



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 02:01 PM EDT

PDB ID : 8G62 / pdb_00008g62
Title : Papain-Like Protease of SARS CoV-2 in complex with remodilin NCGC 390004
Authors : Osipiuk, J.; Tesar, C.; Endres, M.; Jedrzejczak, R.; Luci, D.; Kales, S.; Simonov, A.; Rai, G.; Drayman, N.; Tay, S.; Oakes, S.; Rosner, M.; Chen, B.; Dulin, N.; Solway, J.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID); Center for Structural Biology of Infectious Diseases (CSBID)
Deposited on : 2023-02-14
Resolution : 2.17 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

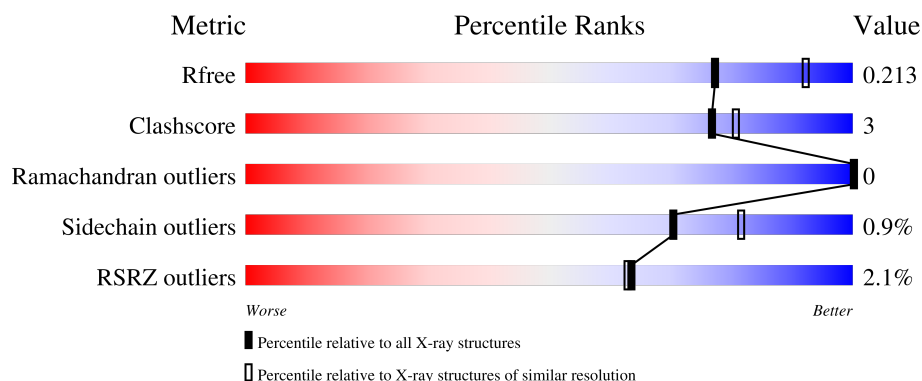
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	318	0% 94% 5%
1	B	318	3% 87% 11%
1	C	318	2% 91% 7%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8110 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 Non-structural protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	5	0
			2527	1609	417	482	19			
1	B	313	Total	C	N	O	S	0	8	0
			2526	1612	417	478	19			
1	C	313	Total	C	N	O	S	0	5	0
			2515	1603	415	478	19			

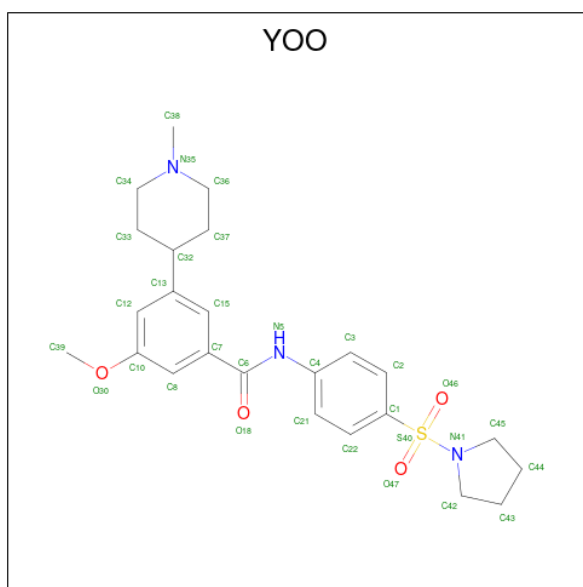
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P0DTC1
A	-1	ASN	-	expression tag	UNP P0DTC1
A	0	ALA	-	expression tag	UNP P0DTC1
B	-2	SER	-	expression tag	UNP P0DTC1
B	-1	ASN	-	expression tag	UNP P0DTC1
B	0	ALA	-	expression tag	UNP P0DTC1
C	-2	SER	-	expression tag	UNP P0DTC1
C	-1	ASN	-	expression tag	UNP P0DTC1
C	0	ALA	-	expression tag	UNP P0DTC1

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 3-methoxy-5-(1-methylpiperidin-4-yl)-N-[4-(pyrrolidine-1-sulfonyl)phenyl]benzamide (CCD ID: YOO) (formula: C₂₄H₃₁N₃O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			49	35	5	7	2		
3	A	1	Total	C	N	O	S	0	0
			32	24	3	4	1		
3	A	1	Total	C	N	O	S	0	0
			32	24	3	4	1		
3	B	1	Total	C	N	O	S	0	1
			49	35	5	7	2		
3	C	1	Total	C	N	O	S	0	0
			32	24	3	4	1		
3	C	1	Total	C	N	O	S	0	1
			49	35	5	7	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

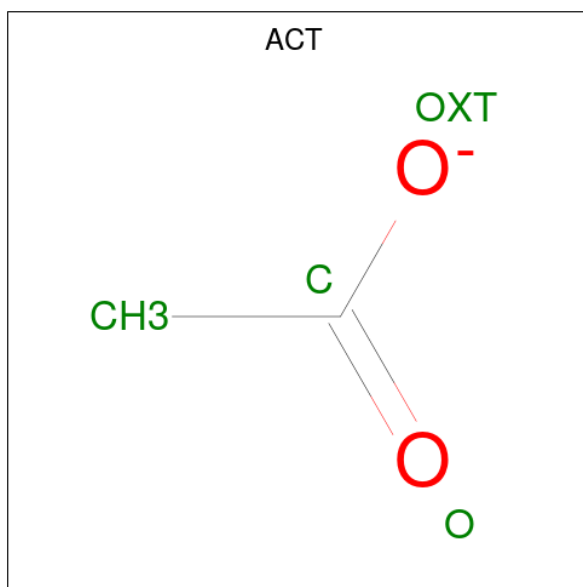
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Cl	0	0
			2	2		
5	C	2	Total	Cl	0	0
			2	2		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	126	Total	O	0	0
			126	126		

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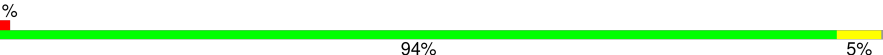
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	75	Total 75	O 75	0	1
7	C	63	Total 63	O 63	0	0

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.

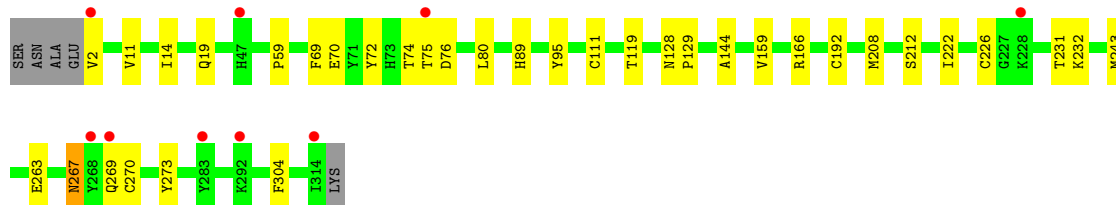
- Molecule 1: Non-structural protein 3

Chain A: 



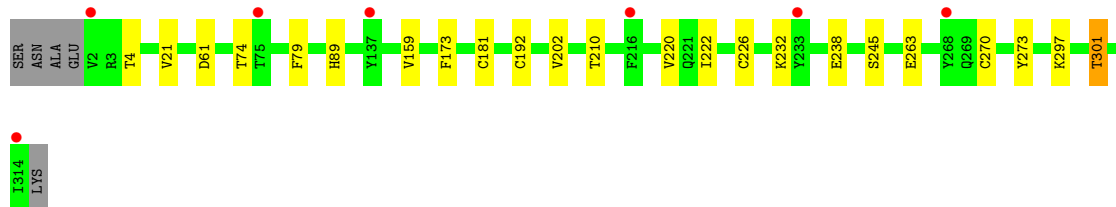
- Molecule 1: Non-structural protein 3

Chain B: 



- Molecule 1: Non-structural protein 3

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	170.02Å 170.02Å 97.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.06 – 2.17 49.06 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.06-2.17) 99.9 (49.06-2.17)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.180 , 0.214 0.184 , 0.213	Depositor DCC
R_{free} test set	3793 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8110	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ZN, YOO, ACT, CL

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	1.00	0/2601	1.25	0/3528
1	B	1.00	0/2610	1.27	3/3539 (0.1%)
1	C	0.97	0/2590	1.26	0/3515
All	All	0.99	0/7801	1.26	3/10582 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	ASP	CB-CA-C	5.98	116.81	110.17
1	B	14	ILE	N-CA-C	-5.32	107.42	111.62
1	B	231	THR	CA-CB-OG1	-5.18	101.83	109.60

