Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 12:38 PM EDT

PDB ID	:	6XVG
Title	:	Human Sirt6 3-318 in complex with ADP-ribose and the activator MDL-801
Authors	:	You, W.; Steegborn, C.
Deposited on	:	2020-01-22
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

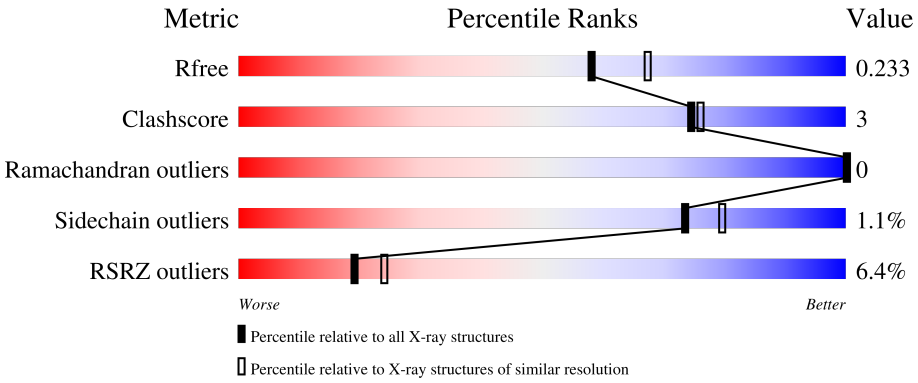
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	316	5% 81% 6% 12%
1	B	316	5% 81% 9% 10%
1	C	316	6% 80% 8% 12%
1	D	316	3% 82% 5% 12%
1	E	316	5% 82% 6% 12%

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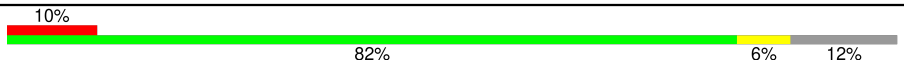
Mol	Chain	Length	Quality of chain
1	F	316	

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
6	SO4	B	409	-	-	X	-

2 Entry composition

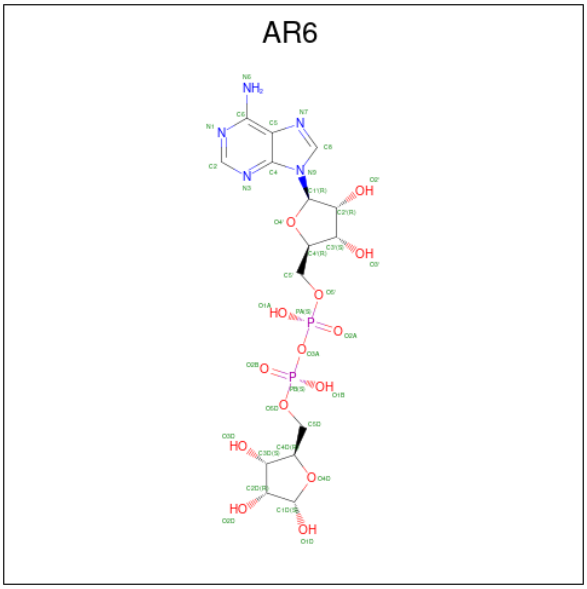
There are 7 unique types of molecules in this entry. The entry contains 13647 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NAD-dependent protein deacetylase sirtuin-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2152	1354	393	394	11			
1	B	284	Total	C	N	O	S	0	0	0
			2199	1383	403	402	11			
1	C	279	Total	C	N	O	S	0	0	0
			2151	1353	390	397	11			
1	D	277	Total	C	N	O	S	0	0	0
			2140	1346	390	393	11			
1	E	279	Total	C	N	O	S	0	0	0
			2149	1353	388	397	11			
1	F	278	Total	C	N	O	S	0	0	0
			2148	1349	390	398	11			

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL [HYDROXY-[[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (three-letter code: AR6) (formula: $C_{15}H_{23}N_5O_{14}P_2$).

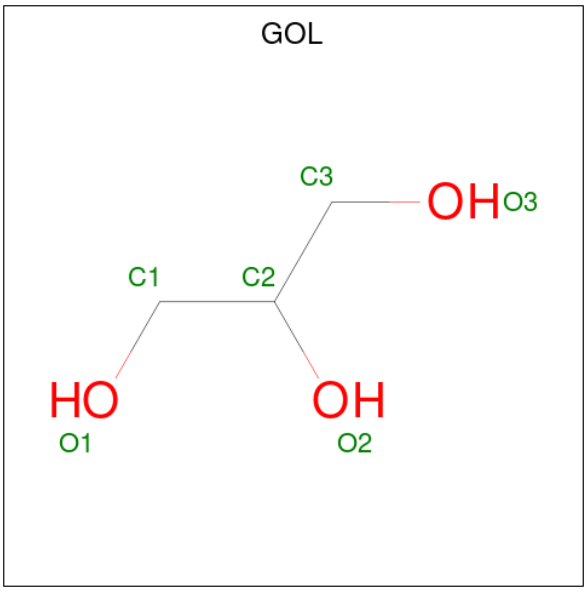


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	C	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	D	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	E	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	F	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

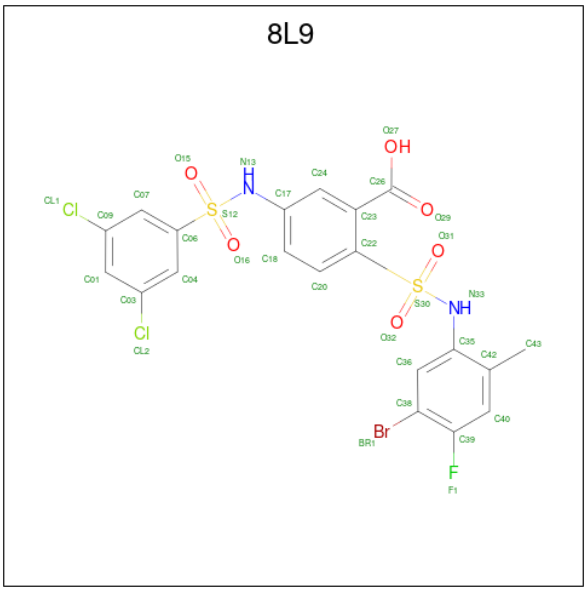
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



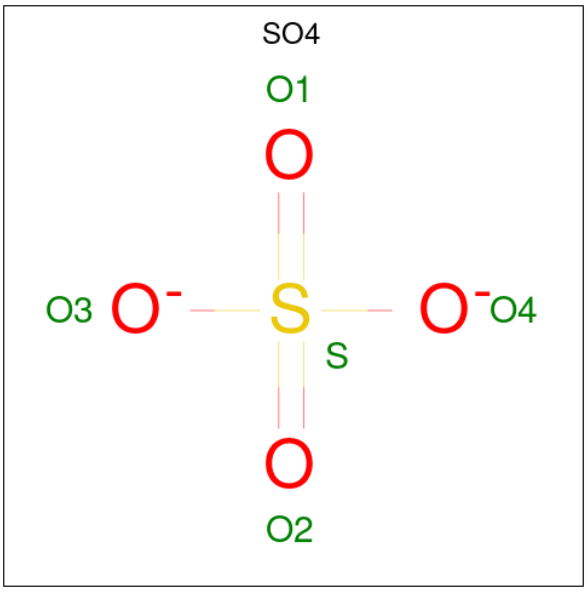
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 5-[[3,5-bis(chloranyl)phenyl]sulfonylamino]-2-[(5-bromanyl-4-fluoranyl-2-methyl-phenyl)sulfamoyl]benzoic acid (three-letter code: 8L9) (formula: $C_{20}H_{14}BrCl_2FN_2O_6S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
5	A	1	Total	Br	C	Cl	F	N	O	S	0	0
			34	1	20	2	1	2	6	2		
5	B	1	Total	Br	C	Cl	F	N	O	S	0	0
			34	1	20	2	1	2	6	2		
5	C	1	Total	Br	C	Cl	F	N	O	S	0	0
			34	1	20	2	1	2	6	2		
5	D	1	Total	Br	C	Cl	F	N	O	S	0	0
			34	1	20	2	1	2	6	2		
5	E	1	Total	Br	C	Cl	F	N	O	S	0	0
			34	1	20	2	1	2	6	2		
5	F	1	Total	Br	C	Cl	F	N	O	S	0	0
			34	1	20	2	1	2	6	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

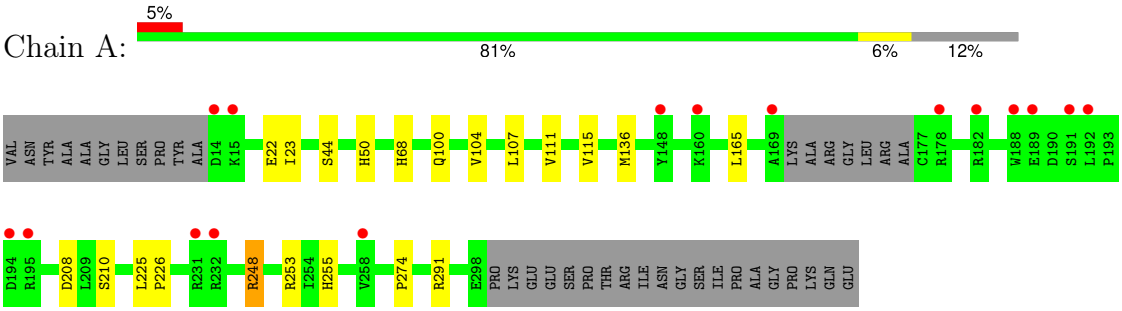
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	29	Total O 29 29	0	0
7	B	32	Total O 32 32	0	0
7	C	40	Total O 40 40	0	0
7	D	29	Total O 29 29	0	0
7	E	25	Total O 25 25	0	0
7	F	14	Total O 14 14	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

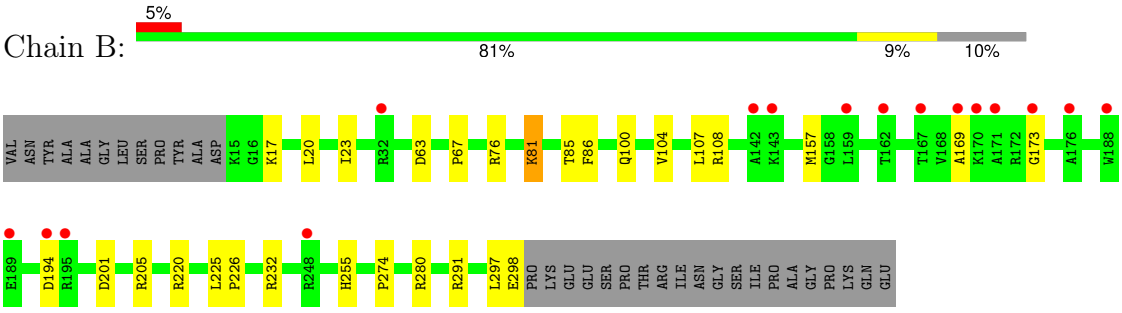
• Molecule 1: NAD-dependent protein deacetylase sirtuin-6

Chain A:



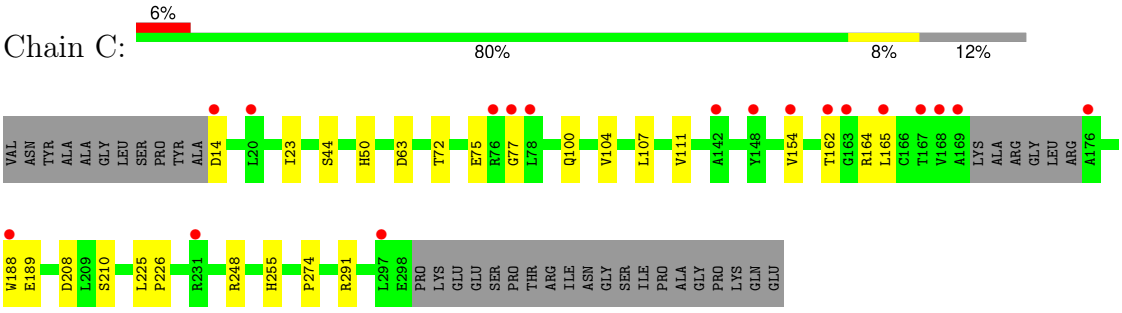
• Molecule 1: NAD-dependent protein deacetylase sirtuin-6

Chain B:



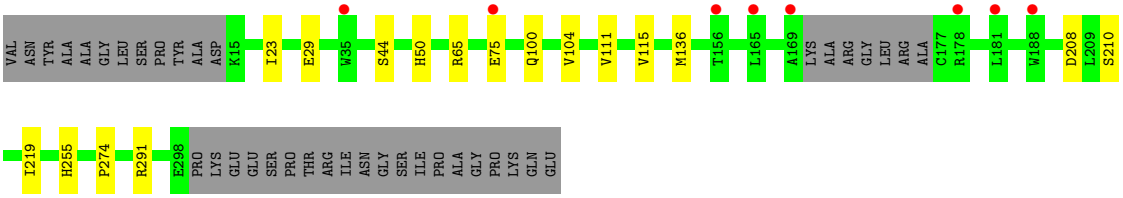
• Molecule 1: NAD-dependent protein deacetylase sirtuin-6

Chain C:

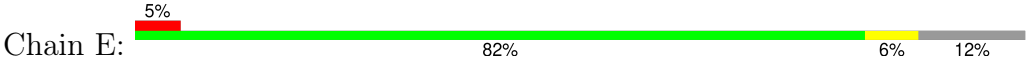


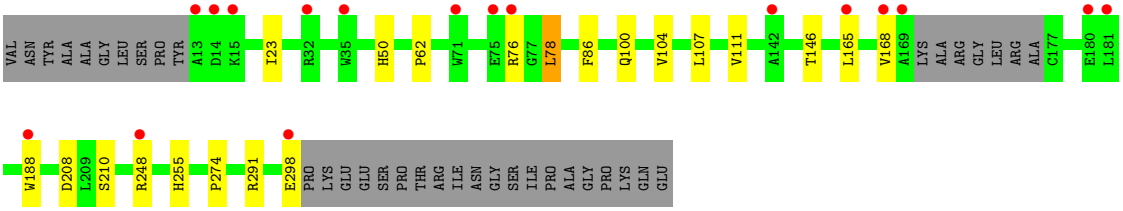
• Molecule 1: NAD-dependent protein deacetylase sirtuin-6

Chain D:

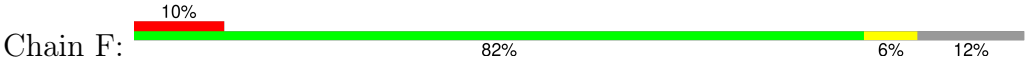


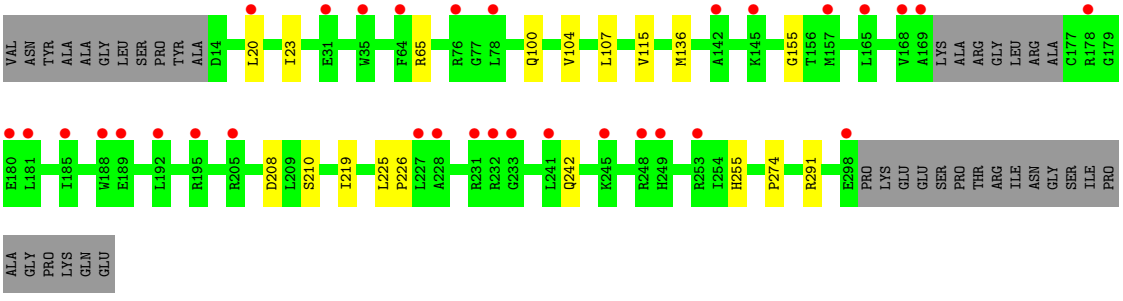
• Molecule 1: NAD-dependent protein deacetylase sirtuin-6





• Molecule 1: NAD-dependent protein deacetylase sirtuin-6





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.51Å 136.53Å 89.87Å 90.00° 117.71° 90.00°	Depositor
Resolution (Å)	46.39 – 2.10 46.39 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.39-2.10) 99.6 (46.39-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.204 , 0.230 0.212 , 0.233	Depositor DCC
R_{free} test set	2101 reflections (1.89%)	wwPDB-VP
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.007 for h,-k,-h-l 0.012 for -h-l,-k,l 0.006 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13647	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8L9, AR6, ZN, GOL, SO4

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	0.67	0/2199	0.81	1/2986 (0.0%)
1	B	0.67	0/2247	0.81	0/3050
1	C	0.66	0/2198	0.81	0/2987
1	D	0.66	0/2187	0.78	0/2972
1	E	0.67	0/2196	0.80	1/2984 (0.0%)
1	F	0.70	2/2195 (0.1%)	0.81	1/2984 (0.0%)
All	All	0.67	2/13222 (0.0%)	0.80	3/17963 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	20	LEU	C-N	8.16	1.49	1.34
1	F	242	GLN	C-N	7.90	1.49	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	208	ASP	CB-CA-C	-6.26	97.89	110.40
1	F	208	ASP	CB-CA-C	-5.68	99.03	110.40
1	A	253	ARG	NE-CZ-NH1	-5.30	117.65	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2152	0	2149	11	0
1	B	2199	0	2206	20	0
1	C	2151	0	2136	17	0
1	D	2140	0	2127	11	0
1	E	2149	0	2136	13	0
1	F	2148	0	2124	9	0
2	A	36	0	21	0	0
2	B	36	0	21	1	0
2	C	36	0	21	1	0
2	D	36	0	21	1	0
2	E	36	0	21	0	0
2	F	36	0	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	2	0
4	C	18	0	24	1	0
4	D	6	0	8	3	0
4	E	12	0	16	2	0
5	A	34	0	0	1	0
5	B	34	0	0	1	0
5	C	34	0	0	1	0
5	D	34	0	0	3	0
5	E	34	0	0	1	0
5	F	34	0	0	1	0
6	A	5	0	0	0	0
6	B	25	0	0	3	0
6	C	5	0	0	0	0
6	D	15	0	0	0	0
6	E	15	0	0	0	0
7	A	29	0	0	0	0
7	B	32	0	0	1	0
7	C	40	0	0	0	0
7	D	29	0	0	0	0
7	E	25	0	0	0	0
7	F	14	0	0	0	0
All	All	13647	0	13068	85	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 3.

