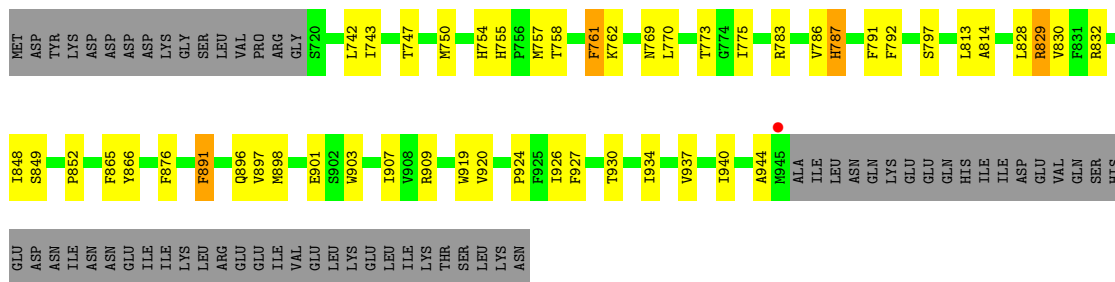


- Molecule 1: Nav1.7 VSD2-NavAb channel chimera protein

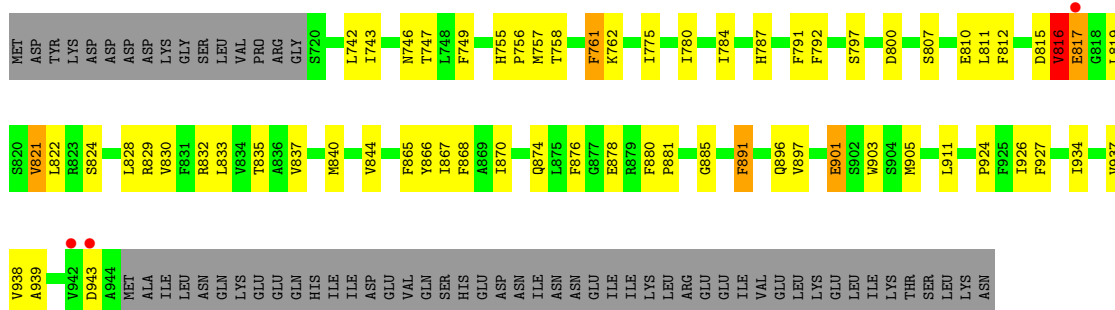


- Molecule 1: Nav1.7 VSD2-NavAb channel chimera protein

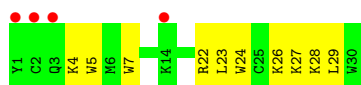




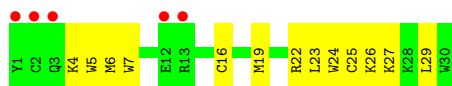
- Molecule 1: Nav1.7 VSD2-NavAb channel chimera protein



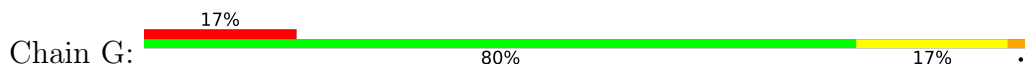
- Molecule 2: Beta/omega-theraphotoxin-Tp2a



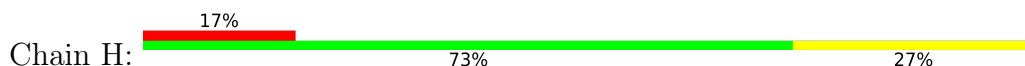
- Molecule 2: Beta/omega-theraphotoxin-Tp2a

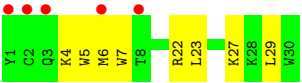


- Molecule 2: Beta/omega-theraphotoxin-Tp2a



- Molecule 2: Beta/omega-theraphotoxin-Tp2a





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	221.22Å 123.53Å 123.99Å 90.00° 124.00° 90.00°	Depositor
Resolution (Å)	36.89 – 3.54 45.85 – 3.54	Depositor EDS
% Data completeness (in resolution range)	81.5 (36.89-3.54) 81.6 (45.85-3.54)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 3.57Å)	Xtriage
Refinement program	PHENIX (dev_2747: ???)	Depositor
R, R_{free}	0.275 , 0.294 0.280 , 0.295	Depositor DCC
R_{free} test set	1376 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	108.8	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for $1/2^*h+1/2^*k+2^*l, 1/2^*h+1/2^*k, -1/2^*h+1/2^*k-l$ 0.018 for $-1/2^*h-3/2^*k-l, -1/2^*h+1/2^*k-l, 1/2^*h+1/2^*k$ 0.035 for $-1/2^*h+3/2^*k-l, 1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k$ 0.035 for $1/2^*h-1/2^*k+2^*l, -1/2^*h+1/2^*k, -1/2^*h-1/2^*k-l$ 0.388 for $-h+k-l, -l, -k$ 0.379 for $-h-k-l, l, k$ 0.037 for $-1/2^*h-1/2^*k+l, -1/2^*h-1/2^*k-l, 1/2^*h-1/2^*k$ 0.022 for $-1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k+l, 1/2^*h+1/2^*k$ 0.038 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.022 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$ 0.397 for $-h-2^*l, -k, l$	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8629	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

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.

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 6OU

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	0.33	0/1875	0.50	0/2554
1	B	0.32	0/1871	0.51	0/2550
1	C	0.32	0/1870	0.51	0/2550
1	D	0.32	0/1860	0.50	0/2536
2	E	0.32	0/270	0.53	0/360
2	F	0.38	0/270	0.59	0/360
2	G	0.32	0/266	0.58	0/356
2	H	0.32	0/270	0.51	0/360
All	All	0.32	0/8552	0.51	0/11626

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	1823	0	1865	60	0
1	B	1819	0	1854	59	0
1	C	1818	0	1845	43	0
1	D	1808	0	1834	47	0
2	E	262	0	254	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	262	0	254	19	0
2	G	258	0	243	10	0
2	H	262	0	254	10	0
3	A	67	0	0	1	0
3	B	69	0	0	0	0
3	C	51	0	0	1	0
3	D	93	0	0	0	0
3	E	13	0	0	0	0
3	F	9	0	0	0	0
3	G	15	0	0	0	0
All	All	8629	0	8403	226	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 13.