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	2527	0	2481	11	0
1	B	2526	0	2492	24	0
1	C	2515	0	2463	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
3	A	113	0	0	1	0
3	B	49	0	0	3	0
3	C	81	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
6	A	12	0	9	1	0
6	B	8	0	6	2	0
6	C	4	0	3	1	0
7	A	126	0	0	1	0
7	B	75	0	0	2	0
7	C	63	0	0	0	0
All	All	8110	0	7454	45	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 (45) 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:B:111:CYS:SG	7:B:643:HOH:O	2.27	0.92
1:B:212:SER:OG	6:B:507:ACT:H1	1.76	0.85
1:B:270:CYS:SG	1:C:232:LYS:NZ	2.56	0.72
1:A:111:CYS:SG	7:A:696:HOH:O	2.48	0.70
3:A:502[B]:YOO:C3	3:A:502[B]:YOO:O18	2.39	0.70
1:A:232:LYS:NZ	1:C:270:CYS:SG	2.60	0.69
1:A:270:CYS:SG	1:B:232:LYS:NZ	2.62	0.67
3:B:502[B]:YOO:C3	3:B:502[B]:YOO:O18	2.45	0.62
3:C:403[B]:YOO:O18	3:C:403[B]:YOO:C21	2.54	0.56
1:B:72:TYR:HB2	1:B:74:THR:HG22	1.88	0.55
1:B:269:GLN:NE2	7:B:603:HOH:O	2.39	0.55
1:B:95:TYR:CD1	1:B:144:ALA:HB3	2.44	0.53
1:B:11:VAL:HB	1:B:80:LEU:HD11	1.90	0.53
1:B:59:PRO:HD3	1:B:80:LEU:HD12	1.90	0.52
1:B:69:PHE:CE1	1:B:75:THR:HG23	2.46	0.51
1:B:208:MET:HE2	3:B:502[A]:YOO:C2	2.40	0.51
1:A:72:TYR:HB2	1:A:74:THR:HG22	1.94	0.49
1:A:119:THR:HG21	1:A:304:PHE:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:HIS:HB2	1:A:159:VAL:HG21	1.95	0.49
1:B:192:CYS:SG	1:B:226:CYS:HB3	2.54	0.48
1:B:267:ASN:CG	1:C:222:ILE:HD12	2.39	0.48
1:C:263:GLU:O	1:C:273:TYR:HA	2.14	0.47
1:B:69:PHE:CZ	1:B:75:THR:CG2	2.98	0.47
1:B:128:ASN:HB2	1:B:129:PRO:HD3	1.95	0.47
1:B:208:MET:HE2	3:B:502[A]:YOO:C3	2.44	0.47
1:B:89:HIS:HB2	1:B:159:VAL:HG21	1.96	0.46
1:B:19:GLN:HE22	6:B:506:ACT:H1	1.82	0.45
1:A:267:ASN:CG	1:B:222:ILE:HD12	2.42	0.45
1:C:173:PHE:HB3	1:C:202:VAL:HG22	1.98	0.44
1:C:210:THR:HG21	1:C:220:VAL:HG11	1.99	0.44
1:C:89:HIS:HB2	1:C:159:VAL:HG21	2.00	0.44
1:C:181:CYS:HA	1:C:238:GLU:O	2.18	0.44
1:A:270:CYS:SG	1:B:232:LYS:CE	3.06	0.43
1:B:119:THR:HG21	1:B:304:PHE:CZ	2.53	0.43
1:C:74:THR:HG21	1:C:79:PHE:CG	2.54	0.43
1:C:4:THR:HA	1:C:21:VAL:O	2.18	0.43
1:C:61:ASP:OD2	6:C:406:ACT:H3	2.19	0.43
1:C:245:SER:HA	1:C:301:THR:O	2.19	0.42
1:A:166:ARG:HA	1:A:243:MET:HE1	2.01	0.42
1:A:226:CYS:SG	1:A:228:LYS:HB2	2.59	0.42
1:B:2:VAL:HG13	1:B:2:VAL:O	2.20	0.41
1:B:263:GLU:O	1:B:273:TYR:HA	2.20	0.41
1:C:192:CYS:SG	1:C:226:CYS:HB3	2.60	0.41
1:A:57:VAL:HG21	6:A:509:ACT:H1	2.02	0.41
1:B:166:ARG:HA	1:B:243:MET:HE1	2.03	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	318/318 (100%)	305 (96%)	13 (4%)	0	100	100
1	B	319/318 (100%)	309 (97%)	10 (3%)	0	100	100
1	C	316/318 (99%)	305 (96%)	11 (4%)	0	100	100
All	All	953/954 (100%)	919 (96%)	34 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/277 (101%)	276 (99%)	3 (1%)	65	77
1	B	281/277 (101%)	279 (99%)	2 (1%)	76	86
1	C	278/277 (100%)	276 (99%)	2 (1%)	76	86
All	All	838/831 (101%)	831 (99%)	7 (1%)	70	83

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LEU
1	A	200	LYS
1	A	228	LYS
1	B	70	GLU
1	B	267	ASN
1	C	297	LYS
1	C	301	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	146	ASN
1	A	156	ASN

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Mol	Chain	Res	Type
1	A	175	HIS
1	B	19	GLN
1	B	97	GLN
1	B	146	ASN
1	B	175	HIS
1	B	186	ASN
1	C	97	GLN
1	C	122	GLN
1	C	146	ASN
1	C	175	HIS
1	C	229	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 11 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	YOO	A	510	-	35,35,35	1.95	10 (28%)	50,50,50	2.27	16 (32%)
3	YOO	B	502[B]	-	35,35,35	2.18	5 (14%)	50,50,50	2.28	12 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	YOO	A	503	-	35,35,35	1.79	4 (11%)	50,50,50	2.15	15 (30%)
6	ACT	A	508	-	3,3,3	0.99	0	3,3,3	0.74	0
3	YOO	C	403[A]	-	35,35,35	2.19	5 (14%)	50,50,50	2.64	23 (46%)
6	ACT	B	507	-	3,3,3	0.87	0	3,3,3	1.18	0
3	YOO	C	403[B]	-	35,35,35	2.22	5 (14%)	50,50,50	2.52	19 (38%)
6	ACT	C	406	-	3,3,3	1.16	0	3,3,3	0.99	0
6	ACT	B	506	-	3,3,3	1.23	0	3,3,3	0.84	0
3	YOO	A	502[A]	-	35,35,35	2.35	6 (17%)	50,50,50	2.75	23 (46%)
6	ACT	A	507	-	3,3,3	1.13	0	3,3,3	0.65	0
3	YOO	A	502[B]	-	35,35,35	2.46	6 (17%)	50,50,50	2.64	21 (42%)
3	YOO	B	502[A]	-	35,35,35	2.08	5 (14%)	50,50,50	2.35	20 (40%)
3	YOO	C	401	-	35,35,35	1.86	3 (8%)	50,50,50	2.26	16 (32%)
6	ACT	A	509	-	3,3,3	1.57	1 (33%)	3,3,3	0.73	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
3	YOO	A	510	-	-	10/26/43/43	0/4/4/4
3	YOO	B	502[B]	-	-	2/26/43/43	0/4/4/4
3	YOO	A	503	-	-	4/26/43/43	0/4/4/4
3	YOO	C	403[A]	-	-	8/26/43/43	0/4/4/4
3	YOO	C	403[B]	-	-	0/26/43/43	0/4/4/4
3	YOO	A	502[A]	-	-	5/26/43/43	0/4/4/4
3	YOO	A	502[B]	-	-	3/26/43/43	0/4/4/4
3	YOO	B	502[A]	-	-	6/26/43/43	0/4/4/4
3	YOO	C	401	-	-	8/26/43/43	0/4/4/4

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502[B]	YOO	C1-S40	-12.04	1.60	1.76
3	B	502[B]	YOO	C1-S40	-11.41	1.61	1.76
3	A	502[A]	YOO	C1-S40	-10.84	1.61	1.76
3	C	403[B]	YOO	C1-S40	-10.73	1.62	1.76
3	B	502[A]	YOO	C1-S40	-10.54	1.62	1.76
3	C	403[A]	YOO	C1-S40	-10.42	1.62	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	YOO	C1-S40	-8.39	1.65	1.76
3	A	503	YOO	C1-S40	-7.52	1.66	1.76
3	A	510	YOO	C1-S40	-6.96	1.67	1.76
3	A	502[A]	YOO	C8-C10	3.94	1.45	1.39
3	A	502[B]	YOO	C8-C10	3.94	1.45	1.39
3	A	503	YOO	O47-S40	3.66	1.47	1.43
3	A	510	YOO	S40-N41	3.32	1.68	1.63
3	A	502[A]	YOO	C13-C32	-3.31	1.45	1.52
3	A	502[B]	YOO	C13-C32	-3.31	1.45	1.52
3	A	502[A]	YOO	C8-C7	3.26	1.44	1.39
3	A	502[B]	YOO	C8-C7	3.26	1.44	1.39
3	A	503	YOO	C7-C6	3.22	1.57	1.50
3	A	510	YOO	O47-S40	3.16	1.46	1.43
3	C	403[A]	YOO	C8-C10	3.05	1.44	1.39
3	C	403[B]	YOO	C8-C10	3.05	1.44	1.39
3	C	403[A]	YOO	C13-C32	-2.96	1.46	1.52
3	C	403[B]	YOO	C13-C32	-2.96	1.46	1.52
3	C	403[A]	YOO	C12-C10	-2.95	1.34	1.39
3	C	403[B]	YOO	C12-C10	-2.95	1.34	1.39
3	A	502[B]	YOO	C4-N5	-2.95	1.35	1.41
3	A	502[A]	YOO	C7-C6	2.91	1.56	1.50
3	C	403[A]	YOO	C12-C13	-2.89	1.34	1.39
3	C	403[B]	YOO	C12-C13	-2.89	1.34	1.39
3	B	502[A]	YOO	C8-C10	2.82	1.43	1.39
3	B	502[B]	YOO	C8-C10	2.82	1.43	1.39
3	A	510	YOO	O46-S40	2.81	1.46	1.43
3	A	510	YOO	C22-C1	2.69	1.43	1.38
3	B	502[A]	YOO	C8-C7	2.62	1.43	1.39
3	B	502[B]	YOO	C8-C7	2.62	1.43	1.39
3	A	510	YOO	C3-C4	2.56	1.43	1.39
3	C	401	YOO	C8-C10	2.54	1.43	1.39
3	A	502[A]	YOO	C12-C13	-2.48	1.35	1.39
3	A	502[B]	YOO	C12-C13	-2.48	1.35	1.39
3	A	503	YOO	C8-C10	2.40	1.42	1.39
3	A	510	YOO	C2-C1	2.32	1.42	1.38
3	B	502[B]	YOO	C4-N5	-2.32	1.37	1.41
3	B	502[A]	YOO	C4-N5	-2.29	1.37	1.41
3	B	502[A]	YOO	C13-C32	-2.26	1.47	1.52
3	B	502[B]	YOO	C13-C32	-2.26	1.47	1.52
3	C	401	YOO	O47-S40	2.18	1.45	1.43
6	A	509	ACT	CH3-C	2.08	1.57	1.49
3	A	510	YOO	C2-C3	2.03	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	510	YOO	C13-C32	-2.01	1.48	1.52
3	A	510	YOO	C8-C10	2.00	1.42	1.39

