Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 10:19 PM JST

PDB ID	:	7EEK / pdb_00007eek
Title	:	Structure of Human serum albumin-Au compound complex
Authors	:	Yang, F.; Zhang, J.Z.
Deposited on	:	2021-03-18
Resolution	:	2.50 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:

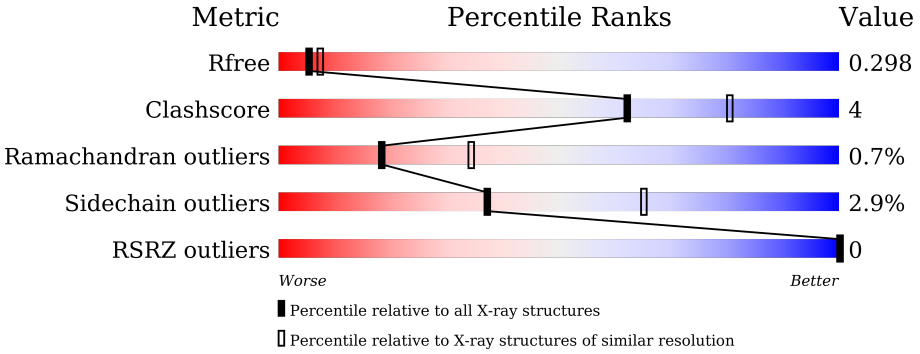
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	583	89% 10% •
1	B	583	88% 11% •

2 Entry composition (i)

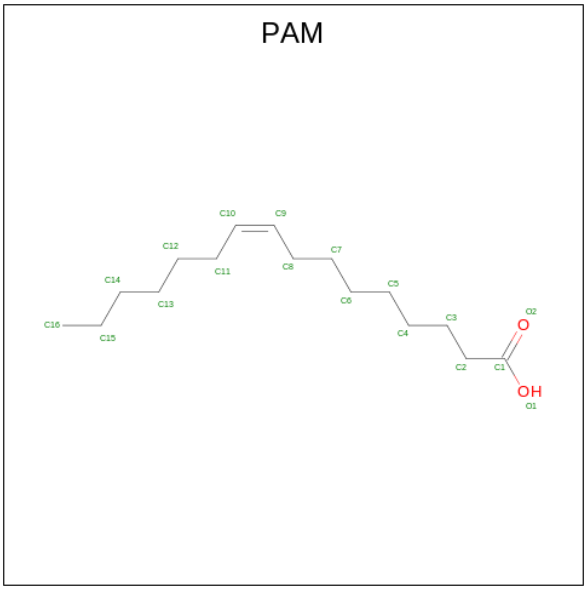
There are 3 unique types of molecules in this entry. The entry contains 9502 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	583	4635	2926	784	884	41	0	0	0
1	B	583	4635	2926	784	884	41	0	0	0

- Molecule 2 is PALMITOLEIC ACID (CCD ID: PAM) (formula: $C_{16}H_{30}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	18	16	2	0	0
2	A	1	18	16	2	0	0
2	A	1	18	16	2	0	0
2	A	1	18	16	2	0	0

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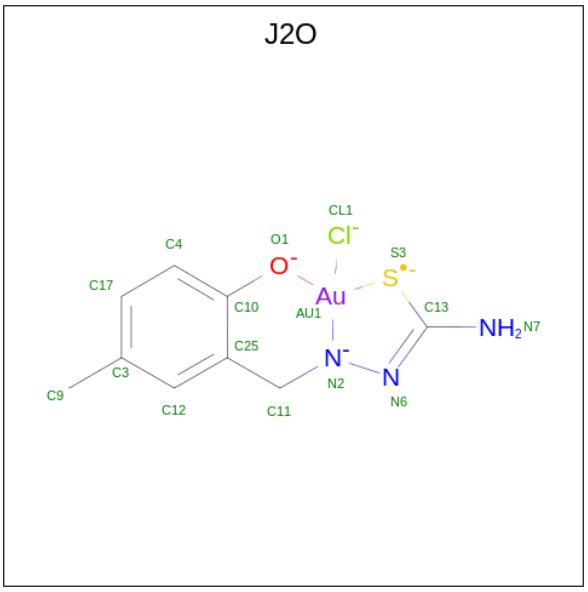
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
2	A	1	16	14	2		0	0
			Total	C	O			
2	A	1	13	11	2		0	0
			Total	C	O			
2	B	1	16	14	2		0	0
			Total	C	O			
2	B	1	13	11	2		0	0
			Total	C	O			
2	B	1	18	16	2		0	0
			Total	C	O			
2	B	1	18	16	2		0	0
			Total	C	O			
2	B	1	18	16	2		0	0
			Total	C	O			
2	B	1	18	16	2		0	0

- Molecule 3 is 3-chloranyl-11-methyl-2-oxa-4-thia-6,7-diaza-3$l^{4}-auratricyclo[7.4.0.0^{3,7}]trideca-1(13),5,9,11-tetraen-5-amine (CCD ID: J2O) (formula: $C_9H_{10}AuClN_3OS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Au	C	N	O	S		
3	A	1	15	1	9	3	1	1	0	0
			Total	Au	C	N	O	S		
3	B	1	15	1	9	3	1	1	0	0

3 Residue-property plots (i)

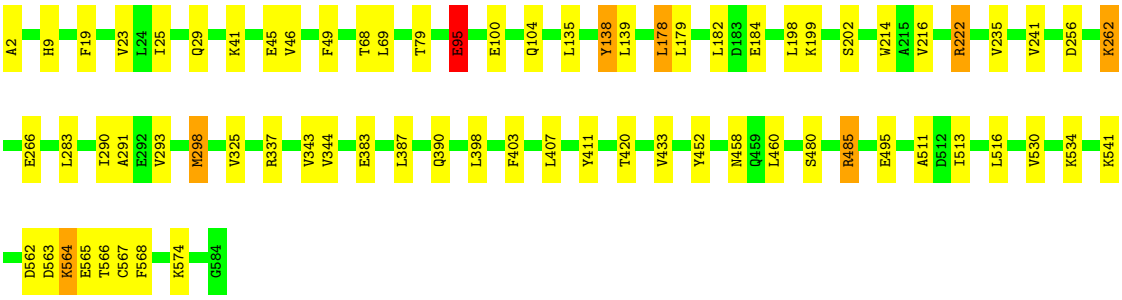
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Serum albumin

Chain A:

- Molecule 1: Serum albumin

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	38.19Å 92.21Å 95.44Å 105.21° 89.68° 100.10°	Depositor
Resolution (Å)	46.10 – 2.50 46.10 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (46.10-2.50) 80.3 (46.10-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.48Å)	Xtriage
Refinement program	PHENIX v1.1	Depositor
R, R_{free}	0.238 , (Not available) 0.237 , 0.298	Depositor DCC
R_{free} test set	1783 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 5.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.159 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9502	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: J2O, PAM

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	0.78	0/4725	1.01	3/6373 (0.0%)
1	B	0.75	0/4725	0.99	2/6373 (0.0%)
All	All	0.76	0/9450	1.00	5/12746 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	564	LYS	N-CA-C	6.22	120.93	107.49
1	A	95	GLU	CA-C-N	-5.85	112.53	119.84
1	A	95	GLU	C-N-CA	-5.85	112.53	119.84
1	B	95	GLU	CA-C-N	-5.38	113.11	119.84
1	B	95	GLU	C-N-CA	-5.38	113.11	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	564	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	B	564	LYS	Peptide

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	4635	0	4557	38	1
1	B	4635	0	4557	39	1
2	A	101	0	154	7	0
2	B	101	0	154	11	0
3	A	15	0	0	1	0
3	B	15	0	0	1	0
All	All	9502	0	9422	78	1