All (85) 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:C:14:ASP:O	1:C:188:TRP:CH2	2.42	0.72
1:B:220:ARG:NH2	6:B:409:SO4:O1	2.23	0.72
1:E:86:PHE:H	4:E:704:GOL:H31	1.55	0.71
1:C:77:GLY:HA3	1:F:155:GLY:O	1.91	0.70
1:D:219:ILE:HD12	1:D:219:ILE:N	2.10	0.67
4:D:403:GOL:C1	5:D:404:8L9:CL2	2.82	0.65
1:B:67:PRO:O	1:B:76:ARG:NH1	2.28	0.65
1:B:201:ASP:O	1:B:205:ARG:HG3	1.97	0.64
1:C:154:VAL:HG13	1:C:162:THR:HG21	1.80	0.62
1:F:104:VAL:O	1:F:291:ARG:NH2	2.31	0.60
4:D:403:GOL:H12	5:D:404:8L9:CL2	2.38	0.59
1:E:146:THR:HG21	1:E:168:VAL:HG21	1.86	0.58
1:E:188:TRP:HA	1:E:188:TRP:CE3	2.39	0.56
1:B:86:PHE:CD2	4:B:403:GOL:H2	2.41	0.55
1:E:298:GLU:N	1:E:298:GLU:OE2	2.40	0.55
1:C:154:VAL:CG1	1:C:162:THR:HG21	2.37	0.54
1:D:219:ILE:HD13	2:D:401:AR6:H5DA	1.90	0.53
1:B:157:MET:SD	5:B:404:8L9:C43	2.97	0.53
1:B:232:ARG:O	1:B:232:ARG:HG2	2.09	0.52
1:B:85:THR:HA	4:B:403:GOL:O2	2.12	0.50
1:C:165:LEU:HD22	1:C:165:LEU:N	2.27	0.50
1:A:165:LEU:N	1:A:165:LEU:HD22	2.27	0.50
1:E:165:LEU:N	1:E:165:LEU:HD22	2.27	0.50
1:E:188:TRP:HA	1:E:188:TRP:HE3	1.78	0.49
1:B:104:VAL:HB	1:B:291:ARG:HB3	1.95	0.48
1:C:72:THR:O	1:C:75:GLU:HG2	2.14	0.47
5:C:1006:8L9:O16	5:C:1006:8L9:C18	2.62	0.47
1:B:20:LEU:H	1:B:20:LEU:HD12	1.80	0.47
1:C:100:GLN:HB2	1:C:274:PRO:HD3	1.97	0.46
1:B:280:ARG:CB	7:B:532:HOH:O	2.63	0.46
1:D:100:GLN:HB2	1:D:274:PRO:HD3	1.98	0.46
1:D:104:VAL:HB	1:D:291:ARG:HB3	1.98	0.46
1:D:44:SER:HB3	1:D:208:ASP:OD1	2.15	0.46
1:D:65:ARG:CZ	1:D:219:ILE:HD11	2.46	0.46
1:F:104:VAL:HB	1:F:291:ARG:HB3	1.97	0.46
1:D:219:ILE:N	1:D:219:ILE:CD1	2.78	0.45
1:E:62:PRO:O	5:E:705:8L9:BR1	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ARG:HG2	6:B:409:SO4:O2	2.16	0.45
1:B:100:GLN:HB2	1:B:274:PRO:HD3	1.98	0.45
5:A:404:8L9:O32	5:A:404:8L9:C36	2.64	0.45
1:C:63:ASP:OD2	2:C:1002:AR6:H8	2.17	0.44
1:C:104:VAL:HB	1:C:291:ARG:HB3	2.00	0.44
1:F:65:ARG:NH2	1:F:219:ILE:HD11	2.32	0.44
1:B:169:ALA:HB1	1:B:173:GLY:HA2	1.99	0.44
1:F:23:ILE:O	1:F:255:HIS:HB3	2.18	0.44
1:F:100:GLN:HB2	1:F:274:PRO:HD3	2.00	0.44
1:A:22:GLU:OE2	1:B:81:LYS:HE3	2.18	0.43
4:D:403:GOL:H11	5:D:404:8L9:CL2	2.55	0.43
1:C:154:VAL:CG1	1:C:162:THR:CG2	2.95	0.43
1:B:63:ASP:OD2	2:B:401:AR6:H8	2.18	0.43
1:E:23:ILE:O	1:E:255:HIS:HB3	2.18	0.43
1:E:100:GLN:HB2	1:E:274:PRO:HD3	2.00	0.43
1:A:23:ILE:O	1:A:255:HIS:HB3	2.18	0.43
1:A:44:SER:HB3	1:A:208:ASP:OD1	2.18	0.43
1:C:44:SER:HB3	1:C:208:ASP:OD1	2.17	0.43
4:C:1004:GOL:H2	4:E:701:GOL:H11	1.99	0.43
1:B:23:ILE:O	1:B:255:HIS:HB3	2.19	0.43
1:A:248:ARG:HH21	1:D:75:GLU:HG2	1.83	0.42
1:C:225:LEU:N	1:C:226:PRO:CD	2.82	0.42
1:A:115:VAL:O	1:A:136:MET:HG2	2.19	0.42
1:C:14:ASP:O	1:C:188:TRP:CZ2	2.71	0.42
1:A:100:GLN:HB2	1:A:274:PRO:HD3	2.02	0.42
1:A:225:LEU:N	1:A:226:PRO:CD	2.83	0.42
1:D:23:ILE:O	1:D:255:HIS:HB3	2.19	0.42
1:E:104:VAL:HB	1:E:291:ARG:HB3	2.01	0.42
1:F:115:VAL:O	1:F:136:MET:HG2	2.20	0.41
1:B:297:LEU:O	1:B:298:GLU:HG3	2.20	0.41
1:A:104:VAL:HB	1:A:291:ARG:HB3	2.02	0.41
1:B:225:LEU:N	1:B:226:PRO:CD	2.84	0.41
1:F:225:LEU:N	1:F:226:PRO:CD	2.83	0.41
1:E:76:ARG:O	1:E:78:LEU:HD22	2.20	0.41
1:A:50:HIS:HA	1:A:111:VAL:O	2.21	0.41
1:C:107:LEU:C	1:C:107:LEU:HD23	2.41	0.41
1:F:107:LEU:HD23	1:F:107:LEU:C	2.42	0.41
1:E:107:LEU:C	1:E:107:LEU:HD23	2.42	0.41
1:E:50:HIS:HA	1:E:111:VAL:O	2.21	0.40
1:A:107:LEU:HD23	1:A:107:LEU:C	2.41	0.40
1:C:23:ILE:O	1:C:255:HIS:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:HIS:HA	1:D:111:VAL:O	2.21	0.40
5:F:403:8L9:C36	5:F:403:8L9:O32	2.68	0.40
1:C:50:HIS:HA	1:C:111:VAL:O	2.21	0.40
1:B:107:LEU:C	1:B:107:LEU:HD23	2.42	0.40
1:C:164:ARG:C	1:C:165:LEU:HD22	2.42	0.40
1:B:108:ARG:HD2	6:B:408:SO4:O2	2.22	0.40
1:D:115:VAL:O	1:D:136:MET:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/316 (87%)	272 (99%)	2 (1%)	0	100	100
1	B	282/316 (89%)	278 (99%)	4 (1%)	0	100	100
1	C	275/316 (87%)	274 (100%)	1 (0%)	0	100	100
1	D	273/316 (86%)	270 (99%)	3 (1%)	0	100	100
1	E	275/316 (87%)	272 (99%)	3 (1%)	0	100	100
1	F	274/316 (87%)	272 (99%)	2 (1%)	0	100	100
All	All	1653/1896 (87%)	1638 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/265 (88%)	229 (99%)	3 (1%)	69	75
1	B	236/265 (89%)	233 (99%)	3 (1%)	69	75
1	C	231/265 (87%)	228 (99%)	3 (1%)	69	75
1	D	230/265 (87%)	228 (99%)	2 (1%)	78	84
1	E	231/265 (87%)	228 (99%)	3 (1%)	69	75
1	F	231/265 (87%)	230 (100%)	1 (0%)	91	94
All	All	1391/1590 (88%)	1376 (99%)	15 (1%)	73	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	210	SER
1	A	248	ARG
1	B	17	LYS
1	B	81	LYS
1	B	194	ASP
1	C	189	GLU
1	C	210	SER
1	C	248	ARG
1	D	29	GLU
1	D	210	SER
1	E	78	LEU
1	E	210	SER
1	E	248	ARG
1	F	210	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	68	HIS
1	F	249	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 6 are monoatomic - leaving 33 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	$\#\|Z\| > 2$
6	SO4	D	407	-	4,4,4	0.33	0	6,6,6	0.13	0
4	GOL	C	1005	-	5,5,5	0.17	0	5,5,5	0.44	0
6	SO4	B	407	-	4,4,4	0.35	0	6,6,6	0.15	0
2	AR6	C	1002	-	35,39,39	0.66	0	42,60,60	0.96	3 (7%)
6	SO4	B	405	-	4,4,4	0.36	0	6,6,6	0.13	0
4	GOL	C	1004	-	5,5,5	0.12	0	5,5,5	0.35	0
6	SO4	E	706	-	4,4,4	0.29	0	6,6,6	0.22	0
6	SO4	D	405	-	4,4,4	0.24	0	6,6,6	0.19	0
2	AR6	B	401	-	35,39,39	0.84	2 (5%)	42,60,60	1.07	4 (9%)
2	AR6	D	401	-	35,39,39	0.75	0	42,60,60	1.15	3 (7%)
4	GOL	C	1001	-	5,5,5	0.09	0	5,5,5	0.26	0
4	GOL	A	403	-	5,5,5	0.22	0	5,5,5	0.44	0
2	AR6	F	401	-	35,39,39	1.04	4 (11%)	42,60,60	0.81	1 (2%)
4	GOL	B	403	-	5,5,5	0.19	0	5,5,5	0.45	0
5	8L9	D	404	-	36,36,36	1.87	9 (25%)	54,55,55	3.56	19 (35%)
6	SO4	B	408	-	4,4,4	0.31	0	6,6,6	0.12	0
5	8L9	E	705	-	36,36,36	1.68	7 (19%)	54,55,55	3.53	11 (20%)
5	8L9	C	1006	-	36,36,36	1.97	10 (27%)	54,55,55	4.22	24 (44%)
6	SO4	B	409	-	4,4,4	0.32	0	6,6,6	0.08	0
2	AR6	E	702	-	35,39,39	0.68	0	42,60,60	1.10	3 (7%)
4	GOL	E	704	-	5,5,5	0.22	0	5,5,5	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	AR6	A	401	-	35,39,39	0.64	0	42,60,60	1.04	3 (7%)
5	8L9	B	404	-	36,36,36	1.99	9 (25%)	54,55,55	3.73	17 (31%)
4	GOL	E	701	-	5,5,5	0.12	0	5,5,5	0.24	0
6	SO4	C	1007	-	4,4,4	0.31	0	6,6,6	0.14	0
6	SO4	E	707	-	4,4,4	0.30	0	6,6,6	0.12	0
5	8L9	F	403	-	36,36,36	2.07	10 (27%)	54,55,55	3.66	18 (33%)
6	SO4	A	405	-	4,4,4	0.32	0	6,6,6	0.10	0
5	8L9	A	404	-	36,36,36	2.06	10 (27%)	54,55,55	3.66	21 (38%)
6	SO4	E	708	-	4,4,4	0.29	0	6,6,6	0.13	0
6	SO4	B	406	-	4,4,4	0.24	0	6,6,6	0.19	0
6	SO4	D	406	-	4,4,4	0.31	0	6,6,6	0.08	0
4	GOL	D	403	-	5,5,5	0.15	0	5,5,5	0.41	0

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
4	GOL	C	1005	-	-	4/4/4/4	-
2	AR6	C	1002	-	-	1/18/54/54	0/4/4/4
4	GOL	C	1004	-	-	4/4/4/4	-
2	AR6	B	401	-	-	0/18/54/54	0/4/4/4
2	AR6	D	401	-	-	1/18/54/54	0/4/4/4
4	GOL	C	1001	-	-	2/4/4/4	-
4	GOL	A	403	-	-	2/4/4/4	-
2	AR6	F	401	-	-	2/18/54/54	0/4/4/4
4	GOL	B	403	-	-	0/4/4/4	-
5	8L9	D	404	-	-	10/26/26/26	0/3/3/3
5	8L9	E	705	-	-	11/26/26/26	0/3/3/3
5	8L9	C	1006	-	-	13/26/26/26	0/3/3/3
2	AR6	E	702	-	-	1/18/54/54	0/4/4/4
4	GOL	E	704	-	-	2/4/4/4	-
2	AR6	A	401	-	-	1/18/54/54	0/4/4/4
5	8L9	B	404	-	-	9/26/26/26	0/3/3/3
4	GOL	E	701	-	-	0/4/4/4	-
5	8L9	F	403	-	-	14/26/26/26	0/3/3/3
5	8L9	A	404	-	-	8/26/26/26	0/3/3/3
4	GOL	D	403	-	-	2/4/4/4	-

