



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 12:07 pm BST

PDB ID : 5HSA
Title : Alcohol Oxidase AOX1 from Pichia Pastoris
Authors : Neumann, P.; Ficner, R.; Feussner, I.; Koch, C.
Deposited on : 2016-01-25
Resolution : 2.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.11
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) : 2.11

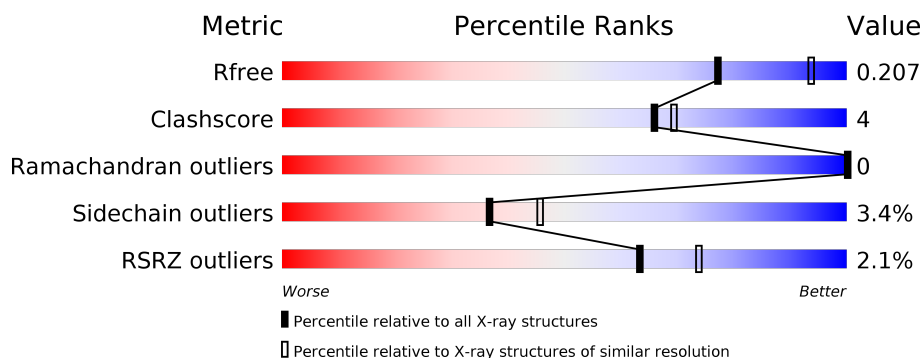
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 on 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	663	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 10%, green 89%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> % 89% 10% • </div> </div>
1	B	663	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 11%, green 88%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 3% 88% 11% • </div> </div>
1	C	663	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, orange 0%, yellow 10%, green 89%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> % 89% 10% • </div> </div>
1	D	663	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 8%, green 90%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 5% 90% 8% • </div> </div>
1	E	663	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 10%, green 89%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> % 89% 10% • </div> </div>
1	F	663	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 9%, green 89%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 2% 89% 9% • </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	663	<div><div>%</div><div><div></div><div>89%</div><div>10%</div></div><div></div></div>
1	H	663	<div><div>4%</div><div><div></div><div>88%</div><div>10%</div></div><div></div></div>

2 Entry composition

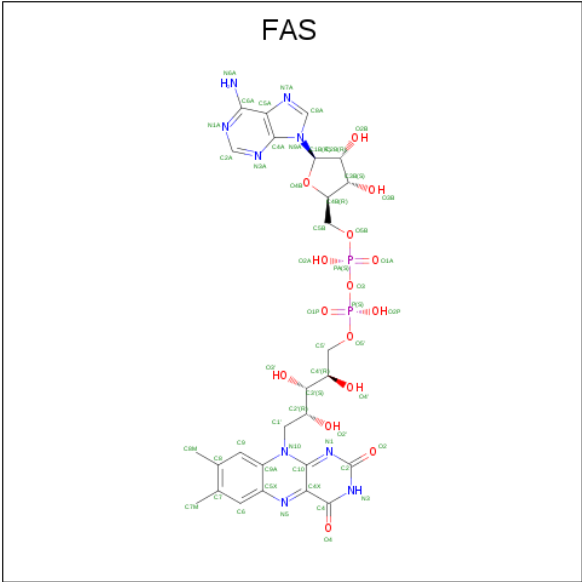
There are 9 unique types of molecules in this entry. The entry contains 44407 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alcohol oxidase 1.

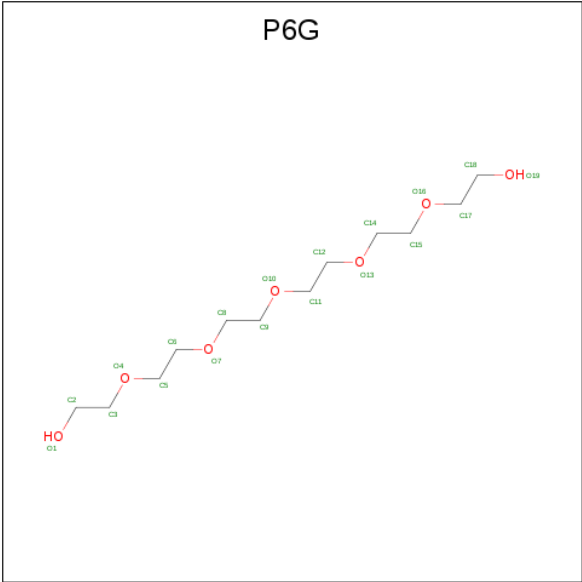
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	B	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	C	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	D	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	E	662	Total	C	N	O	S	0	1	0
			5206	3291	901	988	26			
1	F	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	G	662	Total	C	N	O	S	0	1	0
			5207	3292	901	988	26			
1	H	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			

- Molecule 2 is ARABINO-FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAS) (formula: C₂₇H₃₃N₉O₁₅P₂).