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 4.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ARG:HD2	2:A:604:PAM:H9	1.53	0.91
1:A:254:ALA:HB1	2:A:601:PAM:H42	1.69	0.73
1:B:485:ARG:HD3	2:B:606:PAM:H41	1.71	0.71
1:B:69:LEU:HB3	2:B:603:PAM:H142	1.75	0.68
3:A:607:J2O:AU1	3:A:607:J2O:S3	2.24	0.65
3:B:607:J2O:S3	3:B:607:J2O:AU1	2.24	0.65
1:A:564:LYS:HZ1	1:A:567:CYS:HB3	1.65	0.62
1:A:564:LYS:NZ	1:A:567:CYS:HB3	2.15	0.61
1:B:214:TRP:CD1	1:B:343:VAL:HG11	2.35	0.61
1:A:198:LEU:HD13	1:A:458:ASN:OD1	2.02	0.60
1:A:485:ARG:HD3	2:A:604:PAM:H41	1.85	0.59
1:B:460:LEU:HD11	2:B:605:PAM:H161	1.83	0.59
1:A:287:SER:OG	2:A:601:PAM:O2	2.21	0.59
1:B:46:VAL:HG22	2:B:603:PAM:H151	1.85	0.58
1:B:398:LEU:HD23	1:B:403:PHE:HA	1.87	0.57
1:B:433:VAL:HG22	1:B:452:TYR:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:VAL:HG22	1:A:235:VAL:HG21	1.89	0.55
1:B:68:THR:HA	1:B:95:GLU:HG2	1.89	0.55
1:B:325:VAL:HG22	2:B:604:PAM:H163	1.88	0.54
1:B:222:ARG:NH1	1:B:291:ALA:O	2.40	0.54
1:A:564:LYS:HA	1:A:564:LYS:CE	2.37	0.54
1:B:216:VAL:HG22	1:B:235:VAL:HG21	1.89	0.53
1:A:95:GLU:OE1	1:A:99:ASN:HB2	2.10	0.51
1:A:83:THR:HB	1:A:84:TYR:CD1	2.46	0.51
1:B:2:ALA:HA	1:B:9:HIS:CG	2.46	0.50
1:B:530:VAL:HG12	1:B:534:LYS:HE3	1.92	0.50
1:B:460:LEU:HD11	2:B:605:PAM:C16	2.42	0.49
1:A:2:ALA:HA	1:A:9:HIS:CG	2.48	0.48
1:A:387:LEU:HD21	2:A:603:PAM:H41	1.95	0.48
1:A:31:LEU:HD21	1:A:74:LEU:HD22	1.94	0.48
1:B:198:LEU:HD13	1:B:458:ASN:HD21	1.79	0.47
1:B:19:PHE:O	1:B:23:VAL:HG23	2.13	0.47
1:B:241:VAL:HG22	1:B:256:ASP:HB3	1.97	0.47
1:B:69:LEU:HB3	2:B:603:PAM:C14	2.43	0.47
1:A:12:LYS:HE2	1:A:54:VAL:HG13	1.96	0.47
1:B:138:TYR:CD1	1:B:139:LEU:N	2.83	0.47
1:B:298:MET:SD	1:B:337:ARG:HA	2.55	0.47
1:A:115:LEU:HD11	1:A:141:GLU:HB3	1.97	0.46
1:B:46:VAL:HG22	2:B:603:PAM:C15	2.45	0.46
1:A:68:THR:HA	1:A:95:GLU:HG2	1.97	0.46
1:A:296:ASP:OD1	1:A:297:GLU:N	2.49	0.46
1:A:241:VAL:HG22	1:A:256:ASP:HB3	1.98	0.45
1:A:395:PHE:CD1	1:A:395:PHE:C	2.95	0.45
1:A:198:LEU:HD11	1:A:481:LEU:HD21	1.99	0.45
1:B:49:PHE:CD2	2:B:603:PAM:H162	2.51	0.45
1:B:100:GLU:O	1:B:104:GLN:HG2	2.18	0.45
1:A:23:VAL:HG22	2:A:601:PAM:H132	1.98	0.44
1:A:515:THR:HB	1:B:79:THR:CG2	2.48	0.44
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.53	0.44
1:B:383:GLU:OE1	1:B:485:ARG:NH1	2.51	0.44
1:B:564:LYS:CE	1:B:567:CYS:HB2	2.47	0.44
1:A:21:ALA:HB1	1:A:155:LEU:HD13	2.00	0.43
1:B:2:ALA:HA	1:B:9:HIS:CD2	2.53	0.43
1:B:511:ALA:HA	1:B:568:PHE:CE2	2.54	0.43
1:A:408:LEU:HD13	1:A:427:SER:OG	2.18	0.43
1:B:178:LEU:HD22	1:B:182:LEU:HG	2.00	0.43
1:B:25:ILE:O	1:B:29:GLN:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ILE:HG13	2:A:604:PAM:H112	2.01	0.42
1:A:420:THR:N	1:A:421:PRO:CD	2.82	0.42
1:B:387:LEU:HB3	2:B:606:PAM:H10	2.01	0.42
1:A:138:TYR:CD1	1:A:139:LEU:N	2.87	0.42
1:A:475:LYS:O	1:A:479:GLU:HG2	2.19	0.42
1:A:567:CYS:O	1:A:571:GLU:N	2.52	0.42
1:A:564:LYS:HA	1:A:564:LYS:HE2	2.01	0.42
1:A:237:ASP:O	1:A:241:VAL:HG23	2.20	0.42
1:B:290:ILE:O	1:B:293:VAL:HG12	2.20	0.42
1:B:41:LYS:NZ	1:B:45:GLU:OE1	2.53	0.41
1:A:231:VAL:O	1:A:235:VAL:HG23	2.21	0.41
1:A:433:VAL:HG22	1:A:452:TYR:HB3	2.03	0.41
1:B:420:THR:HG23	1:B:530:VAL:HB	2.03	0.41
1:A:224:PRO:HD2	1:A:296:ASP:HB3	2.03	0.41
1:B:344:VAL:HG21	2:B:606:PAM:H42	2.03	0.41
1:B:135:LEU:O	1:B:138:TYR:HB3	2.21	0.41
1:B:407:LEU:HG	1:B:411:TYR:HE2	1.84	0.40
1:A:383:GLU:OE1	1:A:485:ARG:NH2	2.54	0.40
1:B:262:LYS:HE2	1:B:266:GLU:OE2	2.22	0.40
1:B:513:ILE:HA	1:B:516:LEU:HD12	2.03	0.40
1:A:415:VAL:HG12	1:A:415:VAL:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ASP:OD2	1:B:574:LYS:NZ[1_545]	2.17	0.03

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	581/583 (100%)	553 (95%)	23 (4%)	5 (1%)	14	27
1	B	581/583 (100%)	547 (94%)	31 (5%)	3 (0%)	24	43
All	All	1162/1166 (100%)	1100 (95%)	54 (5%)	8 (1%)	18	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	562	ASP
1	A	563	ASP
1	A	322	ALA
1	A	479	GLU
1	A	268	GLN
1	B	563	ASP
1	A	95	GLU
1	B	95	GLU

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	509/509 (100%)	496 (97%)	13 (3%)	40	68
1	B	509/509 (100%)	492 (97%)	17 (3%)	33	61
All	All	1018/1018 (100%)	988 (97%)	30 (3%)	37	65

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

Mol	Chain	Res	Type
1	A	132	GLU
1	A	138	TYR
1	A	184	GLU
1	A	232	SER
1	A	270	SER
1	A	283	LEU
1	A	378	LYS
1	A	435	SER

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Mol	Chain	Res	Type
1	A	466	LYS
1	A	485	ARG
1	A	495	GLU
1	A	563	ASP
1	A	564	LYS
1	B	138	TYR
1	B	178	LEU
1	B	179	LEU
1	B	184	GLU
1	B	199	LYS
1	B	202	SER
1	B	222	ARG
1	B	262	LYS
1	B	283	LEU
1	B	298	MET
1	B	390	GLN
1	B	480	SER
1	B	485	ARG
1	B	495	GLU
1	B	541	LYS
1	B	565	GLU
1	B	566	THR

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

Mol	Chain	Res	Type
1	A	109	ASN
1	A	130	ASN
1	A	196	GLN
1	A	242	HIS
1	A	338	HIS
1	A	483	ASN
1	B	33	GLN
1	B	483	ASN

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)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PAM	A	604	-	17,17,17	1.03	2 (11%)	17,17,17	1.63	3 (17%)
2	PAM	B	604	-	17,17,17	1.03	1 (5%)	17,17,17	1.05	0
2	PAM	B	606	-	17,17,17	0.96	1 (5%)	17,17,17	1.76	3 (17%)
2	PAM	B	602	-	12,12,17	1.08	1 (8%)	12,12,17	1.01	0
3	J2O	A	607	1	11,17,18	2.49	2 (18%)	12,25,28	1.56	2 (16%)
2	PAM	A	603	-	17,17,17	1.06	1 (5%)	17,17,17	1.19	0
2	PAM	A	605	-	15,15,17	1.04	1 (6%)	15,15,17	1.26	1 (6%)
2	PAM	B	605	-	17,17,17	1.01	1 (5%)	17,17,17	1.39	3 (17%)
2	PAM	A	602	-	17,17,17	0.98	1 (5%)	17,17,17	1.22	2 (11%)
2	PAM	A	601	-	17,17,17	0.96	1 (5%)	17,17,17	1.67	3 (17%)
2	PAM	B	603	-	17,17,17	0.97	1 (5%)	17,17,17	1.33	2 (11%)
2	PAM	B	601	-	15,15,17	1.11	1 (6%)	15,15,17	1.28	2 (13%)
3	J2O	B	607	1	11,17,18	2.39	2 (18%)	12,25,28	1.04	0
2	PAM	A	606	-	12,12,17	1.04	1 (8%)	12,12,17	1.24	1 (8%)

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
2	PAM	A	604	-	-	12/15/15/15	-
2	PAM	B	604	-	-	5/15/15/15	-
2	PAM	B	606	-	-	7/15/15/15	-
2	PAM	B	602	-	-	6/10/10/15	-
3	J2O	A	607	1	-	-	0/2/3/3
2	PAM	A	603	-	-	9/15/15/15	-
2	PAM	A	605	-	-	5/13/13/15	-
2	PAM	B	605	-	-	9/15/15/15	-
2	PAM	A	602	-	-	7/15/15/15	-
2	PAM	A	601	-	-	8/15/15/15	-
2	PAM	B	603	-	-	7/15/15/15	-
2	PAM	B	601	-	-	6/13/13/15	-
3	J2O	B	607	1	-	-	0/2/3/3
2	PAM	A	606	-	-	8/10/10/15	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	607	J2O	C11-N2	-6.50	1.31	1.45
3	B	607	J2O	C11-N2	-6.02	1.32	1.45
3	B	607	J2O	C11-C25	-4.13	1.42	1.51
3	A	607	J2O	C11-C25	-3.99	1.42	1.51
2	A	603	PAM	C10-C9	3.62	1.52	1.31
2	B	601	PAM	C10-C9	3.60	1.52	1.31
2	B	604	PAM	C10-C9	3.56	1.52	1.31
2	B	603	PAM	C10-C9	3.54	1.52	1.31
2	A	602	PAM	C10-C9	3.53	1.52	1.31
2	A	601	PAM	C10-C9	3.49	1.52	1.31
2	A	605	PAM	C10-C9	3.46	1.51	1.31
2	B	605	PAM	C10-C9	3.41	1.51	1.31
2	B	606	PAM	C10-C9	3.40	1.51	1.31
2	A	604	PAM	C10-C9	3.38	1.51	1.31
2	A	606	PAM	C9-C10	2.93	1.51	1.29
2	B	602	PAM	C9-C10	2.91	1.51	1.29
2	A	604	PAM	O2-C1	2.16	1.29	1.22