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	404	8L9	C06-S12	6.08	1.85	1.76
5	F	403	8L9	S12-N13	6.01	1.73	1.63
5	C	1006	8L9	S12-N13	5.49	1.72	1.63
5	D	404	8L9	S12-N13	5.30	1.71	1.63
5	A	404	8L9	S12-N13	4.87	1.71	1.63
5	F	403	8L9	S30-N33	4.69	1.71	1.63
5	B	404	8L9	C06-S12	4.56	1.83	1.76
5	B	404	8L9	S12-N13	4.51	1.70	1.63
5	B	404	8L9	S30-N33	4.46	1.70	1.63
5	E	705	8L9	S12-N13	4.34	1.70	1.63
5	D	404	8L9	C22-S30	4.16	1.83	1.77
5	C	1006	8L9	S30-N33	4.02	1.69	1.63
5	F	403	8L9	C22-S30	4.01	1.83	1.77
5	C	1006	8L9	C06-S12	3.76	1.82	1.76
5	B	404	8L9	O31-S30	3.62	1.47	1.43
5	A	404	8L9	O32-S30	3.61	1.47	1.43
5	A	404	8L9	C22-S30	3.60	1.82	1.77
5	E	705	8L9	S30-N33	3.55	1.69	1.63
5	D	404	8L9	C06-S12	3.52	1.81	1.76
5	B	404	8L9	C22-S30	3.50	1.82	1.77
5	E	705	8L9	C22-S30	3.42	1.82	1.77
5	F	403	8L9	O31-S30	3.37	1.47	1.43
5	E	705	8L9	C06-S12	3.26	1.81	1.76
5	A	404	8L9	O15-S12	3.23	1.47	1.43
5	F	403	8L9	O32-S30	3.13	1.47	1.43
5	F	403	8L9	O15-S12	3.12	1.47	1.43
5	C	1006	8L9	O15-S12	3.09	1.47	1.43
5	D	404	8L9	S30-N33	3.06	1.68	1.63
5	C	1006	8L9	O32-S30	3.06	1.47	1.43
5	B	404	8L9	O32-S30	3.02	1.47	1.43
5	D	404	8L9	O15-S12	2.95	1.47	1.43
5	A	404	8L9	S30-N33	2.93	1.68	1.63
5	F	403	8L9	O16-S12	2.92	1.46	1.43
5	B	404	8L9	O16-S12	2.91	1.46	1.43
5	B	404	8L9	O15-S12	2.91	1.46	1.43
5	E	705	8L9	O32-S30	2.87	1.46	1.43
5	D	404	8L9	O32-S30	2.81	1.46	1.43
5	C	1006	8L9	O16-S12	2.78	1.46	1.43
5	C	1006	8L9	C09-CL1	2.78	1.80	1.74
5	E	705	8L9	O15-S12	2.74	1.46	1.43
2	B	401	AR6	O4D-C1D	2.74	1.46	1.43
5	A	404	8L9	O16-S12	2.74	1.46	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	404	8L9	O31-S30	2.69	1.46	1.43
5	D	404	8L9	O31-S30	2.67	1.46	1.43
5	C	1006	8L9	C22-S30	2.58	1.81	1.77
5	C	1006	8L9	O31-S30	2.56	1.46	1.43
2	F	401	AR6	C1'-N9	-2.50	1.43	1.49
5	B	404	8L9	C23-C26	2.49	1.55	1.49
5	D	404	8L9	O16-S12	2.48	1.46	1.43
5	E	705	8L9	O16-S12	2.46	1.46	1.43
5	F	403	8L9	C06-S12	2.42	1.80	1.76
5	C	1006	8L9	C23-C26	2.29	1.54	1.49
5	F	403	8L9	C09-CL1	2.17	1.79	1.74
2	F	401	AR6	PB-O3A	-2.17	1.57	1.59
5	D	404	8L9	C40-C39	2.15	1.41	1.37
2	F	401	AR6	C8-N7	-2.14	1.30	1.34
2	B	401	AR6	C8-N7	-2.07	1.30	1.34
5	F	403	8L9	C03-CL2	2.07	1.79	1.74
2	F	401	AR6	PA-O3A	-2.05	1.57	1.59
5	A	404	8L9	C23-C22	2.04	1.42	1.40
5	A	404	8L9	C23-C26	2.04	1.54	1.49

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1006	8L9	O16-S12-O15	-17.90	97.78	119.52
5	A	404	8L9	O16-S12-O15	-17.76	97.95	119.52
5	E	705	8L9	O32-S30-O31	-17.68	98.04	119.52
5	F	403	8L9	O32-S30-O31	-16.02	100.07	119.52
5	B	404	8L9	O16-S12-O15	-15.66	100.50	119.52
5	C	1006	8L9	O32-S30-O31	-15.28	100.96	119.52
5	D	404	8L9	O16-S12-O15	-14.72	101.65	119.52
5	E	705	8L9	O16-S12-O15	-14.50	101.91	119.52
5	F	403	8L9	O16-S12-O15	-14.37	102.06	119.52
5	B	404	8L9	O32-S30-O31	-14.34	102.10	119.52
5	A	404	8L9	O32-S30-O31	-13.10	103.62	119.52
5	D	404	8L9	O32-S30-O31	-12.87	103.88	119.52
5	C	1006	8L9	C06-S12-N13	8.84	117.84	106.88
5	B	404	8L9	C06-S12-N13	8.77	117.76	106.88
5	D	404	8L9	C06-S12-N13	8.17	117.01	106.88
5	B	404	8L9	C07-C06-S12	8.05	127.30	119.06
5	C	1006	8L9	C22-S30-N33	-6.97	99.09	107.30
5	C	1006	8L9	C07-C06-S12	6.93	126.15	119.06
5	F	403	8L9	O31-S30-C22	6.02	117.61	107.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	404	8L9	O31-S30-C22	5.93	117.47	107.68
5	F	403	8L9	C22-S30-N33	-5.87	100.39	107.30
5	D	404	8L9	C22-S30-N33	-5.83	100.44	107.30
5	A	404	8L9	C06-S12-N13	5.63	113.86	106.88
5	F	403	8L9	C06-S12-N13	5.28	113.42	106.88
5	E	705	8L9	C06-S12-N13	5.24	113.38	106.88
5	C	1006	8L9	O31-S30-C22	5.19	116.25	107.68
5	F	403	8L9	C42-C35-N33	5.00	125.83	120.32
5	C	1006	8L9	C04-C06-S12	-4.90	114.06	119.06
5	B	404	8L9	C04-C06-S12	-4.71	114.25	119.06
5	D	404	8L9	C24-C23-C22	4.50	122.07	117.55
5	A	404	8L9	C07-C06-S12	4.45	123.61	119.06
5	A	404	8L9	C35-N33-S30	-4.34	109.45	123.34
5	C	1006	8L9	C01-C03-CL2	4.30	124.56	119.17
5	E	705	8L9	O32-S30-C22	4.22	114.64	107.68
5	D	404	8L9	O32-S30-C22	3.92	114.16	107.68
5	E	705	8L9	O31-S30-C22	3.89	114.10	107.68
2	E	702	AR6	O4'-C1'-N9	-3.85	103.64	108.75
5	B	404	8L9	O31-S30-C22	3.66	113.73	107.68
5	A	404	8L9	C03-C04-C06	3.62	121.15	118.12
5	D	404	8L9	C07-C06-S12	3.61	122.76	119.06
5	B	404	8L9	C03-C04-C06	3.61	121.14	118.12
5	A	404	8L9	C09-C07-C06	3.55	121.09	118.12
5	C	1006	8L9	C03-C04-C06	3.48	121.03	118.12
5	F	403	8L9	O32-S30-N33	3.37	114.95	106.74
5	C	1006	8L9	O32-S30-C22	3.37	113.24	107.68
5	C	1006	8L9	C42-C35-N33	3.35	124.01	120.32
5	C	1006	8L9	C17-N13-S12	-3.34	112.56	122.94
5	F	403	8L9	C36-C35-N33	-3.34	113.60	120.84
5	A	404	8L9	C07-C09-CL1	3.32	123.34	119.17
5	D	404	8L9	C07-C09-CL1	-3.30	115.03	119.17
5	B	404	8L9	C22-S30-N33	-3.26	103.46	107.30
5	B	404	8L9	O31-S30-N33	3.24	114.63	106.74
5	D	404	8L9	C01-C03-CL2	3.22	123.20	119.17
5	A	404	8L9	O15-S12-C06	3.21	112.02	107.98
5	A	404	8L9	O16-S12-C06	3.19	112.00	107.98
5	C	1006	8L9	C04-C03-CL2	-3.19	115.17	119.17
5	A	404	8L9	O31-S30-C22	3.16	112.89	107.68
5	C	1006	8L9	O31-S30-N33	3.15	114.42	106.74
5	D	404	8L9	C03-C04-C06	3.15	120.76	118.12
5	F	403	8L9	C01-C03-CL2	3.14	123.11	119.17
5	B	404	8L9	C42-C35-N33	3.10	123.74	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	404	8L9	C01-C09-CL1	3.04	122.98	119.17
5	F	403	8L9	O32-S30-C22	3.03	112.69	107.68
5	B	404	8L9	C35-N33-S30	-3.03	113.65	123.34
5	F	403	8L9	C09-C01-C03	2.91	120.93	117.43
5	C	1006	8L9	O32-S30-N33	2.82	113.60	106.74
5	C	1006	8L9	C18-C17-N13	-2.79	114.15	120.02
2	B	401	AR6	O4'-C1'-N9	-2.77	105.07	108.75
5	E	705	8L9	O32-S30-N33	2.76	113.46	106.74
5	A	404	8L9	O27-C26-C23	2.75	123.09	115.28
5	F	403	8L9	O16-S12-N13	2.73	113.38	106.74
5	D	404	8L9	C04-C03-CL2	-2.68	115.81	119.17
2	C	1002	AR6	O4'-C1'-N9	-2.66	105.22	108.75
2	B	401	AR6	C5-C6-N6	2.64	124.34	120.31
5	A	404	8L9	O27-C26-O29	-2.62	117.72	123.35
5	E	705	8L9	C17-N13-S12	-2.61	114.82	122.94
2	D	401	AR6	O1A-PA-O2A	2.59	124.51	112.44
5	A	404	8L9	C07-C06-C04	-2.59	116.86	120.34
5	F	403	8L9	C20-C22-S30	2.59	121.23	117.51
2	D	401	AR6	C5-C6-N6	2.58	124.24	120.31
5	A	404	8L9	O31-S30-N33	2.56	112.97	106.74
5	E	705	8L9	O16-S12-C06	2.52	111.15	107.98
5	D	404	8L9	C40-C39-C38	-2.50	119.21	122.20
5	B	404	8L9	O32-S30-C22	2.46	111.74	107.68
5	C	1006	8L9	C36-C35-N33	-2.45	115.52	120.84
5	C	1006	8L9	C20-C22-S30	-2.44	114.01	117.51
5	A	404	8L9	C01-C09-CL1	-2.44	116.11	119.17
5	B	404	8L9	O27-C26-C23	2.44	122.20	115.28
2	B	401	AR6	O3A-PA-O2A	-2.43	103.39	110.70
5	A	404	8L9	C04-C03-CL2	2.43	122.21	119.17
2	F	401	AR6	C5-C6-N6	2.42	124.00	120.31
5	C	1006	8L9	O27-C26-O29	-2.42	118.16	123.35
5	C	1006	8L9	C09-C07-C06	2.39	120.13	118.12
5	E	705	8L9	C24-C23-C22	2.38	119.94	117.55
5	D	404	8L9	C43-C42-C35	-2.38	118.53	121.23
5	C	1006	8L9	O27-C26-C23	2.37	122.02	115.28
5	A	404	8L9	O32-S30-C22	2.37	111.59	107.68
5	C	1006	8L9	C07-C09-C01	-2.35	118.78	121.64
2	B	401	AR6	O1A-PA-O2A	2.30	123.17	112.44
5	F	403	8L9	O27-C26-C23	2.30	121.83	115.28
2	A	401	AR6	O3D-C3D-C2D	2.30	119.19	111.82
5	F	403	8L9	C24-C23-C22	2.28	119.84	117.55
2	E	702	AR6	C5-C6-N6	2.28	123.79	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	404	8L9	BR1-C38-C39	2.26	122.85	119.88
2	C	1002	AR6	O1D-C1D-O4D	-2.24	108.27	111.12
5	B	404	8L9	C36-C35-N33	-2.23	116.00	120.84
5	D	404	8L9	O29-C26-C23	-2.21	116.70	121.97
5	B	404	8L9	F1-C39-C40	2.20	123.03	118.64
2	E	702	AR6	O2D-C2D-C1D	2.20	117.96	111.85
5	D	404	8L9	O16-S12-N13	2.20	112.09	106.74
5	C	1006	8L9	C09-C01-C03	2.16	120.03	117.43
5	F	403	8L9	O15-S12-N13	2.15	111.99	106.74
5	A	404	8L9	C24-C23-C22	2.14	119.70	117.55
2	C	1002	AR6	O1A-PA-O2A	2.13	122.37	112.44
5	F	403	8L9	C07-C09-C01	-2.12	119.06	121.64
5	E	705	8L9	C40-C42-C35	2.12	120.65	118.24
5	F	403	8L9	O31-S30-N33	2.12	111.90	106.74
5	A	404	8L9	C17-N13-S12	-2.11	116.39	122.94
5	E	705	8L9	C35-N33-S30	-2.10	116.61	123.34
2	D	401	AR6	O4'-C1'-N9	-2.10	105.96	108.75
5	B	404	8L9	C07-C09-CL1	2.08	121.78	119.17
5	D	404	8L9	C22-C23-C26	-2.07	121.29	124.30
5	C	1006	8L9	O16-S12-N13	2.05	111.73	106.74
2	A	401	AR6	C2D-C3D-C4D	-2.05	98.65	102.61
2	A	401	AR6	O4'-C1'-N9	-2.04	106.04	108.75
5	D	404	8L9	O27-C26-C23	2.00	120.97	115.28
5	B	404	8L9	C01-C09-CL1	-2.00	116.66	119.17

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	AR6	C5D-O5D-PB-O2B
2	E	702	AR6	C5D-O5D-PB-O2B
4	A	403	GOL	C1-C2-C3-O3
4	C	1004	GOL	O1-C1-C2-O2
4	C	1004	GOL	O1-C1-C2-C3
4	C	1004	GOL	C1-C2-C3-O3
4	C	1004	GOL	O2-C2-C3-O3
4	C	1005	GOL	C1-C2-C3-O3
5	C	1006	8L9	C17-N13-S12-O15
5	F	403	8L9	C17-N13-S12-O15
5	F	403	8L9	C17-N13-S12-C06
5	C	1006	8L9	C17-N13-S12-C06
5	A	404	8L9	C07-C06-S12-N13

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Mol	Chain	Res	Type	Atoms
5	A	404	8L9	C04-C06-S12-N13
5	F	403	8L9	C04-C06-S12-N13
5	B	404	8L9	C07-C06-S12-N13
5	F	403	8L9	C07-C06-S12-N13
5	E	705	8L9	C17-N13-S12-O16
5	B	404	8L9	C04-C06-S12-N13
5	C	1006	8L9	C35-N33-S30-O31
5	E	705	8L9	C04-C06-S12-N13
4	C	1005	GOL	O1-C1-C2-O2
5	C	1006	8L9	C17-N13-S12-O16
5	F	403	8L9	C35-N33-S30-O31
5	E	705	8L9	C07-C06-S12-N13
5	D	404	8L9	C07-C06-S12-N13
4	C	1001	GOL	O1-C1-C2-C3
4	C	1005	GOL	O1-C1-C2-C3
4	E	704	GOL	O1-C1-C2-C3
4	A	403	GOL	O2-C2-C3-O3
5	D	404	8L9	C04-C06-S12-N13
5	B	404	8L9	C17-N13-S12-O15
4	C	1005	GOL	O2-C2-C3-O3
5	F	403	8L9	C17-N13-S12-O16
5	F	403	8L9	C22-C23-C26-O27
5	D	404	8L9	C35-N33-S30-O31
5	C	1006	8L9	C35-N33-S30-O32
5	E	705	8L9	C17-N13-S12-C06
5	D	404	8L9	C04-C06-S12-O16
5	E	705	8L9	C17-N13-S12-O15
4	D	403	GOL	O2-C2-C3-O3
5	F	403	8L9	C22-C23-C26-O29
5	C	1006	8L9	C35-N33-S30-C22
5	D	404	8L9	C07-C06-S12-O16
5	F	403	8L9	C24-C23-C26-O27
5	F	403	8L9	C24-C23-C26-O29
5	A	404	8L9	C22-C23-C26-O27
5	A	404	8L9	C22-C23-C26-O29
5	E	705	8L9	C24-C23-C26-O29
5	E	705	8L9	C24-C23-C26-O27
2	A	401	AR6	C5D-O5D-PB-O2B
2	C	1002	AR6	C5D-O5D-PB-O2B
2	F	401	AR6	C5D-O5D-PB-O2B
5	E	705	8L9	C22-C23-C26-O27
5	E	705	8L9	C22-C23-C26-O29

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Mol	Chain	Res	Type	Atoms
5	A	404	8L9	C35-N33-S30-O31
5	F	403	8L9	C35-N33-S30-C22
5	F	403	8L9	C35-N33-S30-O32
5	C	1006	8L9	C23-C22-S30-O31
5	E	705	8L9	C07-C06-S12-O16
5	D	404	8L9	C22-C23-C26-O29
4	D	403	GOL	C1-C2-C3-O3
4	C	1001	GOL	O1-C1-C2-O2
5	E	705	8L9	C04-C06-S12-O16
5	A	404	8L9	C23-C22-S30-O31
5	B	404	8L9	C22-C23-C26-O27
5	C	1006	8L9	C22-C23-C26-O27
5	C	1006	8L9	C22-C23-C26-O29
5	D	404	8L9	C22-C23-C26-O27
5	D	404	8L9	C17-N13-S12-O15
5	C	1006	8L9	C04-C06-S12-O16
5	D	404	8L9	C24-C23-C26-O27
5	B	404	8L9	C22-C23-C26-O29
5	B	404	8L9	C24-C23-C26-O27
5	C	1006	8L9	C07-C06-S12-O16
5	C	1006	8L9	C24-C23-C26-O27
5	D	404	8L9	C24-C23-C26-O29
4	E	704	GOL	O1-C1-C2-O2
5	F	403	8L9	C07-C06-S12-O15
5	F	403	8L9	C04-C06-S12-O15
5	B	404	8L9	C24-C23-C26-O29
5	A	404	8L9	C24-C23-C26-O29
5	C	1006	8L9	C24-C23-C26-O29
5	A	404	8L9	C24-C23-C26-O27
2	F	401	AR6	O4'-C4'-C5'-O5'
5	B	404	8L9	C04-C06-S12-O16
5	B	404	8L9	C07-C06-S12-O16

There are no ring outliers.