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	510	YOO	C1-S40-N41	8.89	118.00	107.28
3	A	502[A]	YOO	C1-S40-N41	8.36	117.36	107.28
3	C	403[A]	YOO	O47-S40-O46	-7.96	107.16	119.59
3	A	503	YOO	C1-S40-N41	7.74	116.61	107.28
3	C	401	YOO	C1-S40-N41	7.65	116.52	107.28
3	B	502[A]	YOO	O47-S40-O46	-7.39	108.05	119.59
3	C	403[B]	YOO	O47-S40-O46	-7.31	108.18	119.59
3	B	502[B]	YOO	C1-S40-N41	7.27	116.05	107.28
3	A	502[A]	YOO	O47-S40-O46	-7.08	108.54	119.59
3	A	502[B]	YOO	C1-S40-N41	7.03	115.77	107.28
3	A	502[B]	YOO	O47-S40-O46	-7.01	108.64	119.59
3	A	510	YOO	O46-S40-N41	-6.00	101.03	106.69
3	B	502[B]	YOO	C45-N41-S40	-5.91	110.29	119.81
3	C	403[A]	YOO	C36-C37-C32	-5.87	104.13	111.00
3	C	403[B]	YOO	C36-C37-C32	-5.87	104.13	111.00
3	A	502[B]	YOO	C45-N41-S40	-5.37	111.14	119.81
3	B	502[B]	YOO	O47-S40-O46	-5.13	111.58	119.59
3	B	502[A]	YOO	C36-N35-C34	5.06	117.60	109.54
3	B	502[B]	YOO	C36-N35-C34	5.06	117.60	109.54
3	C	403[B]	YOO	C42-N41-S40	-4.98	111.78	119.81
3	B	502[B]	YOO	C42-N41-S40	-4.83	112.03	119.81
3	C	403[B]	YOO	C45-N41-S40	-4.79	112.08	119.81
3	C	403[A]	YOO	C1-S40-N41	4.77	113.03	107.28
3	A	502[A]	YOO	C37-C36-N35	4.66	117.21	111.20
3	A	502[B]	YOO	C37-C36-N35	4.66	117.21	111.20
3	C	403[A]	YOO	C42-N41-S40	-4.61	112.37	119.81
3	C	401	YOO	C36-N35-C34	4.48	116.67	109.54
3	B	502[A]	YOO	O47-S40-N41	4.25	110.69	106.69
3	A	510	YOO	C21-C22-C1	4.22	123.55	119.44
3	A	502[B]	YOO	O18-C6-C7	-4.22	112.54	120.90
3	A	502[A]	YOO	C8-C7-C6	4.21	134.30	120.40
3	C	403[A]	YOO	C39-O30-C10	4.20	126.51	117.50
3	C	403[B]	YOO	C39-O30-C10	4.20	126.51	117.50
3	A	503	YOO	C8-C7-C15	-4.15	114.80	119.65
3	C	403[B]	YOO	C1-S40-N41	4.06	112.17	107.28
3	A	502[B]	YOO	C42-N41-S40	-4.00	113.35	119.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502[A]	YOO	C22-C1-S40	4.00	123.71	119.73
3	C	403[A]	YOO	C12-C13-C32	-3.99	111.02	120.88
3	C	403[B]	YOO	C12-C13-C32	-3.99	111.02	120.88
3	C	401	YOO	O47-S40-O46	-3.96	113.41	119.59
3	A	510	YOO	O47-S40-O46	-3.91	113.49	119.59
3	A	502[A]	YOO	C42-N41-S40	-3.89	113.53	119.81
3	A	503	YOO	O47-S40-N41	-3.86	103.05	106.69
3	C	401	YOO	C39-O30-C10	3.85	125.76	117.50
3	C	403[A]	YOO	C8-C7-C15	-3.75	115.26	119.65
3	C	403[B]	YOO	C8-C7-C15	-3.75	115.26	119.65
3	C	401	YOO	C45-N41-S40	-3.72	113.81	119.81
3	C	403[A]	YOO	O47-S40-N41	3.70	110.17	106.69
3	A	502[A]	YOO	C38-N35-C34	-3.70	103.58	110.63
3	A	502[B]	YOO	C38-N35-C34	-3.70	103.58	110.63
3	C	403[A]	YOO	C34-C33-C32	-3.68	106.69	111.00
3	C	403[B]	YOO	C34-C33-C32	-3.68	106.69	111.00
3	A	502[A]	YOO	C36-C37-C32	-3.68	106.70	111.00
3	A	502[B]	YOO	C36-C37-C32	-3.68	106.70	111.00
3	A	503	YOO	C2-C1-C22	-3.65	115.70	120.47
3	C	403[A]	YOO	C2-C1-S40	3.62	123.33	119.73
3	A	502[B]	YOO	O47-S40-N41	3.61	110.09	106.69
3	A	502[A]	YOO	C45-N41-S40	-3.56	114.06	119.81
3	A	510	YOO	C2-C1-S40	3.53	123.24	119.73
3	A	503	YOO	C22-C1-S40	3.52	123.23	119.73
3	C	401	YOO	C37-C36-N35	3.46	115.66	111.20
3	B	502[A]	YOO	C42-N41-S40	-3.44	114.26	119.81
3	A	502[A]	YOO	C15-C13-C12	3.41	122.74	118.09
3	A	502[B]	YOO	C15-C13-C12	3.41	122.74	118.09
3	A	510	YOO	O46-S40-C1	3.40	112.34	108.10
3	C	403[A]	YOO	C45-N41-S40	-3.38	114.35	119.81
3	A	502[B]	YOO	C7-C6-N5	3.33	124.00	115.90
3	B	502[A]	YOO	C45-N41-S40	-3.33	114.43	119.81
3	A	502[A]	YOO	C22-C1-S40	3.32	123.03	119.73
3	A	502[A]	YOO	C15-C7-C6	-3.29	109.52	120.40
3	A	503	YOO	C3-C2-C1	3.27	122.62	119.44
3	C	401	YOO	C2-C1-S40	3.25	122.96	119.73
3	A	503	YOO	C45-N41-S40	-3.24	114.59	119.81
3	A	502[A]	YOO	O47-S40-N41	3.21	109.71	106.69
3	C	403[A]	YOO	C15-C13-C12	3.17	122.42	118.09
3	C	403[B]	YOO	C15-C13-C12	3.17	122.42	118.09
3	C	401	YOO	C21-C22-C1	3.12	122.47	119.44
3	B	502[A]	YOO	C7-C15-C13	3.07	124.11	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502[B]	YOO	C7-C15-C13	3.07	124.11	121.11
3	A	503	YOO	O46-S40-N41	-3.06	103.81	106.69
3	A	510	YOO	C42-N41-S40	-3.05	114.90	119.81
3	A	503	YOO	C7-C15-C13	3.04	124.08	121.11
3	B	502[A]	YOO	C33-C34-N35	3.04	115.12	111.20
3	B	502[B]	YOO	C33-C34-N35	3.04	115.12	111.20
3	C	401	YOO	C36-C37-C32	-3.02	107.46	111.00
3	A	502[A]	YOO	C36-N35-C34	3.02	114.34	109.54
3	A	502[B]	YOO	C36-N35-C34	3.02	114.34	109.54
3	A	503	YOO	C3-C4-C21	-2.99	115.07	119.04
3	B	502[A]	YOO	C3-C2-C1	2.98	122.33	119.44
3	A	502[A]	YOO	C8-C7-C15	-2.97	116.17	119.65
3	A	502[B]	YOO	C8-C7-C15	-2.97	116.17	119.65
3	A	510	YOO	C2-C1-C22	-2.96	116.61	120.47
3	C	403[A]	YOO	C36-N35-C34	2.94	114.22	109.54
3	C	403[B]	YOO	C36-N35-C34	2.94	114.22	109.54
3	A	502[A]	YOO	C37-C32-C33	2.94	116.06	109.68
3	A	502[B]	YOO	C37-C32-C33	2.94	116.06	109.68
3	B	502[A]	YOO	C8-C7-C6	2.93	130.10	120.40
3	A	502[A]	YOO	C39-O30-C10	2.89	123.71	117.50
3	A	502[B]	YOO	C39-O30-C10	2.89	123.71	117.50
3	A	503	YOO	C7-C6-N5	2.88	122.90	115.90
3	C	401	YOO	C2-C1-C22	-2.86	116.73	120.47
3	B	502[A]	YOO	C8-C7-C15	-2.74	116.45	119.65
3	B	502[B]	YOO	C8-C7-C15	-2.74	116.45	119.65
3	C	403[B]	YOO	C7-C6-N5	2.74	122.55	115.90
3	A	503	YOO	C21-C22-C1	2.72	122.09	119.44
3	A	502[A]	YOO	C33-C32-C13	-2.72	106.23	112.67
3	A	502[B]	YOO	C33-C32-C13	-2.72	106.23	112.67
3	A	502[A]	YOO	O30-C10-C12	-2.68	107.22	120.00
3	A	502[B]	YOO	O30-C10-C12	-2.68	107.22	120.00
3	C	401	YOO	C8-C7-C15	-2.67	116.53	119.65
3	C	403[B]	YOO	O47-S40-C1	2.64	111.38	108.10
3	B	502[A]	YOO	C45-N41-C42	-2.61	107.61	111.22
3	C	403[A]	YOO	O46-S40-N41	2.58	109.12	106.69
3	C	403[A]	YOO	C44-C45-N41	2.57	108.12	103.52
3	C	401	YOO	C37-C32-C13	2.56	118.73	112.67
3	A	502[B]	YOO	C4-N5-C6	-2.53	119.95	126.61
3	A	510	YOO	C43-C42-N41	2.52	108.03	103.52
3	C	403[A]	YOO	O30-C10-C12	-2.51	108.01	120.00
3	C	403[B]	YOO	O30-C10-C12	-2.51	108.01	120.00
3	B	502[A]	YOO	O46-S40-N41	2.50	109.04	106.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403[A]	YOO	C43-C42-N41	2.49	107.98	103.52
3	B	502[A]	YOO	O46-S40-C1	2.49	111.20	108.10
3	C	403[A]	YOO	C2-C1-C22	-2.47	117.24	120.47
3	A	503	YOO	C42-N41-S40	-2.46	115.83	119.81
3	C	403[A]	YOO	C45-N41-C42	-2.45	107.83	111.22
3	B	502[A]	YOO	C2-C1-C22	-2.45	117.27	120.47
3	A	502[A]	YOO	C7-C6-N5	2.42	121.77	115.90
3	A	510	YOO	O47-S40-C1	-2.40	105.11	108.10
3	A	510	YOO	O18-C6-C7	-2.40	116.14	120.90
3	C	403[B]	YOO	C43-C42-N41	2.39	107.79	103.52
3	C	401	YOO	C45-N41-C42	-2.35	107.97	111.22
3	C	401	YOO	O46-S40-N41	-2.35	104.47	106.69
3	B	502[B]	YOO	C7-C6-N5	2.34	121.58	115.90
3	A	502[B]	YOO	C44-C45-N41	2.33	107.68	103.52
3	A	510	YOO	C8-C7-C15	-2.31	116.95	119.65
3	C	403[A]	YOO	C15-C13-C32	2.30	126.56	120.88
3	C	403[B]	YOO	C15-C13-C32	2.30	126.56	120.88
3	B	502[A]	YOO	C7-C8-C10	-2.30	117.18	119.56
3	B	502[B]	YOO	C7-C8-C10	-2.30	117.18	119.56
3	A	502[A]	YOO	C43-C42-N41	2.29	107.61	103.52
3	B	502[A]	YOO	C21-C4-N5	2.28	128.08	120.41
3	C	403[B]	YOO	C44-C45-N41	2.25	107.54	103.52
3	C	403[A]	YOO	C21-C22-C1	2.23	121.61	119.44
3	A	502[A]	YOO	C38-N35-C36	-2.22	106.41	110.63
3	A	502[B]	YOO	C38-N35-C36	-2.22	106.41	110.63
3	C	403[A]	YOO	C8-C7-C6	2.21	127.69	120.40
3	B	502[A]	YOO	O30-C10-C12	-2.17	109.67	120.00
3	B	502[B]	YOO	O30-C10-C12	-2.17	109.67	120.00
3	A	510	YOO	C44-C45-N41	2.13	107.33	103.52
3	C	403[A]	YOO	C38-N35-C34	-2.11	106.61	110.63
3	C	403[B]	YOO	C38-N35-C34	-2.11	106.61	110.63
3	A	503	YOO	O18-C6-N5	-2.10	118.41	123.75
3	B	502[A]	YOO	C15-C7-C6	-2.10	113.46	120.40
3	A	502[A]	YOO	O30-C10-C8	2.10	130.03	120.00
3	A	502[B]	YOO	O30-C10-C8	2.10	130.03	120.00
3	B	502[A]	YOO	C36-C37-C32	2.10	113.46	111.00
3	B	502[B]	YOO	C36-C37-C32	2.10	113.46	111.00
3	A	503	YOO	C37-C32-C33	-2.09	105.13	109.68
3	A	510	YOO	C7-C8-C10	2.07	121.69	119.56
3	C	403[B]	YOO	C2-C1-C22	-2.05	117.80	120.47
3	C	401	YOO	C15-C13-C32	-2.04	115.83	120.88
3	A	502[A]	YOO	C44-C45-N41	2.03	107.15	103.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	510	YOO	C37-C32-C33	2.02	114.08	109.68
3	A	510	YOO	C45-N41-C42	-2.02	108.43	111.22
3	C	401	YOO	C7-C6-N5	2.01	120.79	115.90