All (226) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:ASP:OD1	1:A:835:THR:OG1	1.96	0.82
1:D:800:ASP:OD1	1:D:835:THR:OG1	1.97	0.82
2:H:4:LYS:HG2	2:H:5:TRP:H	1.45	0.82
1:C:769:ASN:OD1	1:C:829:ARG:NH2	2.15	0.77
2:H:4:LYS:HG2	2:H:5:TRP:N	2.01	0.75
2:G:4:LYS:HG2	2:G:5:TRP:H	1.54	0.72
2:F:4:LYS:HG2	2:F:5:TRP:H	1.56	0.70
2:G:4:LYS:HG2	2:G:5:TRP:N	2.08	0.69
1:A:759:GLU:O	1:A:761:PHE:N	2.26	0.69
2:F:4:LYS:HG2	2:F:5:TRP:N	2.10	0.66
2:E:4:LYS:HB3	2:E:7:TRP:HD1	1.60	0.66
2:E:4:LYS:HG3	2:E:5:TRP:N	2.11	0.66
2:F:4:LYS:HB3	2:F:7:TRP:CD1	2.30	0.66
1:B:759:GLU:O	1:B:760:GLU:HB2	1.94	0.66
1:A:870:ILE:HD11	1:B:830:VAL:HG21	1.78	0.65
1:A:759:GLU:O	1:A:762:LYS:N	2.29	0.64
1:B:823:ARG:NH1	2:F:22:ARG:NH1	2.47	0.62
1:D:787:HIS:HB2	1:D:791:PHE:HB2	1.81	0.62
2:H:4:LYS:HB3	2:H:7:TRP:CD1	2.35	0.62
2:F:4:LYS:HB3	2:F:7:TRP:HD1	1.65	0.62
1:C:755:HIS:O	1:C:757:MET:N	2.31	0.62
1:B:757:MET:HG3	1:B:758:THR:H	1.67	0.60
1:D:828:LEU:O	1:D:830:VAL:N	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:5:TRP:CD1	2:H:27:LYS:HG3	2.38	0.59
2:G:4:LYS:CG	2:G:5:TRP:H	2.16	0.58
2:G:4:LYS:HB3	2:G:7:TRP:CD1	2.39	0.57
2:H:4:LYS:HB3	2:H:7:TRP:HD1	1.67	0.57
2:E:4:LYS:HG3	2:E:5:TRP:H	1.68	0.57
1:B:815:ASP:HB2	1:B:820:SER:HA	1.88	0.56
1:D:747:THR:HG21	1:D:833:LEU:HD11	1.88	0.56
1:C:828:LEU:O	1:C:830:VAL:N	2.38	0.56
1:A:739:ILE:O	1:A:743:ILE:HG13	2.07	0.55
1:D:743:ILE:HD13	1:D:832:ARG:HB3	1.88	0.55
1:A:865:PHE:HB3	1:A:891:PHE:CE2	2.43	0.54
2:G:4:LYS:HB3	2:G:7:TRP:HD1	1.73	0.53
1:A:787:HIS:O	1:A:789:ILE:N	2.42	0.53
1:C:758:THR:O	1:C:758:THR:HG22	2.09	0.53
1:A:759:GLU:C	1:A:761:PHE:N	2.62	0.53
1:C:754:HIS:O	1:C:757:MET:HB2	2.08	0.53
1:B:823:ARG:HH12	2:F:22:ARG:NH1	2.07	0.53
1:C:909:ARG:NH1	1:D:896:GLN:OE1	2.41	0.53
1:D:742:LEU:CD2	1:D:775:ILE:HG21	2.39	0.53
1:D:821:VAL:HG12	1:D:822:LEU:HD12	1.91	0.53
1:C:743:ILE:HD13	1:C:832:ARG:HB3	1.92	0.52
1:D:816:VAL:HG22	1:D:817:GLU:N	2.24	0.52
1:B:747:THR:HG21	1:B:833:LEU:HD11	1.92	0.52
1:B:934:ILE:HG21	1:C:937:VAL:HG22	1.92	0.52
1:D:758:THR:HG22	1:D:758:THR:O	2.09	0.52
1:D:815:ASP:O	1:D:817:GLU:N	2.43	0.51
1:C:813:LEU:HA	2:G:26:LYS:HB3	1.92	0.51
1:C:757:MET:SD	1:C:762:LYS:HB2	2.50	0.51
2:E:4:LYS:CG	2:E:5:TRP:H	2.24	0.51
2:E:4:LYS:HB3	2:E:7:TRP:CD1	2.42	0.51
1:A:821:VAL:O	1:A:824:SER:HB3	2.11	0.51
1:B:787:HIS:HB2	1:B:790:SER:HB3	1.92	0.51
2:E:4:LYS:CG	2:E:5:TRP:N	2.74	0.50
1:B:870:ILE:HD11	1:C:750:MET:HB3	1.94	0.50
2:G:28:LYS:O	2:G:28:LYS:HG2	2.12	0.50
2:F:27:LYS:HG3	2:F:29:LEU:H	1.76	0.50
1:A:755:HIS:O	1:A:757:MET:N	2.42	0.49
1:A:758:THR:HG22	1:A:758:THR:O	2.12	0.49
1:B:828:LEU:O	1:B:830:VAL:N	2.45	0.49
1:A:878:GLU:HB2	1:B:755:HIS:NE2	2.28	0.49
1:D:757:MET:HG3	1:D:758:THR:H	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:865:PHE:HB3	1:D:891:PHE:CE2	2.48	0.49
2:F:4:LYS:CG	2:F:5:TRP:H	2.24	0.49
1:B:811:LEU:O	2:F:6:MET:HE1	2.13	0.49
1:B:743:ILE:HD13	1:B:776:PHE:CZ	2.48	0.49
1:D:939:ALA:O	1:D:943:ASP:N	2.44	0.49
1:A:827:LEU:HD13	1:D:874:GLN:CB	2.43	0.48
1:B:926:ILE:O	1:B:927:PHE:C	2.52	0.48
1:A:926:ILE:O	1:A:927:PHE:C	2.52	0.48
2:H:4:LYS:CG	2:H:5:TRP:N	2.75	0.48
1:A:742:LEU:CD2	1:A:775:ILE:HG21	2.42	0.48
1:D:821:VAL:O	1:D:824:SER:HB3	2.14	0.48
1:B:759:GLU:CG	1:B:761:PHE:HB2	2.44	0.48
1:C:930:THR:O	1:C:934:ILE:HG12	2.14	0.48
1:A:940:ILE:HG21	1:D:938:VAL:HG21	1.96	0.47
1:A:800:ASP:OD1	1:A:835:THR:CB	2.61	0.47
1:A:907:ILE:HD11	1:D:905:MET:HE1	1.97	0.47
2:F:4:LYS:CG	2:F:5:TRP:N	2.77	0.47
1:B:759:GLU:C	1:B:761:PHE:H	2.18	0.47
1:A:770:LEU:HD12	1:A:811:LEU:HD21	1.96	0.47
1:A:870:ILE:HG22	1:A:887:LEU:HD12	1.95	0.47
1:A:927:PHE:O	1:A:930:THR:HG22	2.14	0.47
1:C:934:ILE:HG21	1:D:937:VAL:HG22	1.97	0.47
2:F:4:LYS:HE3	2:F:7:TRP:HE1	1.80	0.47
1:A:828:LEU:O	1:A:830:VAL:N	2.47	0.47
1:B:852:PRO:HA	1:B:855:LEU:HB2	1.95	0.47
1:C:891:PHE:HB3	3:C:1001:6OU:O17	2.15	0.47
1:C:924:PRO:O	1:C:927:PHE:HB2	2.15	0.47
2:F:6:MET:HE2	2:F:24:TRP:CD1	2.50	0.47
1:D:791:PHE:O	1:D:797:SER:HB2	2.15	0.47
1:D:867:ILE:HG13	1:D:868:PHE:N	2.30	0.47
1:C:761:PHE:C	1:C:761:PHE:CD2	2.88	0.47
1:C:783:ARG:O	1:C:786:VAL:HG22	2.14	0.47
2:E:28:LYS:O	2:E:29:LEU:C	2.53	0.47
1:A:799:PHE:HD2	1:A:835:THR:HG21	1.80	0.46
1:A:870:ILE:HG13	1:A:871:MET:N	2.31	0.46
1:A:905:MET:HE2	1:B:907:ILE:HD11	1.97	0.46
1:D:755:HIS:N	1:D:756:PRO:HD2	2.30	0.46
1:C:757:MET:SD	1:C:761:PHE:CD2	3.08	0.46
1:D:791:PHE:CD2	1:D:797:SER:HB3	2.51	0.46
1:A:745:LEU:CD2	1:A:772:PHE:CZ	2.98	0.46
1:A:876:PHE:N	1:A:876:PHE:CD1	2.84	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:ALA:HB3	2:E:27:LYS:O	2.16	0.46
1:B:757:MET:CG	1:B:758:THR:H	2.27	0.46
1:C:757:MET:SD	1:C:761:PHE:HD2	2.38	0.46
2:H:4:LYS:CG	2:H:5:TRP:H	2.21	0.46
1:A:791:PHE:O	1:A:797:SER:HB2	2.16	0.46
1:A:813:LEU:O	2:E:26:LYS:HD3	2.16	0.45
1:A:870:ILE:CD1	1:B:830:VAL:HG21	2.45	0.45
1:B:742:LEU:HD21	1:B:775:ILE:HG21	1.98	0.45
1:B:934:ILE:CG2	1:C:937:VAL:HG13	2.46	0.45
1:B:759:GLU:HG3	1:B:761:PHE:HB2	1.97	0.45
1:D:755:HIS:O	1:D:757:MET:N	2.48	0.45
1:D:815:ASP:HA	1:D:822:LEU:HD13	1.99	0.45
1:A:743:ILE:HG12	1:A:776:PHE:CZ	2.52	0.45
2:H:29:LEU:HG	2:H:29:LEU:O	2.16	0.45
1:A:931:PHE:O	1:A:934:ILE:CG1	2.64	0.45
1:B:909:ARG:NH1	1:C:896:GLN:OE1	2.50	0.45
1:D:761:PHE:C	1:D:761:PHE:CD2	2.90	0.45
1:D:924:PRO:O	1:D:927:PHE:HB2	2.17	0.45
1:B:876:PHE:N	1:B:876:PHE:CD1	2.84	0.45
1:B:942:VAL:HG22	1:C:944:ALA:HB1	1.98	0.45
1:A:743:ILE:HD13	1:A:832:ARG:CB	2.47	0.45
1:B:830:VAL:HG22	1:B:830:VAL:O	2.16	0.45
1:C:876:PHE:N	1:C:876:PHE:CD1	2.84	0.45
1:A:745:LEU:CD2	1:A:772:PHE:HZ	2.30	0.44
1:D:807:SER:O	1:D:811:LEU:HG	2.17	0.44
1:C:848:ILE:O	1:C:852:PRO:HD3	2.17	0.44
1:A:867:ILE:O	1:A:870:ILE:HG13	2.16	0.44
1:A:869:ALA:O	1:A:873:THR:HG22	2.17	0.44
1:B:812:PHE:HA	2:F:6:MET:HE3	1.98	0.44
1:B:848:ILE:O	1:B:852:PRO:HD3	2.18	0.44
1:B:865:PHE:HB3	1:B:891:PHE:CE1	2.51	0.44
1:C:814:ALA:HB2	2:G:26:LYS:HD2	1.99	0.44
1:D:876:PHE:CD1	1:D:876:PHE:N	2.84	0.44
1:A:755:HIS:N	1:A:756:PRO:CD	2.81	0.44
1:D:800:ASP:OD1	1:D:835:THR:CB	2.66	0.44
1:D:881:PRO:HA	1:D:885:GLY:CA	2.48	0.44
1:D:812:PHE:HB3	2:H:6:MET:CE	2.48	0.44
1:B:755:HIS:N	1:B:756:PRO:HD2	2.33	0.44
1:B:819:LEU:HD13	1:B:821:VAL:HG23	1.99	0.44
1:B:758:THR:HG22	1:B:758:THR:O	2.18	0.43
1:A:755:HIS:CD2	1:D:878:GLU:HG3	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:791:PHE:CE2	1:B:797:SER:HB3	2.52	0.43
1:B:867:ILE:O	1:B:870:ILE:HG22	2.18	0.43
1:D:840:MET:O	1:D:844:VAL:HG23	2.18	0.43
1:D:897:VAL:CG1	1:D:926:ILE:HD11	2.48	0.43
1:C:742:LEU:HD21	1:C:775:ILE:HG21	2.00	0.43
2:F:16:CYS:HB2	2:F:19:MET:CE	2.48	0.43
1:C:742:LEU:CD2	1:C:775:ILE:HG21	2.49	0.43
2:G:29:LEU:O	2:G:29:LEU:HD22	2.19	0.43
1:B:783:ARG:HH22	1:B:841:ARG:HH12	1.65	0.43
2:E:24:TRP:NE1	2:E:26:LYS:HE2	2.33	0.43
1:C:849:SER:O	1:C:852:PRO:HD2	2.19	0.43
1:B:897:VAL:CG1	1:B:926:ILE:HD11	2.49	0.43
1:A:924:PRO:O	1:A:927:PHE:HB2	2.19	0.43
2:F:5:TRP:HD1	2:F:19:MET:HE1	1.84	0.43
1:A:788:ARG:O	1:A:789:ILE:HB	2.19	0.43
1:C:865:PHE:HZ	1:C:898:MET:SD	2.42	0.42
2:E:5:TRP:CD1	2:E:27:LYS:HG3	2.53	0.42
1:B:757:MET:HG3	1:B:758:THR:N	2.34	0.42
1:D:757:MET:CE	1:D:762:LYS:HB2	2.48	0.42
1:B:883:TRP:CH2	1:B:906:GLY:O	2.72	0.42
1:B:905:MET:HE1	1:C:907:ILE:HD11	2.01	0.42
1:C:786:VAL:HG23	1:C:787:HIS:N	2.35	0.42
1:A:901:GLU:HG3	1:D:903:TRP:H	1.85	0.42
1:D:784:ILE:CD1	1:D:792:PHE:HE1	2.33	0.42
2:H:22:ARG:O	2:H:23:LEU:HB3	2.20	0.42
1:A:883:TRP:HB2	1:A:884:PHE:CD2	2.55	0.42
1:B:810:GLU:HG3	1:B:822:LEU:O	2.19	0.42
1:D:816:VAL:O	1:D:817:GLU:HG2	2.19	0.42
1:A:743:ILE:HD13	1:A:832:ARG:HB3	2.02	0.42
1:B:938:VAL:HG21	1:C:940:ILE:HG22	2.02	0.42
1:C:770:LEU:O	1:C:773:THR:HG22	2.19	0.42
1:A:819:LEU:HD13	1:A:821:VAL:HG23	2.01	0.42
1:A:922:PHE:O	1:A:925:PHE:HB3	2.19	0.42
1:B:924:PRO:O	1:B:927:PHE:HB2	2.19	0.42
1:B:927:PHE:O	1:B:928:VAL:C	2.59	0.42
1:D:837:VAL:HG11	1:D:840:MET:HG2	2.02	0.42
1:A:891:PHE:HB3	3:A:1001:6OU:O17	2.20	0.41
1:B:938:VAL:HG11	1:C:940:ILE:HG22	2.02	0.41
1:A:840:MET:O	1:A:844:VAL:HG23	2.21	0.41
1:C:866:TYR:HE1	1:D:747:THR:HG21	1.85	0.41
1:C:897:VAL:HG12	1:C:926:ILE:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:897:VAL:CG1	1:C:926:ILE:HD11	2.50	0.41
1:B:840:MET:O	1:B:844:VAL:HG23	2.20	0.41
1:B:851:ILE:CG2	1:B:852:PRO:HD3	2.51	0.41
1:C:791:PHE:CE1	1:C:797:SER:HB3	2.55	0.41
1:C:866:TYR:CE1	1:D:747:THR:HG21	2.56	0.41
1:D:866:TYR:CZ	1:D:870:ILE:HD11	2.56	0.41
1:A:849:SER:O	1:A:852:PRO:HD2	2.20	0.41
1:A:881:PRO:O	1:A:885:GLY:N	2.48	0.41
1:A:770:LEU:HA	1:A:811:LEU:HD11	2.03	0.41
1:A:848:ILE:O	1:A:851:ILE:HG22	2.20	0.41
1:B:791:PHE:CD2	1:B:797:SER:HB3	2.56	0.41
1:B:811:LEU:O	2:F:6:MET:CE	2.69	0.41
1:A:937:VAL:HG22	1:D:934:ILE:CG2	2.51	0.41
2:F:24:TRP:HE1	2:F:26:LYS:HE2	1.86	0.41
1:A:757:MET:HG3	1:A:758:THR:H	1.85	0.41
1:A:939:ALA:O	1:A:942:VAL:HB	2.21	0.41
1:B:746:ASN:HB2	1:B:772:PHE:CD1	2.56	0.41
2:G:4:LYS:CG	2:G:5:TRP:N	2.73	0.41
1:A:931:PHE:O	1:A:934:ILE:HG13	2.20	0.41
1:B:743:ILE:HD12	1:B:832:ARG:CB	2.51	0.41
1:B:764:VAL:HA	1:B:767:ILE:HD12	2.02	0.41
1:B:866:TYR:CE1	1:C:747:THR:HG21	2.55	0.41
1:C:792:PHE:N	1:C:792:PHE:CD1	2.89	0.41
1:D:810:GLU:HG3	1:D:822:LEU:O	2.21	0.41
2:F:19:MET:SD	2:F:25:CYS:HB3	2.60	0.41
2:F:22:ARG:O	2:F:23:LEU:HB3	2.20	0.41
1:A:878:GLU:O	1:A:879:ARG:HB3	2.21	0.41
1:B:880:PHE:CD1	1:B:911:LEU:HD23	2.55	0.41
1:C:903:TRP:H	1:D:901:GLU:HG3	1.86	0.41
1:C:919:TRP:CE2	1:C:920:VAL:HG23	2.56	0.40
1:D:880:PHE:CE2	1:D:911:LEU:HD23	2.56	0.40
2:E:22:ARG:O	2:E:23:LEU:HB3	2.21	0.40
1:A:759:GLU:O	1:A:760:GLU:C	2.60	0.40
1:A:768:GLY:O	1:A:772:PHE:CD2	2.74	0.40
1:A:901:GLU:OE2	1:A:902:SER:OG	2.35	0.40
1:B:720:SER:O	1:B:724:LEU:HD12	2.21	0.40
1:B:843:ILE:O	1:B:847:LEU:HD13	2.21	0.40
1:B:881:PRO:HA	1:B:885:GLY:CA	2.51	0.40
1:B:919:TRP:CE2	1:B:920:VAL:HG23	2.57	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	223/288 (77%)	207 (93%)	12 (5%)	4 (2%)	8	43
1	B	223/288 (77%)	209 (94%)	11 (5%)	3 (1%)	12	50
1	C	224/288 (78%)	214 (96%)	9 (4%)	1 (0%)	34	71
1	D	223/288 (77%)	210 (94%)	10 (4%)	3 (1%)	12	50
2	E	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
2	F	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
2	G	28/30 (93%)	24 (86%)	4 (14%)	0	100	100
2	H	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
All	All	1005/1272 (79%)	939 (93%)	55 (6%)	11 (1%)	14	54

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	760	GLU
1	A	788	ARG
1	A	789	ILE
1	C	829	ARG
1	A	829	ARG
1	B	816	VAL
1	B	817	GLU
1	B	829	ARG
1	D	816	VAL
1	D	817	GLU
1	D	829	ARG

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	201/265 (76%)	190 (94%)	11 (6%)	21	56
1	B	200/265 (76%)	195 (98%)	5 (2%)	47	76
1	C	199/265 (75%)	195 (98%)	4 (2%)	55	79
1	D	197/265 (74%)	188 (95%)	9 (5%)	27	61
2	E	29/29 (100%)	29 (100%)	0	100	100
2	F	29/29 (100%)	29 (100%)	0	100	100
2	G	28/29 (97%)	27 (96%)	1 (4%)	35	67
2	H	29/29 (100%)	29 (100%)	0	100	100
All	All	912/1176 (78%)	882 (97%)	30 (3%)	38	69

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	746	ASN
1	A	749	PHE
1	A	784	ILE
1	A	791	PHE
1	A	808	LEU
1	A	813	LEU
1	A	816	VAL
1	A	819	LEU
1	A	831	PHE
1	A	891	PHE
1	A	901	GLU
1	B	787	HIS
1	B	821	VAL
1	B	891	PHE
1	B	901	GLU
1	B	931	PHE
1	C	761	PHE
1	C	787	HIS
1	C	891	PHE
1	C	901	GLU
1	D	746	ASN
1	D	749	PHE
1	D	761	PHE
1	D	780	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	816	VAL
1	D	819	LEU
1	D	821	VAL
1	D	891	PHE
1	D	901	GLU
2	G	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

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	6OU	C	1002	-	26,26,48	1.22	3 (11%)	29,31,53	1.12	2 (6%)
3	6OU	C	1001	-	23,23,48	1.59	4 (17%)	27,28,53	1.15	2 (7%)
3	6OU	A	1002	-	26,26,48	1.23	3 (11%)	29,31,53	1.07	2 (6%)
3	6OU	D	1005	-	10,10,48	0.98	0	11,12,53	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6OU	A	1003	-	15,15,48	1.10	0	17,19,53	0.88	0
3	6OU	B	1003	-	17,17,48	1.18	2 (11%)	19,21,53	0.82	1 (5%)
3	6OU	B	1002	-	26,26,48	1.23	3 (11%)	29,31,53	1.12	2 (6%)
3	6OU	D	1001	-	23,23,48	1.59	4 (17%)	27,28,53	1.15	2 (7%)
3	6OU	D	1004	-	16,16,48	1.24	1 (6%)	18,20,53	1.16	1 (5%)
3	6OU	G	101	-	14,14,48	1.49	2 (14%)	16,18,53	1.60	2 (12%)
3	6OU	D	1003	-	13,13,48	0.90	0	14,16,53	0.53	0
3	6OU	E	101	-	12,12,48	1.60	3 (25%)	14,16,53	1.73	1 (7%)
3	6OU	F	101	-	8,8,48	1.05	0	9,10,53	0.44	0
3	6OU	D	1002	-	26,26,48	1.21	3 (11%)	29,31,53	1.05	2 (6%)
3	6OU	A	1001	-	23,23,48	1.57	4 (17%)	27,28,53	1.04	2 (7%)
3	6OU	B	1001	-	23,23,48	1.61	4 (17%)	27,28,53	1.12	2 (7%)

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	6OU	C	1002	-	-	17/30/30/52	-
3	6OU	C	1001	-	-	8/25/25/52	-
3	6OU	A	1002	-	-	20/30/30/52	-
3	6OU	D	1005	-	-	9/10/10/52	-
3	6OU	A	1003	-	-	14/16/16/52	-
3	6OU	B	1003	-	-	10/19/19/52	-
3	6OU	B	1002	-	-	17/30/30/52	-
3	6OU	D	1001	-	-	8/25/25/52	-
3	6OU	D	1004	-	-	8/18/18/52	-
3	6OU	G	101	-	-	8/15/15/52	-
3	6OU	D	1003	-	-	9/14/14/52	-
3	6OU	E	101	-	-	5/13/13/52	-
3	6OU	F	101	-	-	4/8/8/52	-
3	6OU	D	1002	-	-	17/30/30/52	-
3	6OU	A	1001	-	-	7/25/25/52	-
3	6OU	B	1001	-	-	12/25/25/52	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	6OU	P23-O24	4.78	1.66	1.50
3	A	1001	6OU	P23-O24	4.77	1.65	1.50
3	D	1001	6OU	P23-O24	4.74	1.65	1.50
3	C	1001	6OU	P23-O24	4.70	1.65	1.50
3	G	101	6OU	O30-C20	-3.39	1.41	1.47
3	E	101	6OU	O30-C20	-3.28	1.41	1.47
3	D	1004	6OU	O18-C16	2.91	1.41	1.33
3	A	1002	6OU	O18-C16	2.87	1.41	1.33
3	B	1001	6OU	O18-C16	2.86	1.41	1.33
3	D	1001	6OU	O18-C16	2.80	1.41	1.33
3	C	1001	6OU	O18-C16	2.77	1.41	1.33
3	E	101	6OU	O30-C31	2.74	1.41	1.35
3	C	1002	6OU	O18-C16	2.72	1.41	1.33
3	G	101	6OU	O30-C31	2.68	1.41	1.35
3	B	1002	6OU	O18-C16	2.60	1.40	1.33
3	D	1002	6OU	O18-C16	2.59	1.40	1.33
3	B	1001	6OU	O30-C31	2.56	1.41	1.34
3	B	1003	6OU	O18-C16	2.53	1.40	1.33
3	A	1001	6OU	O18-C16	2.50	1.40	1.33
3	D	1002	6OU	O30-C31	2.48	1.41	1.34
3	B	1002	6OU	O30-C31	2.47	1.41	1.34
3	A	1001	6OU	O30-C31	2.47	1.41	1.34
3	A	1002	6OU	O30-C20	-2.44	1.40	1.46
3	C	1002	6OU	O30-C31	2.43	1.41	1.34
3	A	1002	6OU	O30-C31	2.43	1.41	1.34
3	D	1001	6OU	O30-C31	2.36	1.41	1.34
3	C	1001	6OU	O30-C20	-2.36	1.40	1.46
3	C	1001	6OU	O30-C31	2.34	1.40	1.34
3	A	1001	6OU	O30-C20	-2.31	1.40	1.46
3	D	1001	6OU	O30-C20	-2.23	1.41	1.46
3	B	1001	6OU	O30-C20	-2.09	1.41	1.46
3	B	1003	6OU	O18-C19	-2.07	1.40	1.45
3	C	1002	6OU	O30-C20	-2.04	1.41	1.46
3	D	1002	6OU	O30-C20	-2.03	1.41	1.46
3	B	1002	6OU	O30-C20	-2.01	1.41	1.46
3	E	101	6OU	P23-O26	2.00	1.66	1.59