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	606	PAM	C3-C2-C1	4.76	126.48	114.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	604	PAM	C3-C2-C1	4.18	125.01	114.47
2	A	601	PAM	C3-C2-C1	3.34	122.90	114.47
2	A	601	PAM	O1-C1-C2	3.10	124.00	114.03
2	A	605	PAM	C3-C2-C1	3.09	122.27	114.47
3	A	607	J2O	S3-C13-N7	-3.08	112.86	117.71
2	A	604	PAM	C4-C3-C2	3.00	123.97	113.19
3	A	607	J2O	C11-C25-C10	2.92	126.35	120.22
2	A	601	PAM	O1-C1-O2	-2.90	116.08	123.30
2	B	605	PAM	C3-C2-C1	2.86	121.69	114.47
2	B	606	PAM	O1-C1-O2	-2.85	116.19	123.30
2	B	605	PAM	O1-C1-O2	-2.70	116.56	123.30
2	B	605	PAM	C6-C7-C8	2.41	124.28	113.79
2	B	603	PAM	O1-C1-O2	-2.41	117.30	123.30
2	B	606	PAM	C5-C4-C3	2.33	126.25	114.42
2	B	603	PAM	O1-C1-C2	2.31	121.45	114.03
2	B	601	PAM	C3-C2-C1	2.29	120.24	114.47
2	A	606	PAM	O1-C1-C2	2.07	120.68	114.03
2	B	601	PAM	O1-C1-C2	2.06	120.66	114.03
2	A	602	PAM	O1-C1-C2	2.06	120.66	114.03
2	A	604	PAM	O1-C1-C2	2.03	120.54	114.03
2	A	602	PAM	C3-C2-C1	2.01	119.54	114.47

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	603	PAM	C6-C7-C8-C9
2	A	602	PAM	C11-C10-C9-C8
2	B	606	PAM	C3-C4-C5-C6
2	B	605	PAM	C1-C2-C3-C4
2	B	605	PAM	C3-C4-C5-C6
2	A	601	PAM	C1-C2-C3-C4
2	A	602	PAM	C1-C2-C3-C4
2	B	603	PAM	C11-C10-C9-C8
2	B	604	PAM	C11-C12-C13-C14
2	A	601	PAM	C11-C12-C13-C14
2	B	602	PAM	C1-C2-C3-C4
2	B	601	PAM	C5-C6-C7-C8
2	A	603	PAM	C3-C4-C5-C6
2	B	601	PAM	C3-C4-C5-C6
2	B	605	PAM	C5-C6-C7-C8
2	A	604	PAM	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	B	602	PAM	C2-C3-C4-C5
2	A	603	PAM	C4-C5-C6-C7
2	B	605	PAM	C12-C13-C14-C15
2	A	604	PAM	C13-C14-C15-C16
2	A	604	PAM	C10-C11-C12-C13
2	B	601	PAM	C2-C3-C4-C5
2	A	604	PAM	C11-C12-C13-C14
2	A	604	PAM	C9-C10-C11-C12
2	A	602	PAM	C2-C3-C4-C5
2	B	605	PAM	C4-C5-C6-C7
2	B	604	PAM	C10-C11-C12-C13
2	B	604	PAM	C4-C5-C6-C7
2	B	603	PAM	C2-C3-C4-C5
2	A	601	PAM	C7-C8-C9-C10
2	B	605	PAM	C6-C7-C8-C9
2	A	603	PAM	C2-C3-C4-C5
2	B	605	PAM	C11-C10-C9-C8
2	A	601	PAM	C3-C4-C5-C6
2	A	605	PAM	C6-C7-C8-C9
2	A	606	PAM	C6-C7-C8-C9
2	B	603	PAM	C10-C11-C12-C13
2	B	603	PAM	C3-C4-C5-C6
2	B	602	PAM	C3-C4-C5-C6
2	B	603	PAM	C12-C13-C14-C15
2	B	605	PAM	C13-C14-C15-C16
2	A	604	PAM	C11-C10-C9-C8
2	B	606	PAM	C2-C3-C4-C5
2	B	606	PAM	C12-C13-C14-C15
2	A	605	PAM	C11-C10-C9-C8
2	B	606	PAM	C13-C14-C15-C16
2	B	604	PAM	C13-C14-C15-C16
2	A	603	PAM	C13-C14-C15-C16
2	A	604	PAM	C2-C3-C4-C5
2	A	606	PAM	C11-C10-C9-C8
2	A	602	PAM	C12-C13-C14-C15
2	A	605	PAM	C5-C6-C7-C8
2	A	606	PAM	C4-C5-C6-C7
2	A	604	PAM	C5-C6-C7-C8
2	A	601	PAM	C13-C14-C15-C16
2	B	601	PAM	C11-C10-C9-C8
2	B	606	PAM	C7-C8-C9-C10
2	A	601	PAM	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	B	606	PAM	C9-C10-C11-C12
2	A	603	PAM	C1-C2-C3-C4
2	A	604	PAM	C1-C2-C3-C4
2	B	601	PAM	C9-C10-C11-C12
2	A	606	PAM	C3-C4-C5-C6
2	A	603	PAM	O1-C1-C2-C3
2	B	603	PAM	C7-C8-C9-C10
2	A	603	PAM	O2-C1-C2-C3
2	A	604	PAM	C6-C7-C8-C9
2	A	604	PAM	O1-C1-C2-C3
2	A	606	PAM	C2-C3-C4-C5
2	A	601	PAM	O1-C1-C2-C3
2	A	602	PAM	O1-C1-C2-C3
2	A	602	PAM	O2-C1-C2-C3
2	B	602	PAM	O1-C1-C2-C3
2	A	605	PAM	C7-C8-C9-C10
2	A	603	PAM	C9-C10-C11-C12
2	B	603	PAM	C9-C10-C11-C12
2	A	606	PAM	O1-C1-C2-C3
2	B	602	PAM	O2-C1-C2-C3
2	A	606	PAM	C7-C8-C9-C10
2	A	604	PAM	O2-C1-C2-C3
2	B	606	PAM	O2-C1-C2-C3
2	B	605	PAM	O2-C1-C2-C3
2	A	606	PAM	O2-C1-C2-C3
2	A	605	PAM	C11-C12-C13-C14
2	B	601	PAM	C7-C8-C9-C10
2	B	602	PAM	C4-C5-C6-C7
2	A	601	PAM	C9-C10-C11-C12
2	B	604	PAM	C9-C10-C11-C12
2	A	602	PAM	C10-C11-C12-C13

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	PAM	3	0
2	B	604	PAM	1	0
2	B	606	PAM	3	0
3	A	607	J2O	1	0
2	A	603	PAM	1	0
2	B	605	PAM	2	0

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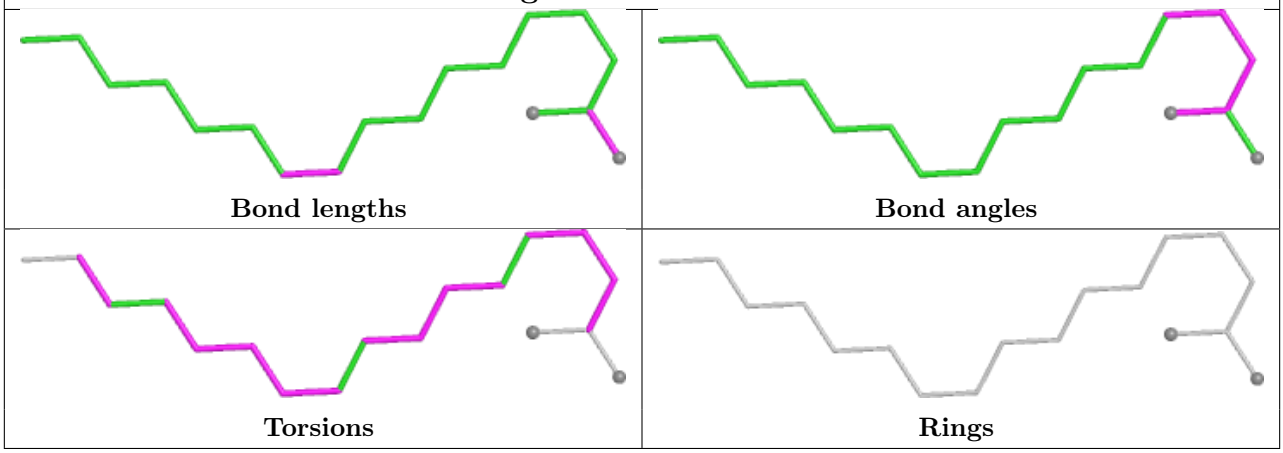
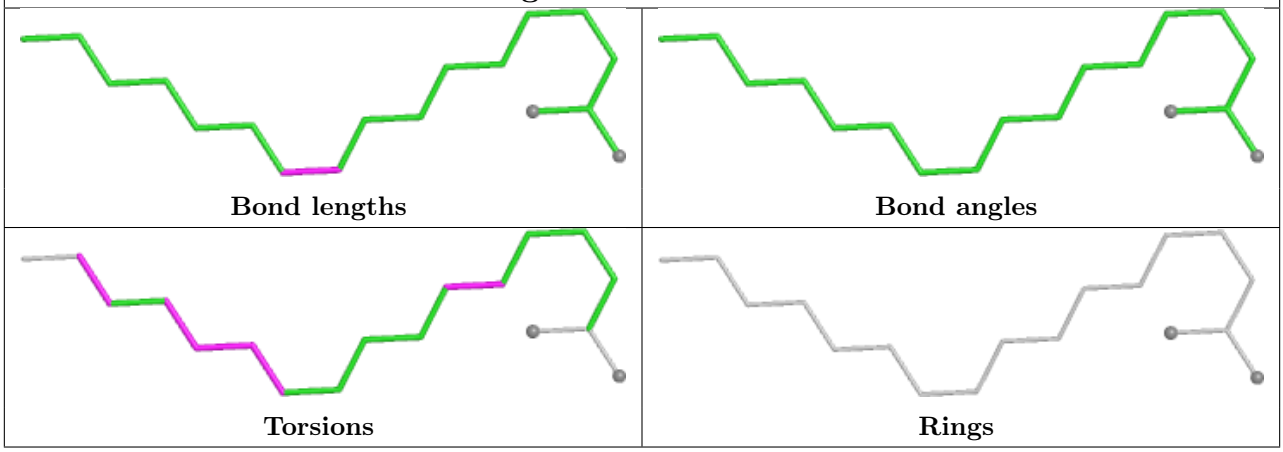
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PAM	3	0
2	B	603	PAM	5	0
3	B	607	J2O	1	0