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	510	YOO	C45-N41-S40-C1
3	C	401	YOO	C42-N41-S40-C1
3	C	403[A]	YOO	C22-C1-S40-N41
3	C	403[A]	YOO	C2-C1-S40-N41
3	A	510	YOO	C12-C10-O30-C39
3	A	510	YOO	C8-C10-O30-C39
3	A	510	YOO	C45-N41-S40-O47
3	B	502[A]	YOO	C42-N41-S40-C1
3	C	401	YOO	C42-N41-S40-O47
3	C	403[A]	YOO	C42-N41-S40-O47
3	C	403[A]	YOO	C42-N41-S40-C1
3	A	502[A]	YOO	C22-C1-S40-N41
3	A	502[A]	YOO	C2-C1-S40-N41
3	C	401	YOO	C12-C10-O30-C39
3	B	502[A]	YOO	C2-C1-S40-N41
3	A	502[B]	YOO	C42-N41-S40-O47
3	C	401	YOO	C8-C10-O30-C39
3	A	503	YOO	C42-N41-S40-O47
3	B	502[A]	YOO	C22-C1-S40-N41
3	A	510	YOO	C42-N41-S40-O47
3	C	401	YOO	C45-N41-S40-O47
3	B	502[A]	YOO	C2-C1-S40-O46
3	B	502[B]	YOO	C42-N41-S40-O47
3	B	502[A]	YOO	C22-C1-S40-O46
3	B	502[A]	YOO	C42-N41-S40-O47
3	A	502[A]	YOO	C2-C1-S40-O47
3	A	502[A]	YOO	C45-N41-S40-O46
3	A	502[A]	YOO	C22-C1-S40-O47
3	A	503	YOO	C42-N41-S40-C1
3	A	510	YOO	C42-N41-S40-C1
3	C	401	YOO	C42-N41-S40-O46
3	C	403[A]	YOO	C22-C1-S40-O46
3	C	403[A]	YOO	C2-C1-S40-O46
3	A	502[B]	YOO	C22-C1-S40-O46

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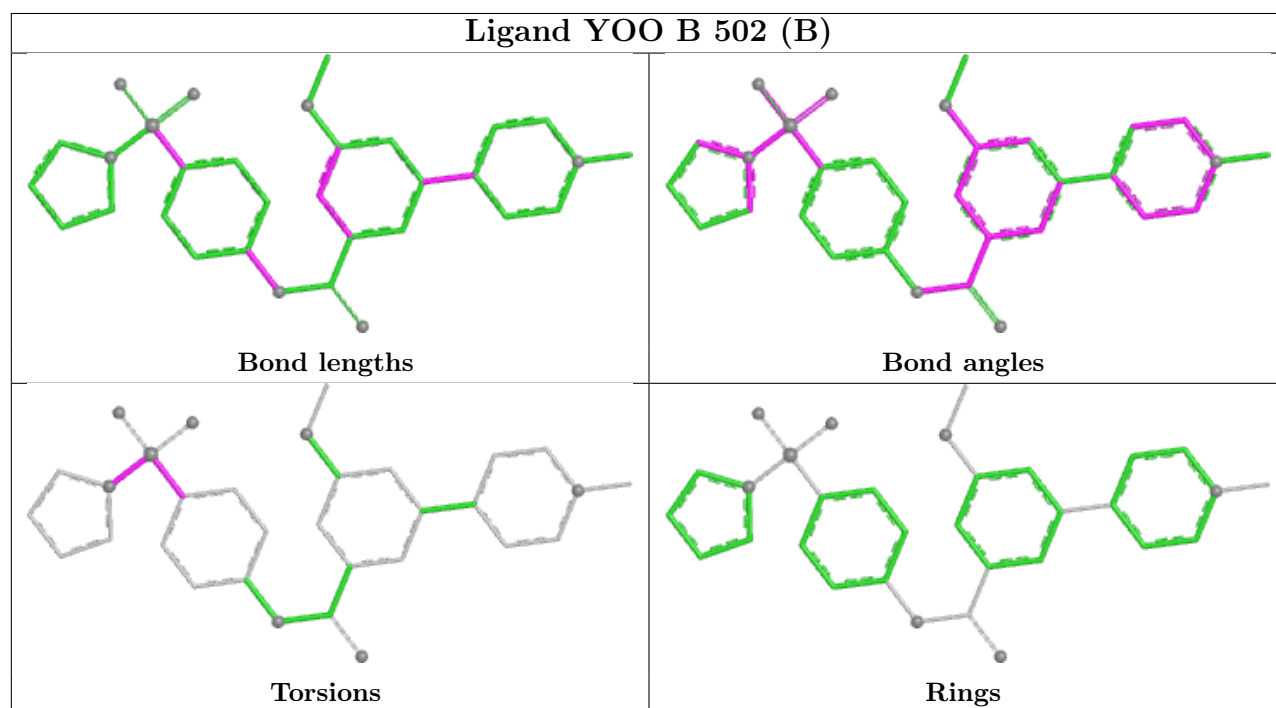
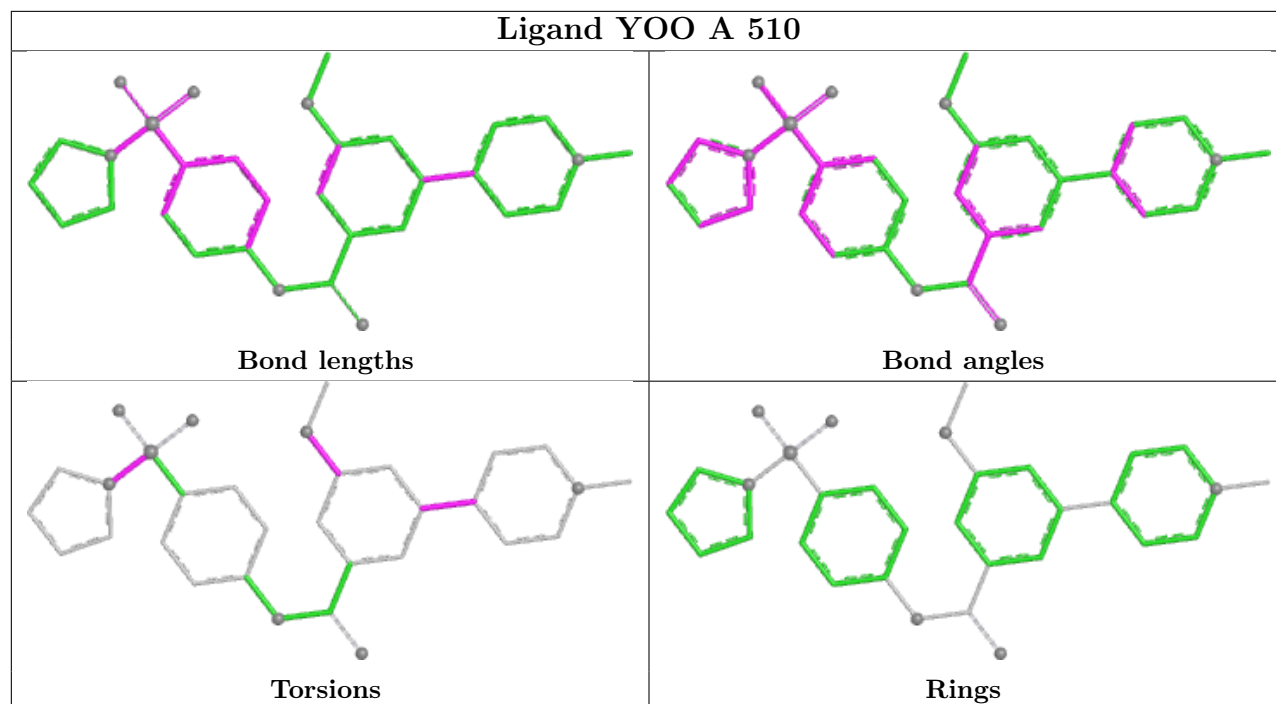
Mol	Chain	Res	Type	Atoms
3	C	403[A]	YOO	C22-C1-S40-O47
3	C	403[A]	YOO	C2-C1-S40-O47
3	A	502[B]	YOO	C2-C1-S40-O46
3	C	401	YOO	C45-N41-S40-C1
3	A	503	YOO	C12-C13-C32-C37
3	A	510	YOO	C15-C13-C32-C37
3	B	502[B]	YOO	C22-C1-S40-O47
3	C	401	YOO	C45-N41-S40-O46
3	A	503	YOO	C15-C13-C32-C37
3	A	510	YOO	C12-C13-C32-C37
3	A	510	YOO	C42-N41-S40-O46
3	A	510	YOO	C45-N41-S40-O46