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	101	6OU	O30-C31-C33	5.40	121.02	111.09
3	G	101	6OU	O30-C31-C33	4.97	120.23	111.09
3	C	1002	6OU	O30-C31-C33	4.46	121.12	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	6OU	O30-C31-C33	4.44	121.08	111.50
3	D	1004	6OU	O18-C16-C15	4.03	121.94	111.38
3	D	1002	6OU	O30-C31-C33	3.98	120.09	111.50
3	D	1001	6OU	O30-C31-C33	3.40	120.28	110.80
3	B	1001	6OU	O30-C31-C33	3.33	120.09	110.80
3	A	1002	6OU	O30-C31-C33	3.24	118.49	111.50
3	A	1002	6OU	O18-C16-C15	3.09	121.61	111.91
3	C	1001	6OU	O30-C31-C33	3.06	119.33	110.80
3	C	1001	6OU	O18-C16-C15	3.03	121.41	111.91
3	D	1001	6OU	O18-C16-C15	2.88	120.96	111.91
3	A	1001	6OU	O18-C16-C15	2.86	120.88	111.91
3	B	1001	6OU	O18-C16-C15	2.85	120.85	111.91
3	A	1001	6OU	O30-C31-C33	2.79	118.57	110.80
3	G	101	6OU	C20-O30-C31	-2.62	113.79	118.31
3	B	1003	6OU	O18-C16-C15	2.48	119.71	111.91
3	D	1002	6OU	O18-C16-C15	2.42	119.51	111.91
3	B	1002	6OU	O18-C16-C15	2.42	119.49	111.91
3	C	1002	6OU	O18-C16-C15	2.27	119.02	111.91

There are no chirality outliers.

All (173) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	6OU	O30-C20-C21-O22
3	A	1002	6OU	C21-O22-P23-O24
3	A	1002	6OU	C21-O22-P23-O25
3	A	1002	6OU	C21-O22-P23-O26
3	A	1002	6OU	C27-O26-P23-O24
3	A	1002	6OU	C27-O26-P23-O25
3	A	1002	6OU	O26-C27-C28-N29
3	A	1003	6OU	C20-C19-O18-C16
3	A	1003	6OU	O18-C19-C20-C21
3	A	1003	6OU	C21-O22-P23-O24
3	A	1003	6OU	C21-O22-P23-O25
3	A	1003	6OU	O26-C27-C28-N29
3	B	1001	6OU	C21-O22-P23-O24
3	B	1001	6OU	C21-O22-P23-O25
3	B	1001	6OU	C21-O22-P23-O26
3	B	1002	6OU	C27-O26-P23-O25
3	B	1002	6OU	C28-C27-O26-P23
3	B	1002	6OU	C33-C31-O30-C20
3	B	1003	6OU	C27-O26-P23-O22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	1003	6OU	C27-O26-P23-O24
3	B	1003	6OU	C27-O26-P23-O25
3	B	1003	6OU	O26-C27-C28-N29
3	C	1001	6OU	C21-O22-P23-O26
3	C	1002	6OU	C21-O22-P23-O25
3	C	1002	6OU	C27-O26-P23-O24
3	C	1002	6OU	C27-O26-P23-O25
3	C	1002	6OU	O26-C27-C28-N29
3	C	1002	6OU	C33-C31-O30-C20
3	D	1002	6OU	C19-C20-O30-C31
3	D	1002	6OU	C33-C31-O30-C20
3	D	1003	6OU	O18-C19-C20-C21
3	D	1003	6OU	O18-C19-C20-O30
3	D	1003	6OU	C27-O26-P23-O24
3	D	1003	6OU	C27-O26-P23-O25
3	D	1004	6OU	C15-C16-O18-C19
3	D	1004	6OU	O17-C16-O18-C19
3	D	1004	6OU	O18-C19-C20-C21
3	D	1004	6OU	O26-C27-C28-N29
3	D	1005	6OU	C21-O22-P23-O24
3	D	1005	6OU	C21-O22-P23-O25
3	D	1005	6OU	C21-O22-P23-O26
3	D	1005	6OU	C27-O26-P23-O22
3	D	1005	6OU	C27-O26-P23-O24
3	D	1005	6OU	C27-O26-P23-O25
3	D	1005	6OU	O26-C27-C28-N29
3	E	101	6OU	C21-O22-P23-O24
3	E	101	6OU	C27-O26-P23-O24
3	E	101	6OU	C27-O26-P23-O25
3	F	101	6OU	C21-O22-P23-O25
3	F	101	6OU	C27-O26-P23-O22
3	F	101	6OU	C27-O26-P23-O24
3	F	101	6OU	O26-C27-C28-N29
3	G	101	6OU	C21-O22-P23-O24
3	G	101	6OU	C21-O22-P23-O25
3	G	101	6OU	O26-C27-C28-N29
3	G	101	6OU	O32-C31-O30-C20
3	G	101	6OU	C33-C31-O30-C20
3	B	1002	6OU	O32-C31-O30-C20
3	C	1002	6OU	O32-C31-O30-C20
3	D	1002	6OU	O32-C31-O30-C20
3	A	1003	6OU	C15-C16-O18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1003	6OU	O18-C19-C20-O30
3	D	1004	6OU	O18-C19-C20-O30
3	B	1002	6OU	C34-C35-C36-C37
3	A	1002	6OU	C33-C31-O30-C20
3	D	1001	6OU	C13-C14-C15-C16
3	C	1002	6OU	C34-C35-C36-C37
3	A	1002	6OU	C31-C33-C34-C35
3	C	1002	6OU	C31-C33-C34-C35
3	D	1002	6OU	C31-C33-C34-C35
3	A	1003	6OU	O17-C16-O18-C19
3	B	1002	6OU	C31-C33-C34-C35
3	A	1002	6OU	O32-C31-O30-C20
3	B	1003	6OU	O18-C19-C20-O30
3	A	1002	6OU	C27-O26-P23-O22
3	A	1003	6OU	C21-O22-P23-O26
3	A	1003	6OU	C27-O26-P23-O22
3	B	1002	6OU	C21-O22-P23-O26
3	B	1002	6OU	C27-O26-P23-O22
3	C	1002	6OU	C21-O22-P23-O26
3	C	1002	6OU	C27-O26-P23-O22
3	D	1002	6OU	C21-O22-P23-O26
3	D	1003	6OU	C27-O26-P23-O22
3	E	101	6OU	C21-O22-P23-O26
3	G	101	6OU	C21-O22-P23-O26
3	B	1002	6OU	C19-C20-O30-C31
3	C	1002	6OU	C19-C20-O30-C31
3	A	1002	6OU	C33-C34-C35-C36
3	A	1001	6OU	C10-C11-C12-C13
3	C	1001	6OU	C13-C14-C15-C16
3	D	1001	6OU	C10-C11-C12-C13
3	B	1001	6OU	C19-C20-C21-O22
3	B	1002	6OU	C35-C36-C37-C38
3	B	1001	6OU	O18-C19-C20-C21
3	B	1001	6OU	C13-C14-C15-C16
3	D	1002	6OU	C33-C34-C35-C36
3	C	1002	6OU	C13-C14-C15-C16
3	A	1002	6OU	C34-C35-C36-C37
3	C	1001	6OU	C33-C31-O30-C20
3	D	1001	6OU	C33-C31-O30-C20
3	C	1001	6OU	O32-C31-O30-C20
3	D	1001	6OU	O32-C31-O30-C20
3	A	1001	6OU	C19-C20-C21-O22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	1001	6OU	C10-C11-C12-C13
3	A	1001	6OU	C33-C31-O30-C20
3	D	1005	6OU	C19-C20-C21-O22
3	B	1002	6OU	C13-C14-C15-C16
3	D	1002	6OU	C15-C16-O18-C19
3	C	1001	6OU	C08-C09-C10-C11
3	A	1002	6OU	C15-C16-O18-C19
3	A	1002	6OU	C19-C20-C21-O22
3	B	1002	6OU	C19-C20-C21-O22
3	A	1001	6OU	O32-C31-O30-C20
3	D	1002	6OU	C34-C35-C36-C37
3	D	1002	6OU	O17-C16-O18-C19
3	A	1001	6OU	O30-C20-C21-O22
3	B	1001	6OU	O30-C20-C21-O22
3	D	1003	6OU	C19-C20-C21-O22
3	B	1001	6OU	C08-C09-C10-C11
3	D	1003	6OU	C20-C21-O22-P23
3	A	1002	6OU	O17-C16-O18-C19
3	D	1002	6OU	O30-C31-C33-C34
3	C	1002	6OU	C19-C20-C21-O22
3	D	1002	6OU	C19-C20-C21-O22
3	A	1002	6OU	C19-C20-O30-C31
3	D	1001	6OU	O18-C19-C20-C21
3	G	101	6OU	C20-C21-O22-P23
3	B	1002	6OU	O30-C20-C21-O22
3	D	1003	6OU	C20-C19-O18-C16
3	A	1002	6OU	C35-C36-C37-C38
3	B	1002	6OU	C36-C37-C38-C39
3	A	1003	6OU	C27-O26-P23-O24
3	B	1002	6OU	C21-O22-P23-O25
3	B	1003	6OU	C21-O22-P23-O25
3	C	1002	6OU	C21-O22-P23-O24
3	D	1002	6OU	C21-O22-P23-O24
3	E	101	6OU	C21-O22-P23-O25
3	D	1001	6OU	C19-C20-C21-O22
3	G	101	6OU	C28-C27-O26-P23
3	C	1001	6OU	O30-C20-C21-O22
3	C	1002	6OU	O30-C20-C21-O22
3	D	1001	6OU	O30-C20-C21-O22
3	D	1003	6OU	O30-C20-C21-O22
3	B	1002	6OU	O30-C31-C33-C34
3	B	1001	6OU	O18-C19-C20-O30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	1002	6OU	O30-C31-C33-C34
3	A	1001	6OU	O17-C16-O18-C19
3	B	1003	6OU	O17-C16-O18-C19
3	B	1001	6OU	C19-C20-O30-C31
3	A	1003	6OU	C20-C21-O22-P23
3	B	1003	6OU	C15-C16-O18-C19
3	B	1001	6OU	C10-C11-C12-C13
3	D	1002	6OU	C27-O26-P23-O22
3	D	1004	6OU	C21-O22-P23-O26
3	D	1004	6OU	C27-O26-P23-O22
3	A	1003	6OU	C19-C20-C21-O22
3	A	1001	6OU	C15-C16-O18-C19
3	A	1002	6OU	O18-C19-C20-O30
3	C	1002	6OU	C36-C37-C38-C39
3	D	1001	6OU	C08-C09-C10-C11
3	B	1003	6OU	O18-C19-C20-C21
3	A	1002	6OU	O30-C31-C33-C34
3	C	1001	6OU	C19-C20-C21-O22
3	D	1002	6OU	C36-C37-C38-C39
3	B	1003	6OU	C19-C20-C21-O22
3	D	1002	6OU	O32-C31-C33-C34
3	D	1002	6OU	C21-O22-P23-O25
3	D	1004	6OU	C27-O26-P23-O24
3	B	1002	6OU	O26-C27-C28-N29
3	B	1001	6OU	C21-C20-O30-C31
3	D	1002	6OU	C28-C27-O26-P23
3	D	1005	6OU	C20-C21-O22-P23
3	A	1003	6OU	O30-C20-C21-O22

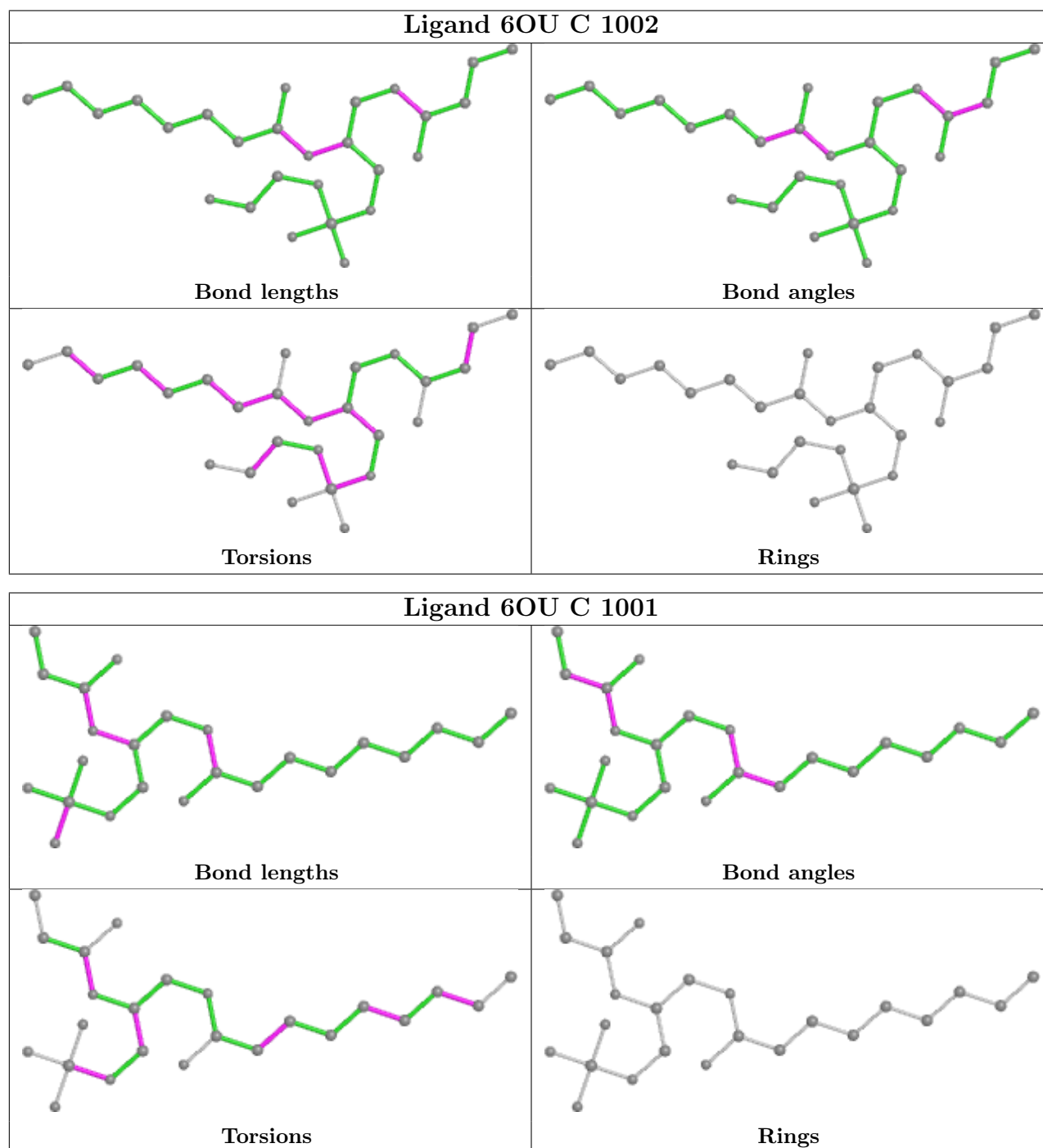
There are no ring outliers.

