



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2021 – 06:11 PM GMT

PDB ID : 7AAI
Title : Crystal structure of Human serum albumin in complex with perfluorooctanoic acid (PFOA) at 2.10 Angstrom Resolution
Authors : Maso, L.; Liberi, S.; Trande, M.; Angelini, A.; Cendron, L.
Deposited on : 2020-09-04
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.17
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) : 2.17

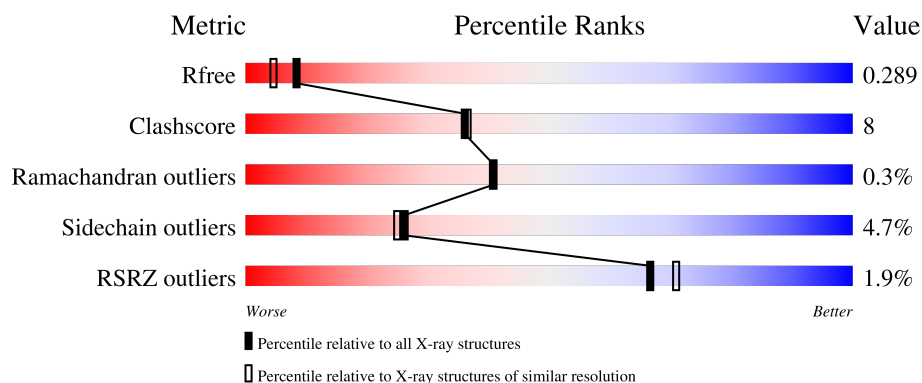
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.10 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 $\leq 5\%$. 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	AAA	584	

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
8	EDO	AAA	618	-	-	X	-

2 Entry composition [i](#)

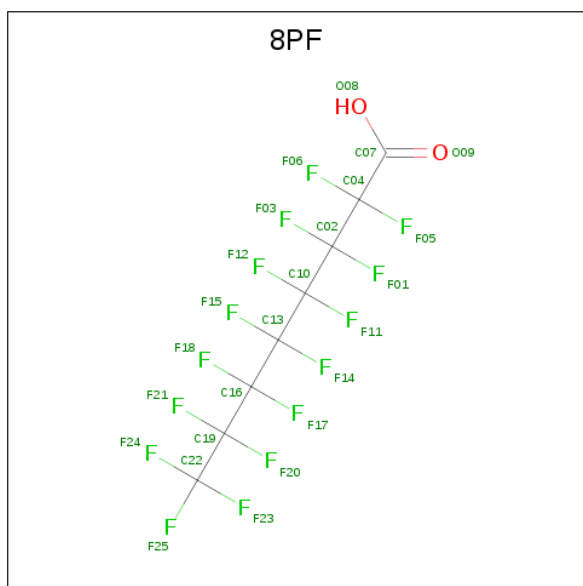
There are 9 unique types of molecules in this entry. The entry contains 4990 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	581	Total	C	N	O	S	0	3	0
			4650	2934	785	890	41			

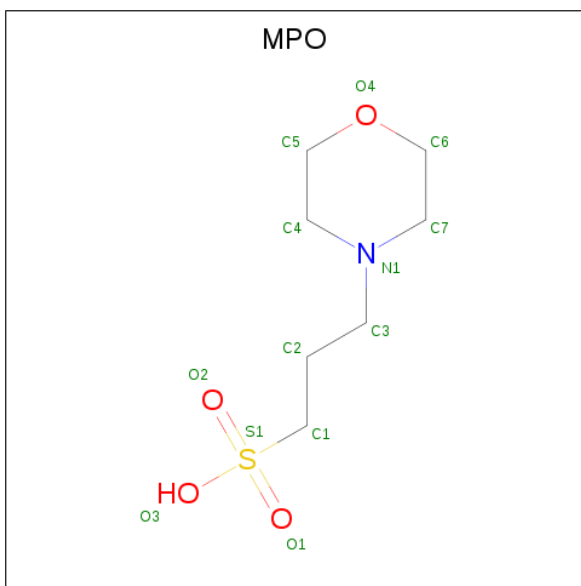
- Molecule 2 is pentadecafluorooctanoic acid (three-letter code: 8PF) (formula: $C_8HF_{15}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	F	O	0	0
			25	8	15	2		
2	AAA	1	Total	C	F	O	0	0
			25	8	15	2		
2	AAA	1	Total	C	F	O	0	0
			25	8	15	2		
2	AAA	1	Total	C	F	O	0	0
			25	8	15	2		

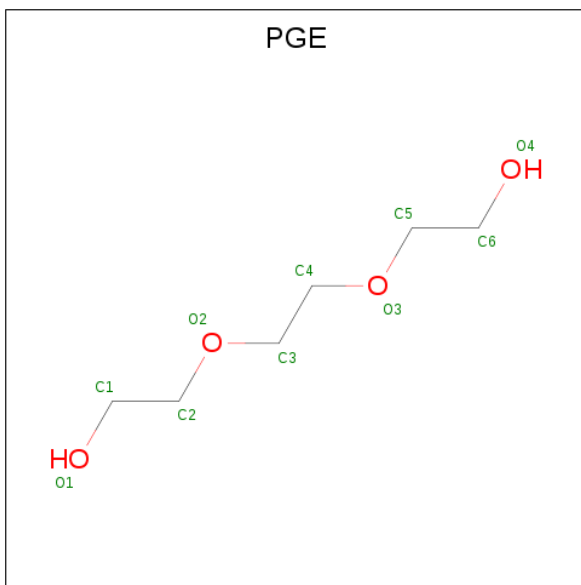
- Molecule 3 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO)

(formula: $C_7H_{15}NO_4S$).



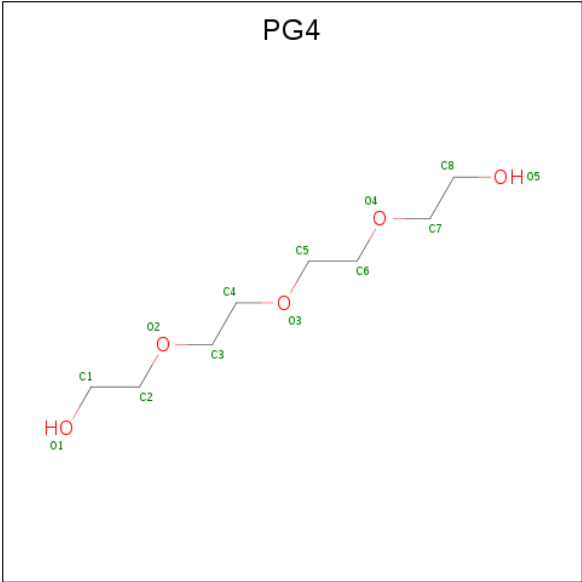
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