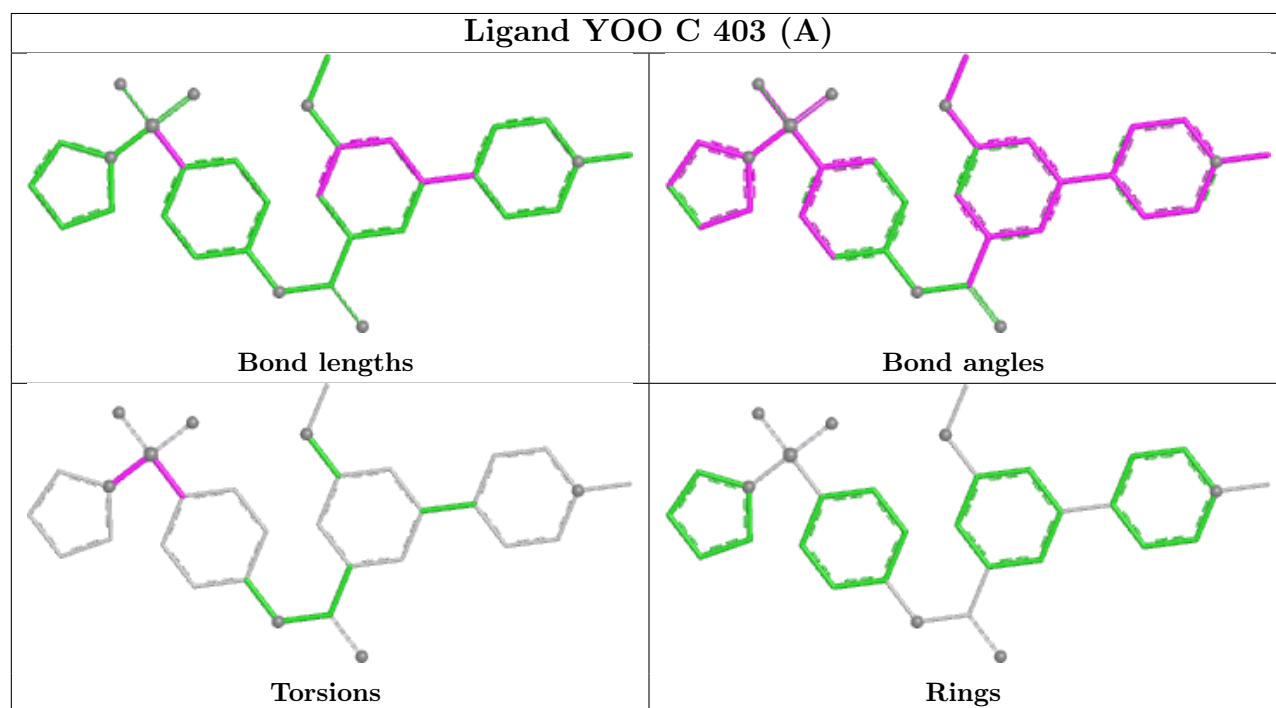
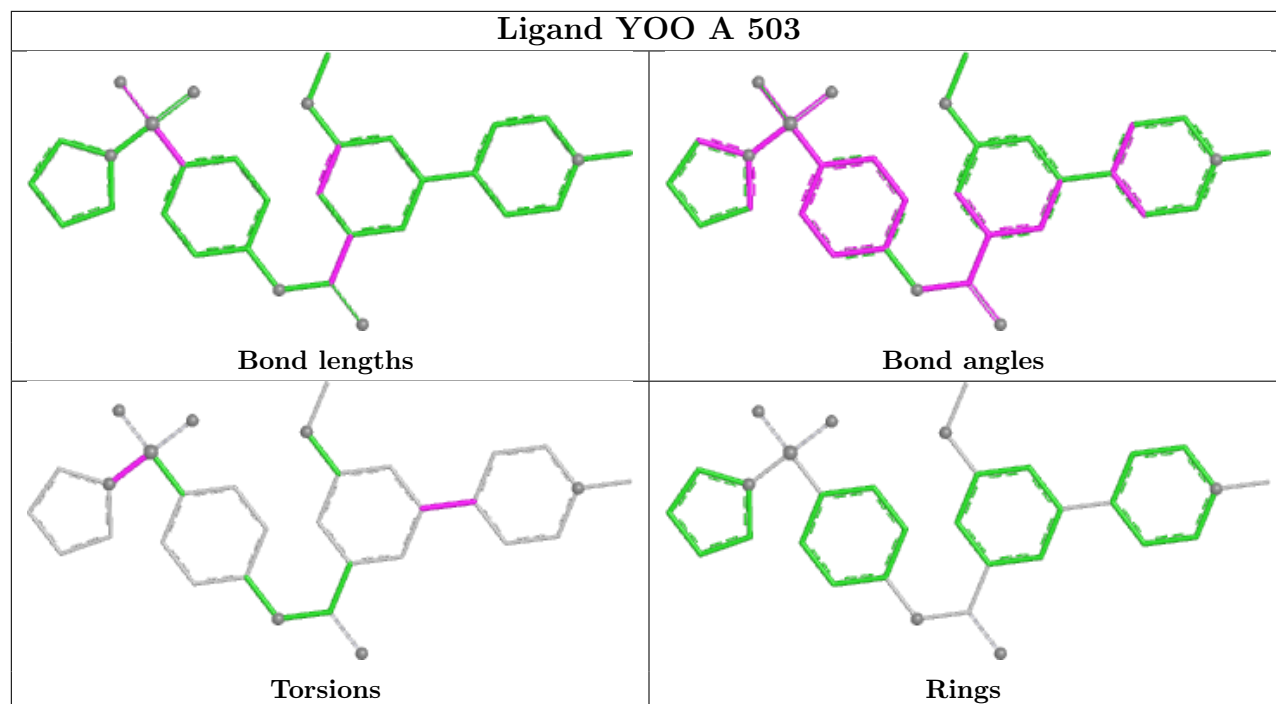
There are no ring outliers.

8 monomers are involved in 9 short contacts:

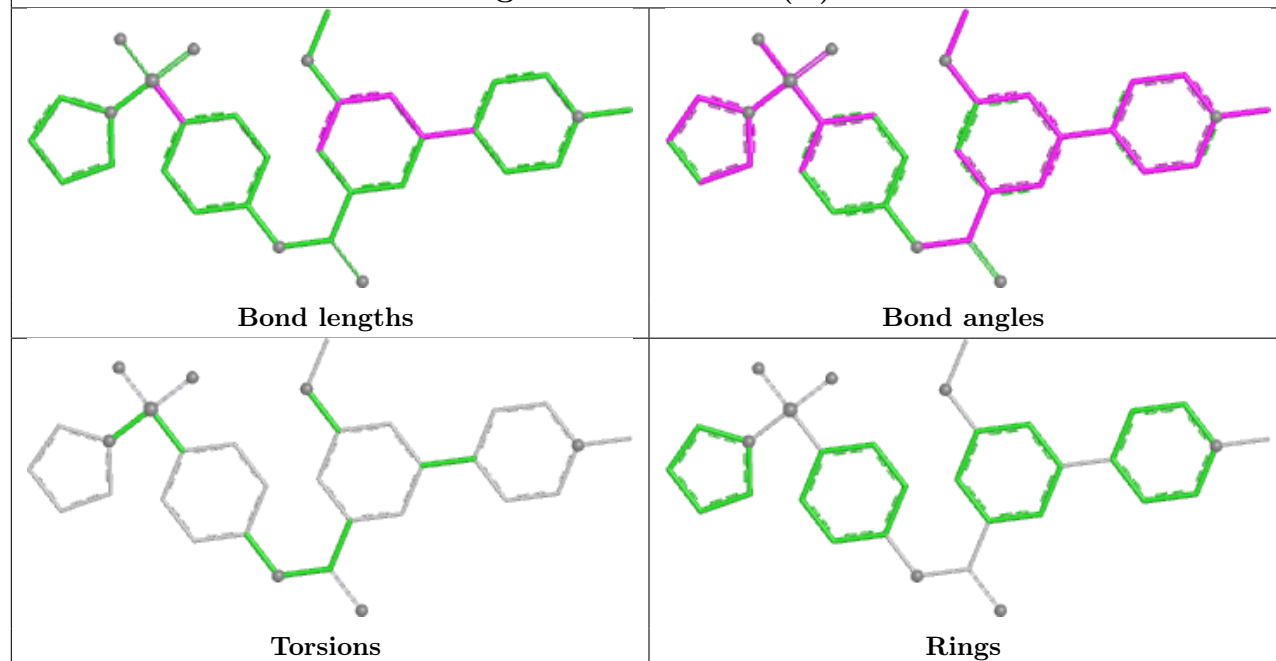
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502[B]	YOO	1	0
6	B	507	ACT	1	0
3	C	403[B]	YOO	1	0
6	C	406	ACT	1	0
6	B	506	ACT	1	0
3	A	502[B]	YOO	1	0
3	B	502[A]	YOO	2	0
6	A	509	ACT	1	0

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.