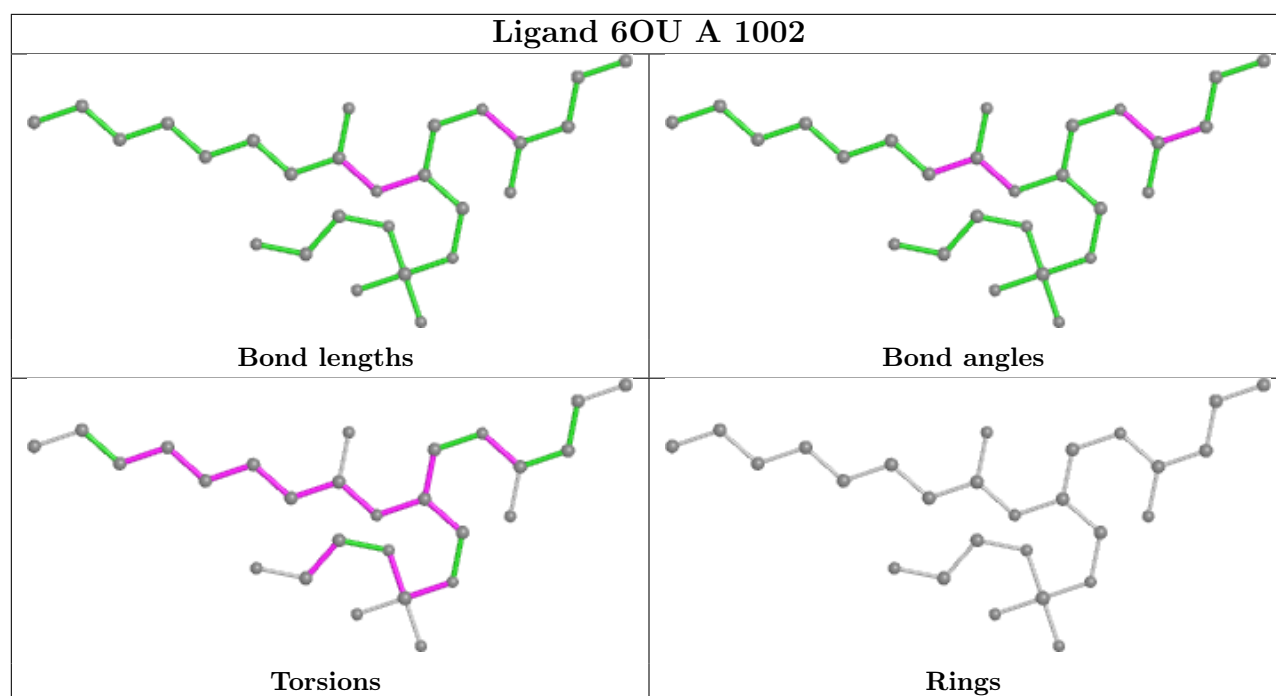
2 monomers are involved in 2 short contacts:

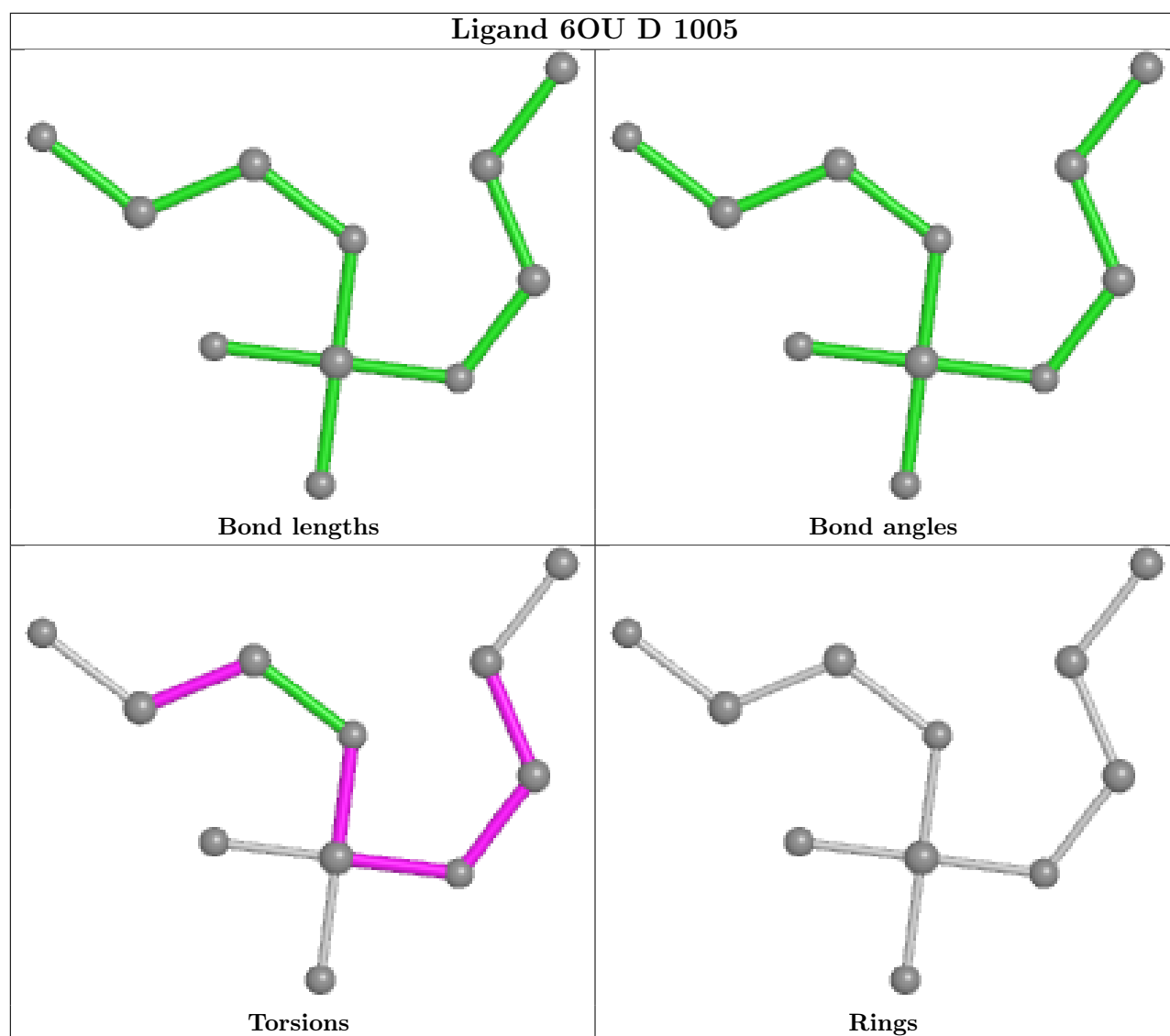
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1001	6OU	1	0
3	A	1001	6OU	1	0

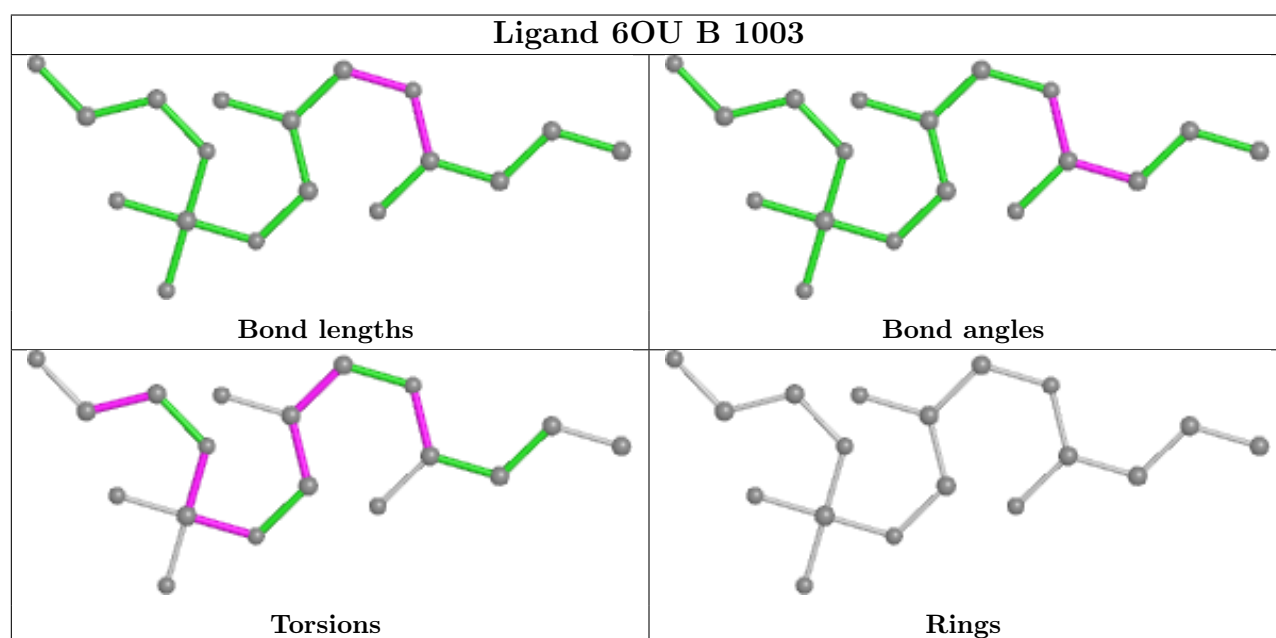
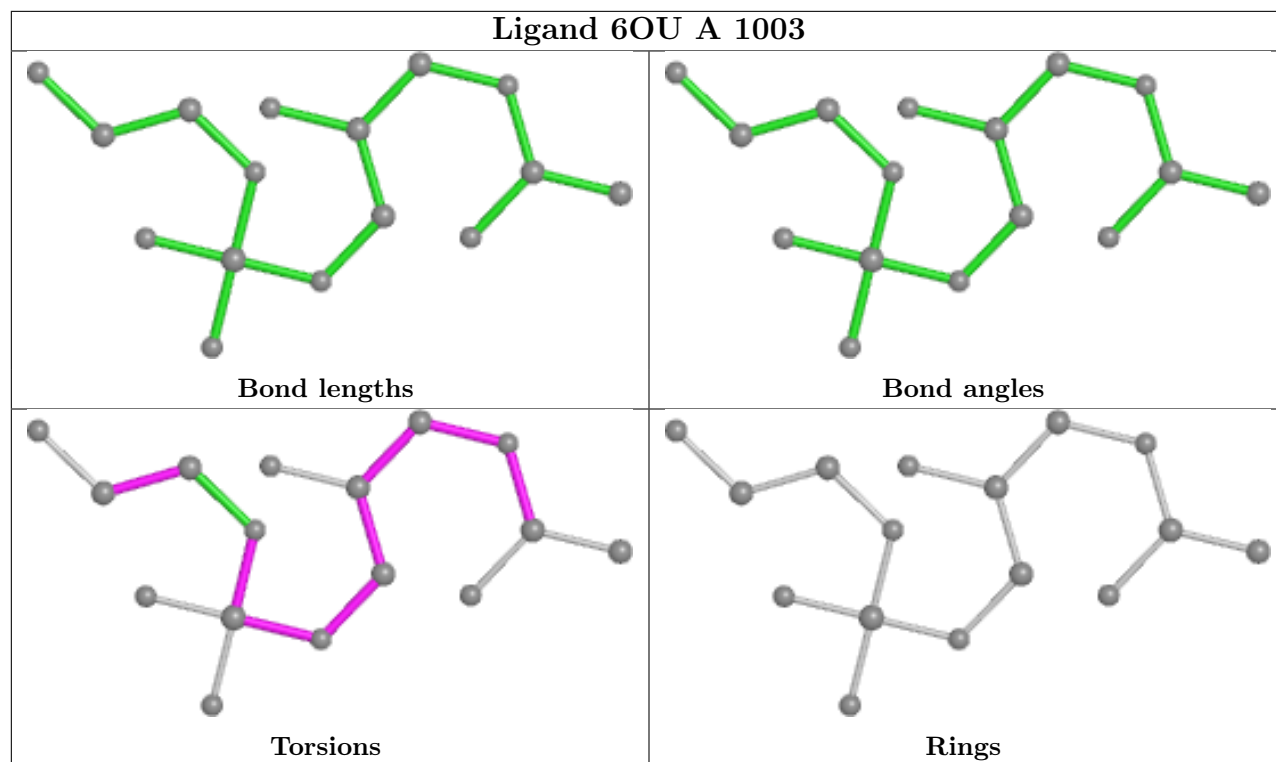
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