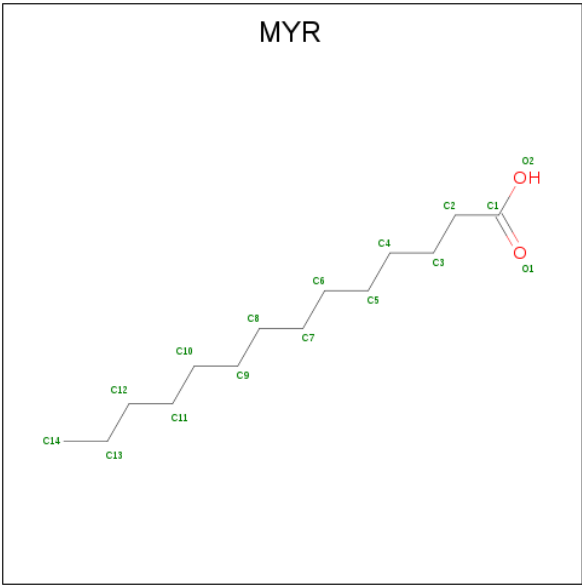
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is MYRISTIC ACID (three-letter code: MYR) (formula: C₁₄H₂₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	C	O	0	0
			16	14	2		
6	AAA	1	Total	C	O	0	0
			16	14	2		
6	AAA	1	Total	C	O	0	0
			16	14	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	C	O	0	0
			16	14	2		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	AAA	1	Total	C	O	0	0
			8	6	2		
7	AAA	1	Total	C	O	0	0
			8	6	2		
7	AAA	1	Total	C	O	0	0
			8	6	2		
7	AAA	1	Total	C	O	0	0
			8	6	2		
7	AAA	1	Total	C	O	0	0
			8	6	2		
7	AAA	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	AAA	1	Total	C	O	0	0
			4	2	2		

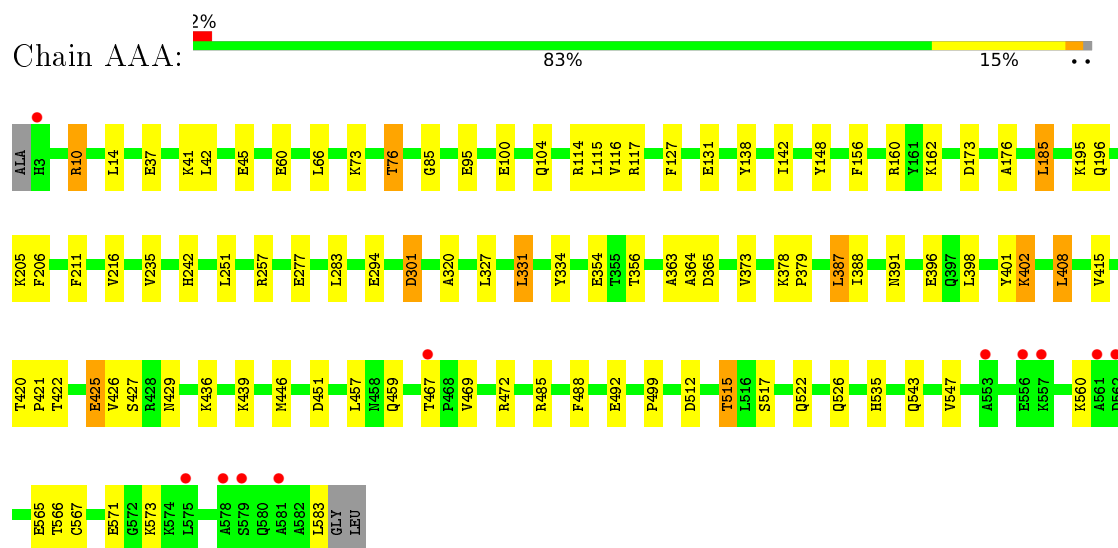
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AAA	88	Total	O	0	0
			88	88		

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: Albumin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.79Å 38.51Å 95.59Å 90.00° 104.95° 90.00°	Depositor
Resolution (Å)	46.22 – 2.10 46.18 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.22-2.10) 100.0 (46.18-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.12-2829	Depositor
R, R_{free}	0.217 , 0.289 0.217 , 0.289	Depositor DCC
R_{free} test set	1887 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4990	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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: PGE, EDO, MPO, PG4, MPD, MYR, 8PF

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	AAA	0.74	0/4740	0.87	0/6393