16 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1002	AR6	1	0
4	C	1004	GOL	1	0
2	B	401	AR6	1	0
2	D	401	AR6	1	0
4	B	403	GOL	2	0

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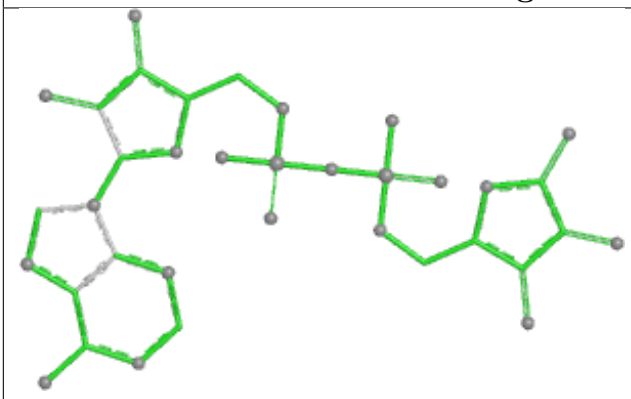
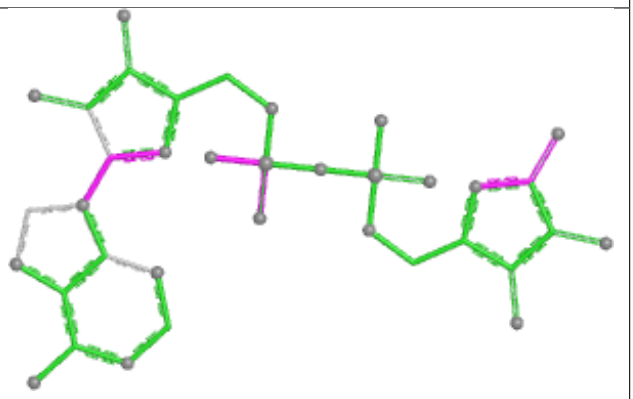
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	404	8L9	3	0
6	B	408	SO4	1	0
5	E	705	8L9	1	0
5	C	1006	8L9	1	0
6	B	409	SO4	2	0
4	E	704	GOL	1	0
5	B	404	8L9	1	0
4	E	701	GOL	1	0
5	F	403	8L9	1	0
5	A	404	8L9	1	0
4	D	403	GOL	3	0

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 then 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.

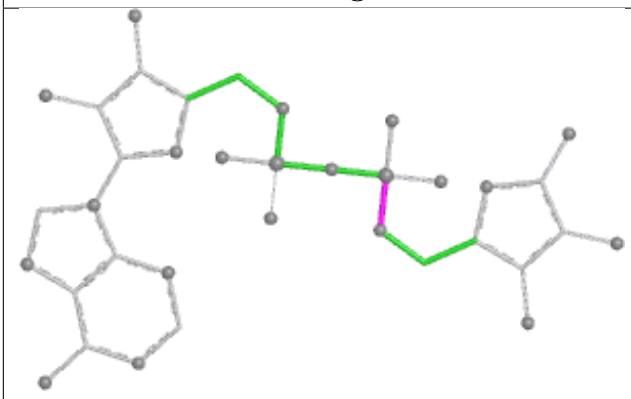
Ligand AR6 C 1002



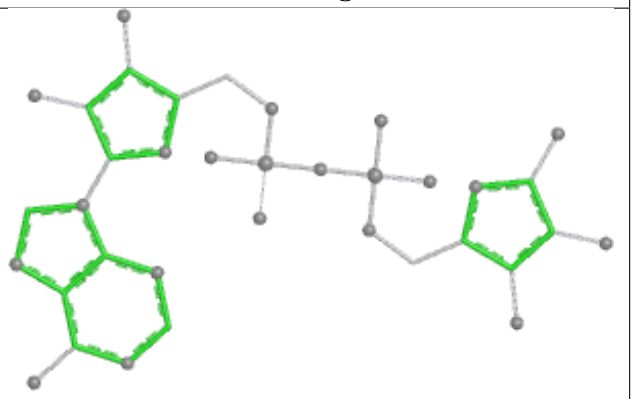
Bond lengths



Bond angles

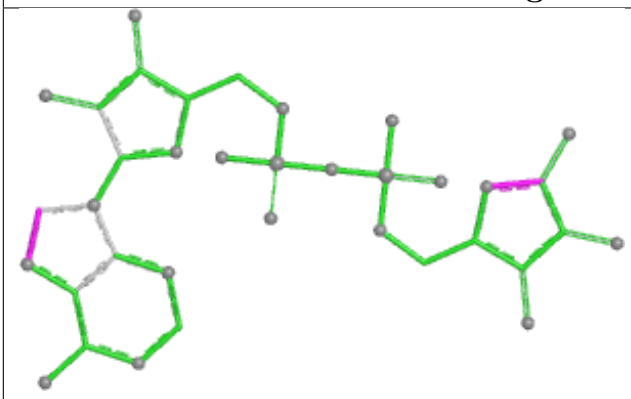


Torsions

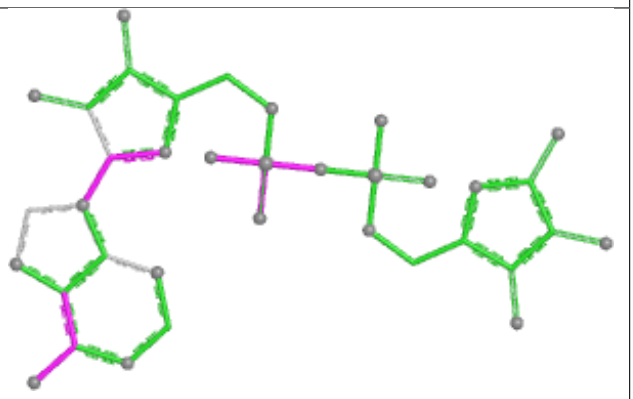


Rings

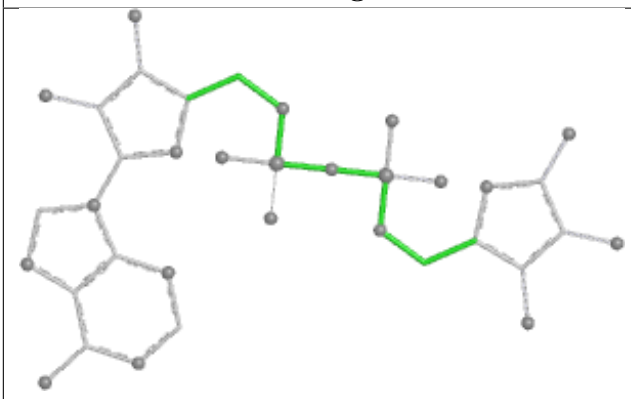
Ligand AR6 B 401



Bond lengths



Bond angles



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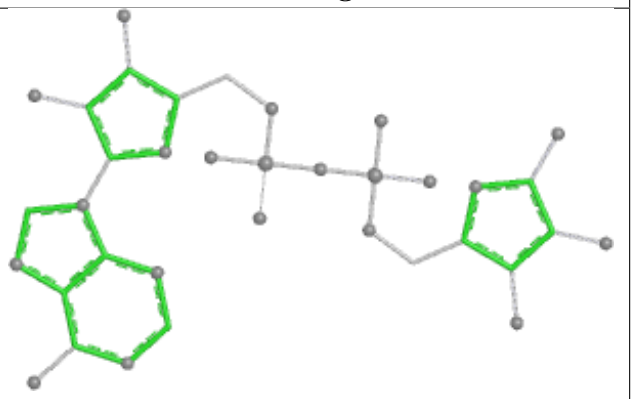
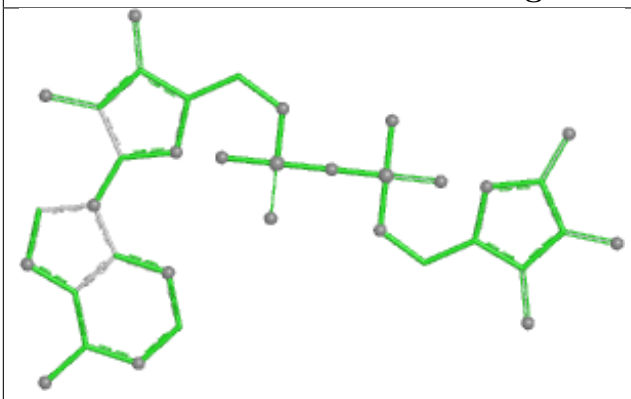
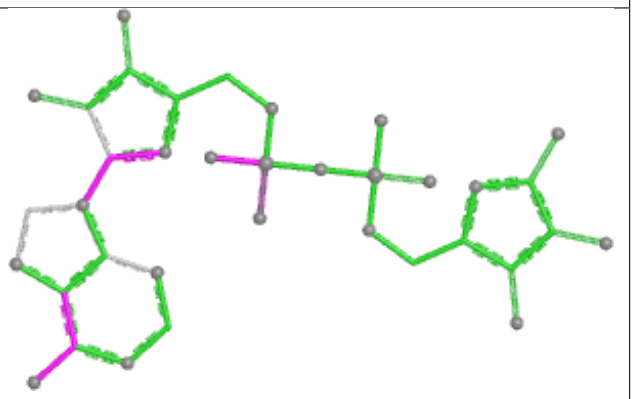


Rings

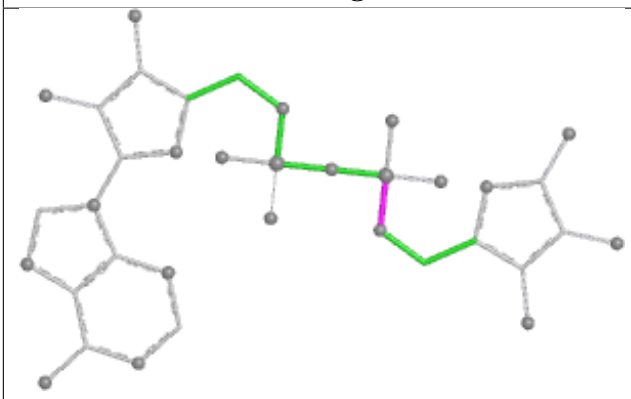
Ligand AR6 D 401



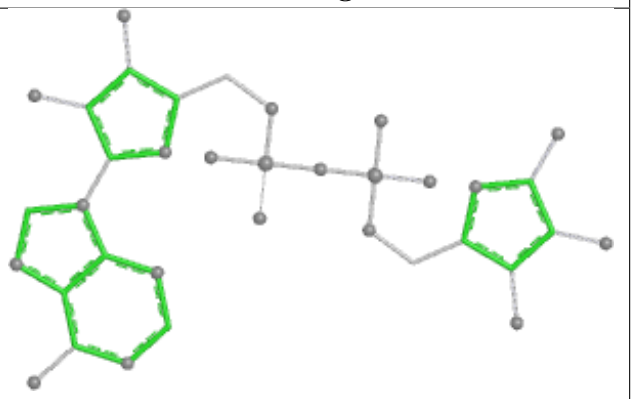
Bond lengths



Bond angles

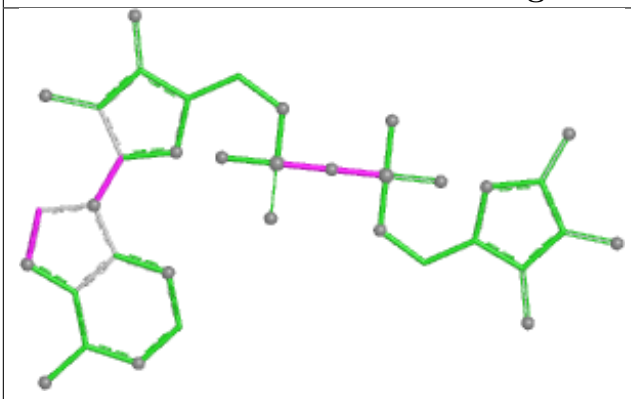


Torsions

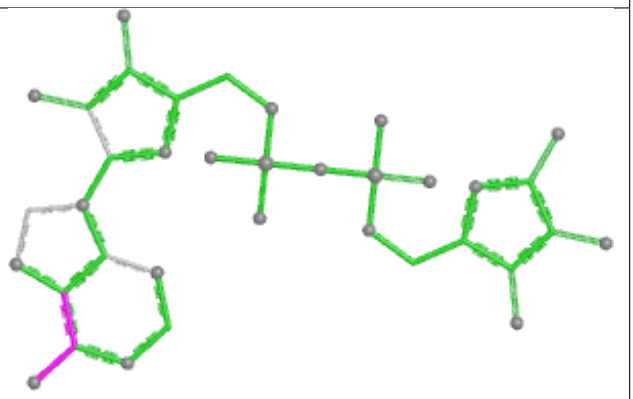


Rings

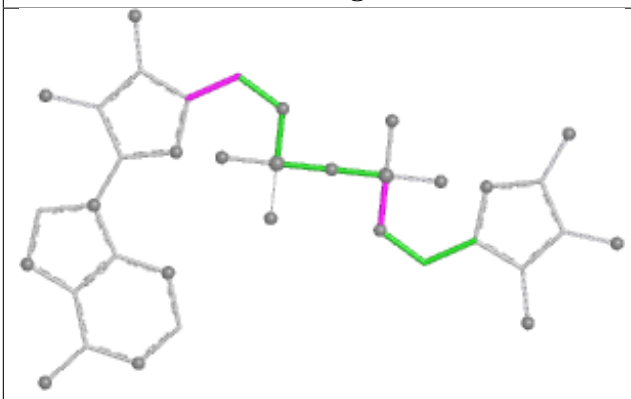
Ligand AR6 F 401



Bond lengths



Bond angles



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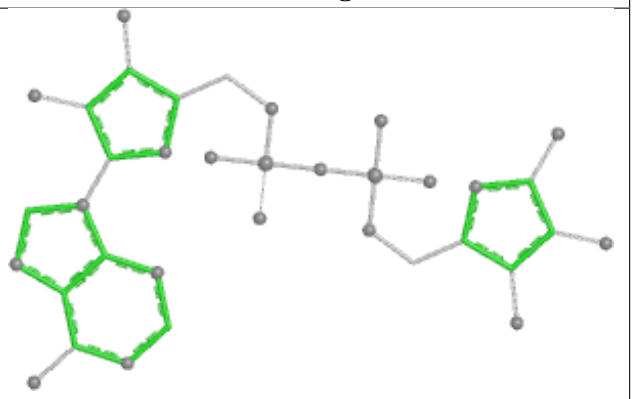
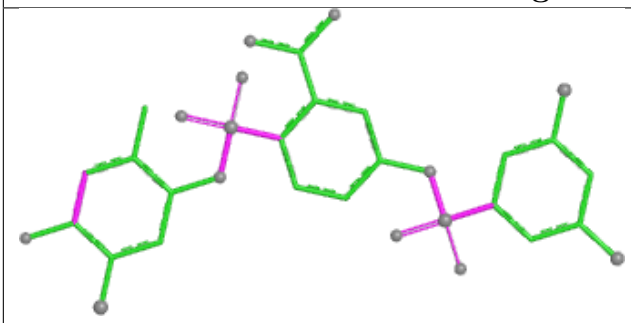
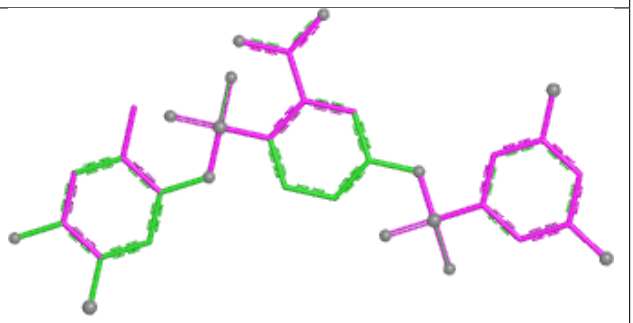