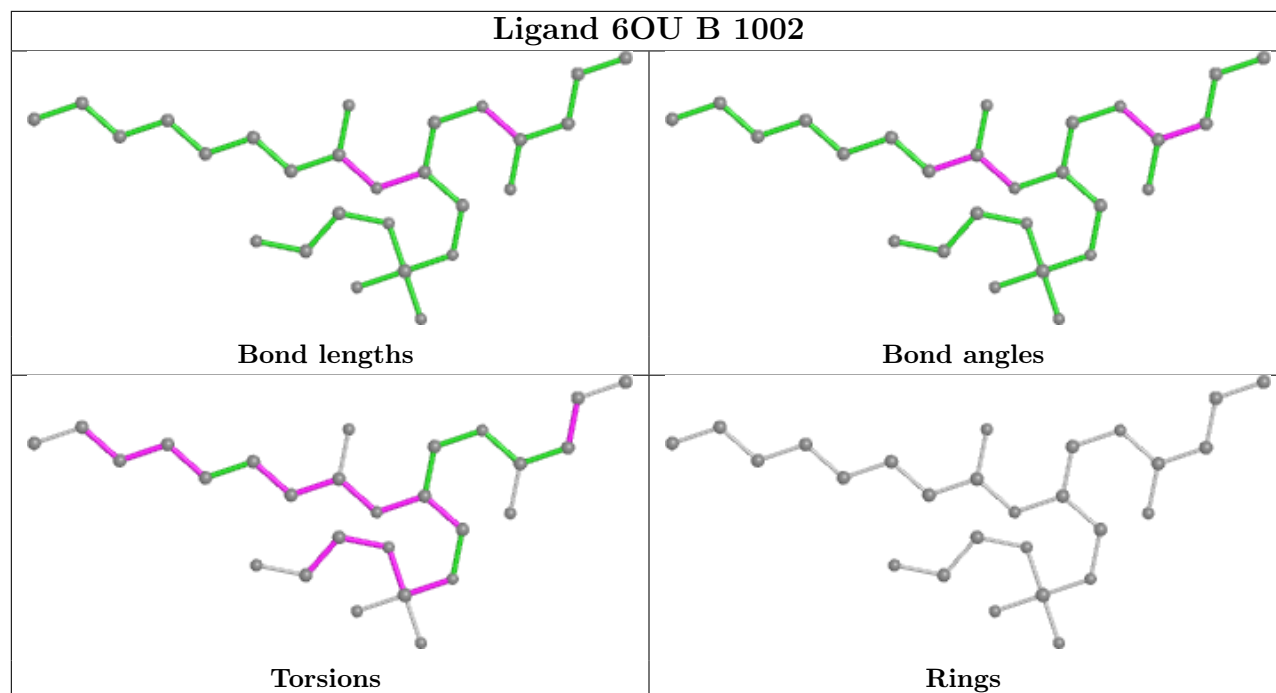




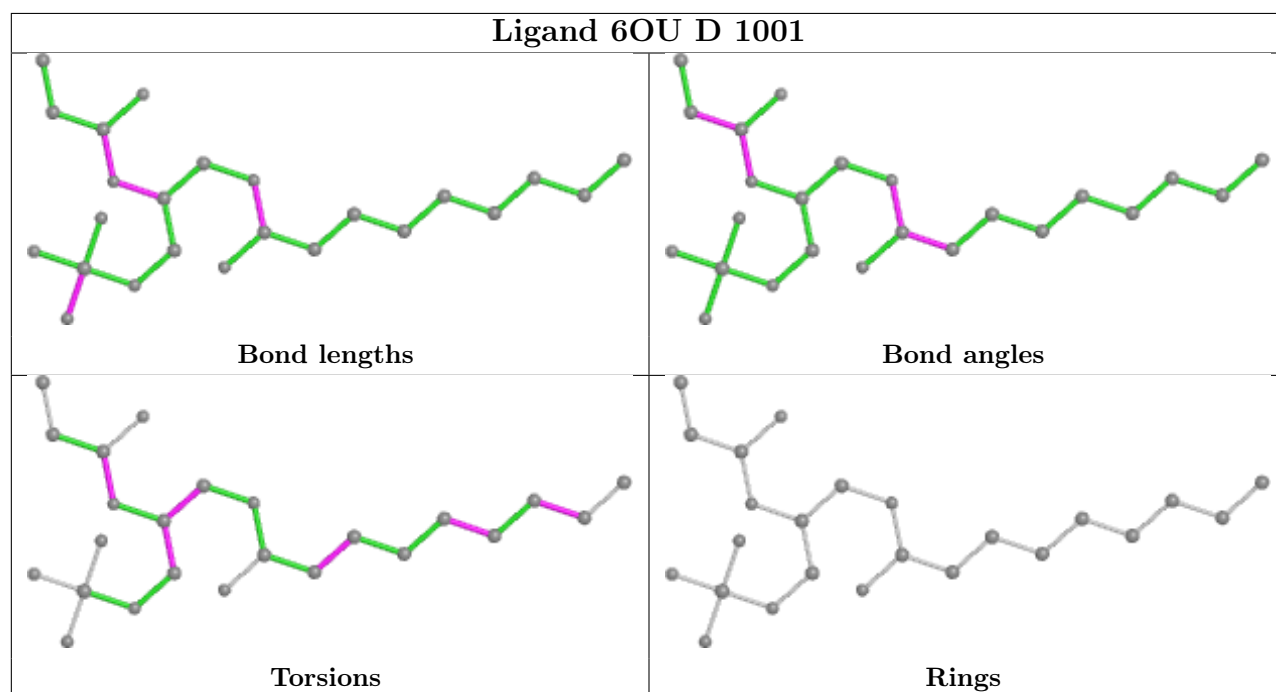


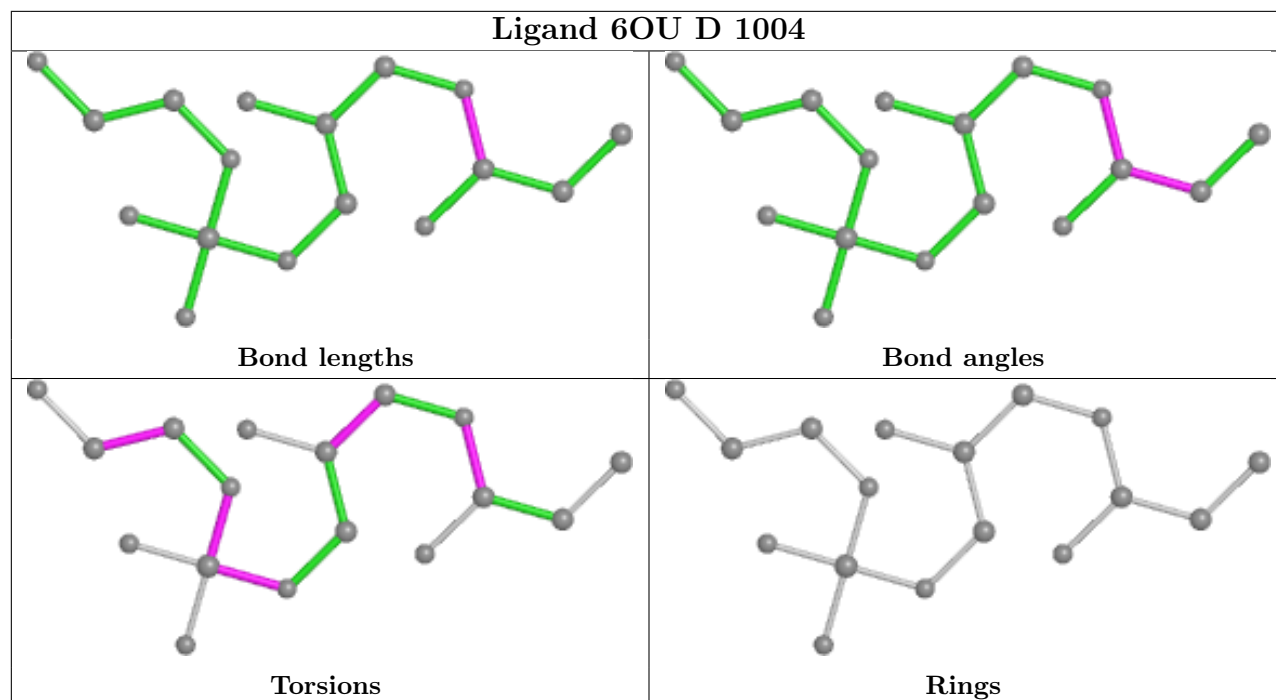


Ligand 6OU B 1002

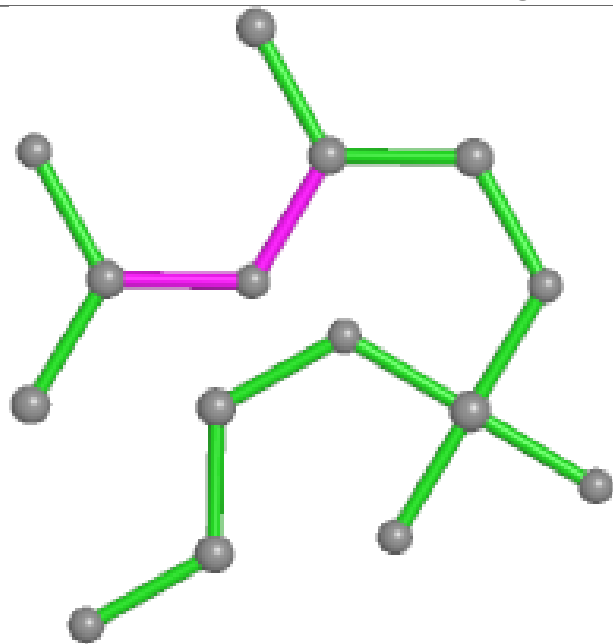


Ligand 6OU D 1001

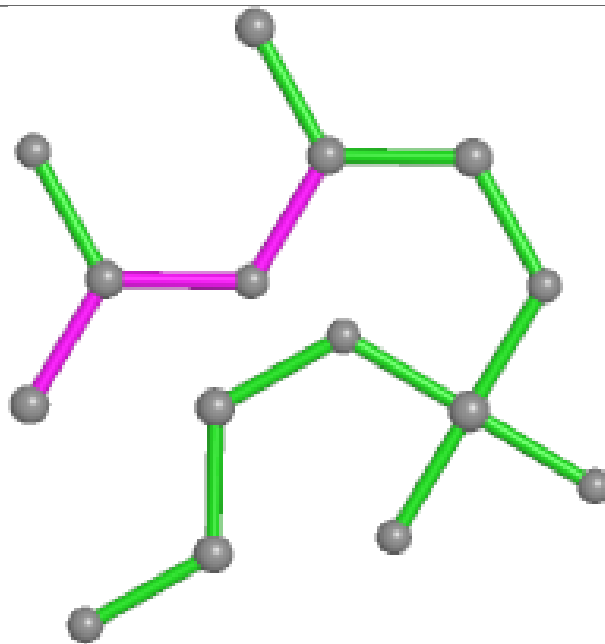




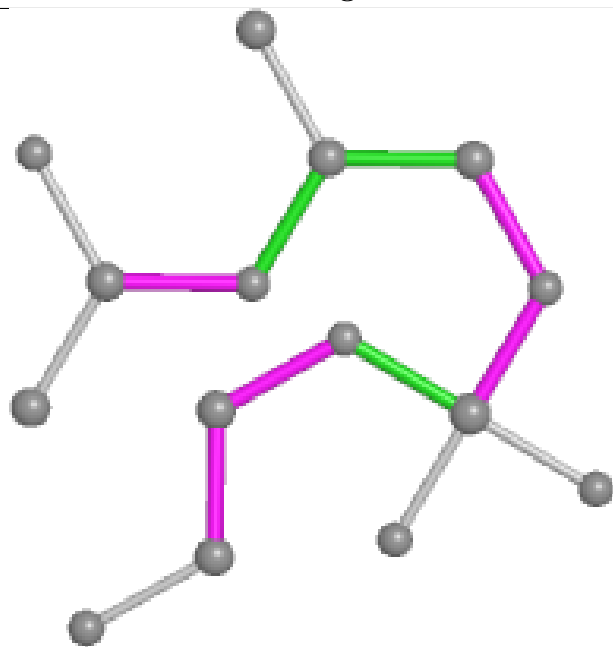
Ligand 6OU G 101



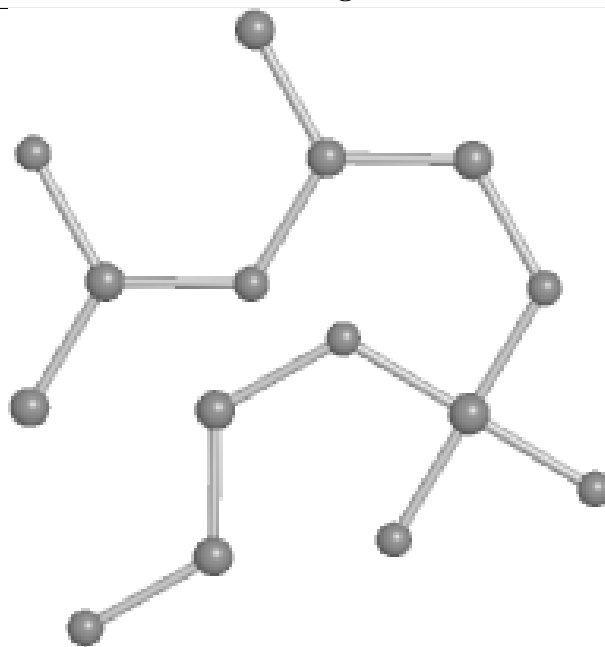
Bond lengths



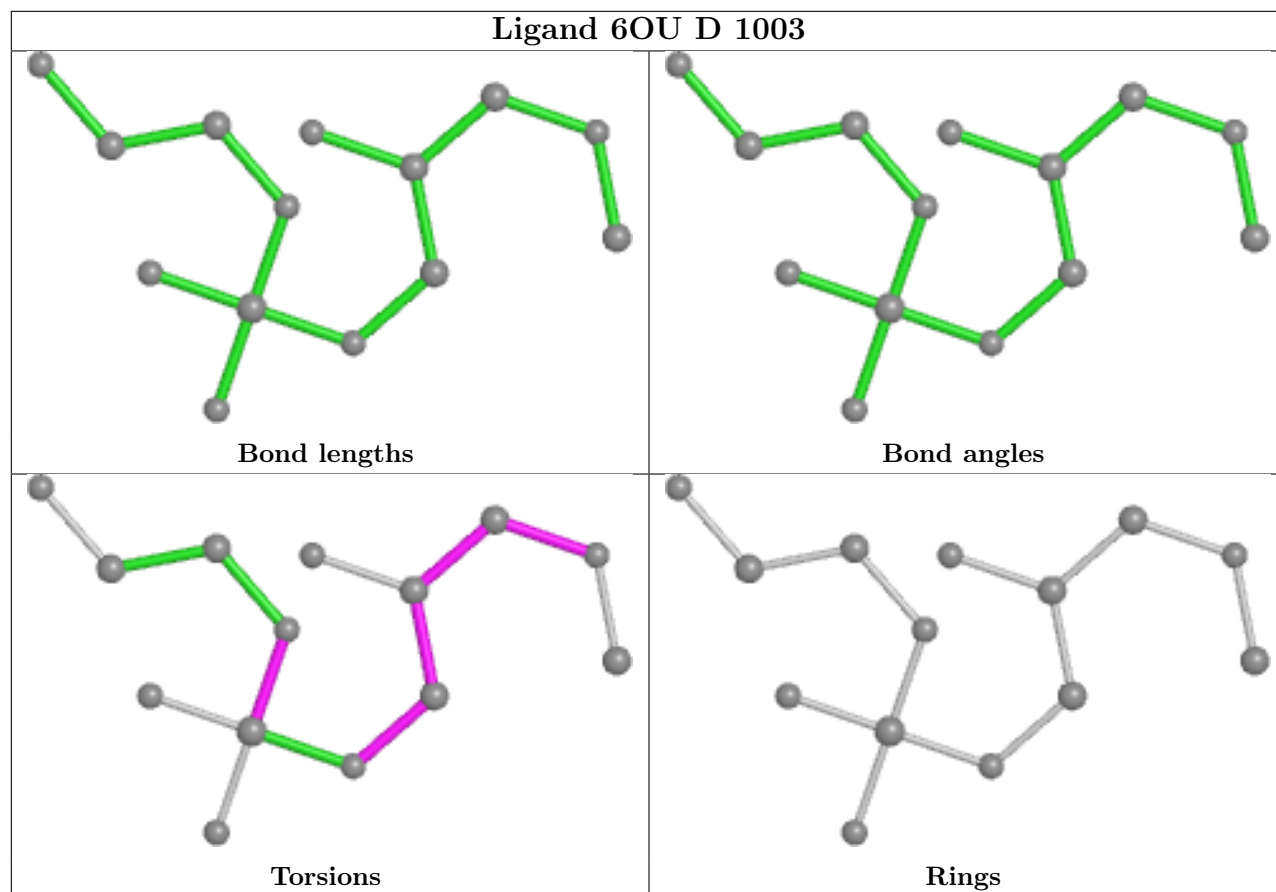
Bond angles



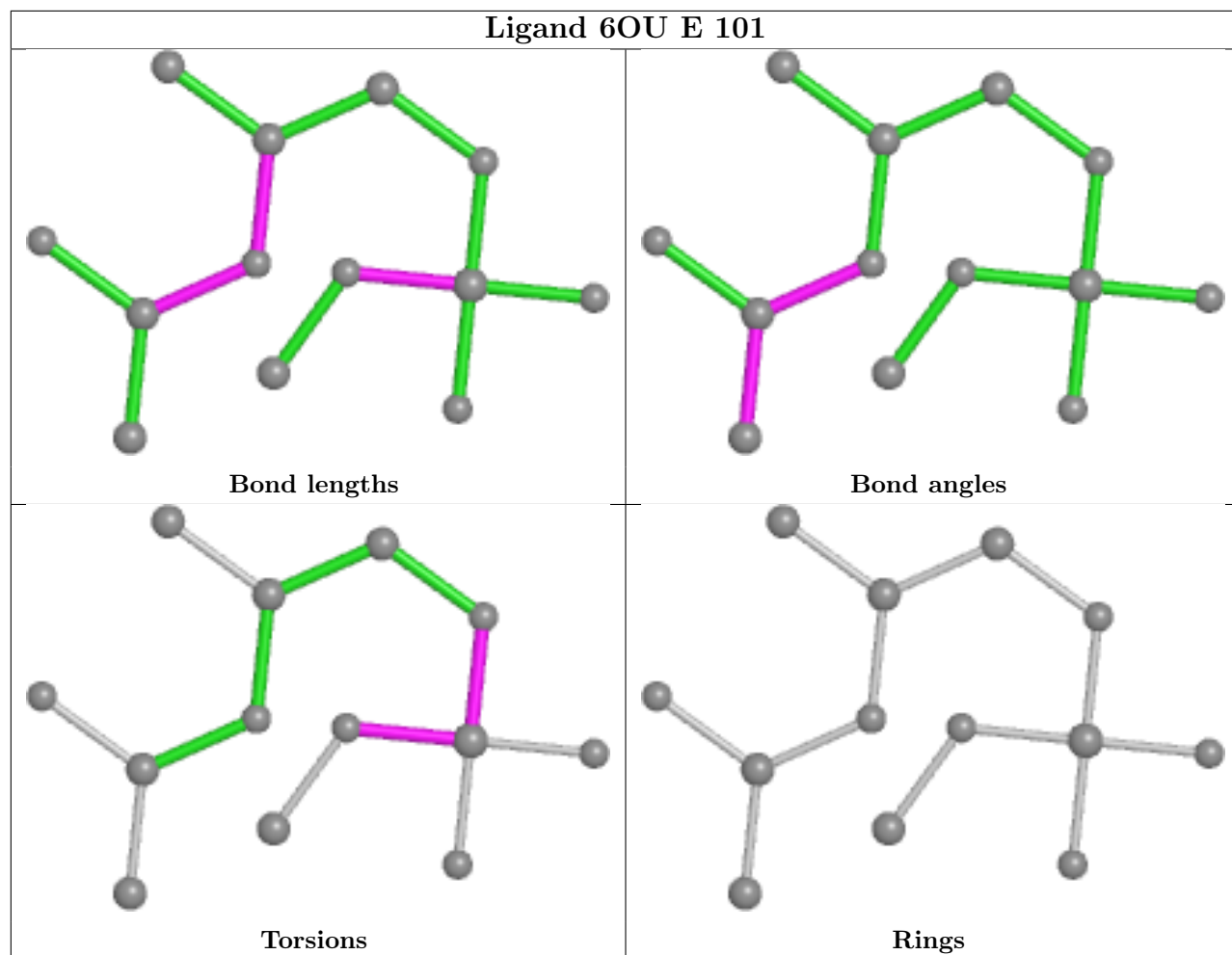
Torsions



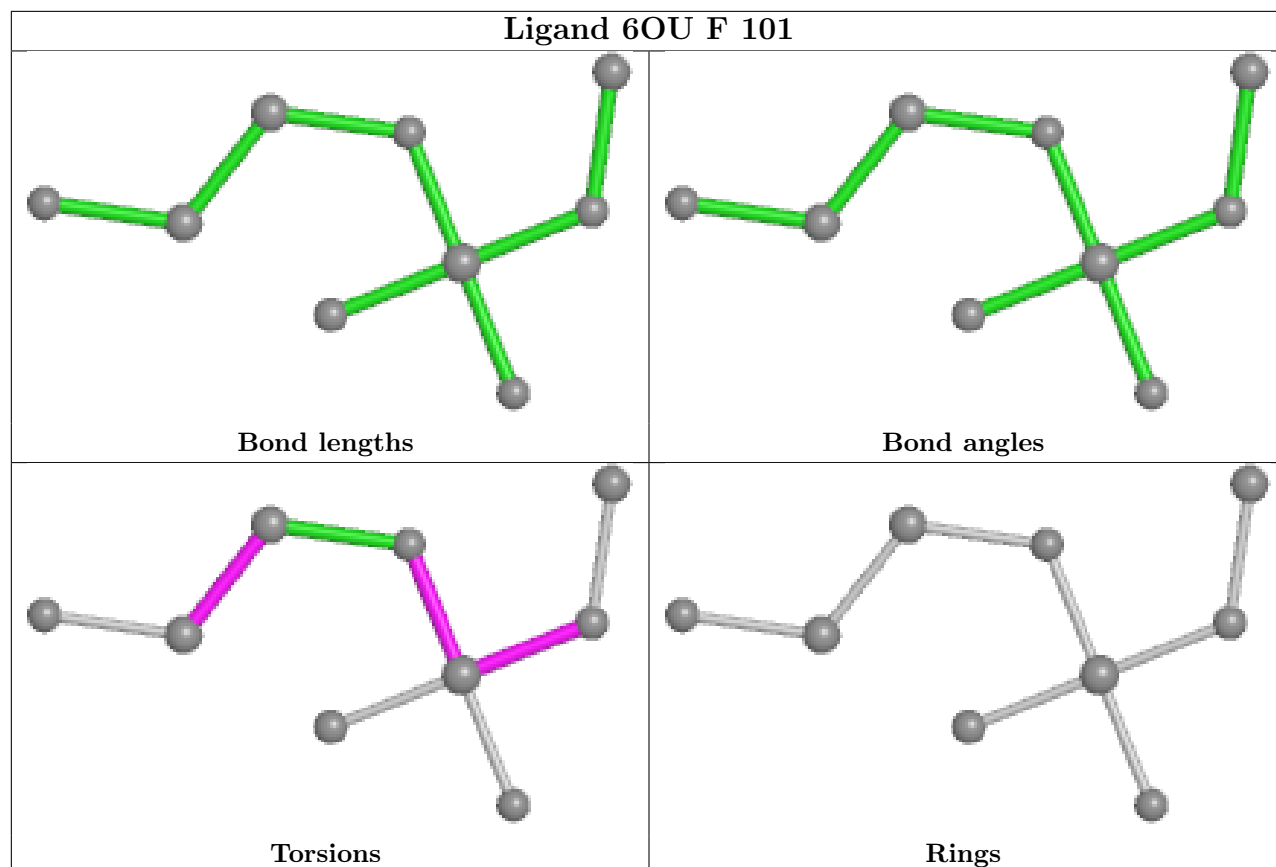
Rings



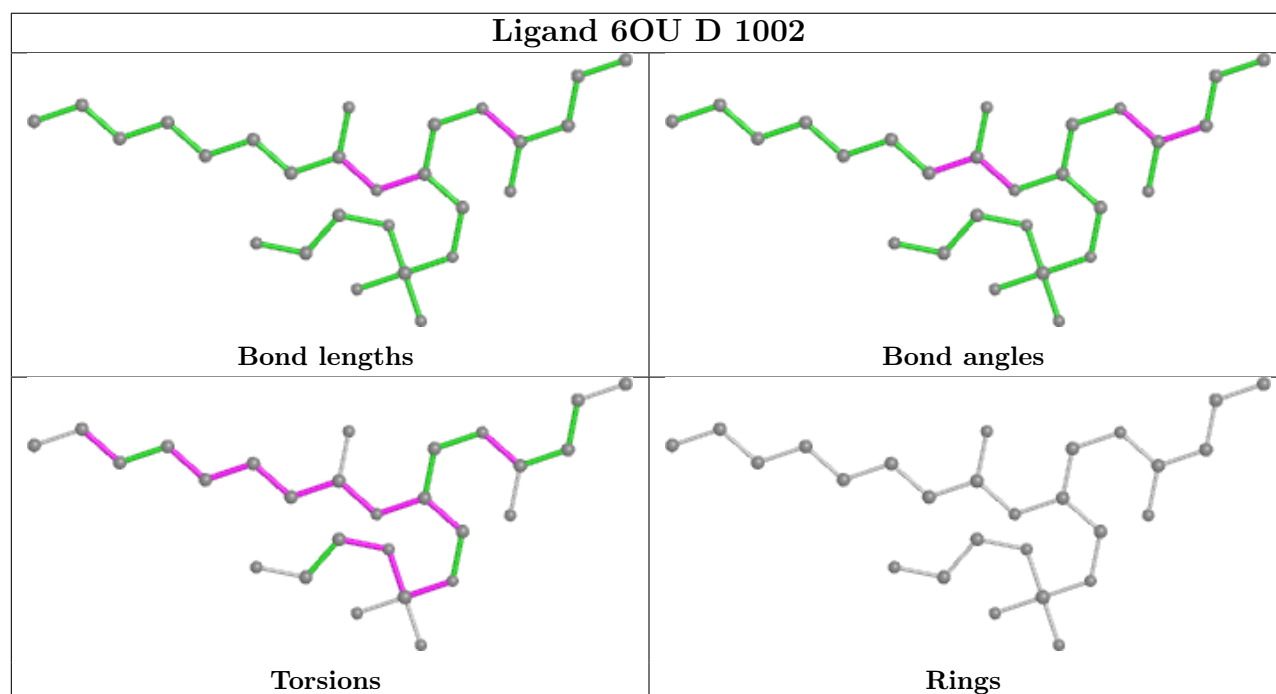
Ligand 6OU E 101

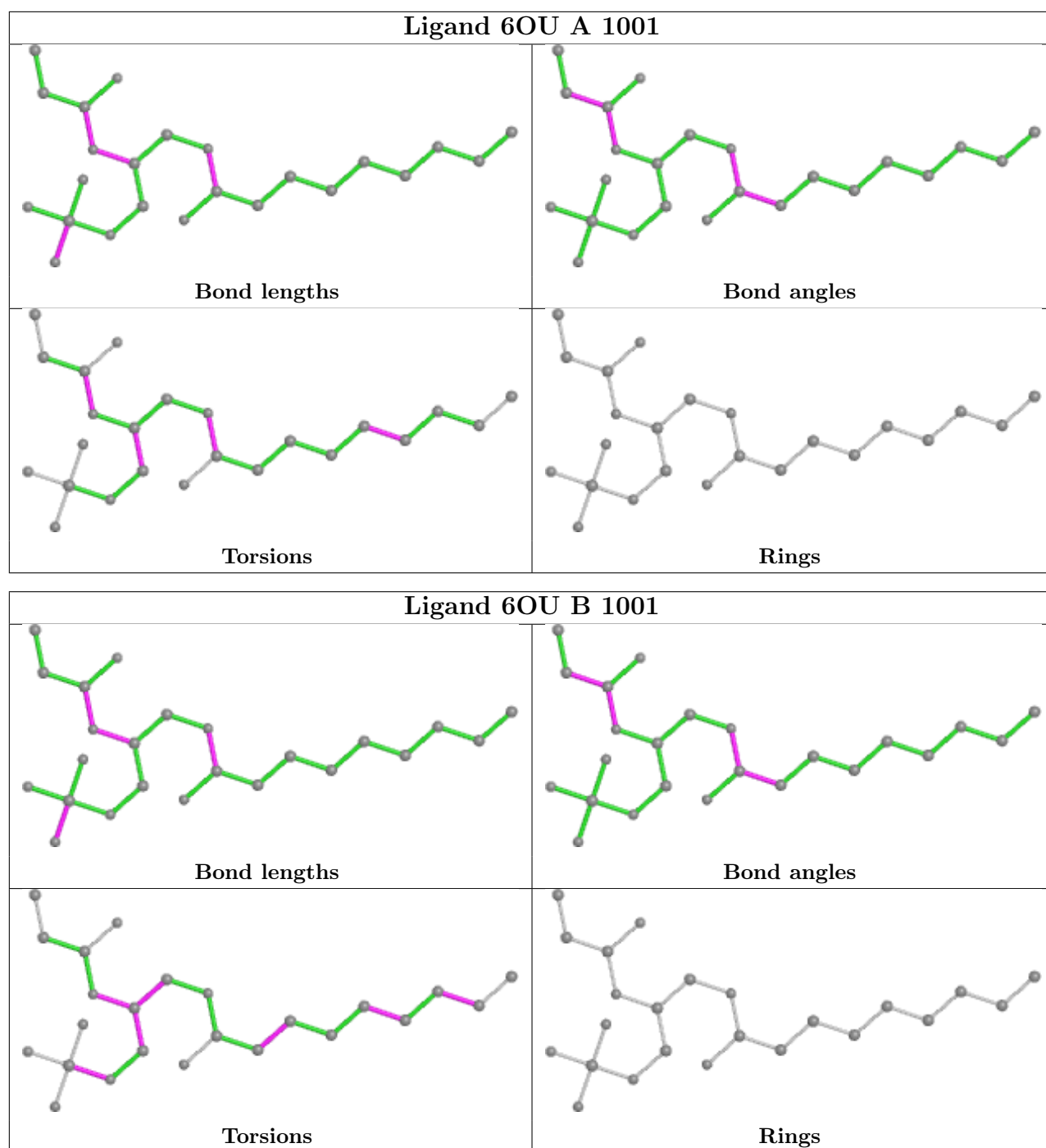


Ligand 6OU F 101



Ligand 6OU D 1002





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	225/288 (78%)	-0.43	3 (1%) 77 65	48, 121, 219, 285	0
1	B	225/288 (78%)	-0.51	1 (0%) 92 87	40, 126, 197, 276	0
1	C	226/288 (78%)	-0.49	1 (0%) 92 87	41, 117, 190, 262	0
1	D	225/288 (78%)	-0.41	3 (1%) 77 65	34, 120, 206, 274	0
2	E	30/30 (100%)	0.39	4 (13%) 3 3	86, 208, 268, 293	0
2	F	30/30 (100%)	1.02	5 (16%) 1 1	103, 230, 318, 377	0
2	G	30/30 (100%)	0.52	5 (16%) 1 1	121, 217, 265, 272	0
2	H	30/30 (100%)	0.50	5 (16%) 1 1	109, 221, 266, 284	0