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	4650	0	4565	73	0
2	AAA	100	0	0	2	0
3	AAA	13	0	15	0	0
4	AAA	10	0	14	4	0
5	AAA	13	0	18	3	0
6	AAA	64	0	108	3	0
7	AAA	48	0	84	8	0
8	AAA	4	0	6	8	0
9	AAA	88	0	0	2	0
All	All	4990	0	4810	78	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (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:AAA:257:ARG:HH11	5:AAA:607:PG4:H41	1.38	0.87
1:AAA:364:ALA:HB3	8:AAA:618:EDO:H12	1.66	0.76
1:AAA:364:ALA:N	8:AAA:618:EDO:H11	2.01	0.75
1:AAA:485:ARG:HB2	7:AAA:615:MPD:H12	1.67	0.75
1:AAA:301:ASP:OD1	1:AAA:301:ASP:N	2.26	0.69
7:AAA:616:MPD:HM1	7:AAA:616:MPD:H52	1.75	0.69
1:AAA:567:CYS:O	1:AAA:571:GLU:HB3	1.92	0.68
1:AAA:205:LYS:HD3	1:AAA:206:PHE:CZ	2.31	0.65
1:AAA:543:GLN:HB3	1:AAA:583:LEU:CD2	2.28	0.64
1:AAA:41:LYS:HD3	1:AAA:45:GLU:OE1	1.98	0.63
1:AAA:396:GLU:OE2	1:AAA:396:GLU:HA	1.99	0.61
1:AAA:251:LEU:HG	7:AAA:612:MPD:H13	1.85	0.59
1:AAA:364:ALA:N	8:AAA:618:EDO:C1	2.66	0.59
1:AAA:547:VAL:HG21	1:AAA:583:LEU:HD11	1.85	0.58
1:AAA:467:THR:HG22	1:AAA:467:THR:O	2.01	0.58
1:AAA:251:LEU:H	7:AAA:612:MPD:H13	1.68	0.58
1:AAA:408:LEU:HD13	1:AAA:427:SER:CB	2.33	0.58
1:AAA:408:LEU:HD21	1:AAA:526:GLN:HB3	1.85	0.57
1:AAA:485:ARG:CB	7:AAA:615:MPD:H12	2.34	0.55
1:AAA:257:ARG:HD2	5:AAA:607:PG4:H42	1.88	0.54
1:AAA:114:ARG:NH2	1:AAA:116:VAL:HG12	2.23	0.53
1:AAA:363:ALA:HB1	8:AAA:618:EDO:H22	1.91	0.53
1:AAA:512:ASP:O	1:AAA:515:THR:HG22	2.09	0.53
1:AAA:41:LYS:CD	1:AAA:45:GLU:OE1	2.56	0.52
1:AAA:257:ARG:HD2	5:AAA:607:PG4:C4	2.41	0.51
1:AAA:365:ASP:H	8:AAA:618:EDO:C1	2.24	0.51
1:AAA:138:TYR:O	1:AAA:142:ILE:HG12	2.11	0.51
1:AAA:211:PHE:CE2	1:AAA:242:HIS:CD2	2.99	0.50
1:AAA:148:TYR:HB3	4:AAA:606:PGE:H5	1.93	0.50
1:AAA:425:GLU:OE1	1:AAA:429:ASN:ND2	2.44	0.50
1:AAA:388:ILE:HG13	6:AAA:609:MYR:H62	1.92	0.50
1:AAA:422:THR:O	1:AAA:426:VAL:HG23	2.12	0.50
1:AAA:408:LEU:HD13	1:AAA:427:SER:HB2	1.95	0.49
1:AAA:457:LEU:HD12	7:AAA:615:MPD:HM2	1.94	0.49
1:AAA:543:GLN:HB3	1:AAA:583:LEU:HD23	1.96	0.47
1:AAA:415:VAL:O	1:AAA:415:VAL:HG23	2.14	0.47
1:AAA:148:TYR:HB3	4:AAA:606:PGE:C5	2.45	0.47
1:AAA:131:GLU:OE1	1:AAA:162:LYS:NZ	2.47	0.47
4:AAA:606:PGE:C1	4:AAA:606:PGE:C4	2.93	0.46
1:AAA:95:GLU:HA	1:AAA:95:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:388:ILE:HD11	1:AAA:446:MET:HG3	1.96	0.46
1:AAA:251:LEU:H	7:AAA:612:MPD:C1	2.28	0.46
1:AAA:420:THR:N	1:AAA:421:PRO:CD	2.79	0.45
1:AAA:573:LYS:HE3	1:AAA:573:LYS:HA	1.98	0.45
1:AAA:515:THR:O	1:AAA:515:THR:HG23	2.15	0.45
1:AAA:363:ALA:HB1	8:AAA:618:EDO:H11	1.97	0.45
1:AAA:387:LEU:HD13	1:AAA:391:ASN:ND2	2.32	0.44
1:AAA:66:LEU:HD23	1:AAA:66:LEU:HA	1.83	0.44
1:AAA:398:LEU:HB3	1:AAA:402:LYS:HB2	1.98	0.43
1:AAA:499:PRO:HB3	1:AAA:535:HIS:O	2.18	0.43
1:AAA:401:TYR:CE1	1:AAA:522:GLN:HG2	2.54	0.43
1:AAA:73:LYS:O	1:AAA:76:THR:HB	2.19	0.42
7:AAA:612:MPD:O4	7:AAA:612:MPD:H12	2.18	0.42
1:AAA:363:ALA:C	8:AAA:618:EDO:H11	2.39	0.42
1:AAA:364:ALA:CB	8:AAA:618:EDO:H12	2.44	0.42
1:AAA:356:THR:HG21	1:AAA:373:VAL:CG2	2.50	0.42
1:AAA:387:LEU:HD21	9:AAA:767:HOH:O	2.20	0.42
1:AAA:488:PHE:HB3	2:AAA:601:8PF:F17	2.09	0.42
1:AAA:156:PHE:CZ	1:AAA:160:ARG:HD2	2.55	0.42
1:AAA:185:LEU:HD12	1:AAA:185:LEU:HA	1.91	0.41
1:AAA:127:PHE:CE1	1:AAA:131:GLU:HG3	2.56	0.41
6:AAA:609:MYR:H132	6:AAA:609:MYR:H82	2.02	0.41
1:AAA:387:LEU:CD1	1:AAA:391:ASN:ND2	2.84	0.41
1:AAA:10:ARG:HD2	1:AAA:10:ARG:HA	1.87	0.41
1:AAA:115:LEU:HD12	1:AAA:115:LEU:HA	1.85	0.41
1:AAA:320:ALA:HB2	9:AAA:716:HOH:O	2.20	0.41
1:AAA:42:LEU:HD22	1:AAA:73:LYS:HD3	2.02	0.41
1:AAA:196:GLN:HB3	4:AAA:606:PGE:C6	2.50	0.41
1:AAA:100:GLU:O	1:AAA:104:GLN:HG2	2.21	0.41
1:AAA:117:ARG:NH2	6:AAA:611:MYR:O1	2.53	0.41
2:AAA:603:8PF:F17	2:AAA:603:8PF:F11	2.19	0.41
1:AAA:331:LEU:HD23	1:AAA:331:LEU:HA	1.91	0.40
1:AAA:472:ARG:NH2	1:AAA:492:GLU:O	2.54	0.40
1:AAA:327:LEU:HD11	1:AAA:354:GLU:HG3	2.03	0.40
1:AAA:378:LYS:HB3	1:AAA:379:PRO:CD	2.51	0.40
1:AAA:195:LYS:HE2	1:AAA:451:ASP:OD1	2.22	0.40
1:AAA:216:VAL:HG22	1:AAA:235:VAL:HG21	2.04	0.40
1:AAA:173:ASP:OD2	1:AAA:176:ALA:HB2	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	AAA	582/584 (100%)	559 (96%)	21 (4%)	2 (0%)	41	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	517	SER
1	AAA	85	GLY

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	AAA	512/510 (100%)	487 (95%)	25 (5%)	25	23

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	10	ARG
1	AAA	14	LEU
1	AAA	37[A]	GLU
1	AAA	37[B]	GLU
1	AAA	60	GLU
1	AAA	76	THR
1	AAA	185	LEU
1	AAA	277	GLU
1	AAA	283	LEU

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Mol	Chain	Res	Type
1	AAA	294	GLU
1	AAA	301	ASP
1	AAA	331	LEU
1	AAA	334	TYR
1	AAA	387	LEU
1	AAA	402	LYS
1	AAA	408	LEU
1	AAA	425	GLU
1	AAA	436	LYS
1	AAA	439	LYS
1	AAA	459	GLN
1	AAA	469	VAL
1	AAA	515	THR
1	AAA	560	LYS
1	AAA	565	GLU
1	AAA	566	THR