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 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 PAM A 604



Ligand PAM B 604



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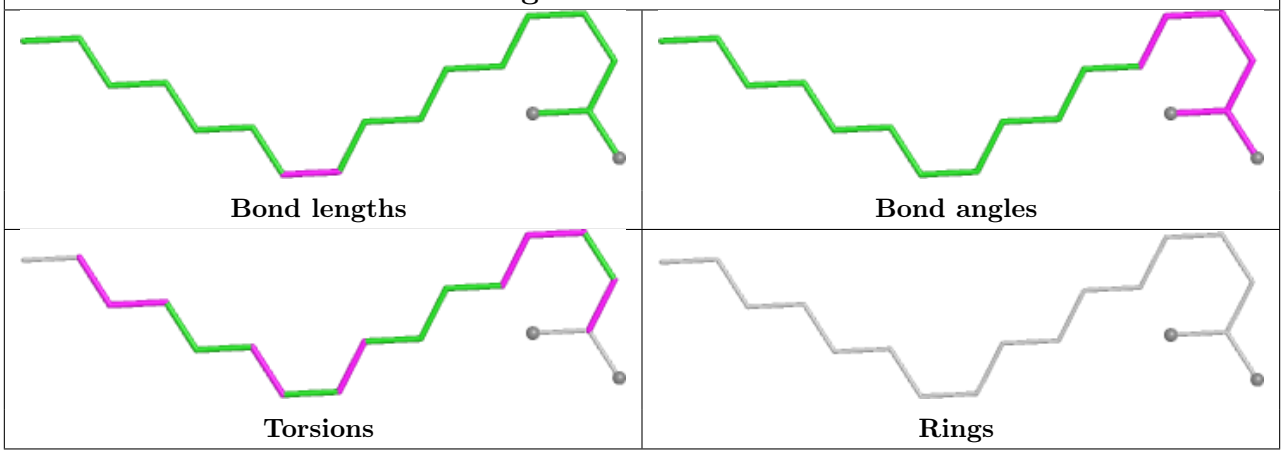

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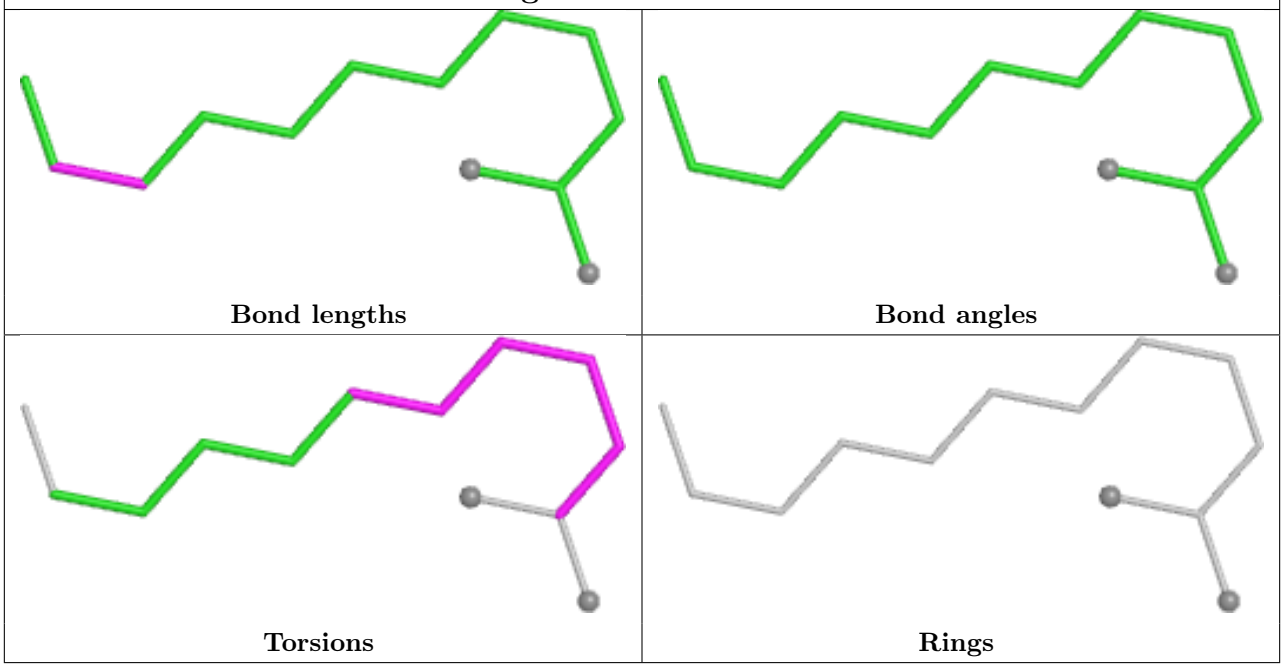
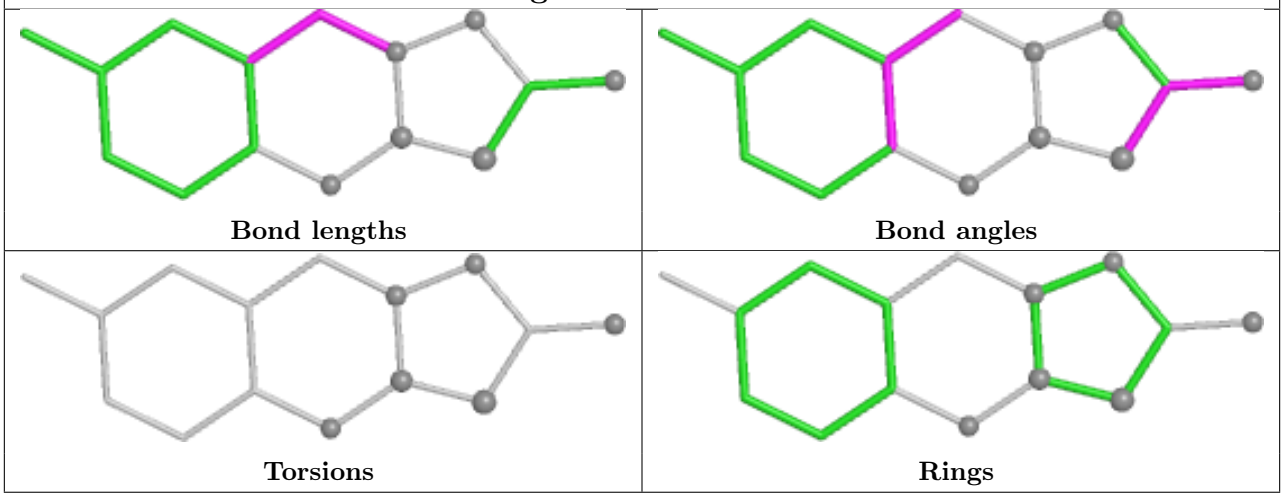
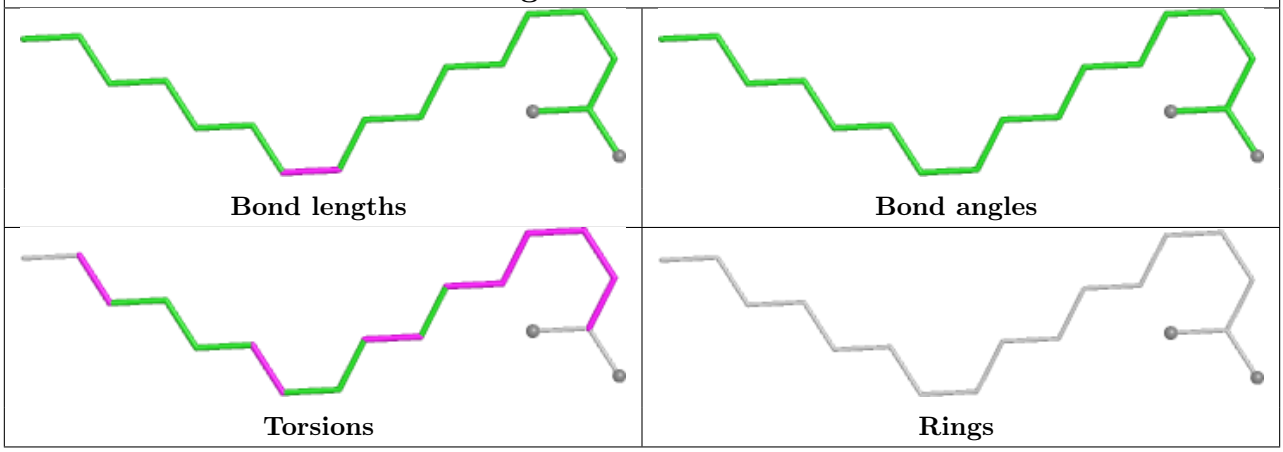