Rings

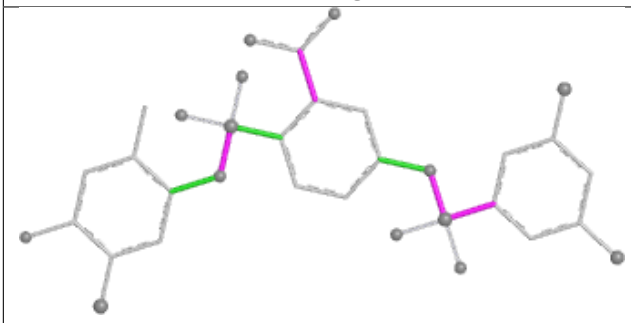
Ligand 8L9 D 404



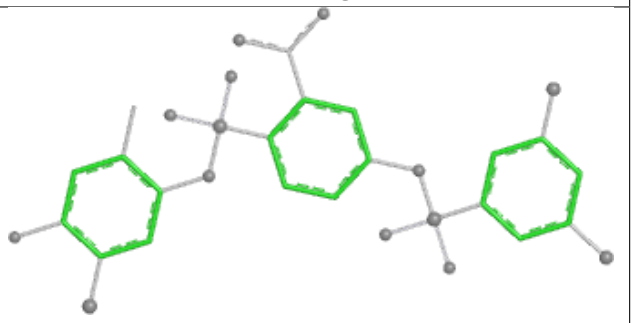
Bond lengths



Bond angles

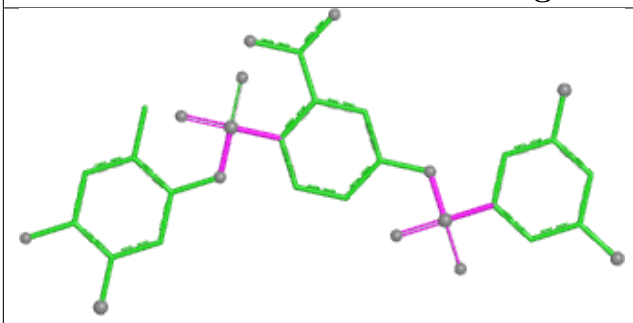


Torsions

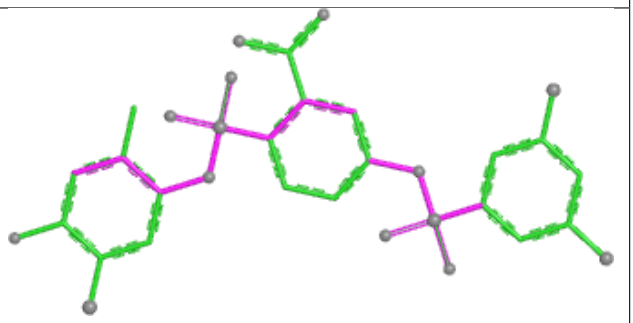


Rings

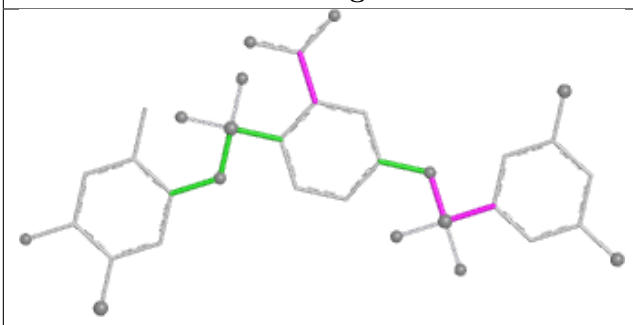
Ligand 8L9 E 705



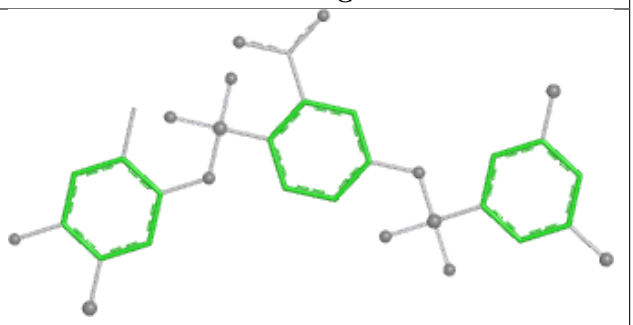
Bond lengths



Bond angles

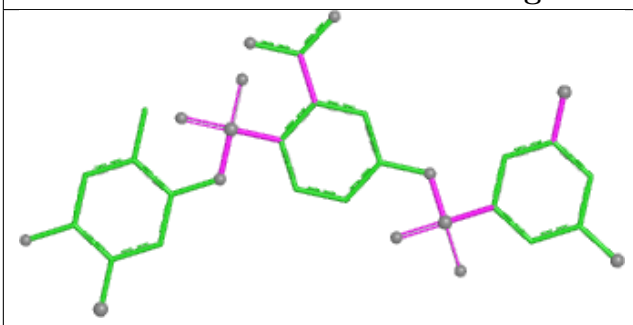


Torsions

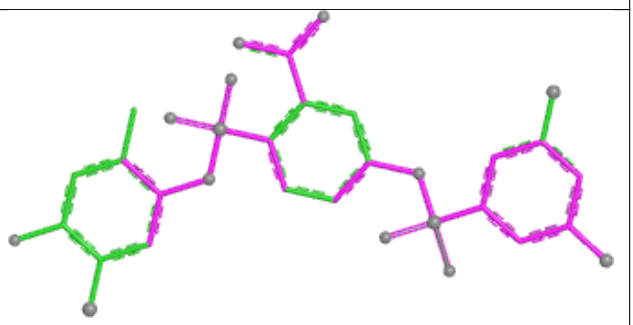


Rings

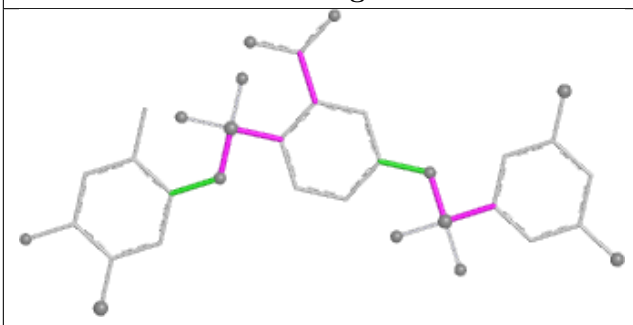
Ligand 8L9 C 1006



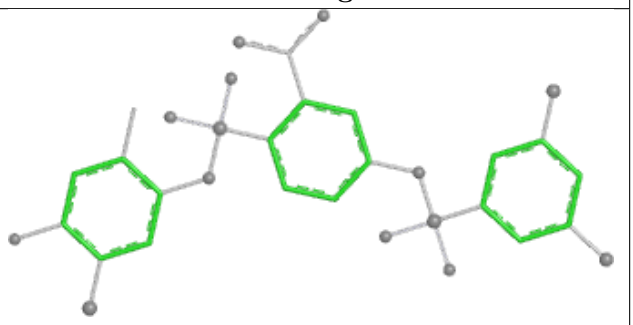
Bond lengths



Bond angles

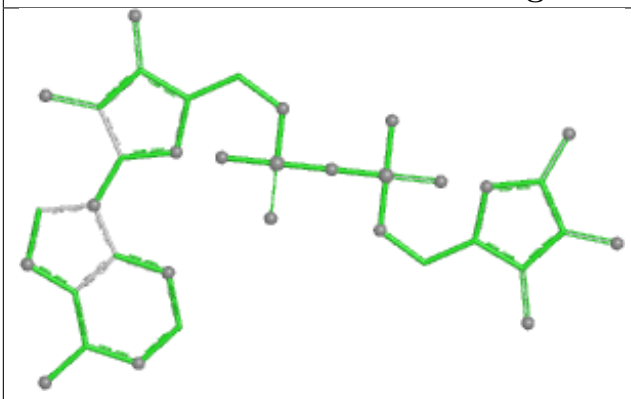


Torsions

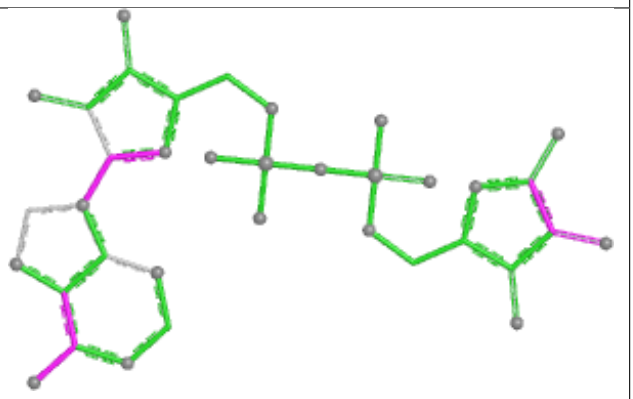


Rings

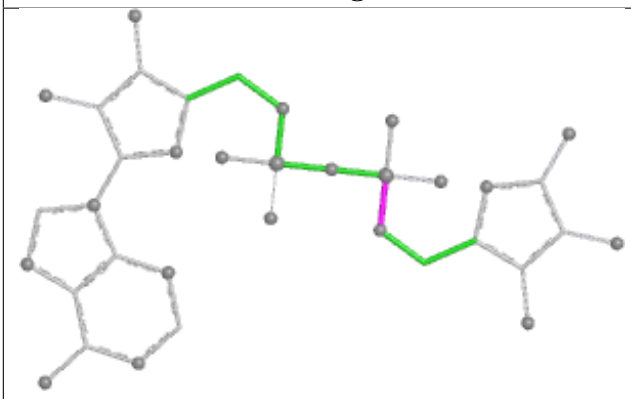
Ligand AR6 E 702



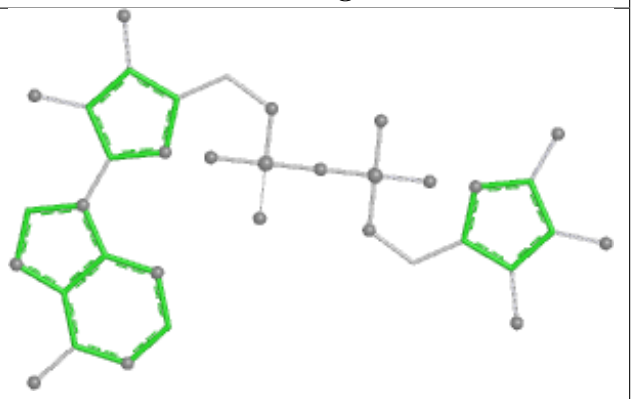
Bond lengths



Bond angles

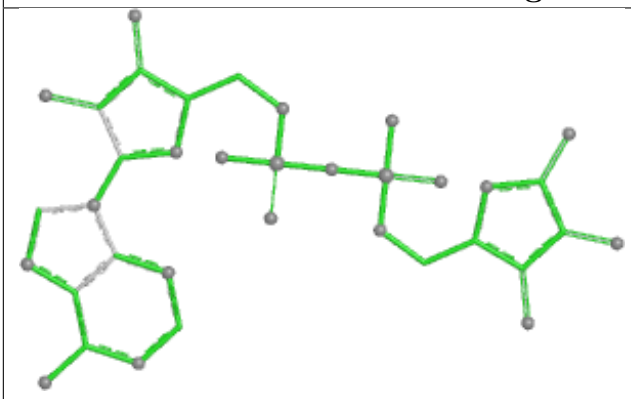


Torsions

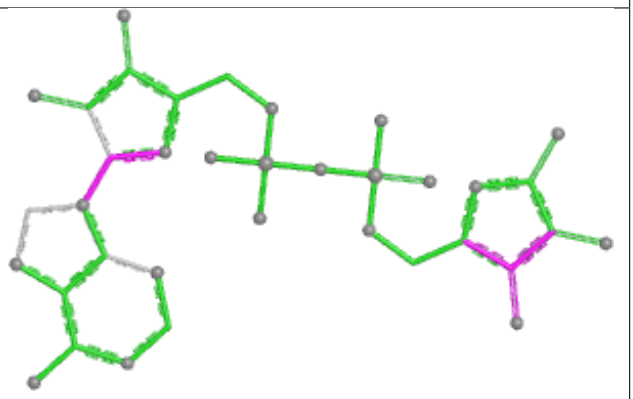


Rings

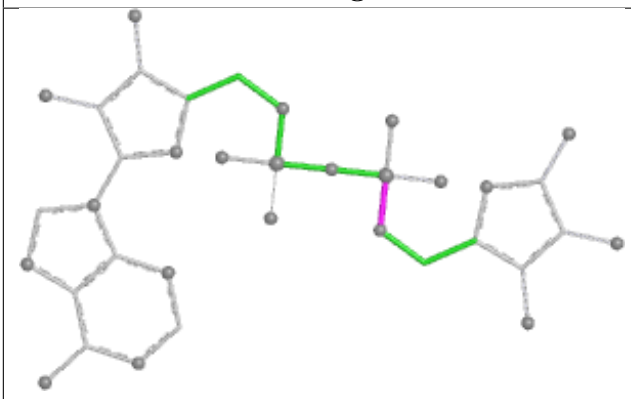
Ligand AR6 A 401



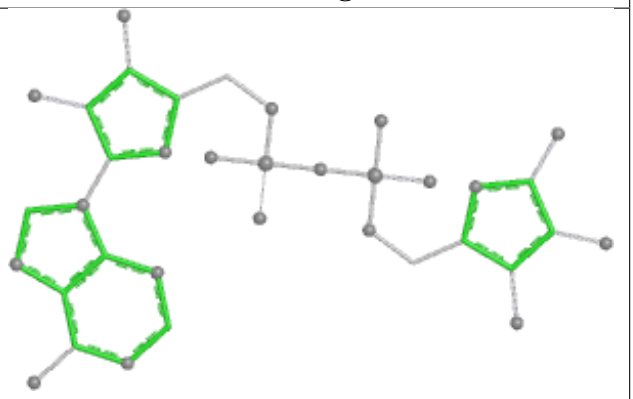
Bond lengths



Bond angles

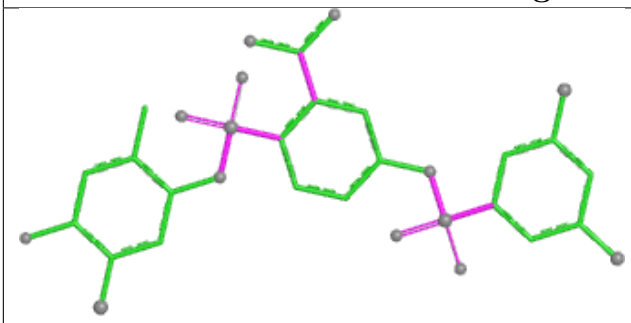


Torsions

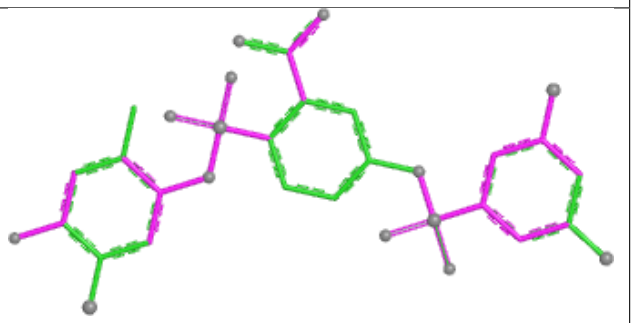


Rings

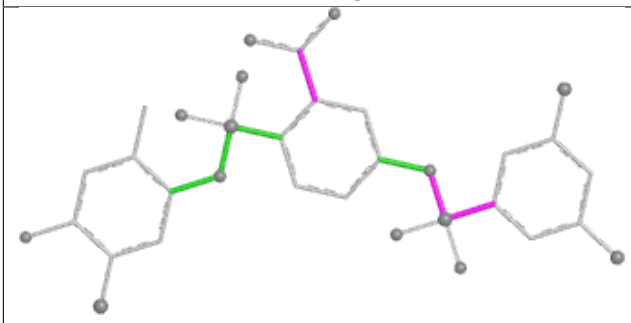
Ligand 8L9 B 404



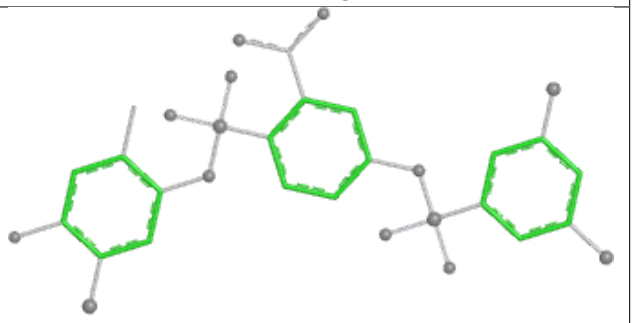
Bond lengths



Bond angles

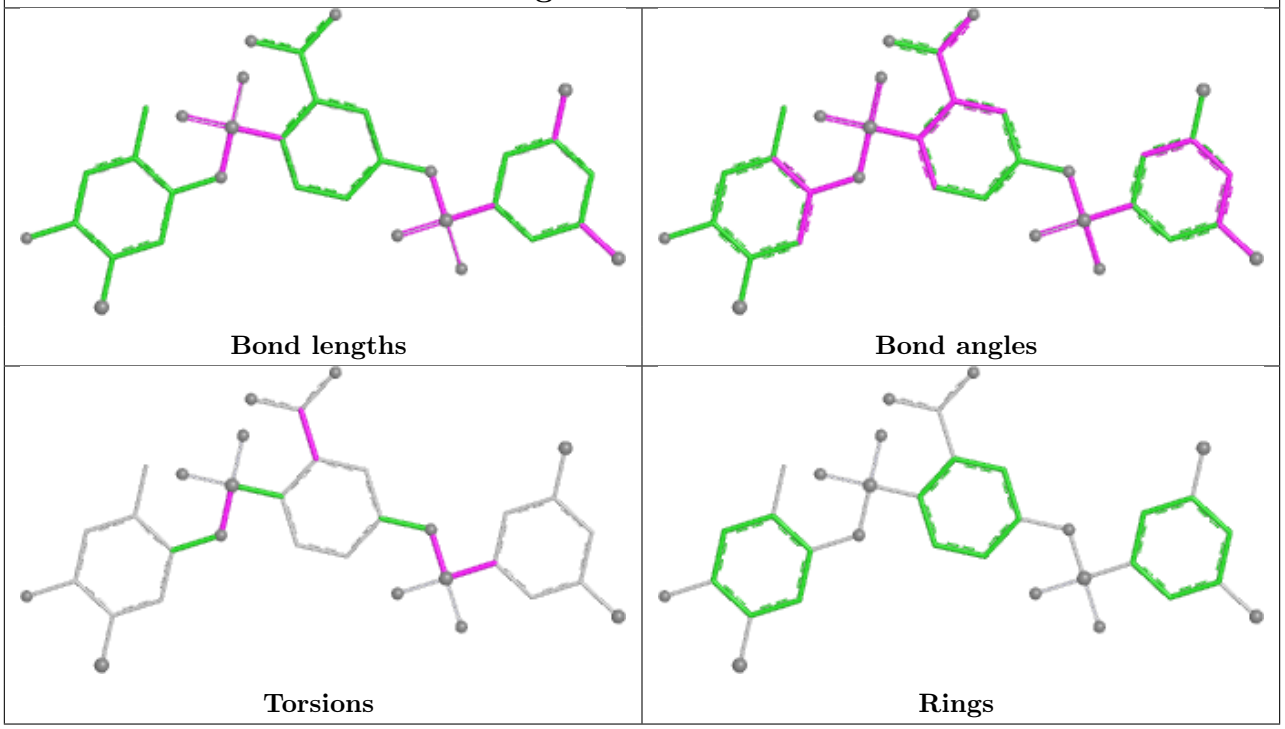


Torsions

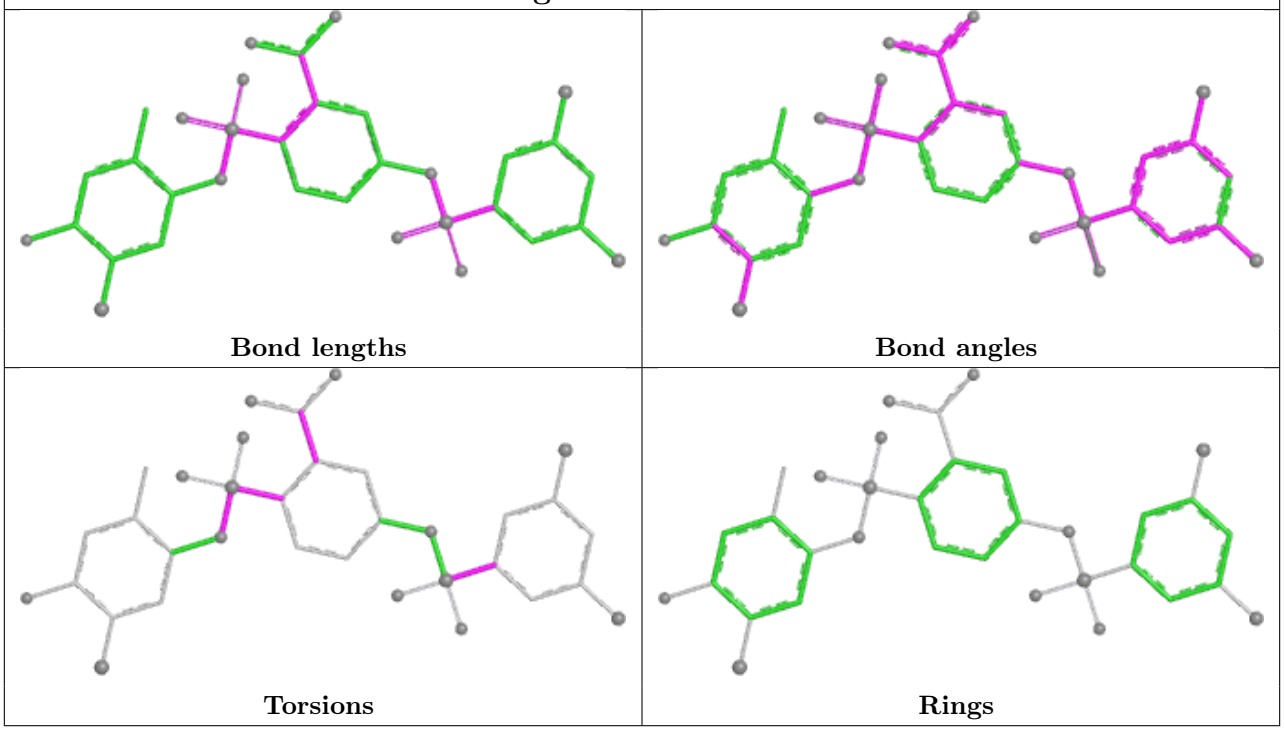


Rings

Ligand 8L9 F 403



Ligand 8L9 A 404



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, 95^{th} 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	278/316 (87%)	0.48	16 (5%)	23	28	34, 48, 84, 133	0
1	B	284/316 (89%)	0.35	16 (5%)	24	29	36, 50, 78, 123	0
1	C	279/316 (88%)	0.47	18 (6%)	18	23	34, 48, 91, 140	0
1	D	277/316 (87%)	0.28	8 (2%)	51	57	36, 52, 79, 117	0
1	E	279/316 (88%)	0.53	17 (6%)	21	26	37, 57, 90, 123	0
1	F	278/316 (87%)	0.60	32 (11%)	4	6	43, 62, 92, 121	0
All	All	1675/1896 (88%)	0.45	107 (6%)	19	24	34, 53, 87, 140	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	ASP	10.8
1	A	188	TRP	8.2
1	E	169	ALA	7.8
1	C	176	ALA	6.5
1	F	178	ARG	6.2
1	E	13	ALA	5.8
1	E	75	GLU	5.7
1	B	188	TRP	5.6
1	E	14	ASP	5.3
1	C	14	ASP	5.2
1	F	298	GLU	4.5
1	D	188	TRP	4.4
1	E	188	TRP	4.4
1	B	176	ALA	4.3
1	D	169	ALA	4.1
1	F	76	ARG	4.1
1	C	169	ALA	4.1
1	C	188	TRP	4.0
1	B	170	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	297	LEU	3.9
1	B	169	ALA	3.6
1	F	227	LEU	3.5
1	C	77	GLY	3.5
1	F	165	LEU	3.5
1	C	148	TYR	3.5
1	F	169	ALA	3.5
1	E	165	LEU	3.5
1	A	195	ARG	3.5
1	A	231	ARG	3.4
1	E	142	ALA	3.4
1	F	228	ALA	3.4
1	D	178	ARG	3.4
1	B	143	LYS	3.4
1	F	142	ALA	3.3
1	F	185	ILE	3.2
1	B	248	ARG	3.2
1	E	15	LYS	3.1
1	F	232	ARG	3.1
1	D	181	LEU	3.1
1	C	168	VAL	3.1
1	F	245	LYS	3.1
1	F	233	GLY	3.1
1	B	189	GLU	3.0
1	A	189	GLU	3.0
1	F	205	ARG	3.0
1	E	180	GLU	2.9
1	C	231	ARG	2.9
1	F	248	ARG	2.9
1	F	231	ARG	2.9
1	C	165	LEU	2.9