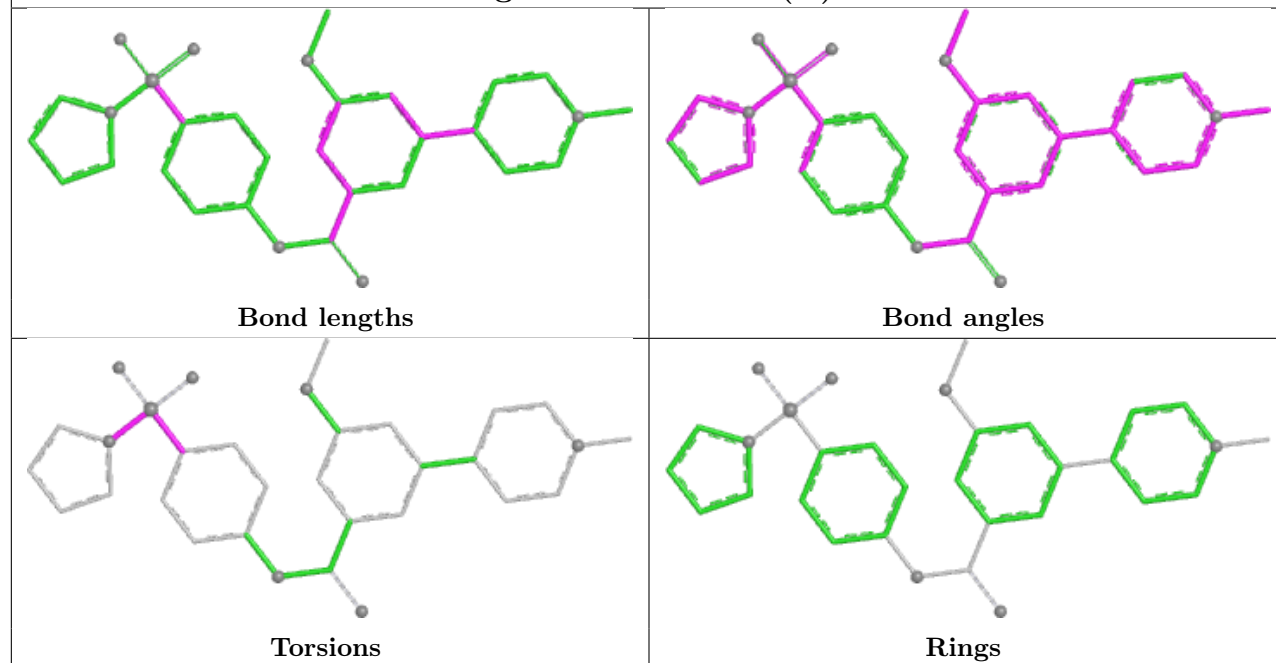




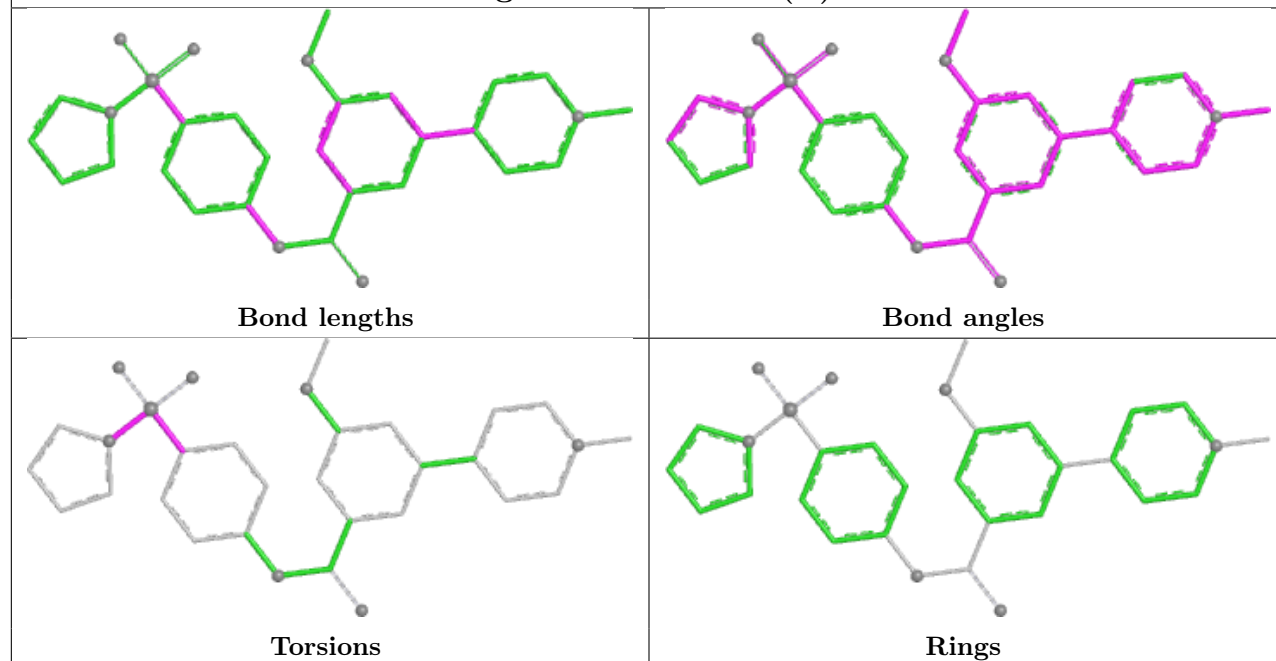
Ligand YOO C 403 (B)



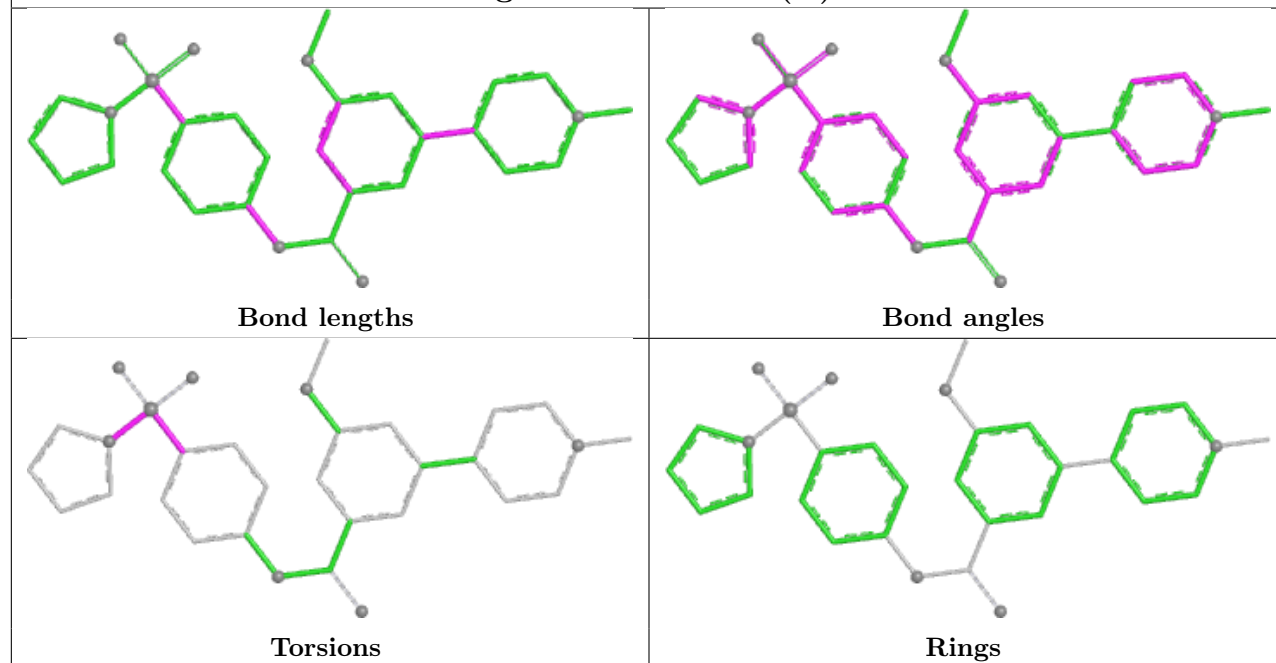
Ligand YOO A 502 (A)

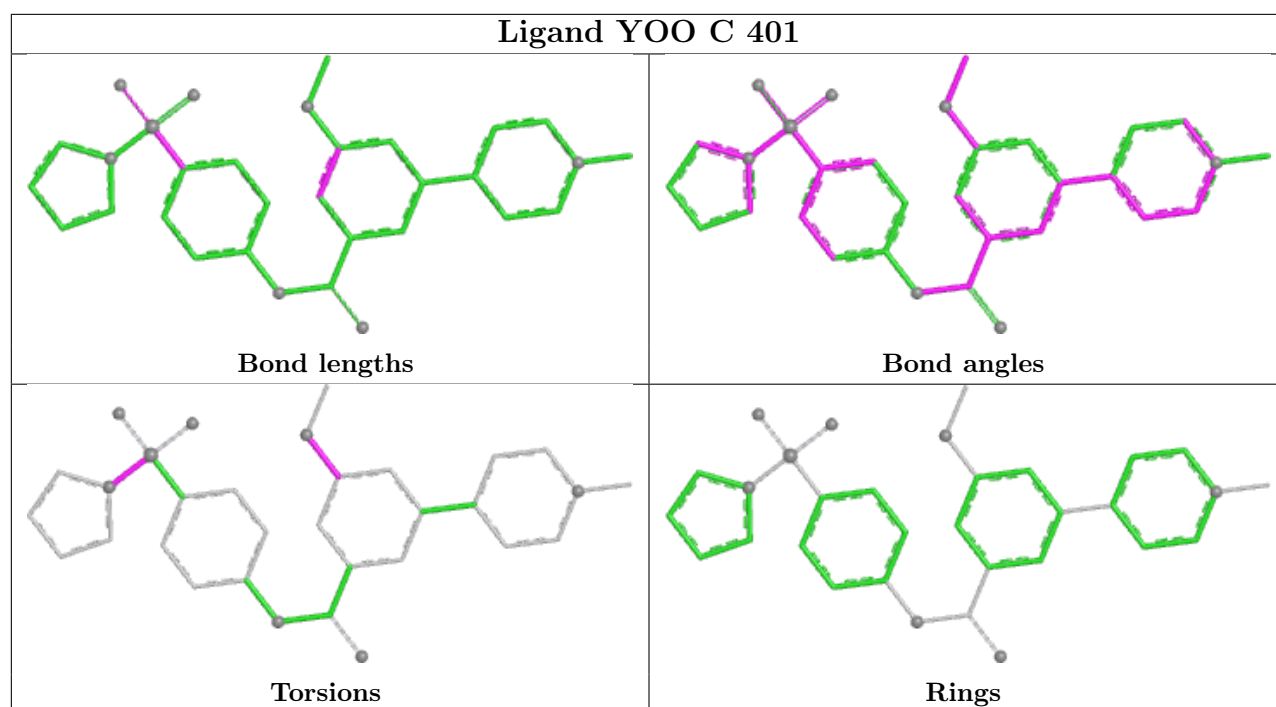


Ligand YOO A 502 (B)