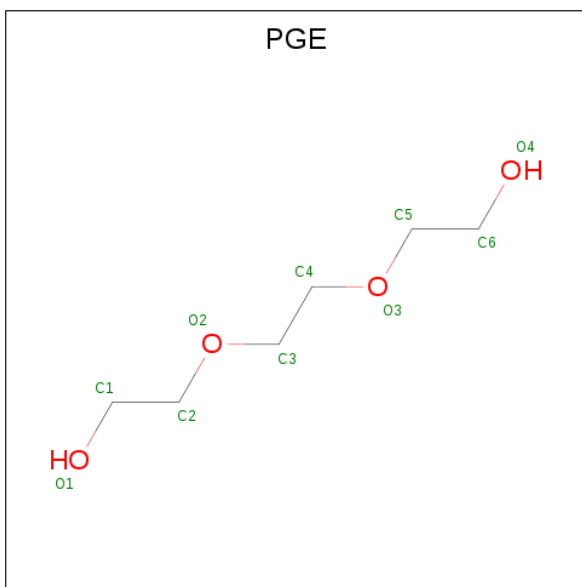
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			19	12	7		
3	B	1	Total	C	O	0	0
			19	12	7		
3	B	1	Total	C	O	0	0
			19	12	7		
3	C	1	Total	C	O	0	0
			19	12	7		
3	C	1	Total	C	O	0	0
			19	12	7		
3	D	1	Total	C	O	0	0
			19	12	7		
3	E	1	Total	C	O	0	0
			19	12	7		
3	F	1	Total	C	O	0	0
			19	12	7		
3	F	1	Total	C	O	0	0
			19	12	7		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		
4	E	1	Total	C	O	0	0
			10	6	4		
4	G	1	Total	C	O	0	0
			10	6	4		
4	G	1	Total	C	O	0	0
			10	6	4		
4	H	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	1
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		
6	E	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		
6	C	2	Total	Ca	0	0
			2	2		
6	A	1	Total	Ca	0	0
			1	1		
6	F	1	Total	Ca	0	0
			1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	1
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Cl	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	358	Total	O	0	2
			359	359		
9	B	226	Total	O	0	1
			226	226		
9	C	325	Total	O	0	3
			325	325		
9	D	178	Total	O	0	2
			178	178		
9	E	356	Total	O	0	0
			356	356		
9	F	300	Total	O	0	0
			300	300		

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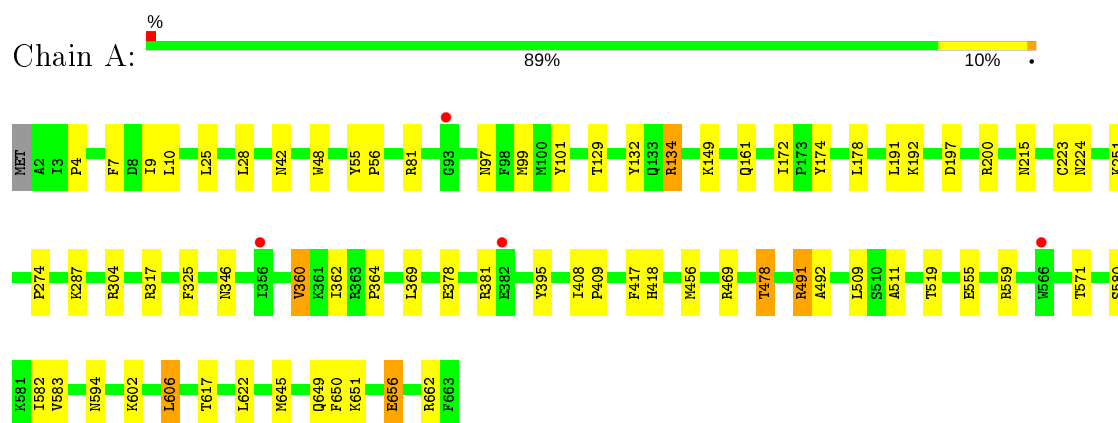
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	211	Total 211	O 211	0	0
9	H	129	Total 129	O 129	0	0