1	F	168	VAL	2.9
1	C	76	ARG	2.9
1	F	249	HIS	2.9
1	A	178	ARG	2.8
1	F	78	LEU	2.8
1	A	232	ARG	2.7
1	F	64	PHE	2.7
1	F	157	MET	2.7
1	A	160	LYS	2.7
1	F	181	LEU	2.7
1	B	159	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	189	GLU	2.6
1	D	35	TRP	2.6
1	E	181	LEU	2.6
1	B	162	THR	2.5
1	F	188	TRP	2.5
1	C	142	ALA	2.5
1	A	191	SER	2.5
1	E	168	VAL	2.5
1	F	192	LEU	2.4
1	D	75	GLU	2.4
1	A	15	LYS	2.4
1	C	162	THR	2.4
1	E	76	ARG	2.4
1	A	169	ALA	2.4
1	B	142	ALA	2.4
1	F	35	TRP	2.4
1	A	182	ARG	2.3
1	B	32	ARG	2.3
1	C	20	LEU	2.3
1	E	32	ARG	2.3
1	A	194	ASP	2.2
1	F	241	LEU	2.2
1	C	167	THR	2.2
1	F	253	ARG	2.2
1	F	180	GLU	2.2
1	C	78	LEU	2.2
1	B	194	ASP	2.2
1	E	35	TRP	2.2
1	D	165	LEU	2.1
1	C	163	GLY	2.1
1	E	71	TRP	2.1
1	B	195	ARG	2.1
1	D	156	THR	2.1
1	E	298	GLU	2.1
1	B	171	ALA	2.1
1	F	31	GLU	2.1
1	A	258	VAL	2.1
1	C	154	VAL	2.1
1	E	248	ARG	2.1
1	B	173	GLY	2.1
1	A	148	TYR	2.0
1	F	195	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	192	LEU	2.0
1	B	167	THR	2.0
1	F	20	LEU	2.0
1	F	145	LYS	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	403	6/6	0.55	0.18	75,80,87,89	0
4	GOL	E	704	6/6	0.64	0.24	70,73,77,89	0
4	GOL	B	403	6/6	0.70	0.25	61,78,81,81	0
4	GOL	E	701	6/6	0.72	0.17	78,93,102,110	0
4	GOL	C	1004	6/6	0.80	0.12	75,85,91,91	0
5	8L9	F	403	34/34	0.80	0.26	92,130,180,193	0
6	SO4	C	1007	5/5	0.80	0.30	107,109,115,126	0
5	8L9	B	404	34/34	0.81	0.24	96,118,149,156	0
4	GOL	C	1005	6/6	0.81	0.38	61,68,73,76	0
4	GOL	D	403	6/6	0.81	0.21	72,77,79,83	0
4	GOL	C	1001	6/6	0.84	0.16	72,79,86,88	0
5	8L9	E	705	34/34	0.85	0.23	81,117,156,156	0
6	SO4	E	707	5/5	0.85	0.34	88,89,106,122	0
6	SO4	A	405	5/5	0.87	0.20	91,105,114,121	0
5	8L9	A	404	34/34	0.89	0.18	74,86,130,156	0
5	8L9	D	404	34/34	0.90	0.20	81,97,135,167	0
6	SO4	B	409	5/5	0.90	0.24	98,105,109,110	0
6	SO4	D	406	5/5	0.91	0.24	95,108,117,117	0
5	8L9	C	1006	34/34	0.91	0.24	78,108,156,157	0

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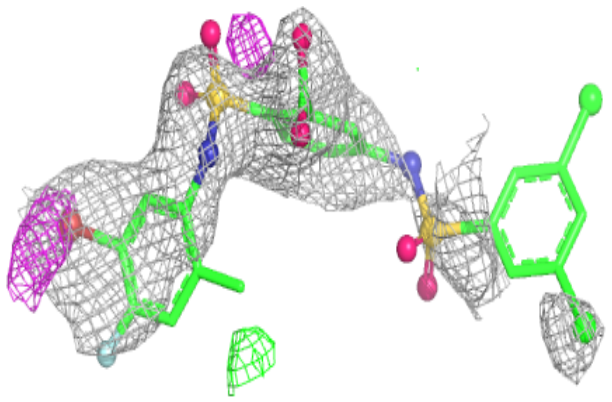
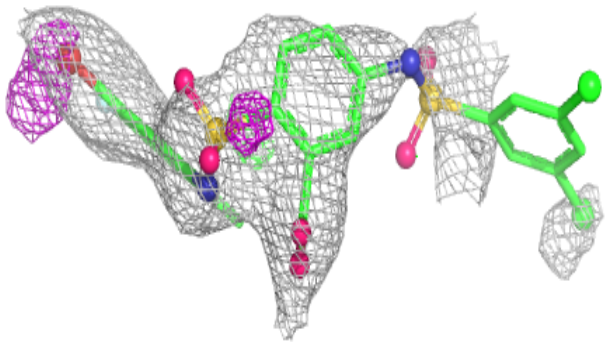
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	E	708	5/5	0.91	0.21	92,106,118,120	0
6	SO4	B	408	5/5	0.92	0.18	82,94,96,101	0
6	SO4	D	407	5/5	0.92	0.17	100,106,112,115	0
6	SO4	B	407	5/5	0.93	0.15	81,90,94,101	0
6	SO4	B	405	5/5	0.94	0.23	77,80,84,95	0
3	ZN	E	703	1/1	0.95	0.07	77,77,77,77	0
6	SO4	B	406	5/5	0.95	0.16	71,79,96,100	0
2	AR6	F	401	36/36	0.97	0.10	47,55,71,72	0
3	ZN	A	402	1/1	0.97	0.07	66,66,66,66	0
6	SO4	E	706	5/5	0.97	0.12	63,65,79,92	0
2	AR6	E	702	36/36	0.97	0.11	44,51,63,65	0
6	SO4	D	405	5/5	0.97	0.16	71,78,87,93	0
3	ZN	C	1003	1/1	0.98	0.09	63,63,63,63	0
2	AR6	A	401	36/36	0.98	0.11	32,38,47,55	0
3	ZN	F	402	1/1	0.98	0.07	79,79,79,79	0
2	AR6	B	401	36/36	0.98	0.12	35,42,50,60	0
2	AR6	D	401	36/36	0.98	0.10	42,45,52,53	0
3	ZN	D	402	1/1	0.99	0.06	68,68,68,68	0
3	ZN	B	402	1/1	0.99	0.07	60,60,60,60	0
2	AR6	C	1002	36/36	0.99	0.11	33,40,50,57	0