Ligand YOO B 502 (A)





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	315/318 (99%)	-0.10	4 (1%) 75 75	31, 50, 73, 86	5 (1%)
1	B	313/318 (98%)	0.07	9 (2%) 53 53	34, 56, 82, 113	8 (2%)
1	C	313/318 (98%)	0.05	7 (2%) 62 61	34, 60, 82, 99	5 (1%)
All	All	941/954 (98%)	0.01	20 (2%) 63 63	31, 56, 80, 113	18 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	ALA	4.9
1	A	268	TYR	3.6
1	A	314	ILE	3.0
1	B	268	TYR	2.9
1	C	2	VAL	2.8
1	A	233	TYR	2.6
1	B	2	VAL	2.6
1	B	47[A]	HIS	2.5
1	B	314	ILE	2.5
1	B	283	TYR	2.4
1	C	216	PHE	2.4
1	B	292	LYS	2.4
1	C	233	TYR	2.3
1	C	75	THR	2.3
1	B	228[A]	LYS	2.3
1	B	75	THR	2.2
1	C	314	ILE	2.2
1	B	269	GLN	2.1
1	C	137[A]	TYR	2.0
1	C	268	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

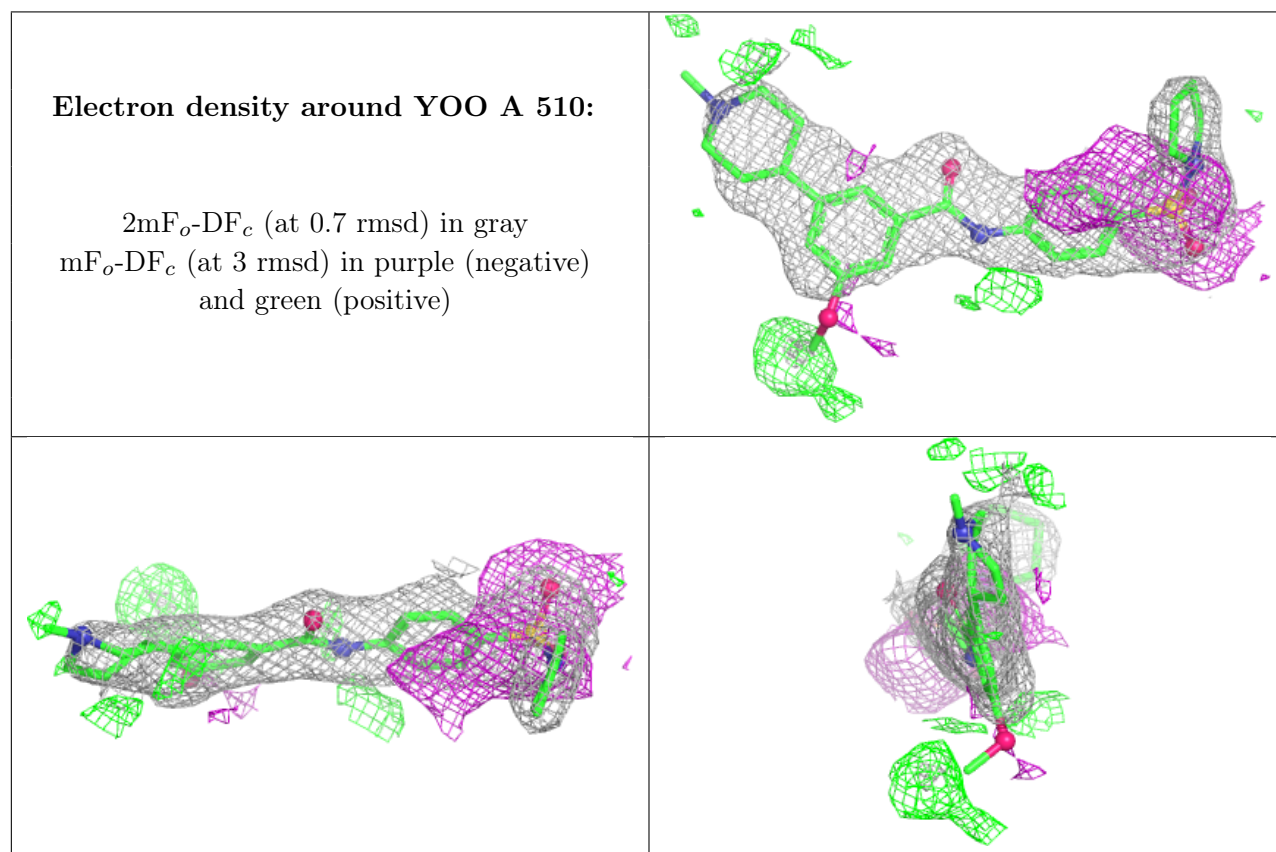
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

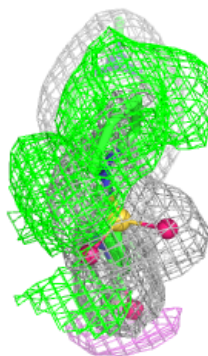
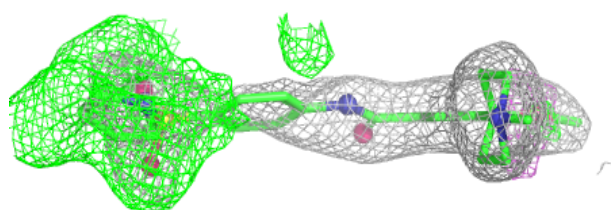
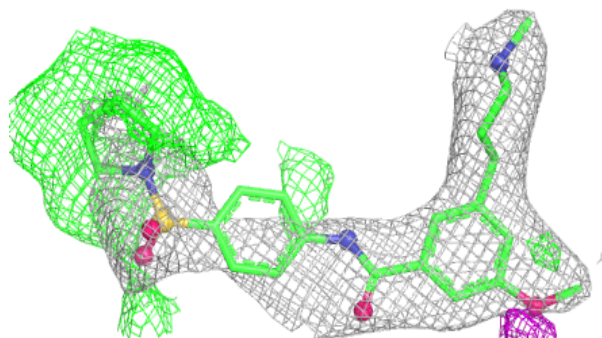
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ACT	B	506	4/4	0.67	0.24	69,70,74,77	0
6	ACT	A	509	4/4	0.77	0.22	63,71,71,72	0
3	YOO	A	510	32/32	0.77	0.22	72,85,96,100	0
3	YOO	C	403[A]	32/32	0.81	0.27	59,84,106,111	17
3	YOO	C	403[B]	32/32	0.81	0.27	59,69,75,77	17
4	NA	B	503	1/1	0.83	0.14	69,69,69,69	0
3	YOO	C	401	32/32	0.83	0.19	76,83,108,111	0
4	NA	A	504	1/1	0.83	0.11	62,62,62,62	0
6	ACT	C	406	4/4	0.85	0.15	66,67,71,77	0
3	YOO	B	502[A]	32/32	0.86	0.24	60,82,107,108	17
3	YOO	B	502[B]	32/32	0.86	0.24	60,71,77,77	17
3	YOO	A	502[B]	32/32	0.87	0.20	51,69,83,85	17
3	YOO	A	502[A]	32/32	0.87	0.20	51,71,94,95	17
6	ACT	A	507	4/4	0.91	0.12	67,72,75,79	0
6	ACT	B	507	4/4	0.91	0.12	56,57,59,63	0
3	YOO	A	503	32/32	0.91	0.15	62,72,93,96	0
5	CL	A	506	1/1	0.92	0.15	75,75,75,75	0
5	CL	B	504	1/1	0.95	0.08	76,76,76,76	0
6	ACT	A	508	4/4	0.95	0.13	54,57,57,60	0
5	CL	C	404	1/1	0.96	0.10	86,86,86,86	0
5	CL	C	405	1/1	0.96	0.07	84,84,84,84	0
5	CL	B	505	1/1	0.97	0.10	55,55,55,55	0
5	CL	A	505	1/1	0.98	0.14	48,48,48,48	0
2	ZN	B	501	1/1	0.99	0.03	69,69,69,69	0
2	ZN	C	402	1/1	1.00	0.02	70,70,70,70	0
2	ZN	A	501	1/1	1.00	0.02	71,71,71,71	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.