Ligand J2O A 607



Ligand PAM A 603



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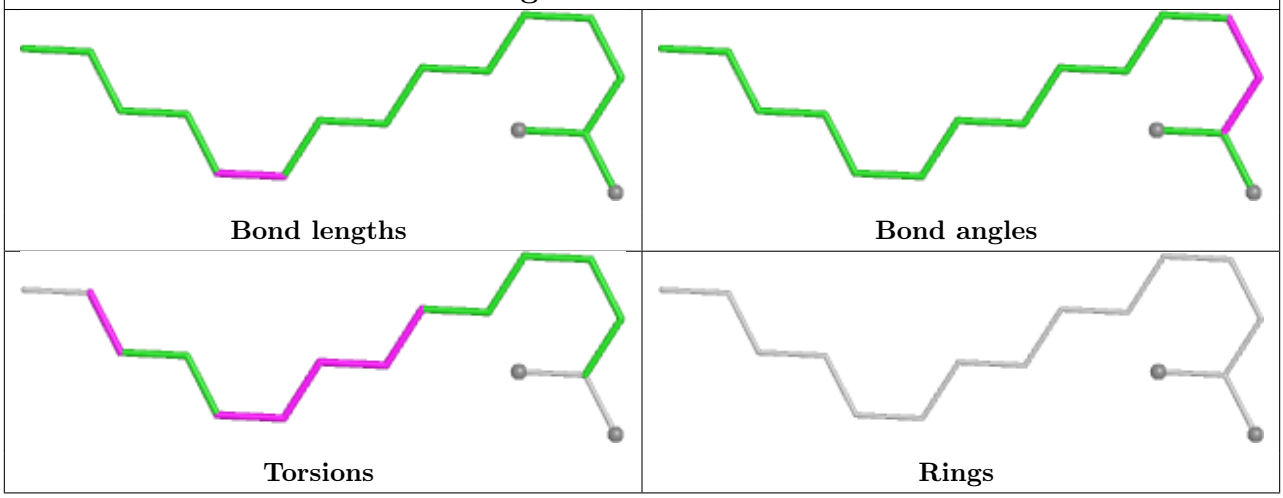

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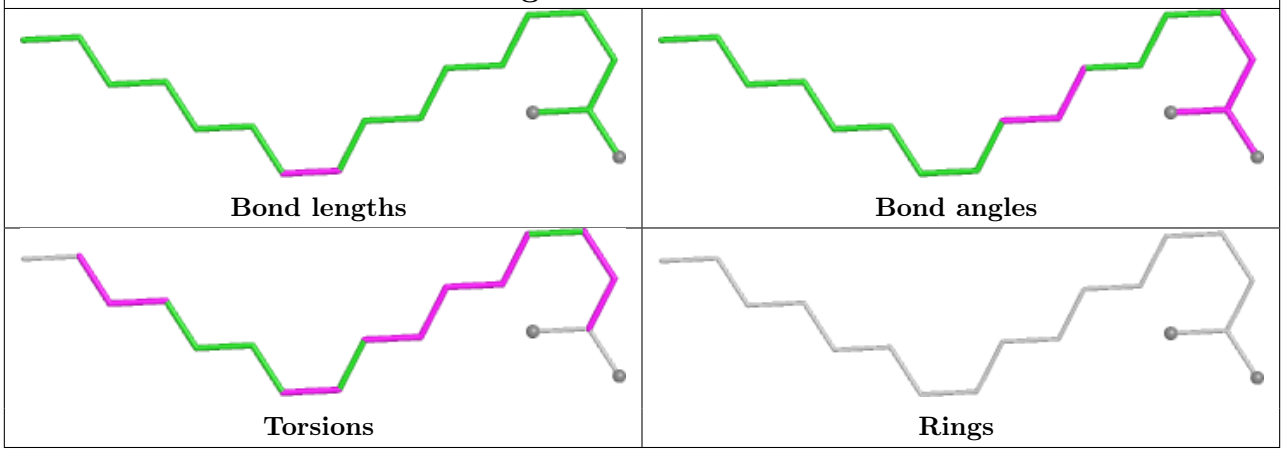

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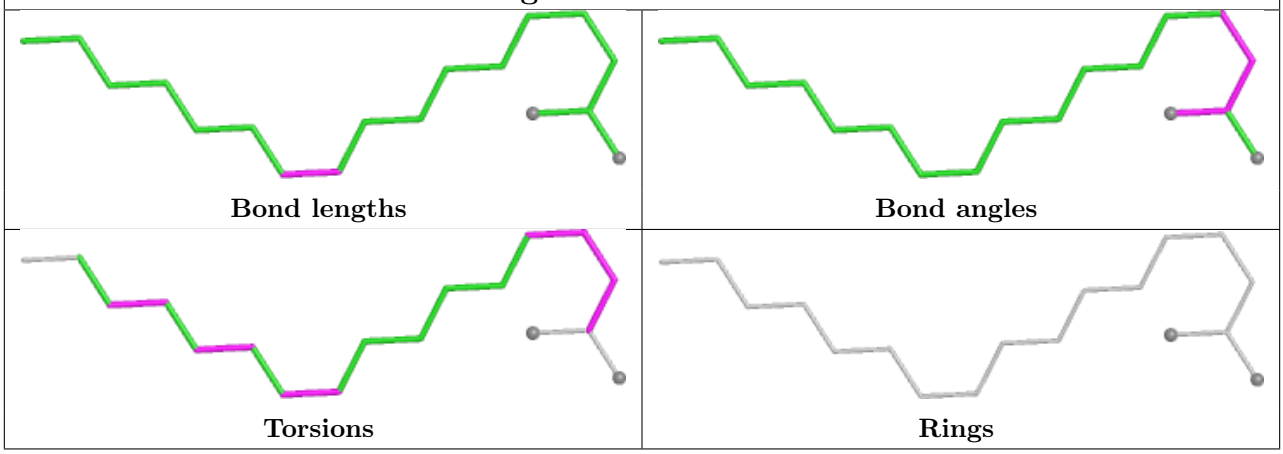

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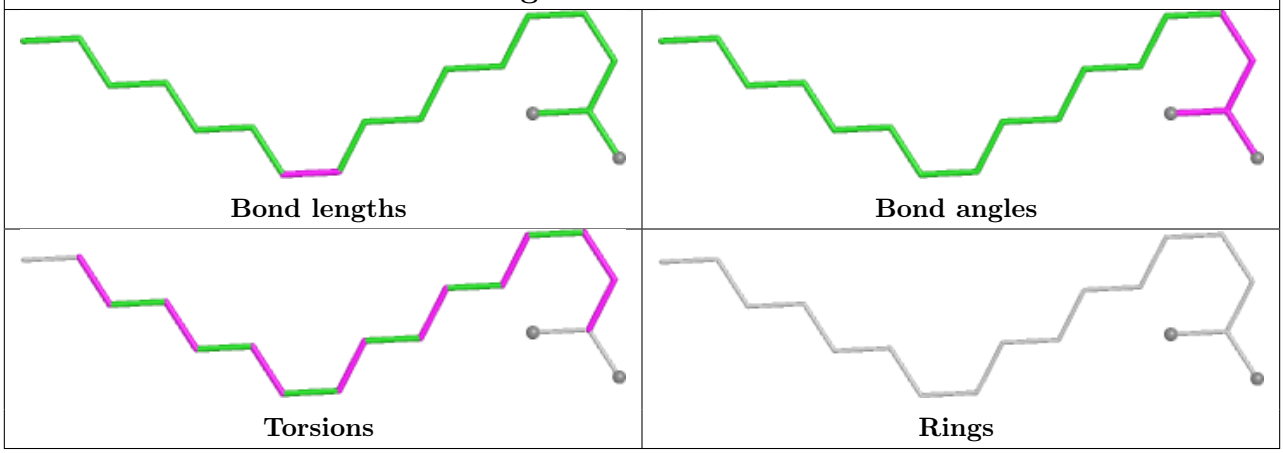

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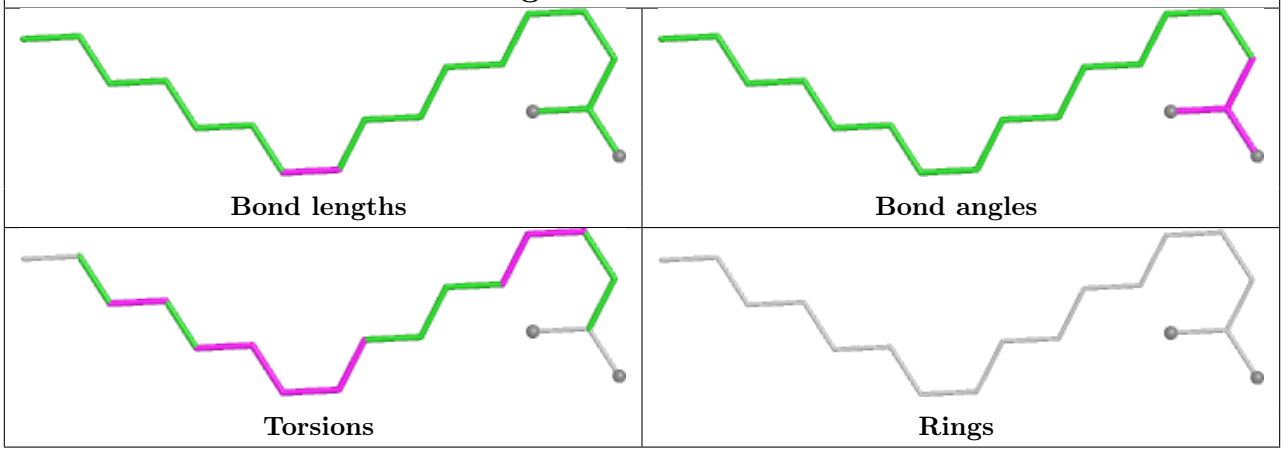