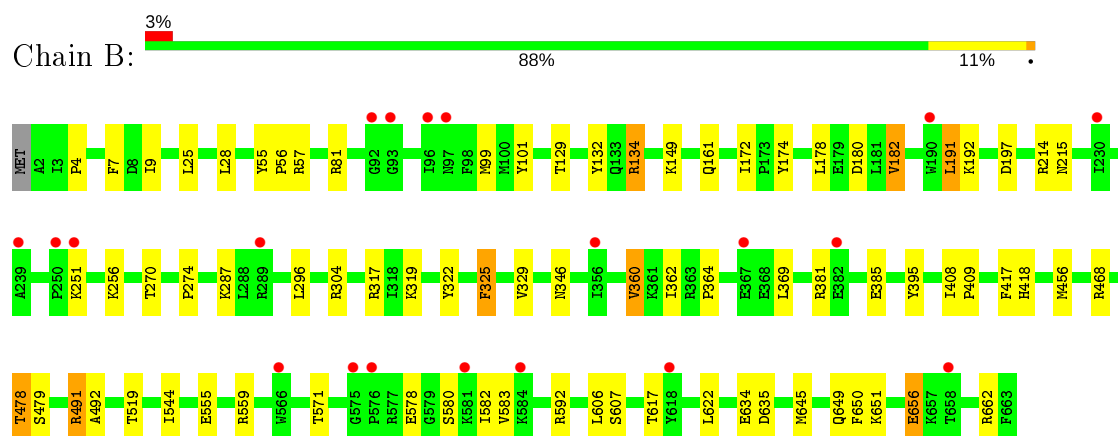
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

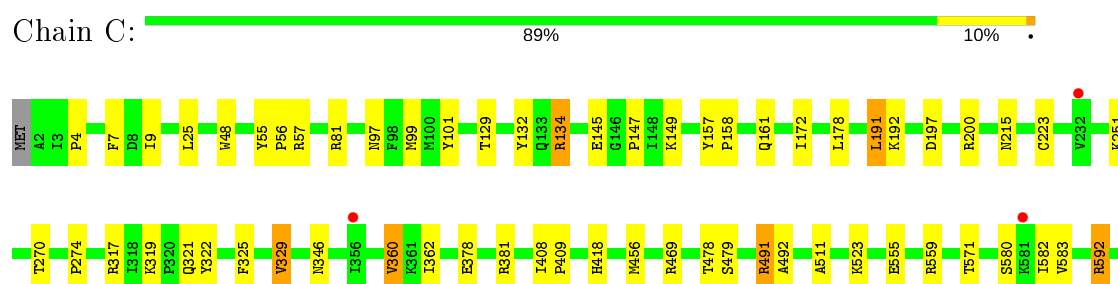
• Molecule 1: Alcohol oxidase 1



• Molecule 1: Alcohol oxidase 1

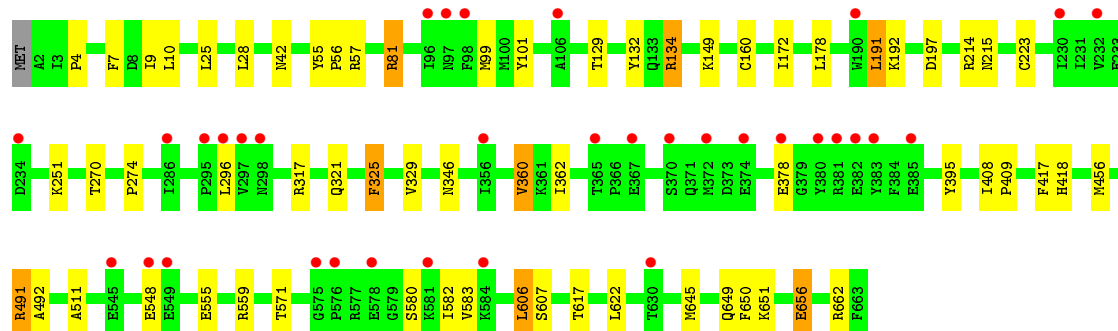
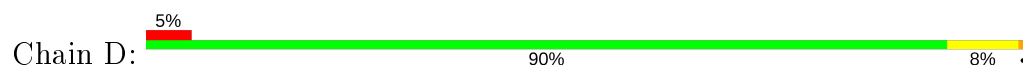