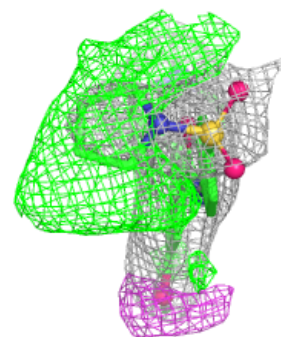
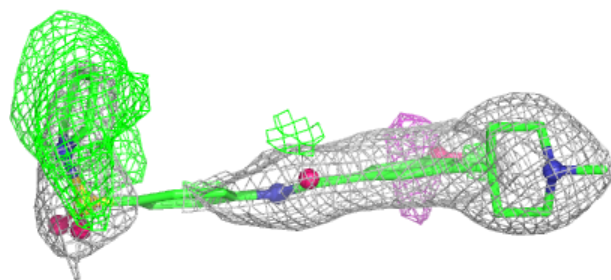
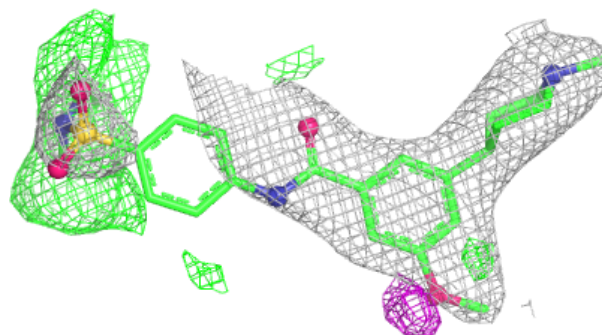


Electron density around YOO C 403 (A):

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

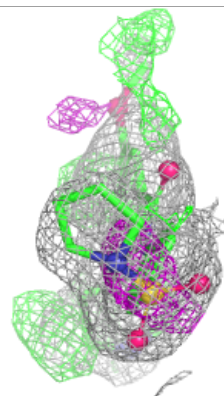
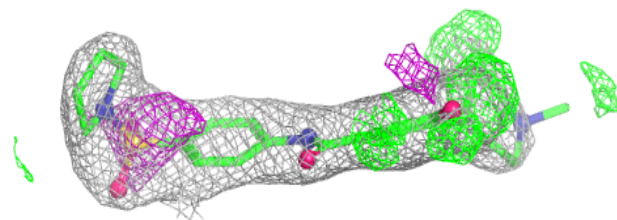
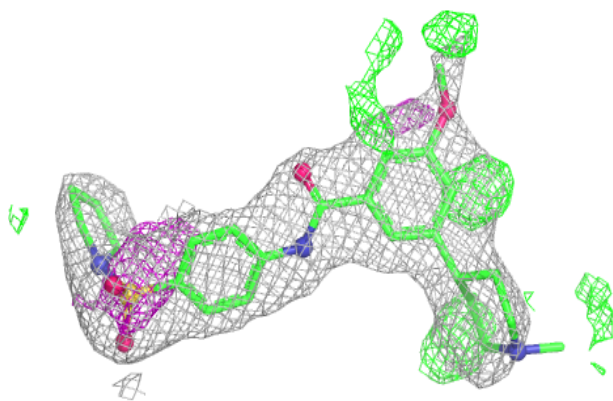
**Electron density around YOO C 403 (B):**

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

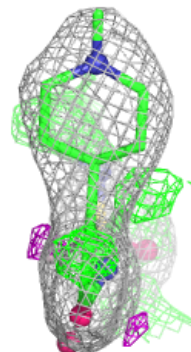
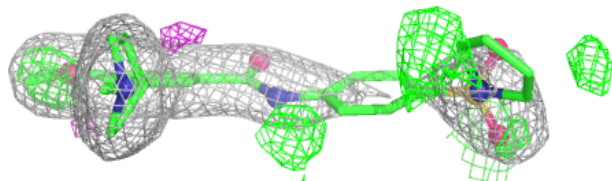
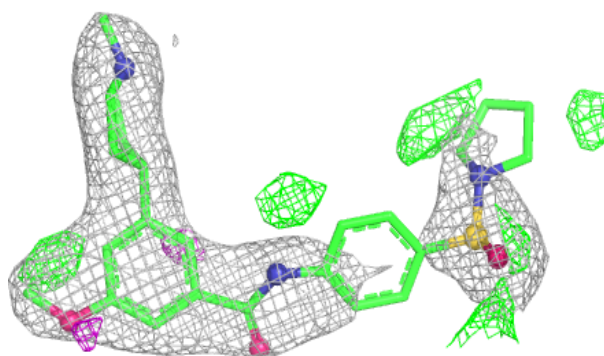


Electron density around YOO C 401:

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

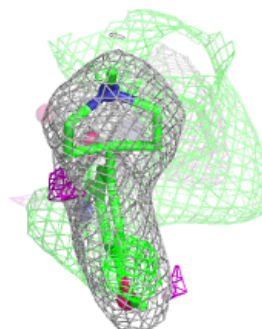
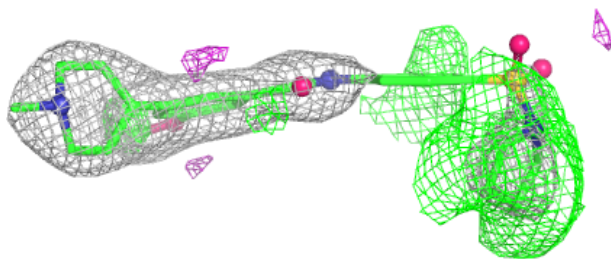
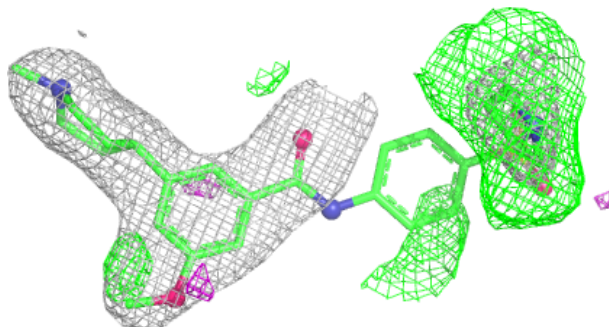
**Electron density around YOO B 502 (A):**

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

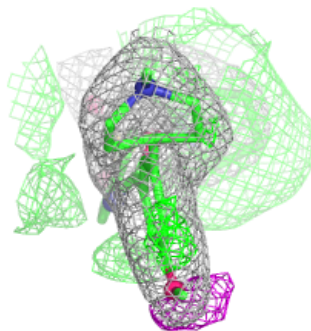
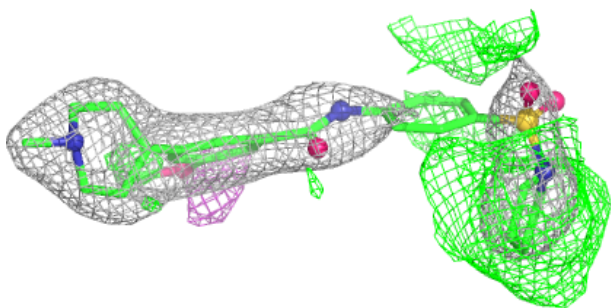
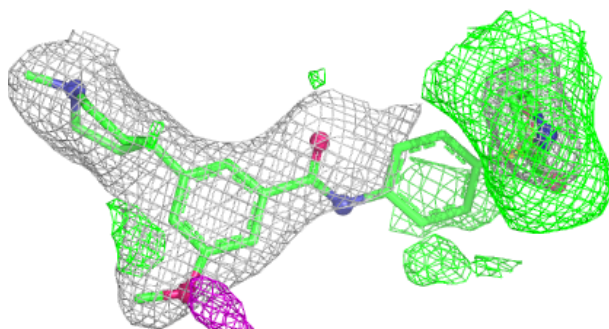


Electron density around YOO B 502 (B):

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

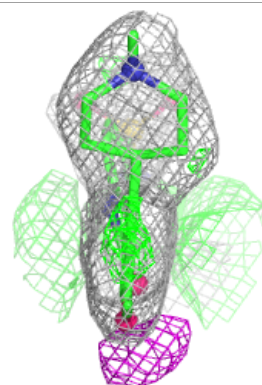
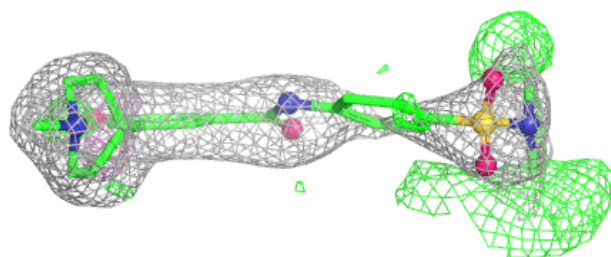
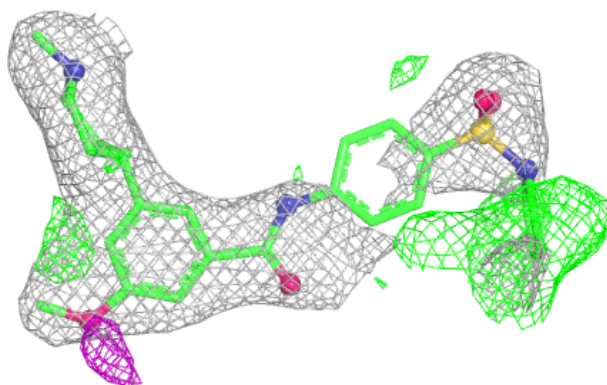
**Electron density around YOO A 502 (B):**

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

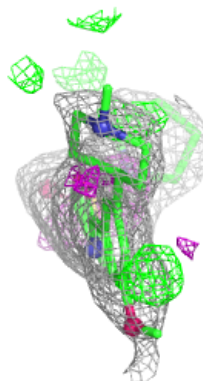
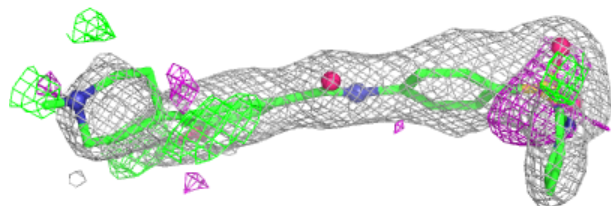
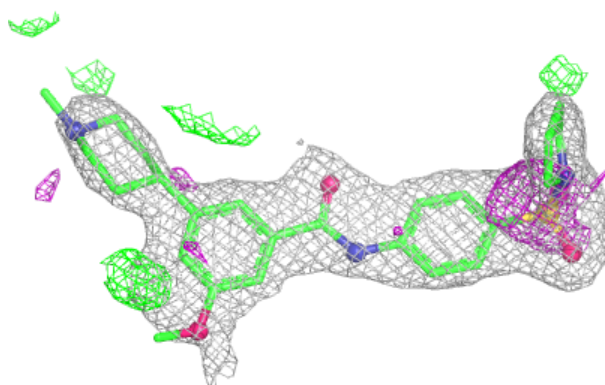


Electron density around YOO A 502 (A):

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

**Electron density around YOO A 503:**

$2mF_o-DF_c$ (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.