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

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MPO	AAA	605	-	13,13,13	0.62	1 (7%)	17,17,17	1.90	3 (17%)
2	8PF	AAA	604	-	21,24,24	0.67	0	40,45,45	1.62	8 (20%)
2	8PF	AAA	601	-	21,24,24	0.94	0	40,45,45	0.86	2 (5%)
5	PG4	AAA	607	-	12,12,12	0.15	0	11,11,11	0.13	0
7	MPD	AAA	616	-	7,7,7	0.21	0	9,10,10	0.63	0
6	MYR	AAA	611	-	12,15,15	0.30	0	11,15,15	0.20	0
6	MYR	AAA	610	-	12,15,15	0.21	0	11,15,15	0.22	0
7	MPD	AAA	615	-	7,7,7	0.24	0	9,10,10	0.56	0
8	EDO	AAA	618	-	3,3,3	0.27	0	2,2,2	0.95	0
7	MPD	AAA	614	-	7,7,7	0.27	0	9,10,10	0.47	0
2	8PF	AAA	603	-	21,24,24	0.55	0	40,45,45	1.50	7 (17%)
7	MPD	AAA	612	-	7,7,7	0.28	0	9,10,10	0.84	0
7	MPD	AAA	617	-	7,7,7	0.31	0	9,10,10	0.51	0
2	8PF	AAA	602	-	21,24,24	0.59	0	40,45,45	1.15	2 (5%)
4	PGE	AAA	606	-	9,9,9	0.25	0	8,8,8	0.17	0
6	MYR	AAA	609	-	12,15,15	0.24	0	11,15,15	0.19	0
6	MYR	AAA	608	-	12,15,15	0.25	0	11,15,15	0.20	0
7	MPD	AAA	613	-	7,7,7	0.13	0	9,10,10	0.49	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	MPO	AAA	605	-	-	7/7/15/15	0/1/1/1
2	8PF	AAA	604	-	-	23/54/60/60	-
2	8PF	AAA	601	-	-	17/54/60/60	-
5	PG4	AAA	607	-	-	7/10/10/10	-
7	MPD	AAA	616	-	-	1/5/5/5	-
6	MYR	AAA	611	-	-	5/11/13/13	-
6	MYR	AAA	610	-	-	8/11/13/13	-
7	MPD	AAA	615	-	-	2/5/5/5	-
8	EDO	AAA	618	-	-	1/1/1/1	-
7	MPD	AAA	614	-	-	1/5/5/5	-
2	8PF	AAA	603	-	-	27/54/60/60	-
7	MPD	AAA	612	-	-	3/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MPD	AAA	617	-	-	2/5/5/5	-
2	8PF	AAA	602	-	-	16/54/60/60	-
4	PGE	AAA	606	-	-	3/7/7/7	-
6	MYR	AAA	609	-	-	8/11/13/13	-
6	MYR	AAA	608	-	-	5/11/13/13	-
7	MPD	AAA	613	-	-	0/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	605	MPO	O3-S1	2.09	1.55	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	605	MPO	C3-N1-C7	4.91	123.79	111.23
3	AAA	605	MPO	C3-N1-C4	4.51	122.76	111.23
2	AAA	602	8PF	F06-C04-F05	4.31	114.71	106.15
2	AAA	604	8PF	F06-C04-C02	-4.16	100.22	107.25
2	AAA	604	8PF	C04-C02-C10	-4.14	107.81	116.84
2	AAA	603	8PF	F25-C22-F24	3.35	117.77	107.53
2	AAA	603	8PF	F05-C04-C02	3.19	112.65	107.25
2	AAA	603	8PF	C02-C04-C07	-3.12	106.29	114.29
2	AAA	604	8PF	F05-C04-C02	2.89	112.13	107.25
2	AAA	603	8PF	F03-C02-F01	2.78	119.33	107.27
3	AAA	605	MPO	O3-S1-C1	-2.71	101.39	105.77
2	AAA	603	8PF	F01-C02-C04	-2.55	102.96	108.20
2	AAA	604	8PF	C02-C04-C07	2.55	120.84	114.29
2	AAA	603	8PF	F14-C13-C10	2.47	117.76	108.01
2	AAA	604	8PF	F01-C02-C10	2.43	117.59	108.01
2	AAA	604	8PF	F21-C19-C22	2.33	116.78	106.63
2	AAA	604	8PF	F24-C22-F23	-2.16	100.93	107.53
2	AAA	602	8PF	C04-C02-C10	-2.14	112.17	116.84
2	AAA	601	8PF	F15-C13-C10	-2.08	99.83	108.01
2	AAA	603	8PF	F21-C19-C22	-2.05	97.71	106.63
2	AAA	604	8PF	F25-C22-C19	-2.02	101.01	110.34
2	AAA	601	8PF	F01-C02-C04	-2.02	104.06	108.20

There are no chirality outliers.

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	601	8PF	C10-C02-C04-F06
2	AAA	601	8PF	C10-C02-C04-C07
2	AAA	601	8PF	F01-C02-C04-C07
2	AAA	602	8PF	F03-C02-C04-C07
2	AAA	603	8PF	C13-C16-C19-C22
2	AAA	603	8PF	C10-C02-C04-F06
2	AAA	603	8PF	C10-C02-C04-C07
3	AAA	605	MPO	C2-C1-S1-O1
3	AAA	605	MPO	C2-C1-S1-O2
3	AAA	605	MPO	C1-C2-C3-N1
7	AAA	612	MPD	C1-C2-C3-C4
7	AAA	616	MPD	C2-C3-C4-O4
2	AAA	603	8PF	F17-C16-C19-C22
2	AAA	602	8PF	F01-C02-C04-F05
2	AAA	603	8PF	C13-C16-C19-F21
5	AAA	607	PG4	O1-C1-C2-O2
2	AAA	602	8PF	C04-C02-C10-C13
2	AAA	603	8PF	C02-C10-C13-C16
2	AAA	604	8PF	F18-C16-C19-F20
3	AAA	605	MPO	C2-C3-N1-C7
4	AAA	606	PGE	O2-C3-C4-O3
2	AAA	603	8PF	F12-C10-C13-F14
5	AAA	607	PG4	O3-C5-C6-O4
2	AAA	602	8PF	F03-C02-C10-F11
3	AAA	605	MPO	C2-C1-S1-O3
2	AAA	603	8PF	F12-C10-C13-C16
5	AAA	607	PG4	O2-C3-C4-O3
2	AAA	604	8PF	F17-C16-C19-F21
2	AAA	603	8PF	F03-C02-C10-F11
2	AAA	604	8PF	F18-C16-C19-F21
2	AAA	604	8PF	F01-C02-C10-F12
2	AAA	604	8PF	C13-C16-C19-F20
5	AAA	607	PG4	O4-C7-C8-O5
2	AAA	601	8PF	F15-C13-C16-F17
2	AAA	602	8PF	F03-C02-C10-C13
3	AAA	605	MPO	C2-C3-N1-C4
2	AAA	604	8PF	F17-C16-C19-F20
2	AAA	601	8PF	F03-C02-C04-C07
2	AAA	602	8PF	F01-C02-C04-C07
2	AAA	603	8PF	F01-C02-C04-C07
2	AAA	603	8PF	F03-C02-C04-C07
2	AAA	602	8PF	C04-C02-C10-F11
2	AAA	603	8PF	F12-C10-C13-F15

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Mol	Chain	Res	Type	Atoms
2	AAA	604	8PF	F21-C19-C22-F25
6	AAA	611	MYR	C3-C4-C5-C6
2	AAA	603	8PF	C02-C10-C13-F14
2	AAA	604	8PF	C13-C16-C19-F21
6	AAA	611	MYR	C11-C10-C9-C8
6	AAA	608	MYR	C2-C3-C4-C5
6	AAA	610	MYR	C9-C10-C11-C12
2	AAA	604	8PF	F18-C16-C19-C22
2	AAA	604	8PF	C04-C02-C10-C13
2	AAA	602	8PF	F03-C02-C10-F12
2	AAA	601	8PF	F15-C13-C16-F18
2	AAA	604	8PF	F17-C16-C19-C22
2	AAA	604	8PF	C04-C02-C10-F12
6	AAA	609	MYR	C2-C3-C4-C5
6	AAA	610	MYR	C10-C11-C12-C13
2	AAA	604	8PF	F01-C02-C10-F11
2	AAA	603	8PF	F03-C02-C10-F12
6	AAA	609	MYR	C11-C10-C9-C8
6	AAA	610	MYR	C6-C7-C8-C9
2	AAA	604	8PF	F03-C02-C10-F11
2	AAA	601	8PF	C10-C02-C04-F05
2	AAA	604	8PF	F03-C02-C10-F12
2	AAA	602	8PF	F01-C02-C10-F11
2	AAA	603	8PF	F18-C16-C19-F20
6	AAA	609	MYR	C6-C7-C8-C9
6	AAA	608	MYR	C9-C10-C11-C12
2	AAA	601	8PF	F15-C13-C16-C19
2	AAA	603	8PF	F11-C10-C13-F14
2	AAA	604	8PF	C13-C16-C19-C22
2	AAA	601	8PF	F14-C13-C16-F18
6	AAA	611	MYR	C4-C5-C6-C7
2	AAA	603	8PF	F03-C02-C10-C13
6	AAA	608	MYR	C10-C11-C12-C13
2	AAA	604	8PF	F21-C19-C22-F24
6	AAA	609	MYR	C11-C12-C13-C14
2	AAA	604	8PF	C04-C02-C10-F11
2	AAA	603	8PF	F17-C16-C19-F20
4	AAA	606	PGE	C1-C2-O2-C3
2	AAA	602	8PF	F03-C02-C04-F05
6	AAA	610	MYR	C5-C6-C7-C8
2	AAA	602	8PF	C04-C02-C10-F12
2	AAA	603	8PF	F17-C16-C19-F21