All	All	1021/1272 (80%)	-0.34	27 (2%) 56 42	34, 130, 240, 377	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1	TYR	18.0
2	E	1	TYR	11.9
2	G	2	CYS	9.2
2	F	2	CYS	7.9
1	A	943	ASP	5.9
2	H	1	TYR	5.8
1	C	945	MET	5.7
2	E	2	CYS	4.9
2	G	14	LYS	4.2
1	D	942	VAL	4.1
2	G	1	TYR	3.7
1	B	942	VAL	3.7
1	A	944	ALA	3.4
2	H	8	THR	3.3
2	F	12	GLU	3.3
2	G	11	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	14	LYS	3.1
2	F	13	ARG	3.0
2	G	17	GLU	2.7
2	H	2	CYS	2.6
1	A	808	LEU	2.6
1	D	817	GLU	2.5
2	H	3	GLN	2.5
2	E	3	GLN	2.4
2	H	6	MET	2.3
2	F	3	GLN	2.2
1	D	943	ASP	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(\AA^2)	Q<0.9
3	6OU	E	101	13/49	0.64	0.52	134,181,291,318	0
3	6OU	D	1005	11/49	0.66	0.86	129,194,338,351	0
3	6OU	A	1002	27/49	0.72	0.22	62,151,197,230	0
3	6OU	F	101	9/49	0.72	0.24	125,183,312,330	0
3	6OU	C	1002	27/49	0.74	0.25	42,161,191,220	0
3	6OU	G	101	15/49	0.75	0.40	153,203,290,293	0
3	6OU	D	1002	27/49	0.77	0.24	35,150,204,281	0
3	6OU	D	1004	17/49	0.84	0.19	75,105,178,210	0
3	6OU	B	1002	27/49	0.85	0.20	52,100,150,177	0
3	6OU	A	1003	16/49	0.87	0.16	74,109,213,219	0
3	6OU	B	1003	18/49	0.88	0.15	34,142,217,261	0
3	6OU	D	1001	24/49	0.88	0.23	55,93,118,180	0

Continued on next page...