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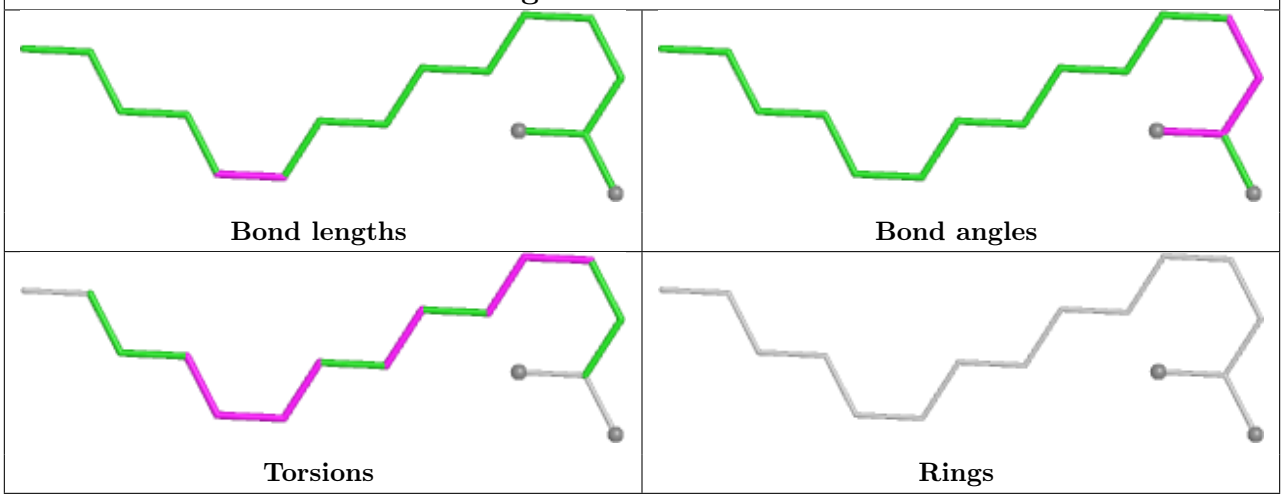
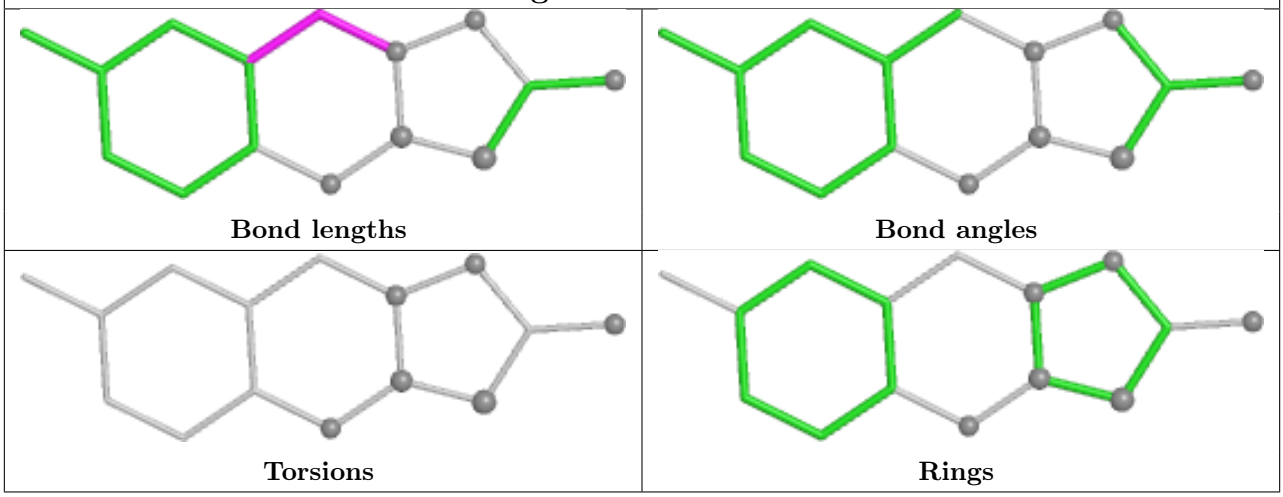
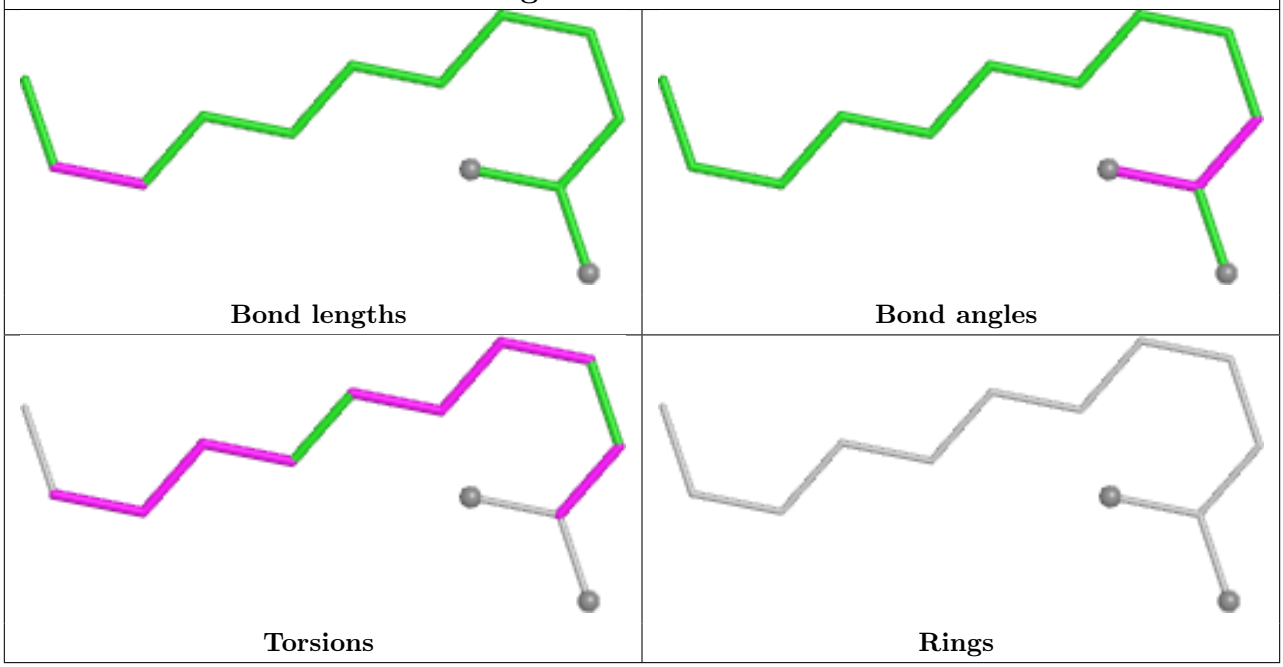


Ligand J2O B 607



Ligand PAM A 606



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	583/583 (100%)	-1.40	0	100	100	16, 32, 58, 106	0
1	B	583/583 (100%)	-1.40	0	100	100	17, 33, 57, 109	0
All	All	1166/1166 (100%)	-1.40	0	100	100	16, 33, 58, 109	0

There are no RSRZ outliers to report.

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(Å^2)	Q<0.9
2	PAM	A	606	13/18	0.98	0.07	52,56,57,58	0
2	PAM	B	602	13/18	0.98	0.07	52,56,57,58	0
2	PAM	B	603	18/18	0.98	0.06	37,47,55,56	0
2	PAM	B	605	18/18	0.98	0.07	52,57,60,61	0
3	J2O	A	607	15/16	0.98	0.10	123,146,175,196	0
3	J2O	B	607	15/16	0.98	0.07	121,136,156,183	0
2	PAM	B	601	16/18	0.99	0.04	36,38,50,51	0

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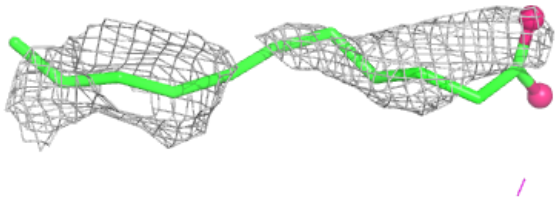
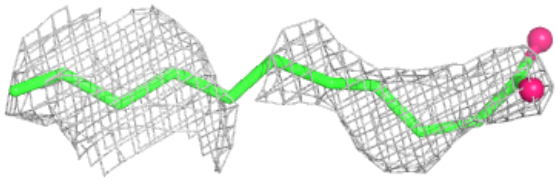
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PAM	A	602	18/18	0.99	0.04	33,38,54,55	0
2	PAM	A	603	18/18	0.99	0.06	38,43,55,57	0
2	PAM	B	604	18/18	0.99	0.04	39,46,50,53	0
2	PAM	A	604	18/18	0.99	0.05	35,41,44,44	0
2	PAM	B	606	18/18	0.99	0.06	36,42,44,48	0
2	PAM	A	605	16/18	0.99	0.04	32,37,44,44	0
2	PAM	A	601	18/18	0.99	0.04	30,33,35,36	0

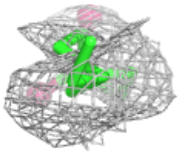
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PAM A 606:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