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Mol	Chain	Res	Type	Atoms
6	AAA	611	MYR	C11-C12-C13-C14
6	AAA	609	MYR	C3-C4-C5-C6
2	AAA	602	8PF	F01-C02-C10-C13
2	AAA	603	8PF	C02-C10-C13-F15
2	AAA	601	8PF	F01-C02-C04-F05
2	AAA	604	8PF	F21-C19-C22-F23
2	AAA	603	8PF	F18-C16-C19-C22
2	AAA	601	8PF	F14-C13-C16-F17
2	AAA	601	8PF	F03-C02-C04-F05
2	AAA	604	8PF	F20-C19-C22-F25
7	AAA	612	MPD	O2-C2-C3-C4
7	AAA	617	MPD	O2-C2-C3-C4
2	AAA	603	8PF	F11-C10-C13-C16
2	AAA	601	8PF	C10-C13-C16-C19
5	AAA	607	PG4	C5-C6-O4-C7
2	AAA	603	8PF	C13-C16-C19-F20
2	AAA	602	8PF	F01-C02-C10-F12
2	AAA	603	8PF	F11-C10-C13-F15
2	AAA	604	8PF	F01-C02-C10-C13
6	AAA	610	MYR	C3-C4-C5-C6
5	AAA	607	PG4	C6-C5-O3-C4
5	AAA	607	PG4	C8-C7-O4-C6
6	AAA	610	MYR	C11-C12-C13-C14
7	AAA	617	MPD	C1-C2-C3-C4
2	AAA	602	8PF	F01-C02-C04-F06
6	AAA	609	MYR	C10-C11-C12-C13
2	AAA	601	8PF	F14-C13-C16-C19
2	AAA	603	8PF	C04-C02-C10-F11
2	AAA	601	8PF	F03-C02-C04-F06
2	AAA	602	8PF	F03-C02-C04-F06
2	AAA	601	8PF	C10-C13-C16-F18
6	AAA	610	MYR	C2-C3-C4-C5
8	AAA	618	EDO	O1-C1-C2-O2
6	AAA	608	MYR	C11-C10-C9-C8
2	AAA	604	8PF	F03-C02-C10-C13
2	AAA	601	8PF	C10-C13-C16-F17
3	AAA	605	MPO	S1-C1-C2-C3
6	AAA	608	MYR	C11-C12-C13-C14
2	AAA	603	8PF	C04-C02-C10-C13
2	AAA	604	8PF	C16-C19-C22-F25
2	AAA	603	8PF	C04-C02-C10-F12
6	AAA	609	MYR	C9-C10-C11-C12

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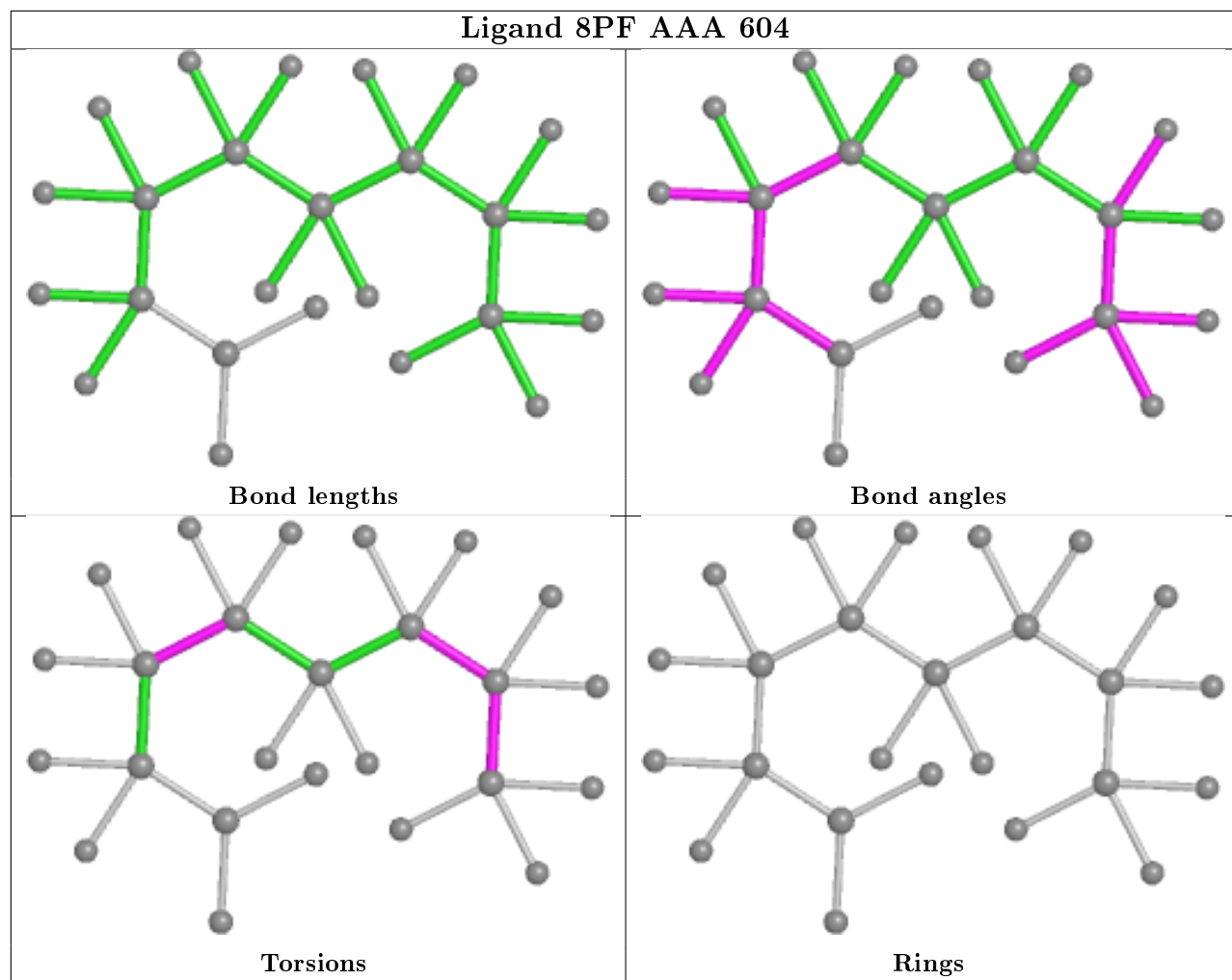
Mol	Chain	Res	Type	Atoms
4	AAA	606	PGE	O1-C1-C2-O2
6	AAA	610	MYR	C1-C2-C3-C4
6	AAA	611	MYR	C1-C2-C3-C4
7	AAA	614	MPD	C2-C3-C4-C5
7	AAA	615	MPD	C2-C3-C4-C5
2	AAA	602	8PF	C10-C02-C04-F05
6	AAA	609	MYR	C4-C5-C6-C7
7	AAA	612	MPD	C2-C3-C4-O4
7	AAA	615	MPD	C2-C3-C4-O4