• Molecule 1: Alcohol oxidase 1

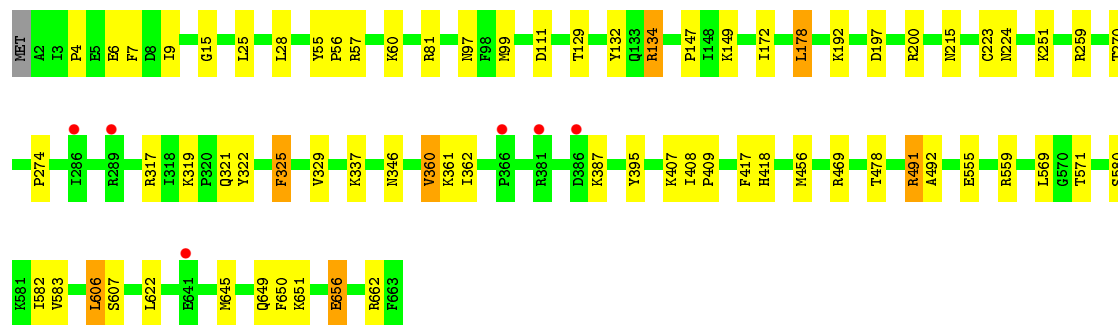
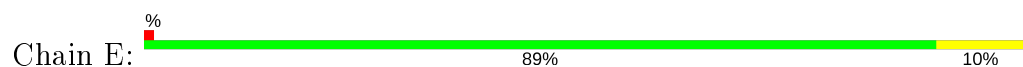




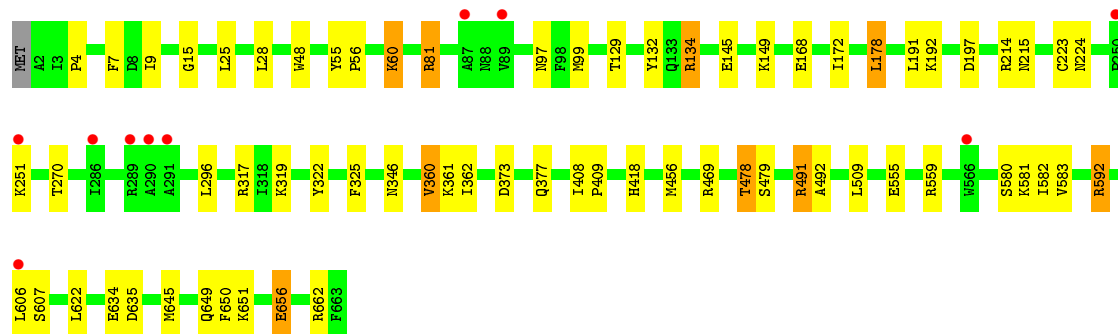
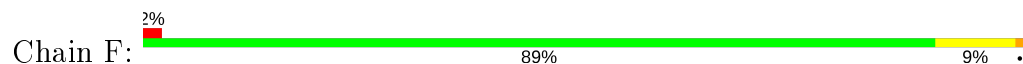
• Molecule 1: Alcohol oxidase 1