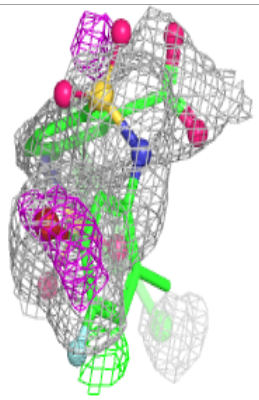
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8L9 F 403:

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

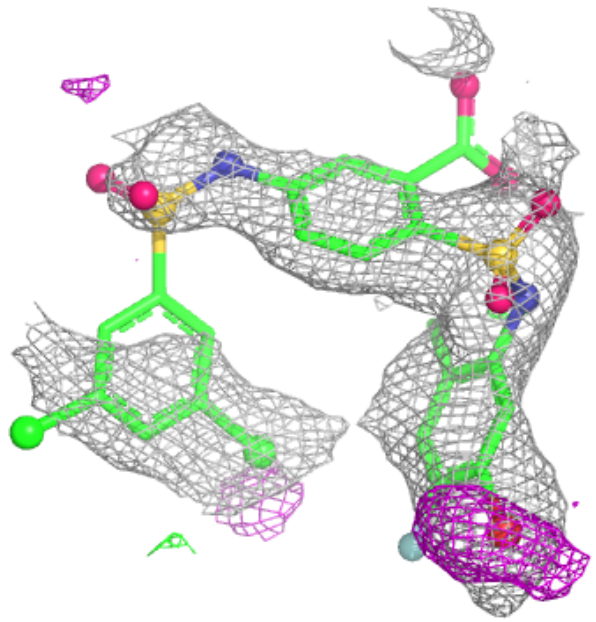


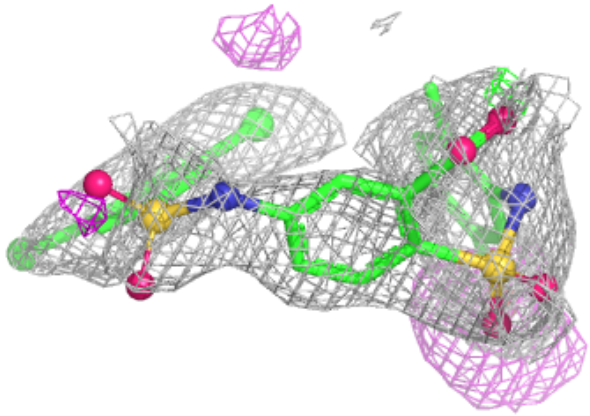


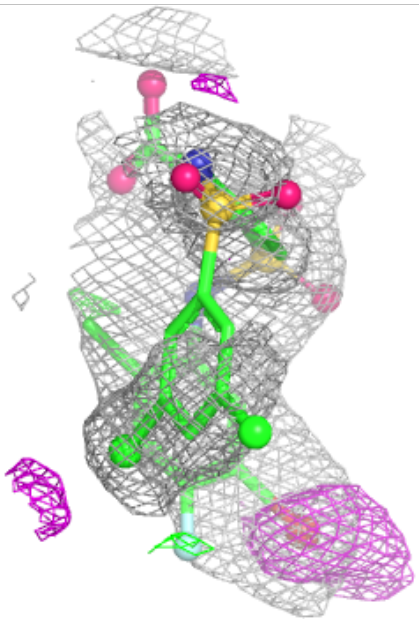


Electron density around 8L9 B 404:

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

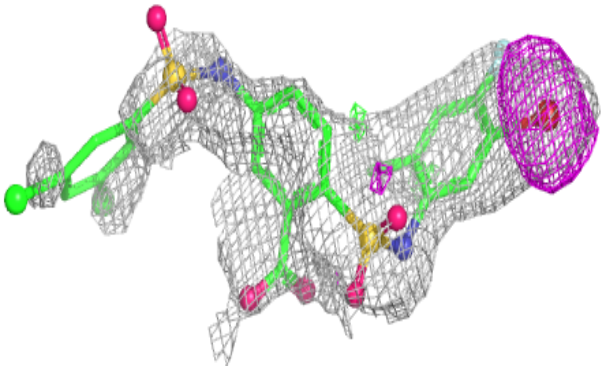


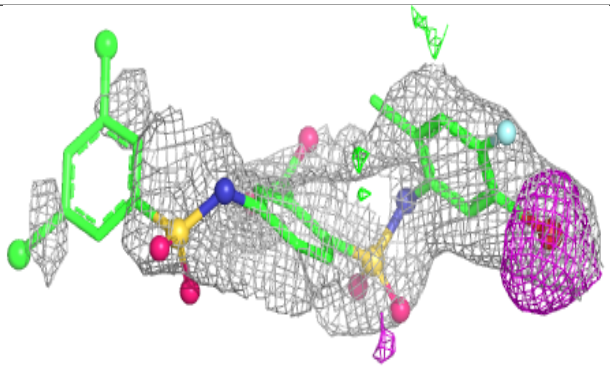


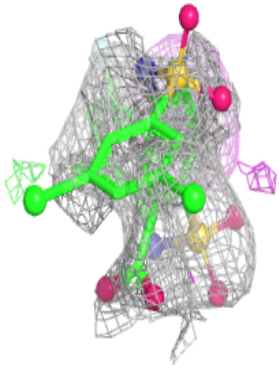


Electron density around 8L9 E 705:

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

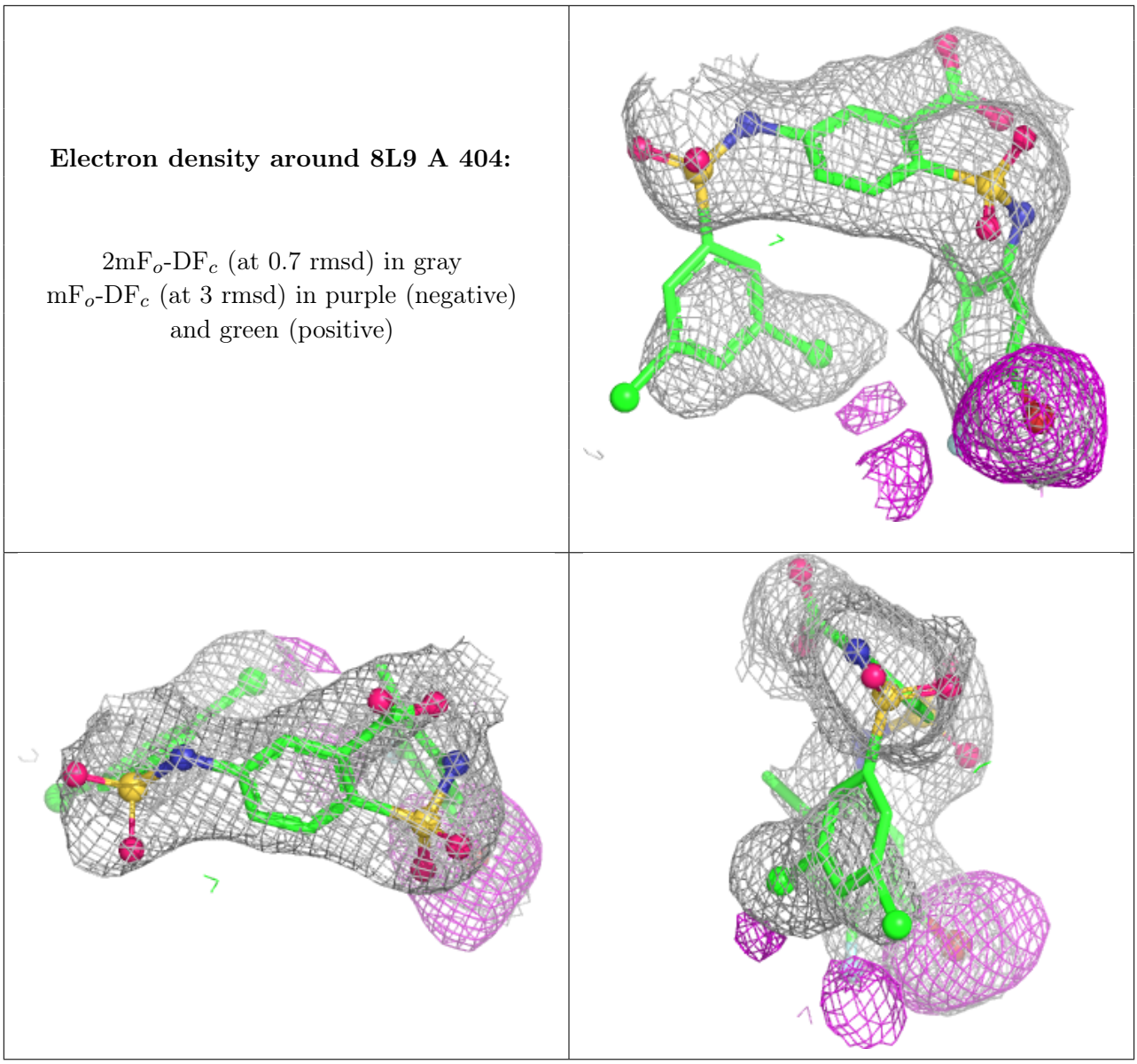






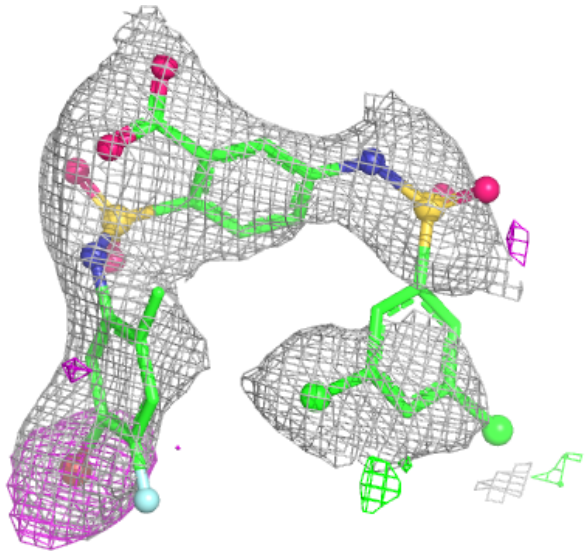
Electron density around 8L9 A 404:

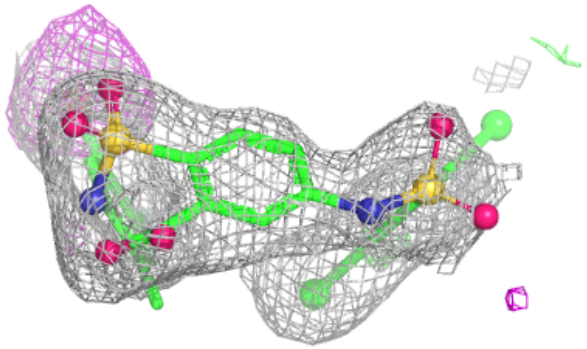
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

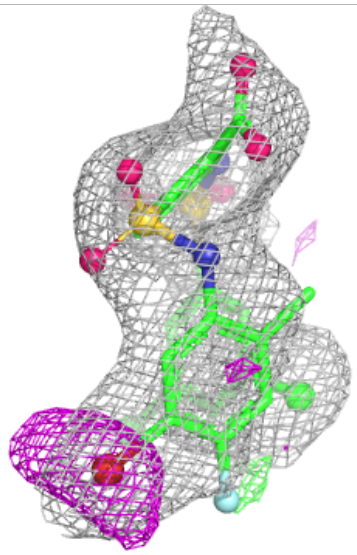


Electron density around 8L9 D 404:

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

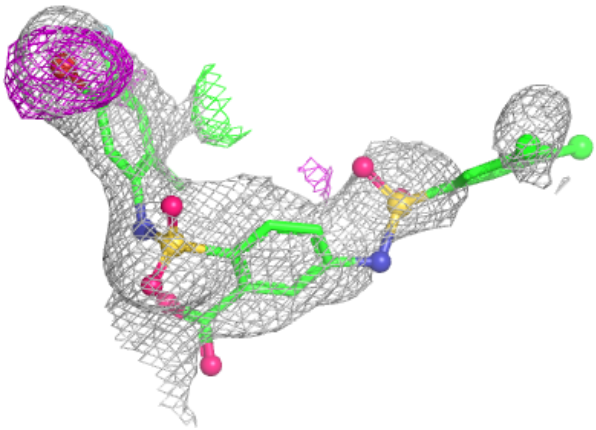


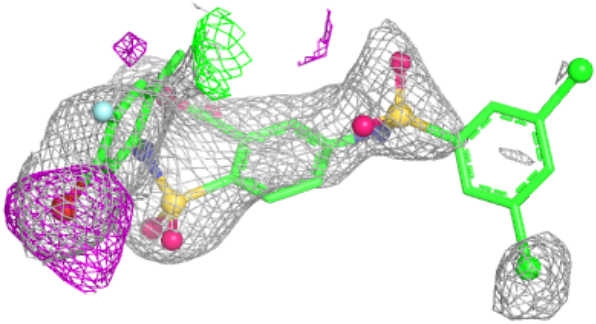


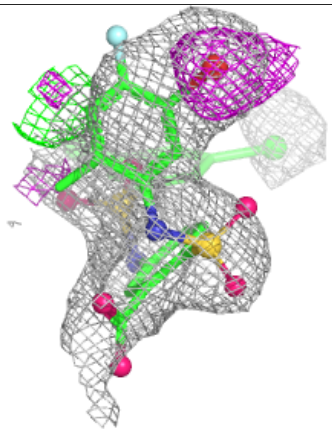


Electron density around 8L9 C 1006:

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

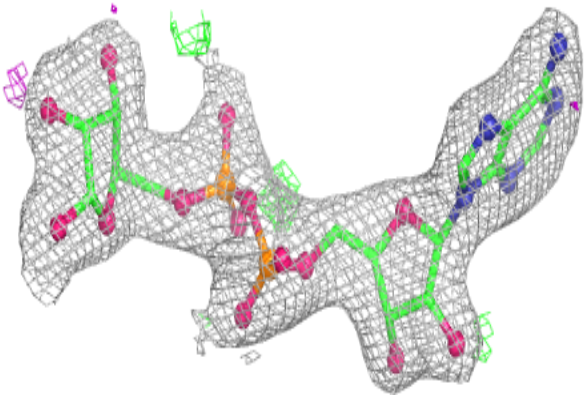


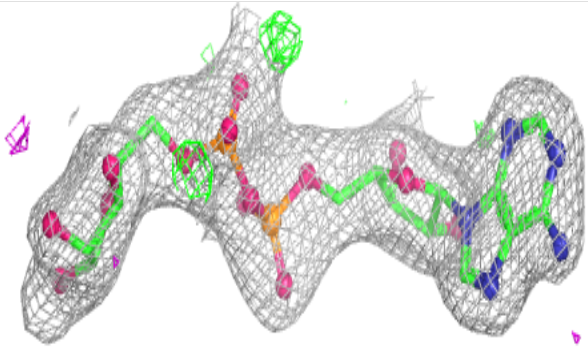


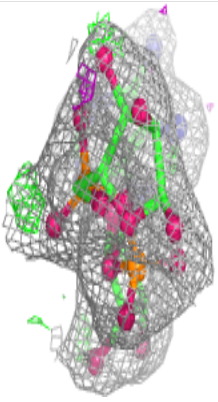


Electron density around AR6 F 401:

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

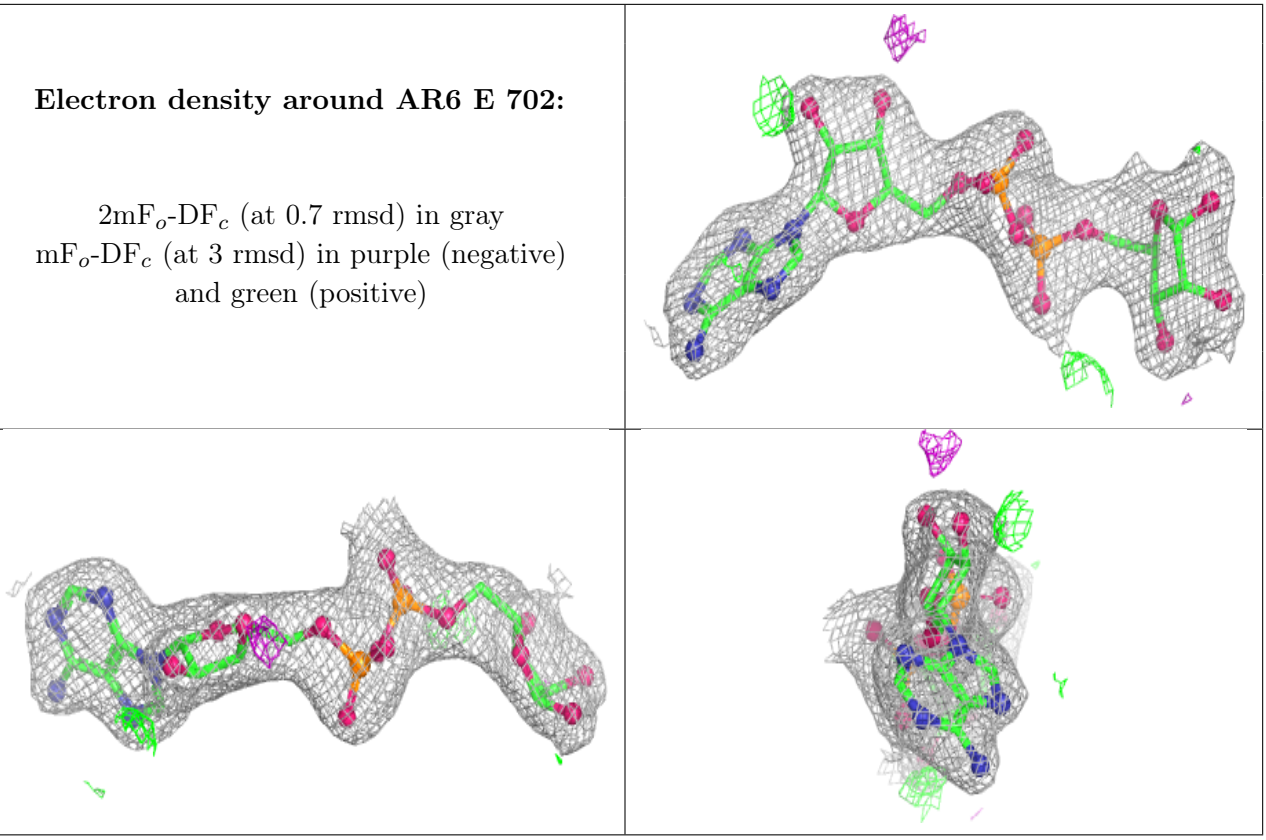






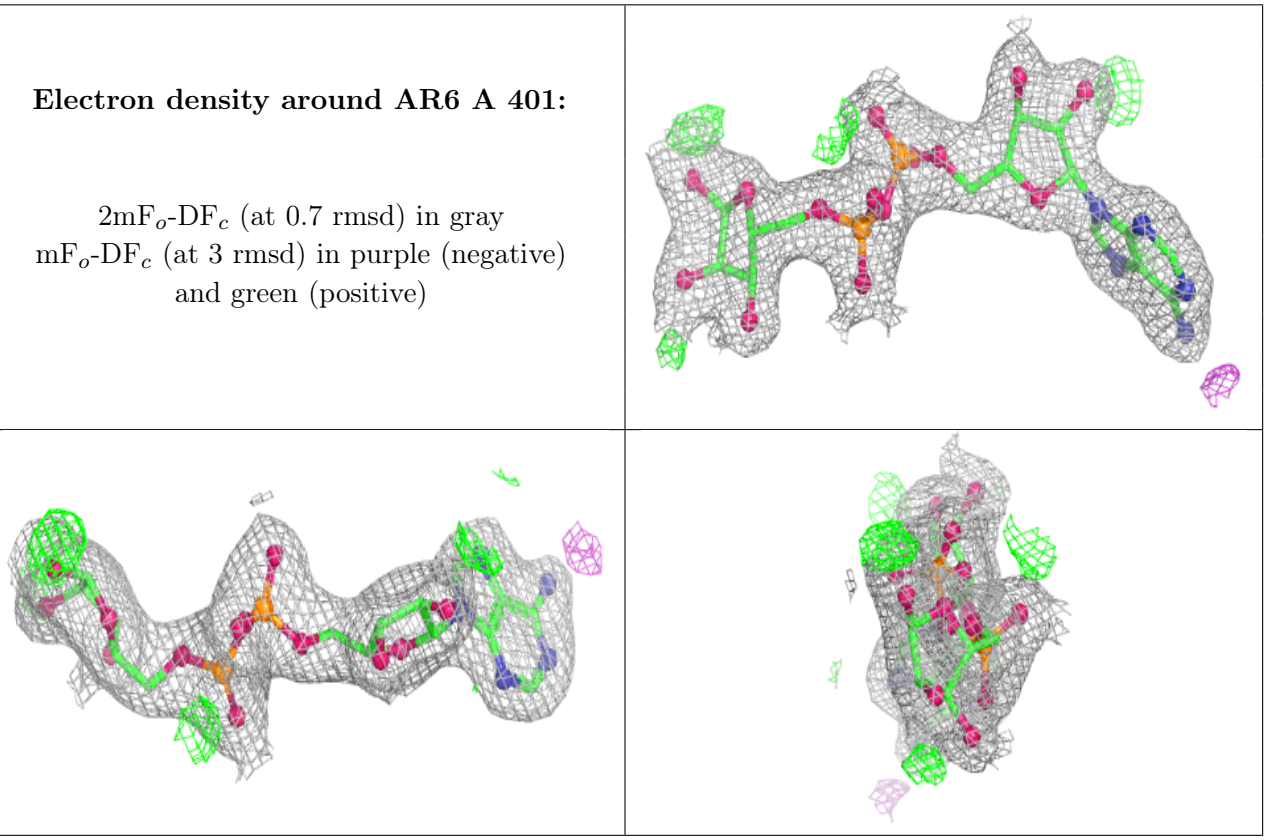
Electron density around AR6 E 702:

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



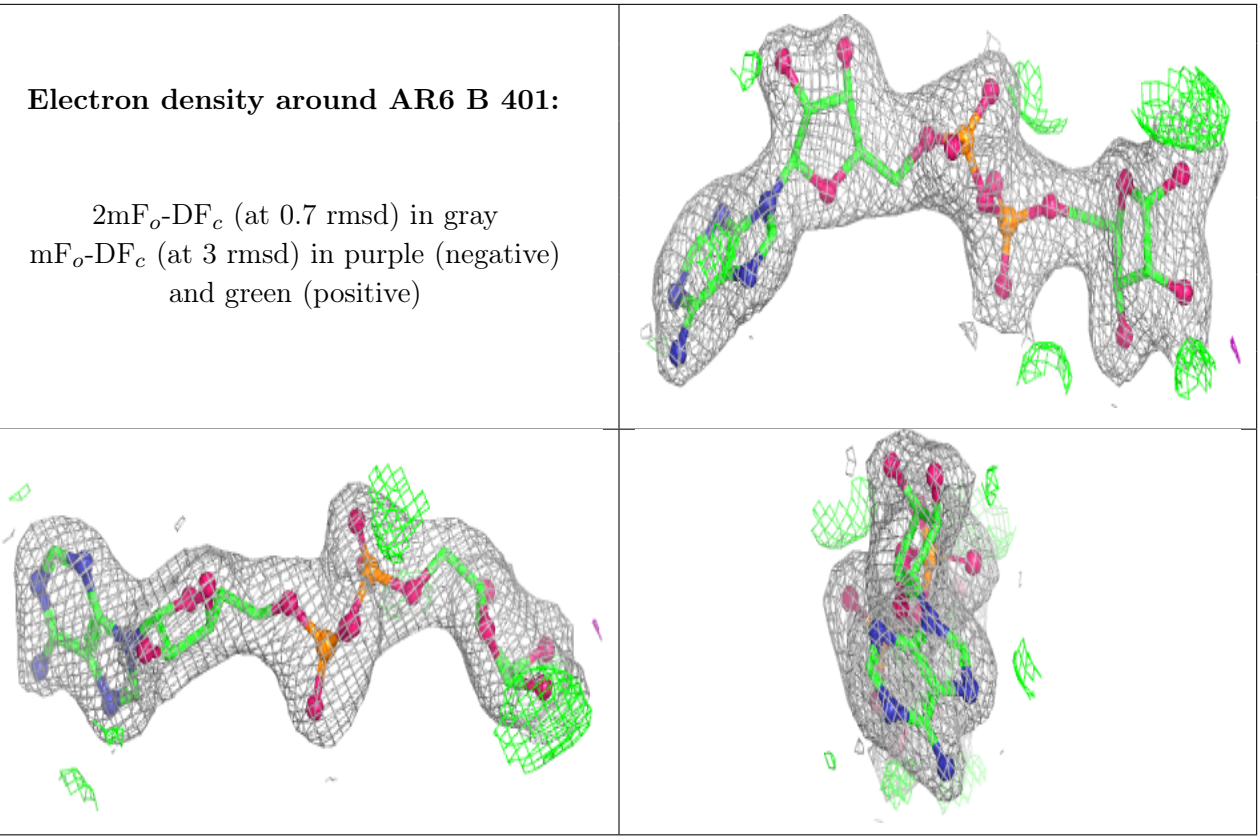
Electron density around AR6 A 401:

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



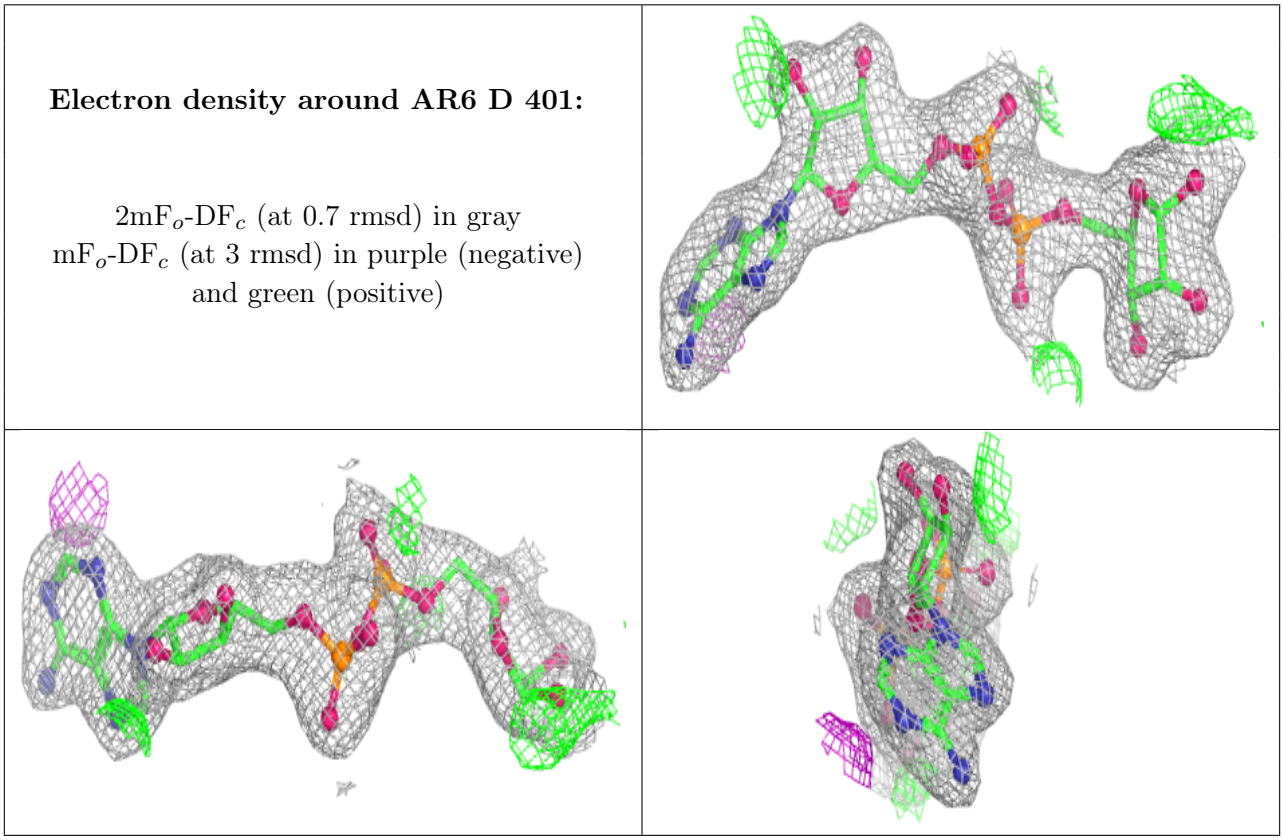
Electron density around AR6 B 401:

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



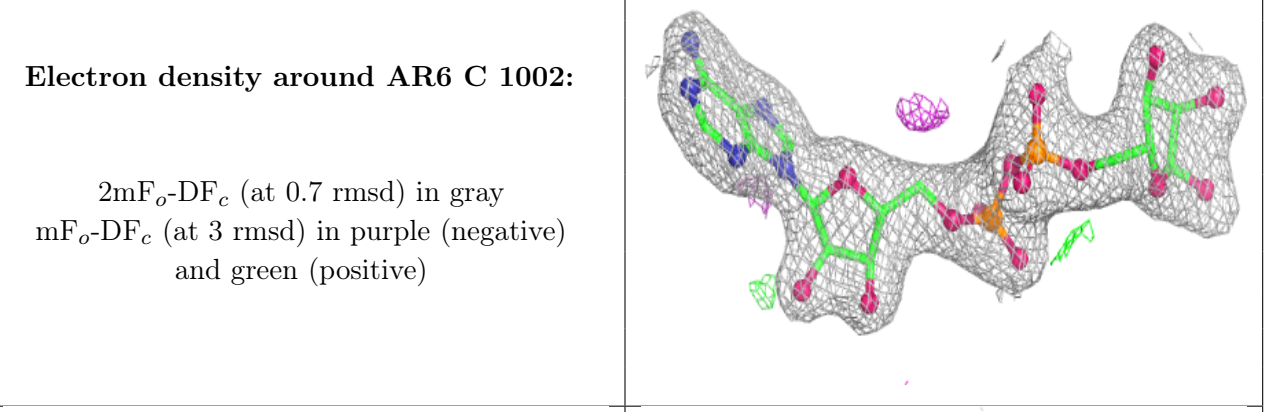
Electron density around AR6 D 401:

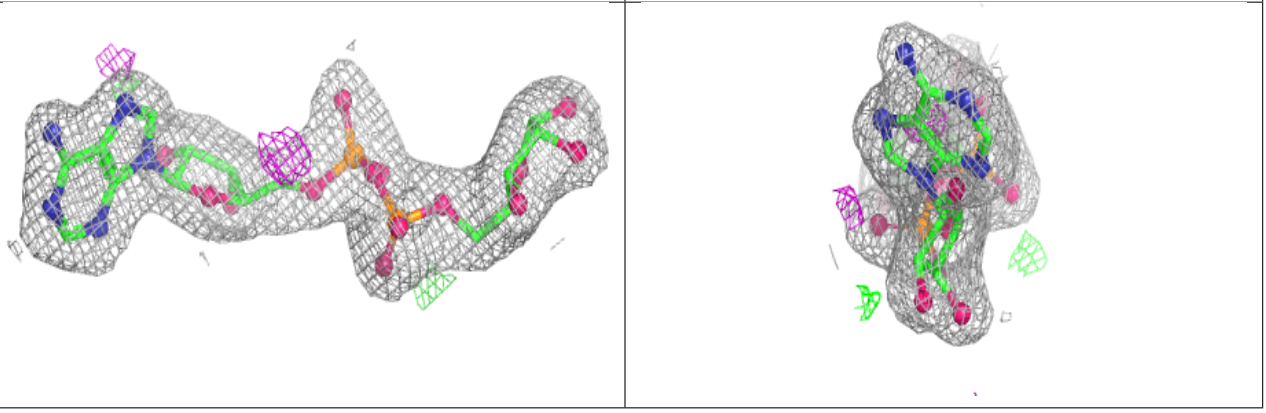
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around AR6 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)





6.5 Other polymers (i)

There are no such residues in this entry.