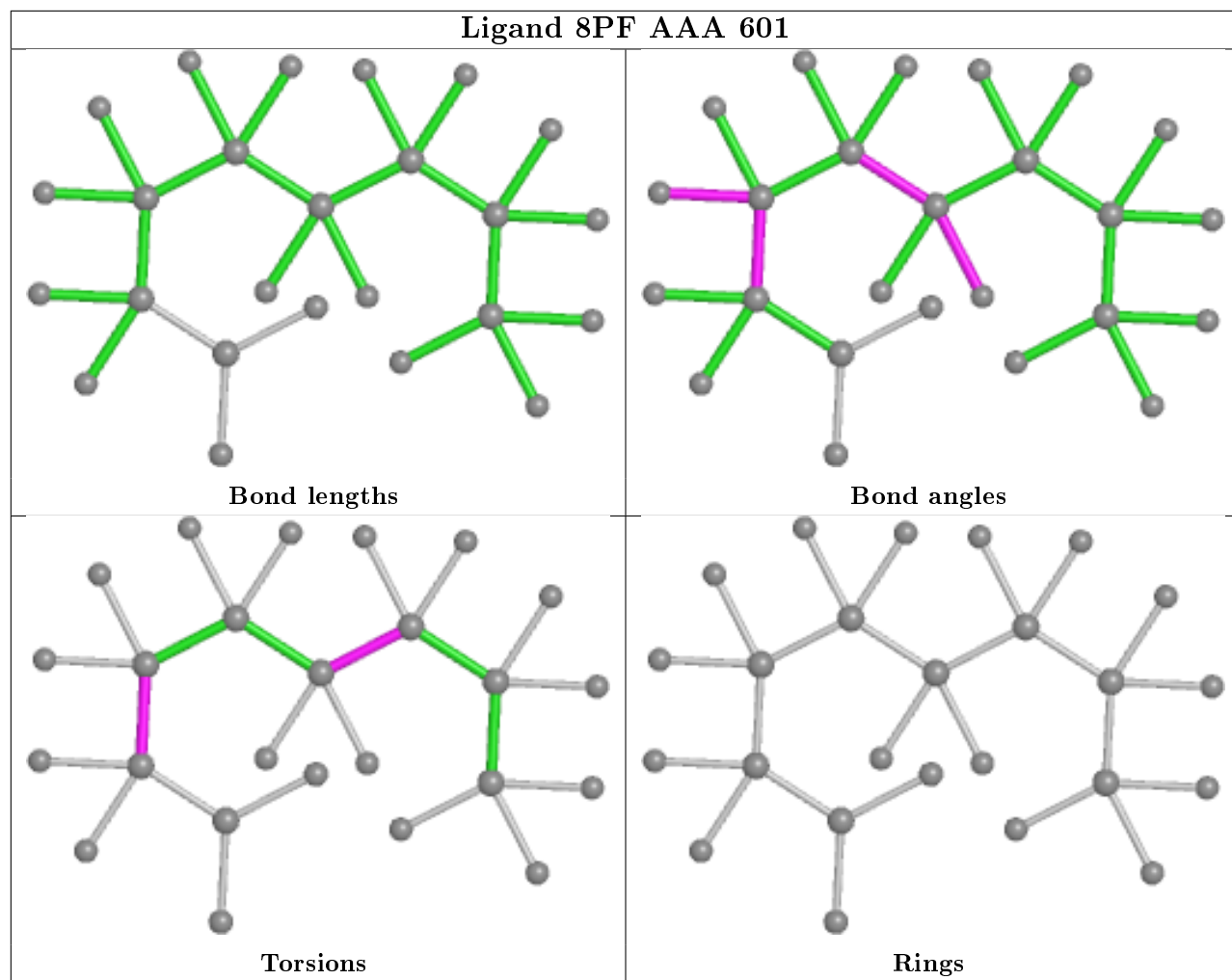
There are no ring outliers.

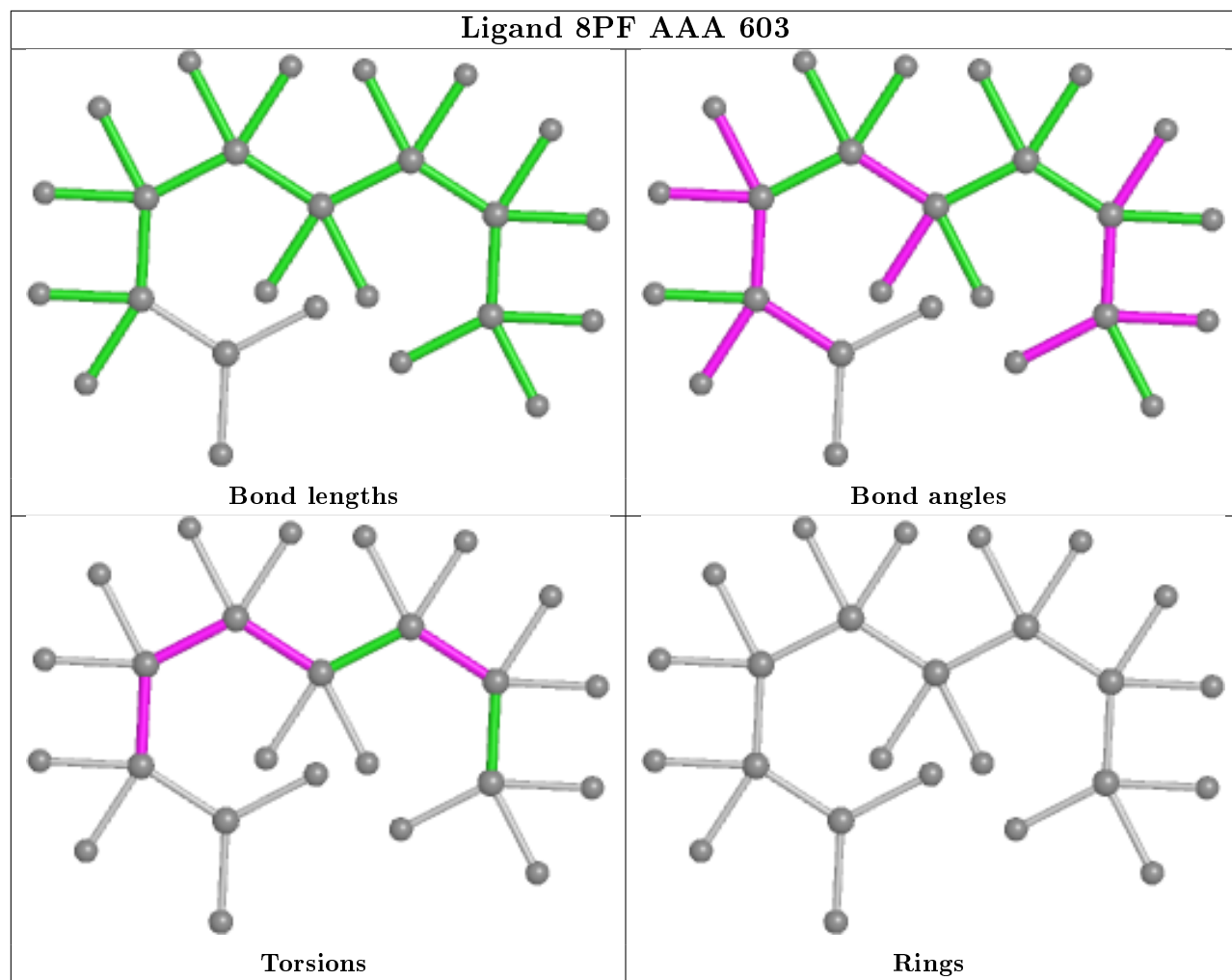
10 monomers are involved in 28 short contacts:

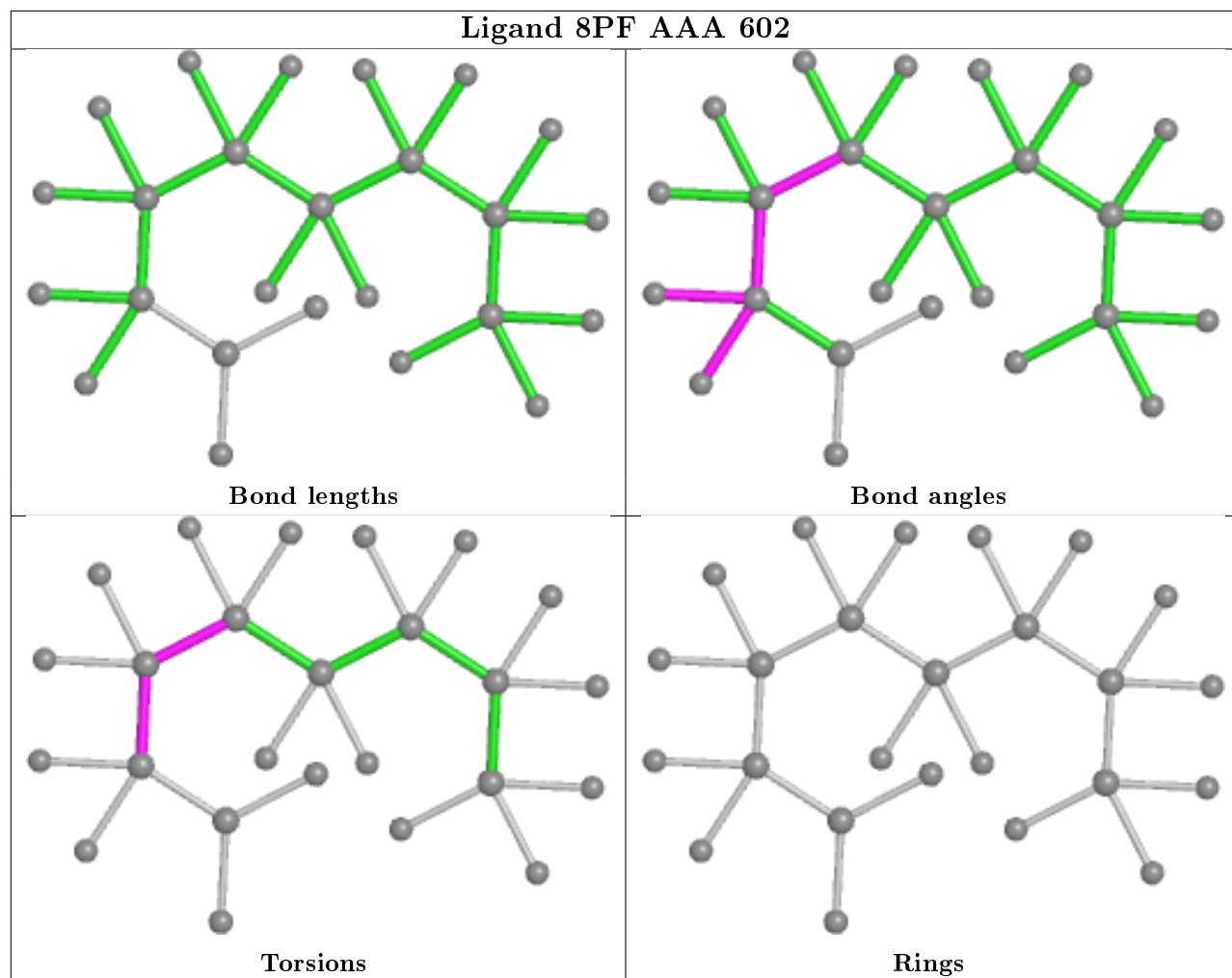
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	601	8PF	1	0
5	AAA	607	PG4	3	0
7	AAA	616	MPD	1	0
6	AAA	611	MYR	1	0
7	AAA	615	MPD	3	0
8	AAA	618	EDO	8	0
2	AAA	603	8PF	1	0
7	AAA	612	MPD	4	0
4	AAA	606	PGE	4	0
6	AAA	609	MYR	2	0

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.









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	AAA	581/584 (99%)	-0.05	11 (1%) 66 71	28, 48, 83, 120	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	553	ALA	3.9
1	AAA	561	ALA	3.5
1	AAA	562	ASP	3.1
1	AAA	575	LEU	3.0
1	AAA	557	LYS	2.8
1	AAA	556	GLU	2.7
1	AAA	579	SER	2.7
1	AAA	578	ALA	2.7
1	AAA	467	THR	2.4
1	AAA	581	ALA	2.3
1	AAA	3	HIS	2.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

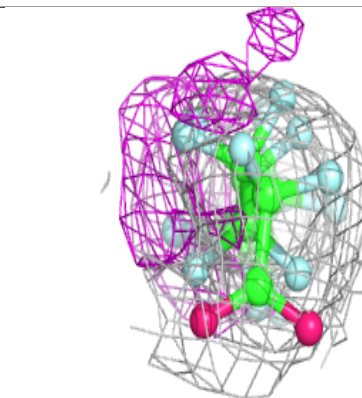
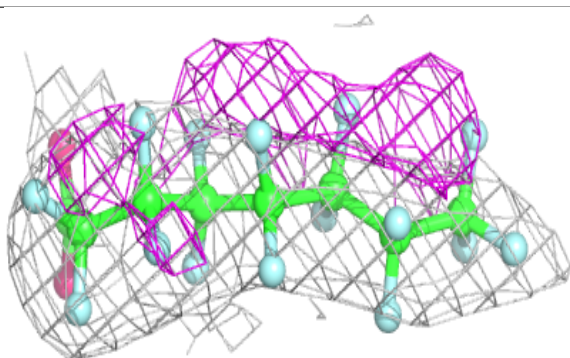
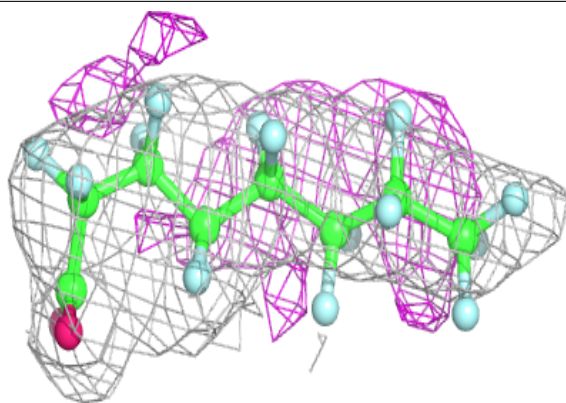
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	EDO	AAA	618	4/4	0.74	0.15	48,51,54,57	0
5	PG4	AAA	607	13/13	0.78	0.20	61,70,79,81	0
3	MPO	AAA	605	13/13	0.79	0.19	72,79,121,128	0
4	PGE	AAA	606	10/10	0.79	0.21	81,91,95,98	0
6	MYR	AAA	610	16/16	0.83	0.24	54,66,96,98	0
6	MYR	AAA	611	16/16	0.86	0.19	45,60,74,75	0
6	MYR	AAA	608	16/16	0.86	0.16	36,53,58,59	0
7	MPD	AAA	616	8/8	0.88	0.29	81,88,94,103	0
2	8PF	AAA	601	25/25	0.89	0.34	57,100,120,144	0
7	MPD	AAA	617	8/8	0.90	0.21	63,64,71,71	0
7	MPD	AAA	613	8/8	0.90	0.16	44,46,49,50	0
7	MPD	AAA	614	8/8	0.93	0.14	41,47,60,72	0
2	8PF	AAA	603	25/25	0.93	0.12	60,76,85,105	0
7	MPD	AAA	615	8/8	0.94	0.22	66,71,78,88	0
2	8PF	AAA	604	25/25	0.94	0.15	65,82,91,104	0
6	MYR	AAA	609	16/16	0.94	0.17	39,59,67,70	0
2	8PF	AAA	602	25/25	0.94	0.12	72,83,98,118	0
7	MPD	AAA	612	8/8	0.95	0.14	32,46,49,51	0