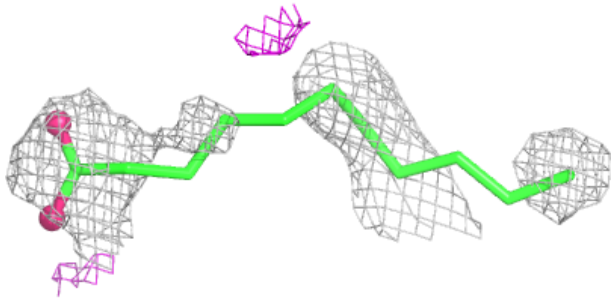


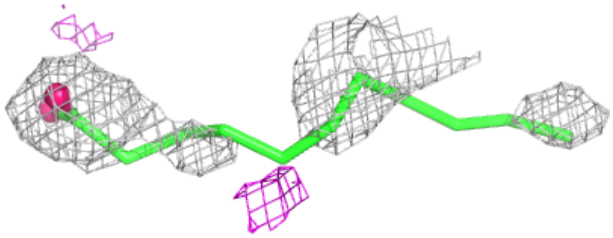


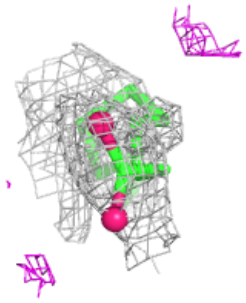


Electron density around PAM B 602:

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

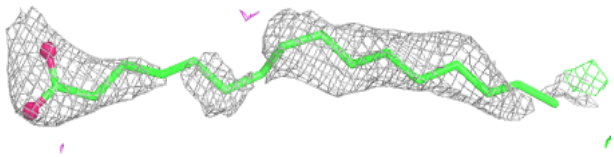


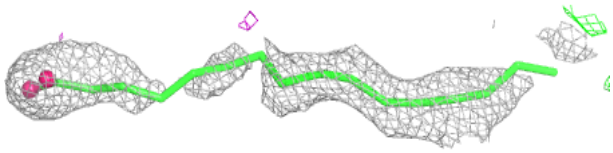


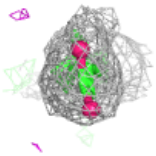


Electron density around PAM B 603:

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

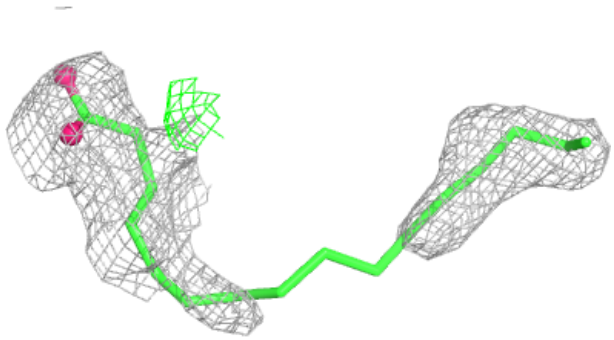


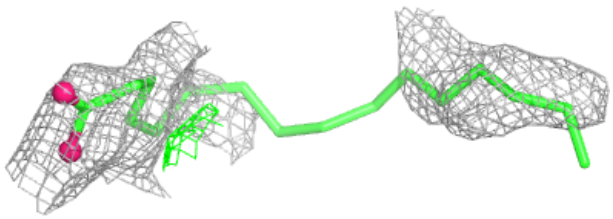


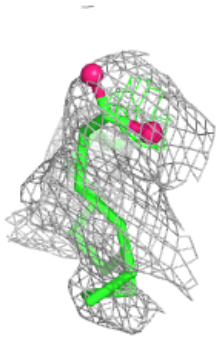


Electron density around PAM B 605:

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

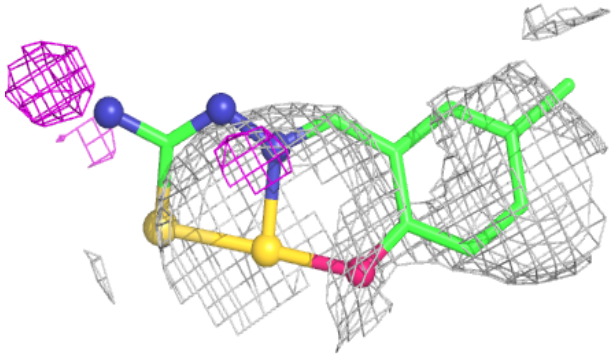


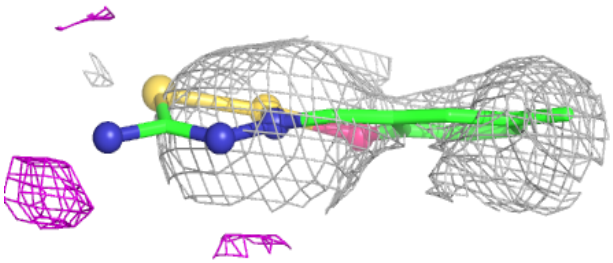


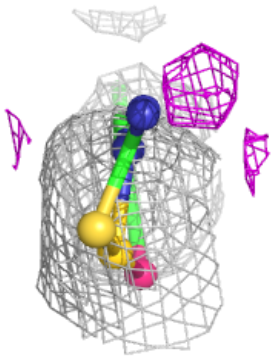


Electron density around J2O A 607:

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

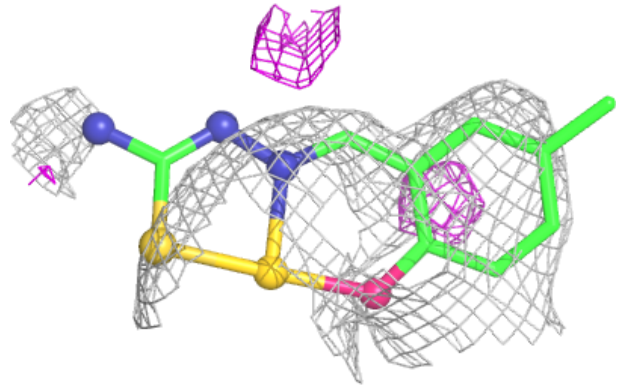


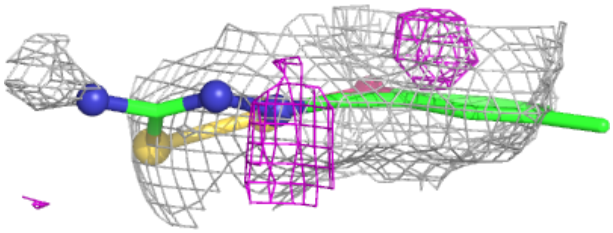


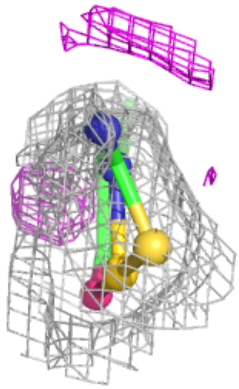


Electron density around J2O B 607:

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

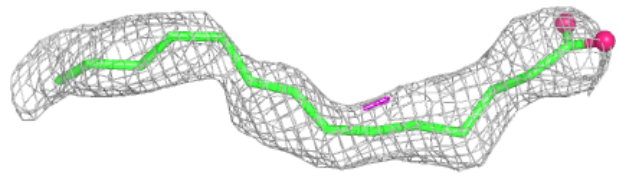


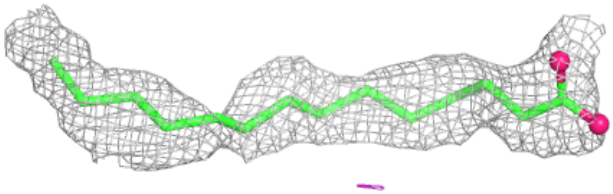


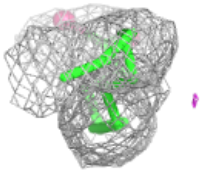


Electron density around PAM B 601:

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

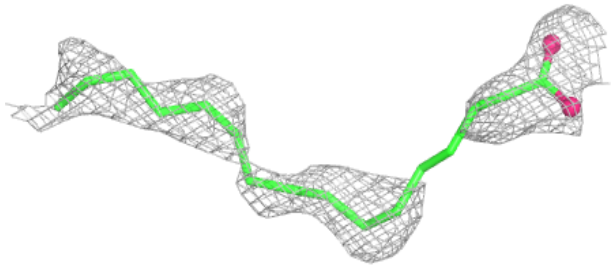


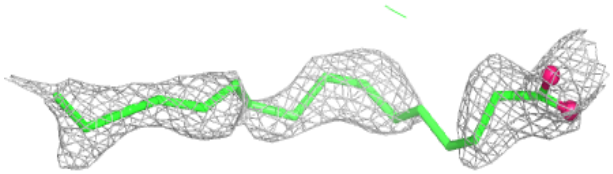


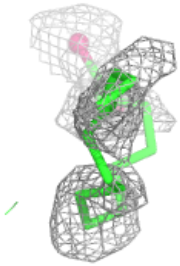


Electron density around PAM A 602:

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

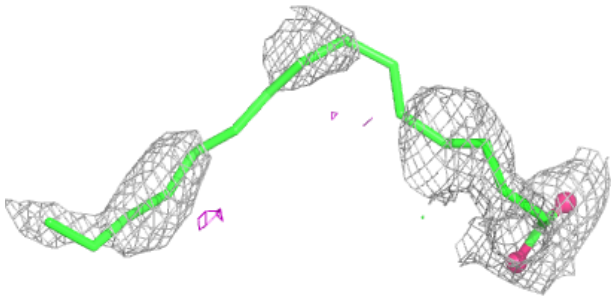


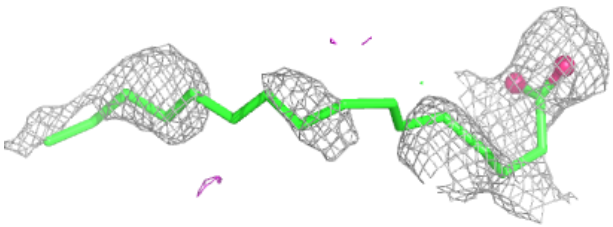


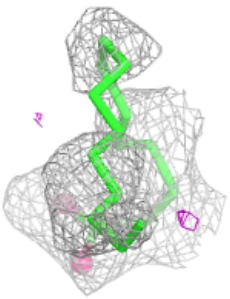


Electron density around PAM A 603:

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

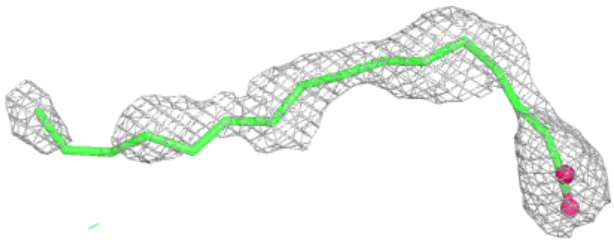


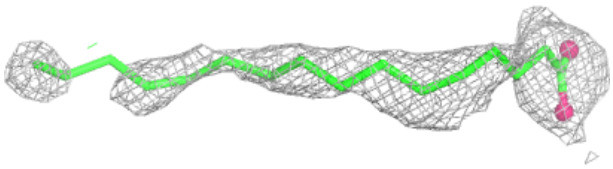


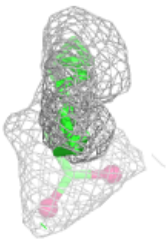


Electron density around PAM B 604:

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

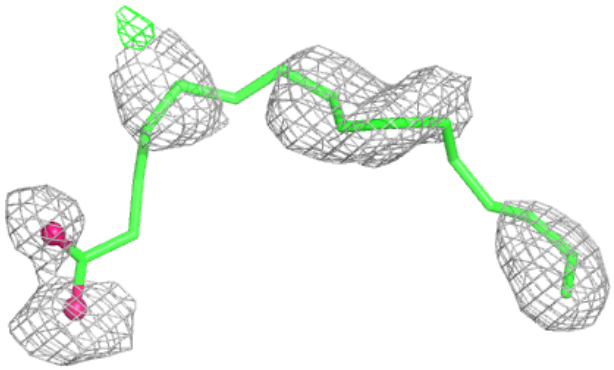


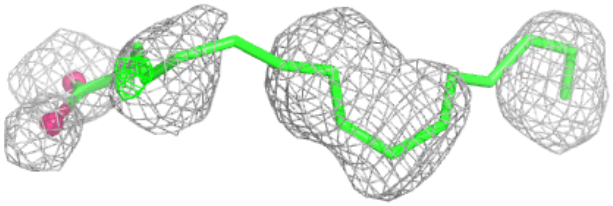


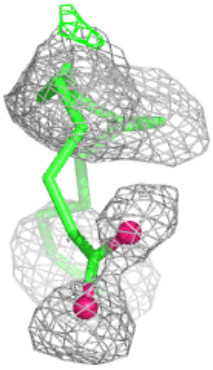


Electron density around PAM A 604:

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

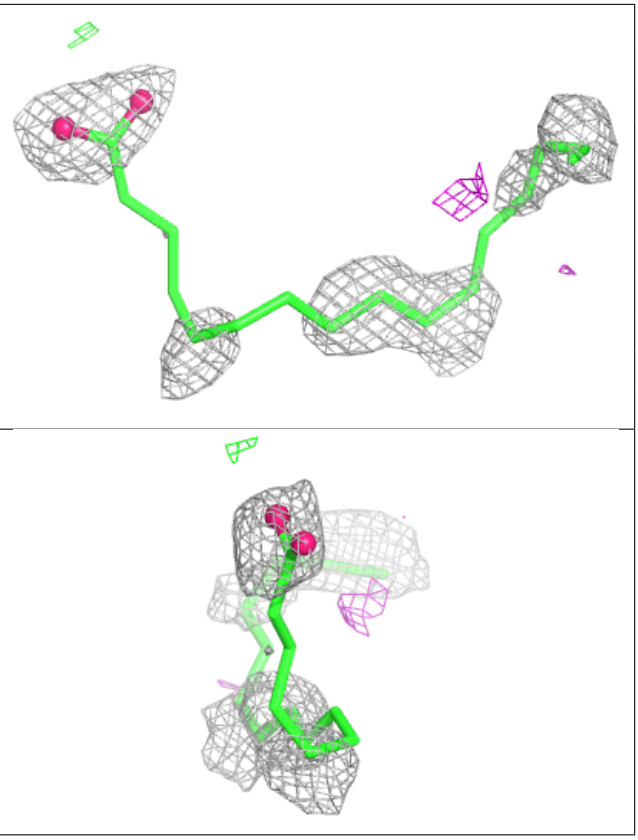






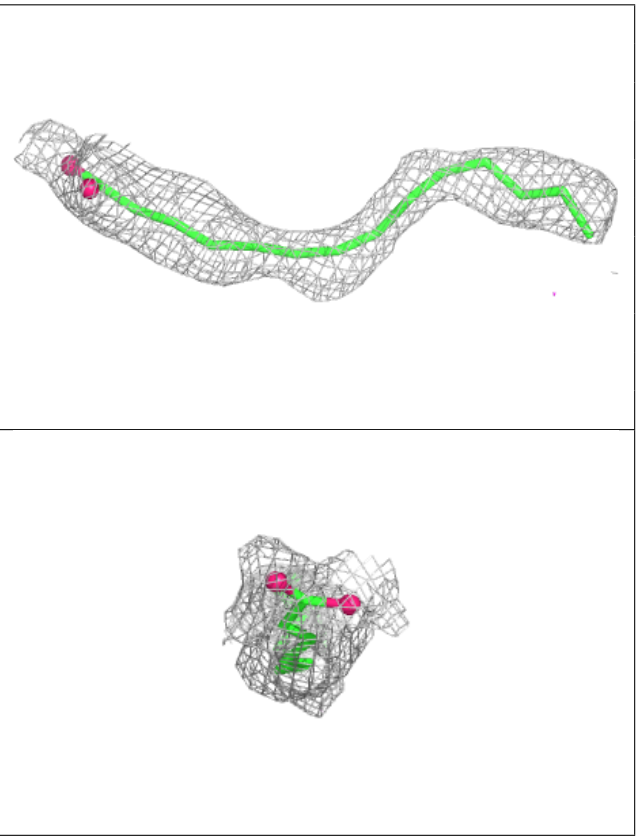
Electron density around PAM B 606:

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



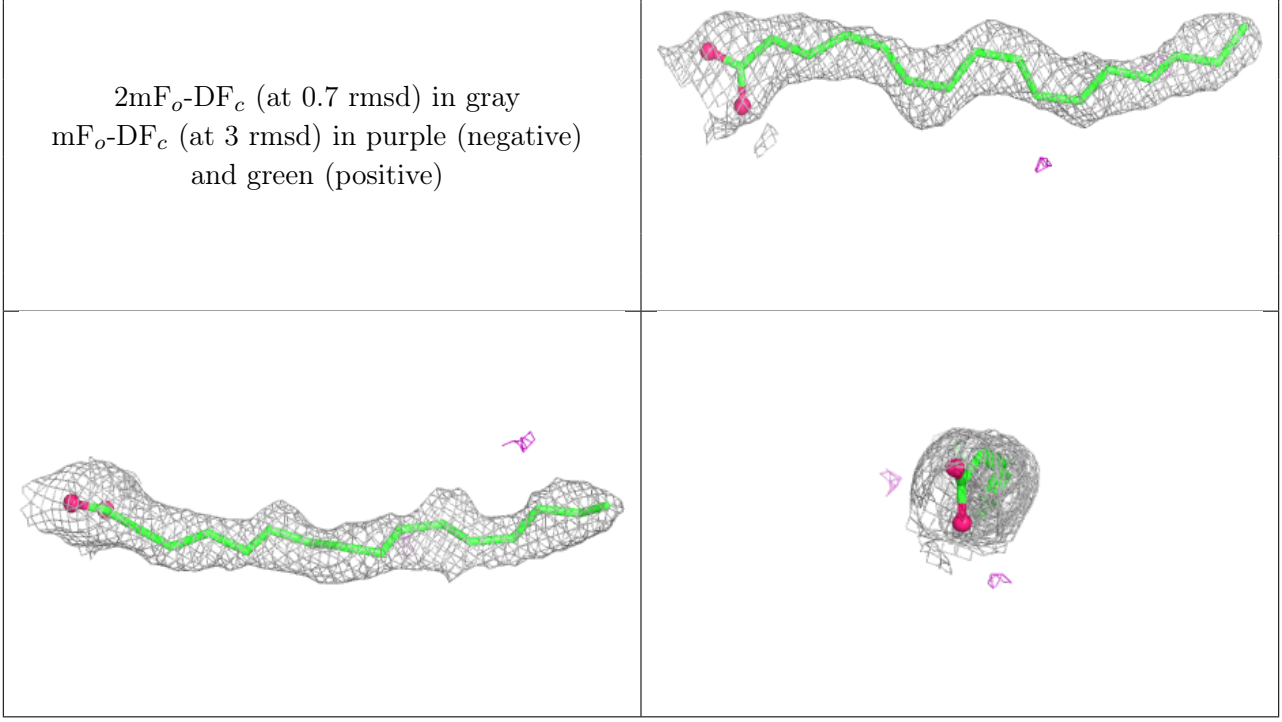
Electron density around PAM A 605:

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



Electron density around PAM A 601:

$2mF_o$-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.