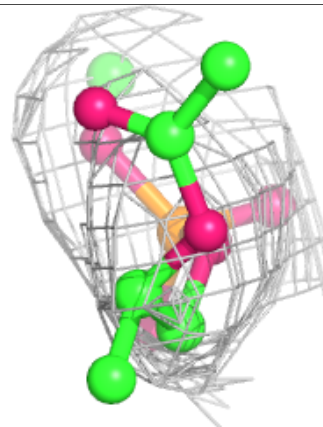
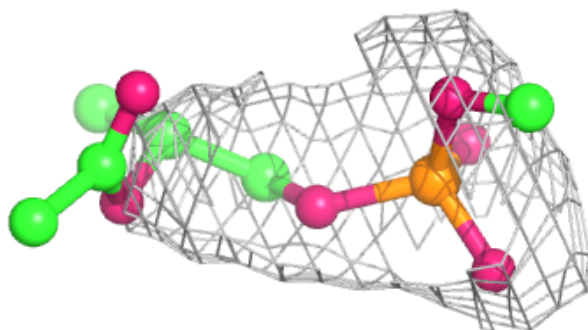
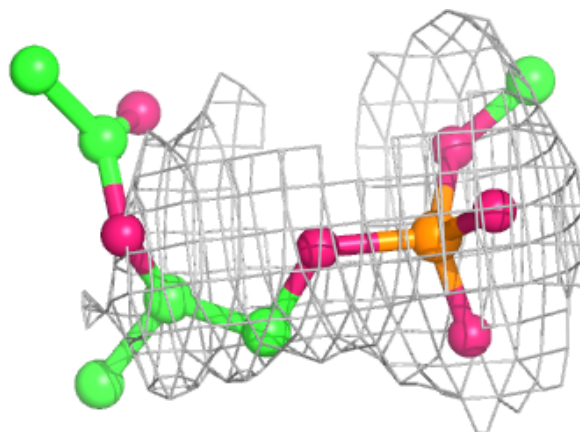
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	6OU	D	1003	14/49	0.89	0.13	29,127,176,188	0
3	6OU	B	1001	24/49	0.89	0.26	23,77,144,196	0
3	6OU	C	1001	24/49	0.90	0.27	59,87,132,202	0
3	6OU	A	1001	24/49	0.91	0.19	47,77,103,196	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.

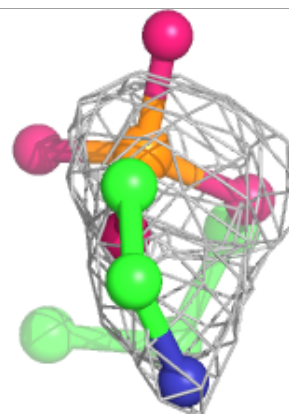
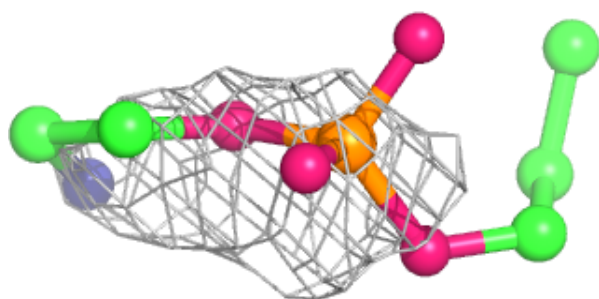
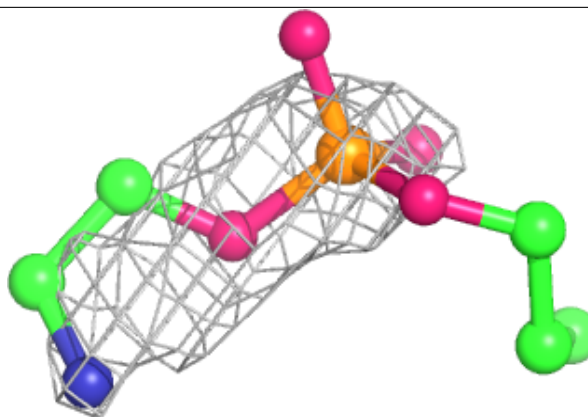
Electron density around 6OU E 101:

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

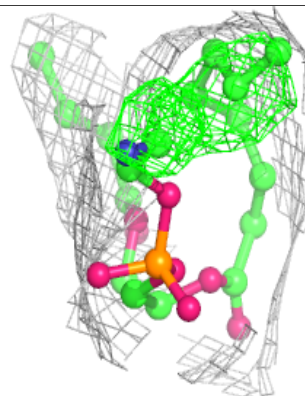
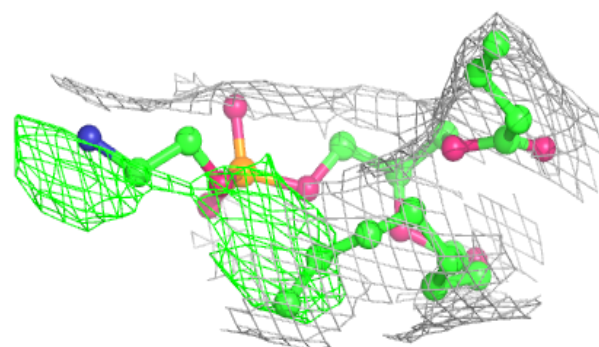
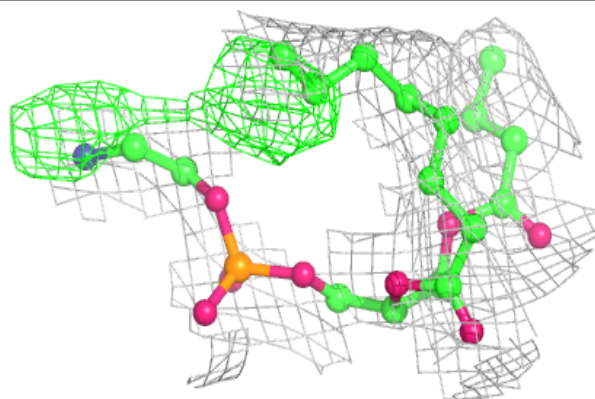


Electron density around 6OU D 1005:

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

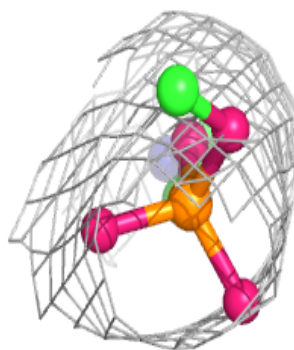
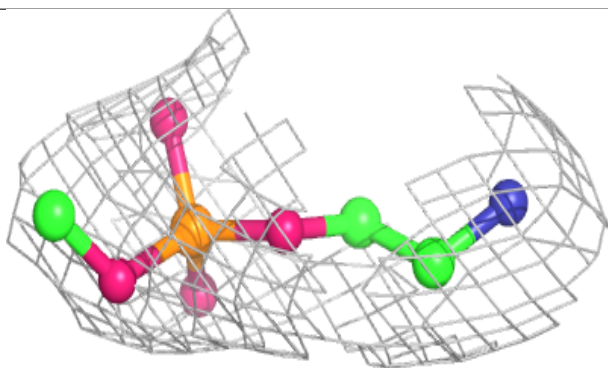
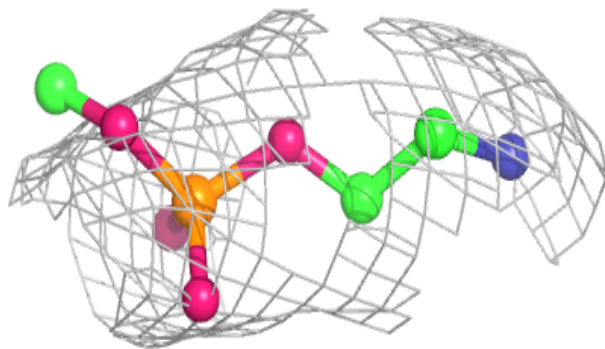
**Electron density around 6OU A 1002:**

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

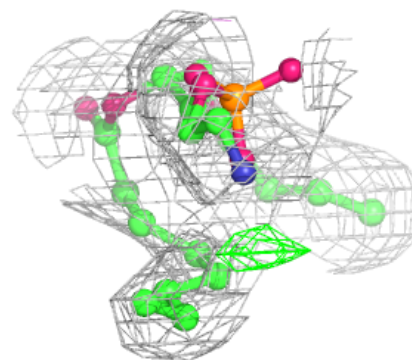
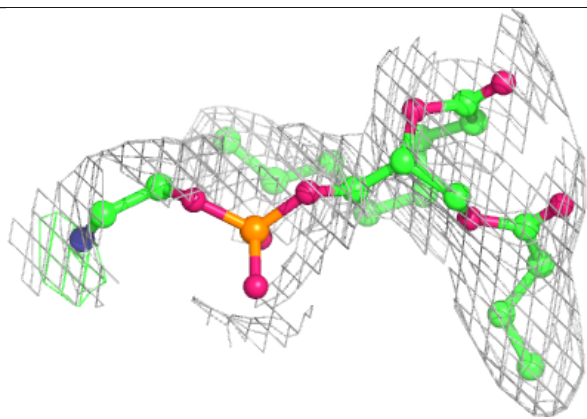
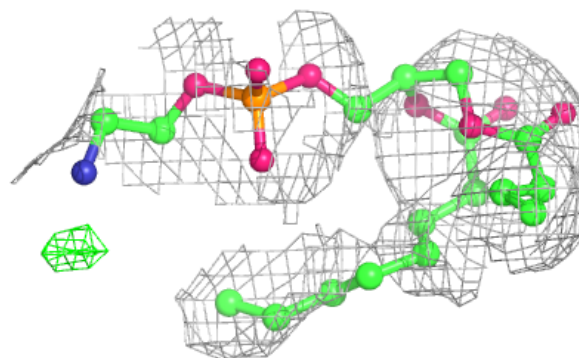


Electron density around 6OU F 101:

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

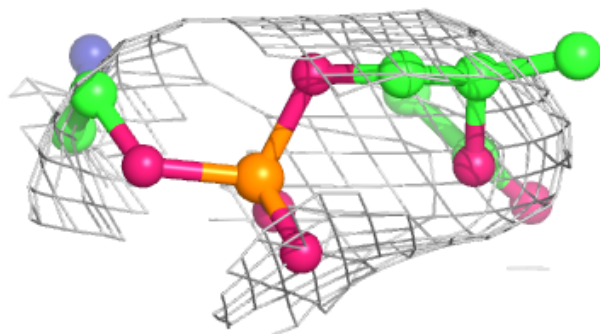
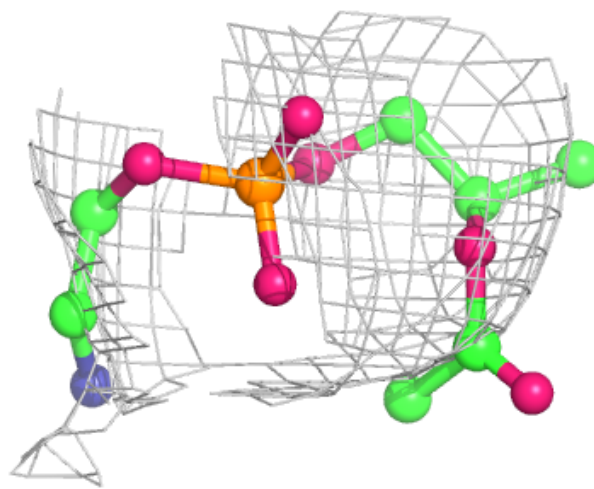
**Electron density around 6OU C 1002:**

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



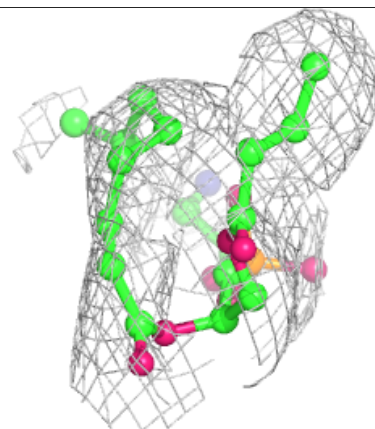
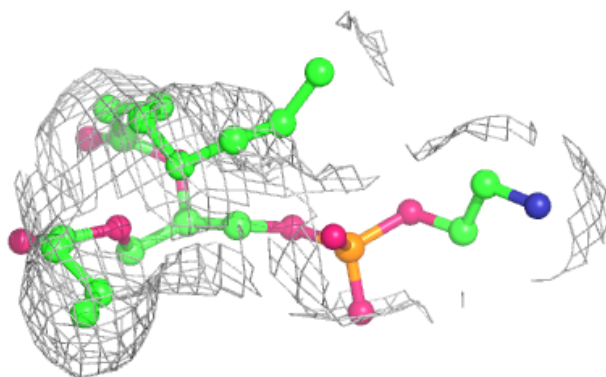
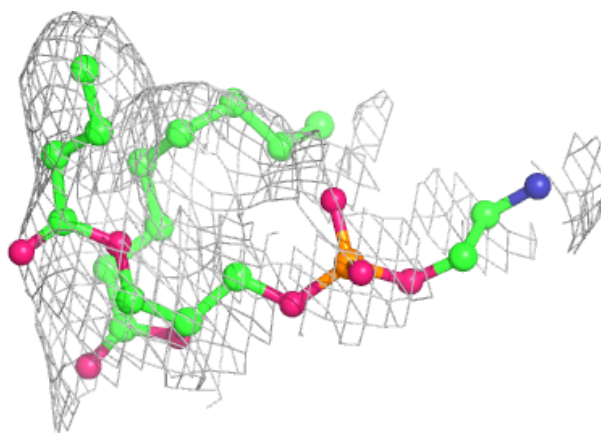
Electron density around 6OU G 101:

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

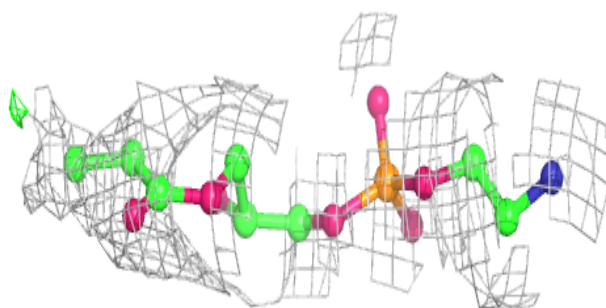
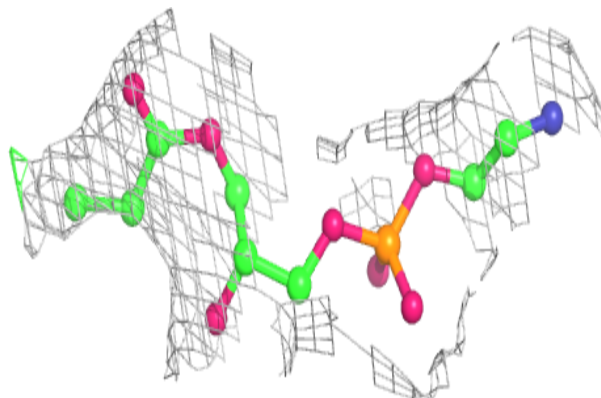


Electron density around 6OU D 1002:

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

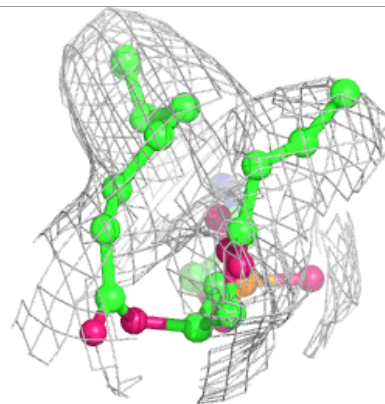
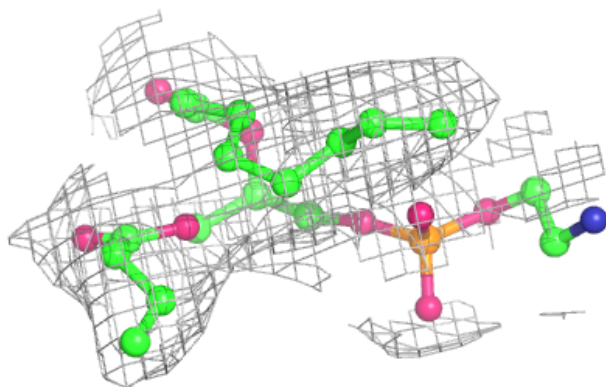
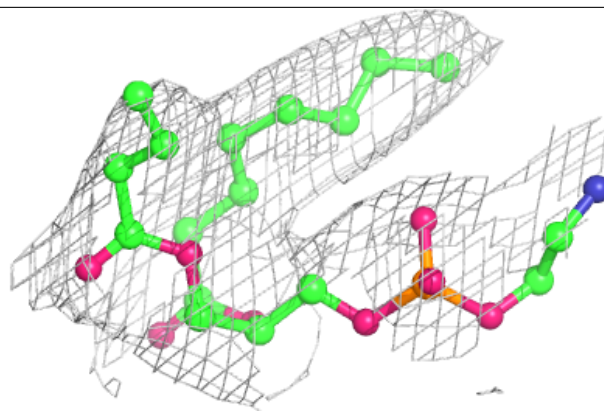
**Electron density around 6OU D 1004:**

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

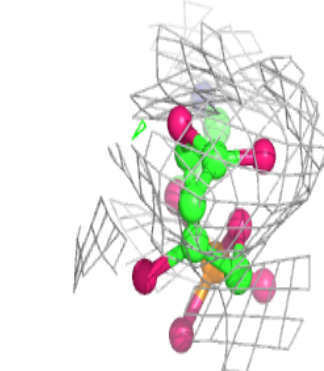
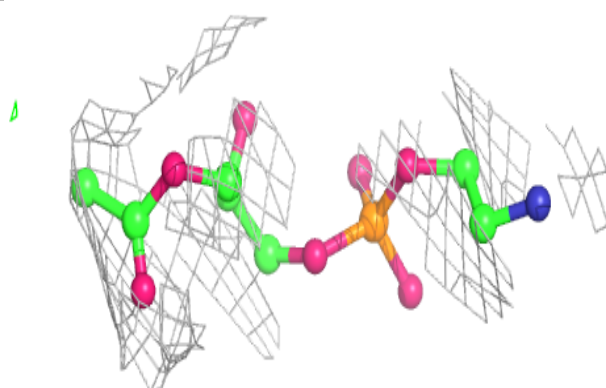
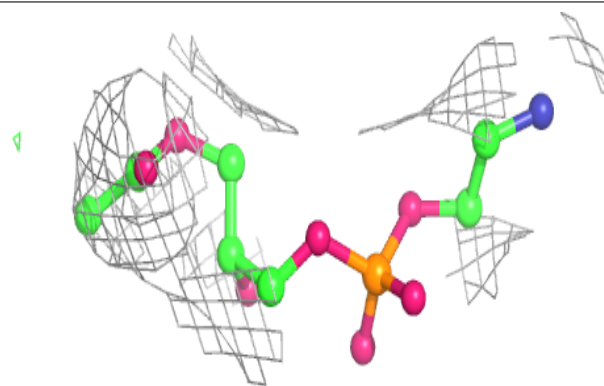


Electron density around 6OU B 1002:

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

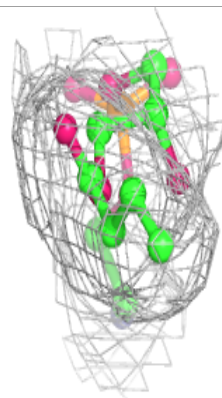
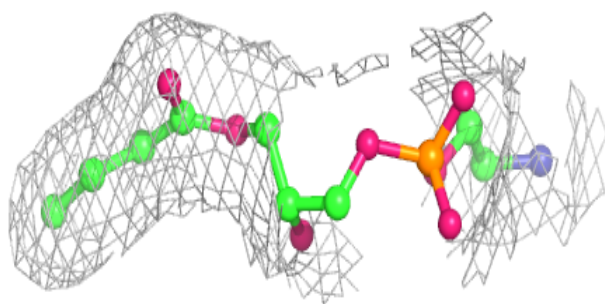
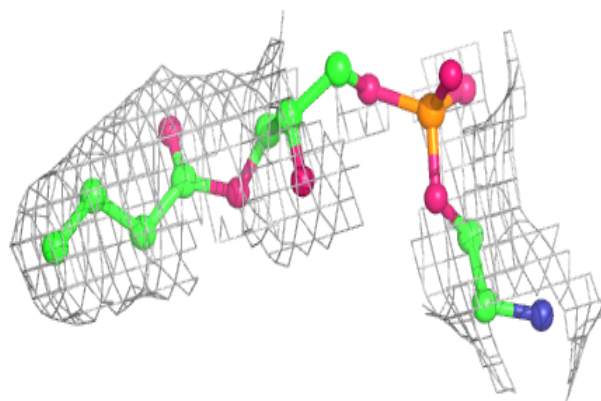
**Electron density around 6OU A 1003:**

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

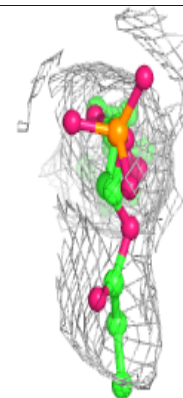
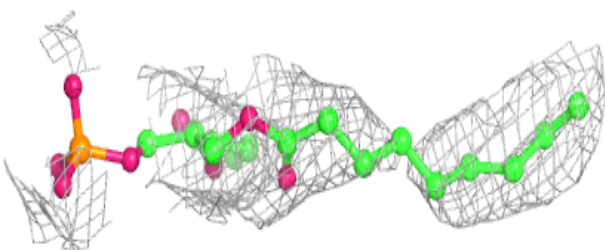
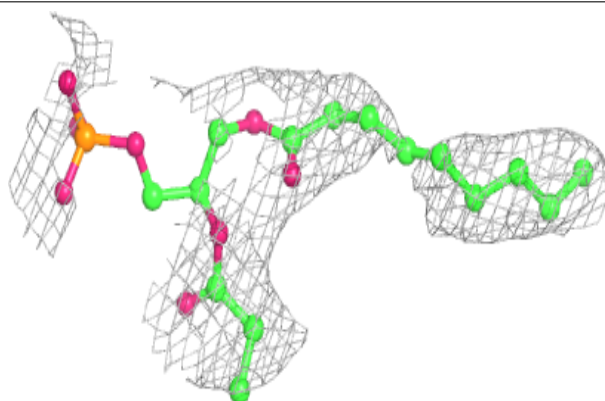


Electron density around 6OU B 1003:

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

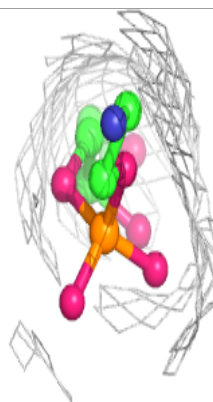
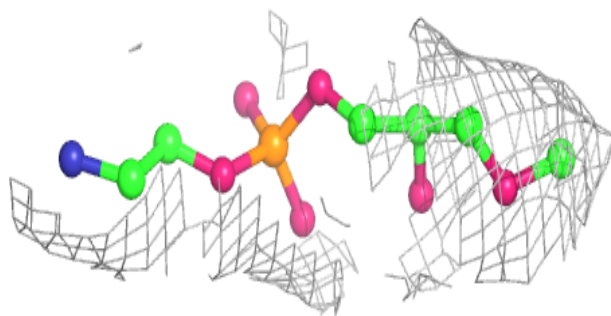
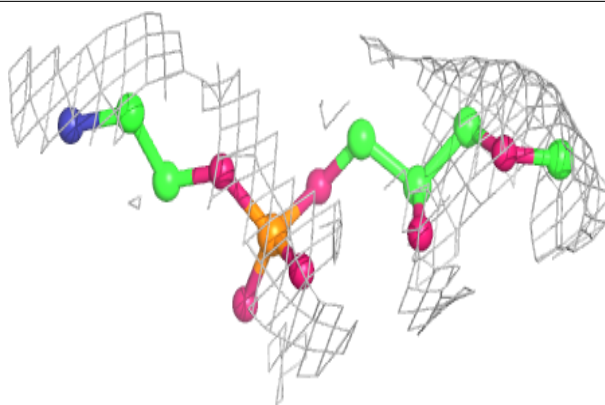
**Electron density around 6OU D 1001:**

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

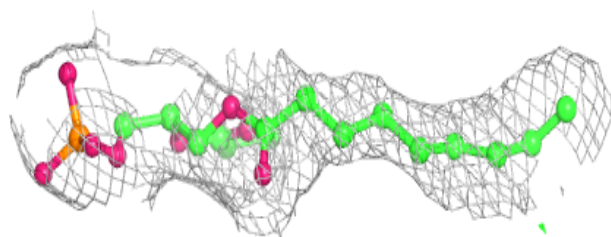
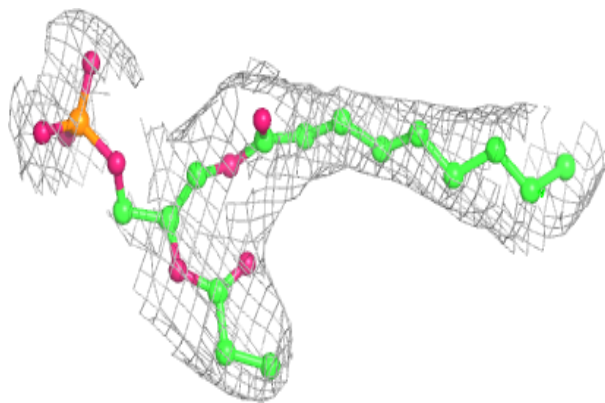


Electron density around 6OU D 1003:

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

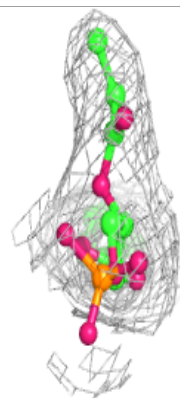
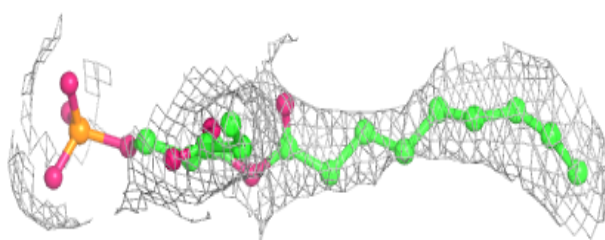
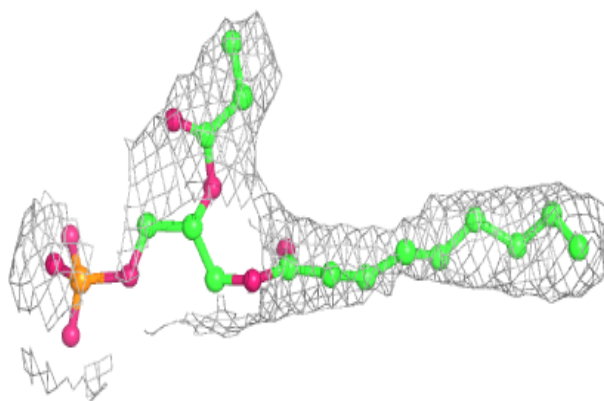
**Electron density around 6OU B 1001:**

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

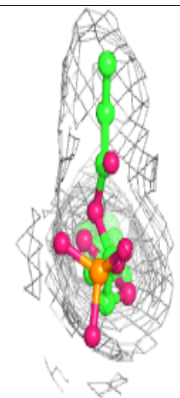
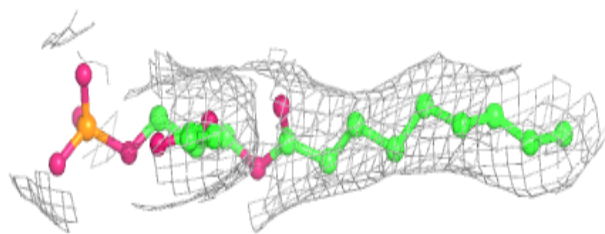
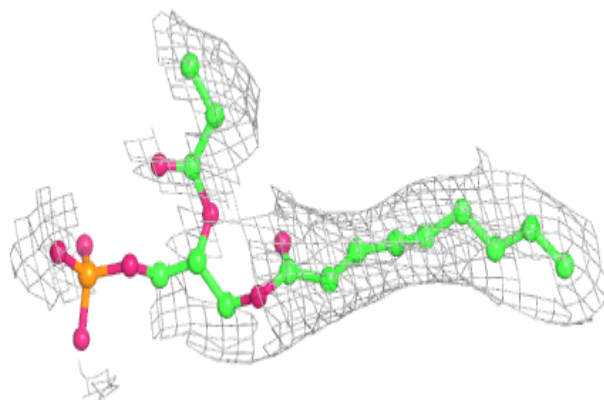


Electron density around 6OU C 1001:

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

**Electron density around 6OU A 1001:**

$2mF_o-DF_c$ (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.