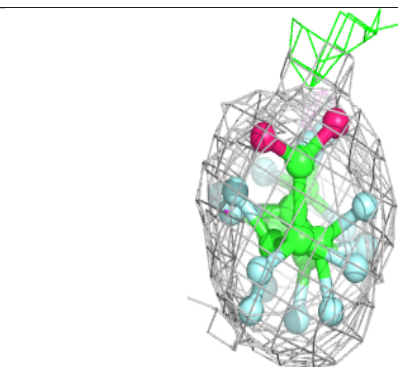
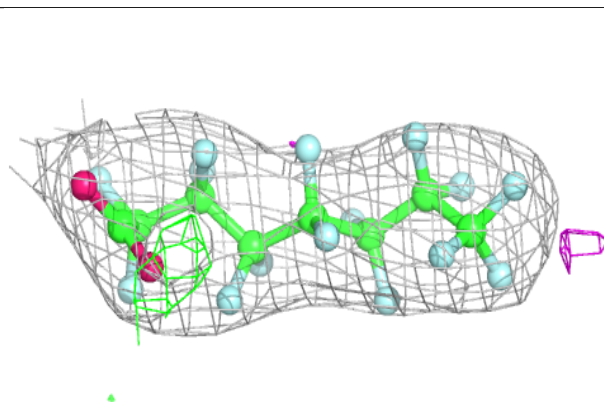
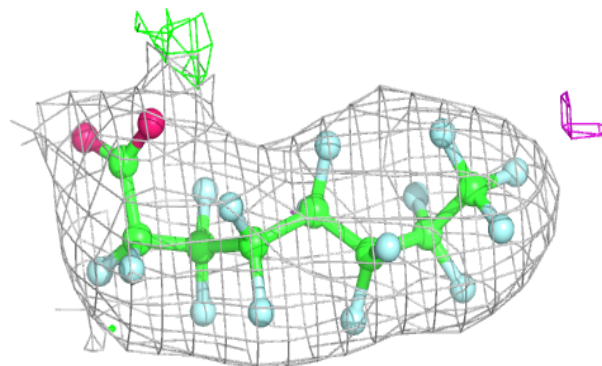
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8PF AAA 601:

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

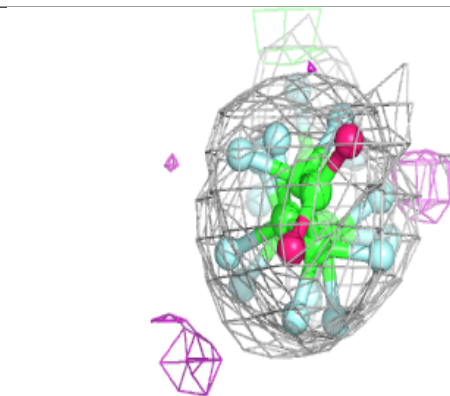
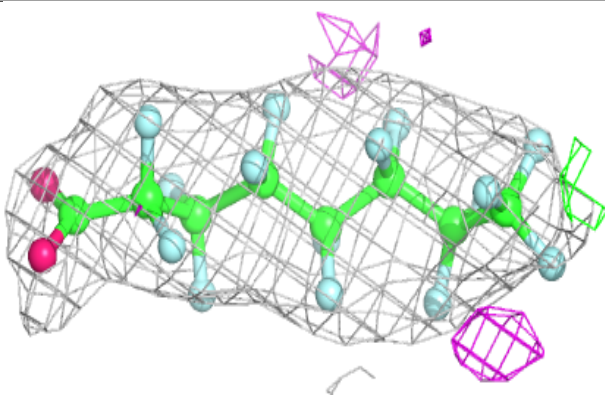
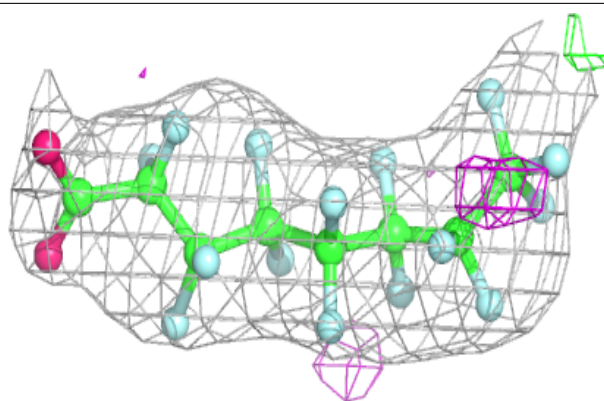
**Electron density around 8PF AAA 603:**

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

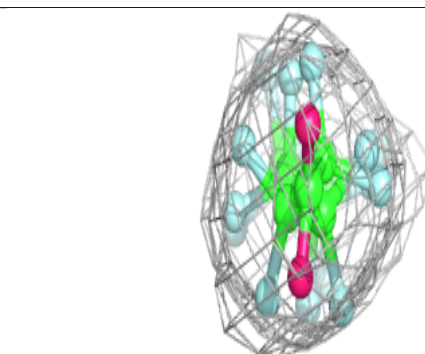
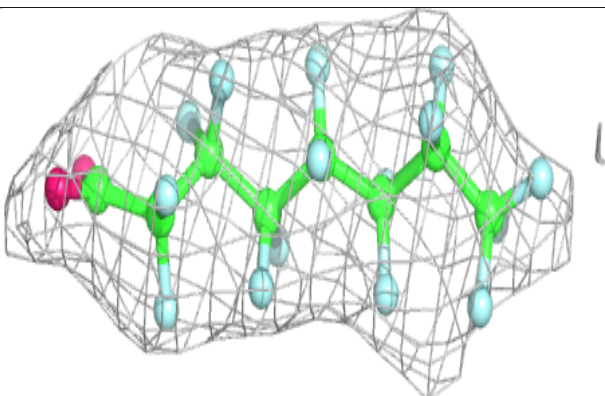
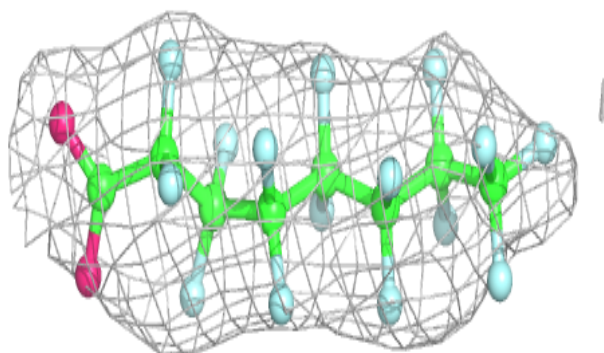


Electron density around 8PF AAA 604:

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

**Electron density around 8PF AAA 602:**

$2mF_o-DF_c$ (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.