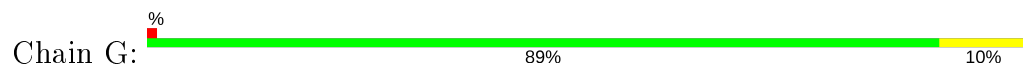
• Molecule 1: Alcohol oxidase 1

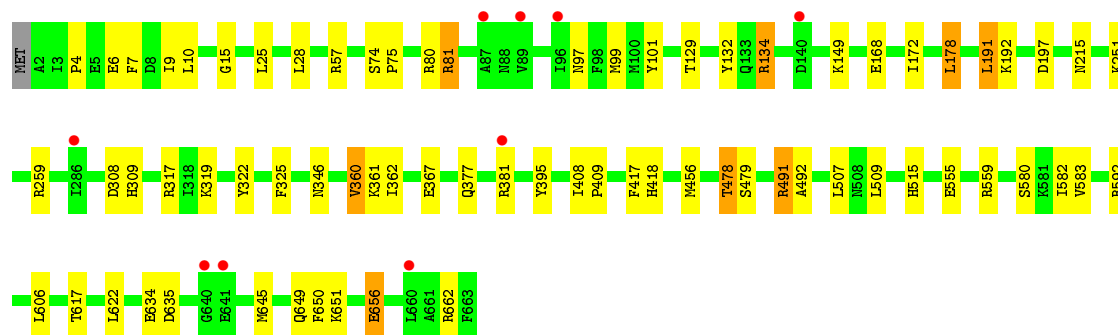


• Molecule 1: Alcohol oxidase 1

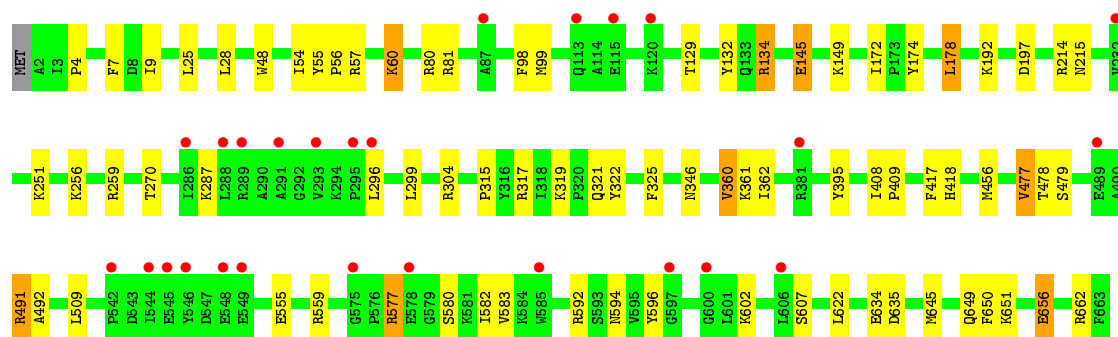
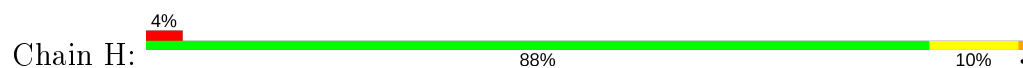


• Molecule 1: Alcohol oxidase 1





• Molecule 1: Alcohol oxidase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.10Å 165.19Å 164.31Å 90.00° 95.67° 90.00°	Depositor
Resolution (Å)	40.88 – 2.35 45.67 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.88-2.35) 98.7 (45.67-2.35)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.9.162	Depositor
R, R_{free}	0.177 , 0.205 0.182 , 0.207	Depositor DCC
R_{free} test set	12283 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	44407	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: GOL, PGE, CL, FAS, PO4, P6G, CA

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	0.29	0/5341	0.46	0/7245
1	B	0.27	0/5341	0.46	0/7245
1	C	0.29	0/5341	0.47	0/7245
1	D	0.26	0/5341	0.45	0/7245
1	E	0.30	0/5348	0.47	0/7255
1	F	0.28	0/5341	0.46	0/7245
1	G	0.27	0/5349	0.46	0/7256
1	H	0.26	0/5341	0.45	0/7245
All	All	0.28	0/42743	0.46	0/57981

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5199	0	5013	45	0
1	B	5199	0	5013	43	0
1	C	5199	0	5013	50	0
1	D	5199	0	5013	36	0
1	E	5206	0	5021	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	5199	0	5013	45	0
1	G	5207	0	5023	45	0
1	H	5199	0	5013	47	0
2	A	53	0	31	2	0
2	B	53	0	31	0	0
2	C	53	0	31	2	0
2	D	53	0	31	1	0
2	E	53	0	31	3	0
2	F	53	0	31	3	0
2	G	53	0	31	3	0
2	H	53	0	31	1	0
3	A	19	0	26	1	0
3	B	38	0	52	10	0
3	C	38	0	52	13	0
3	D	19	0	26	1	0
3	E	19	0	26	4	0
3	F	38	0	52	8	0
4	A	10	0	14	2	0
4	B	20	0	28	1	0
4	C	10	0	14	1	0
4	D	10	0	14	0	0
4	E	10	0	14	0	0
4	G	20	0	28	0	0
4	H	10	0	14	1	0
5	A	5	0	0	1	0
5	F	5	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
7	C	6	0	8	0	0
7	F	6	0	8	2	0
8	C	1	0	0	0	0
9	A	359	0	0	3	0
9	B	226	0	0	2	0
9	C	325	0	0	4	0
9	D	178	0	0	3	0
9	E	356	0	0	3	0
9	F	300	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	G	211	0	0	0	0
9	H	129	0	0	1	0
All	All	44407	0	40746	334	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 4.

The worst 5 of 334 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:223:CYS:H	3:B:702:P6G:H62	1.36	0.89
3:C:703:P6G:H111	1:D:42:ASN:HD22	1.48	0.77
1:C:479:SER:HB2	3:F:702:P6G:H62	1.66	0.75
1:C:649:GLN:NE2	1:C:651:LYS:HG2	2.03	0.73
5:F:704:PO4:O3	9:F:801:HOH:O	2.08	0.71

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	660/663 (100%)	637 (96%)	23 (4%)	0	100	100
1	B	660/663 (100%)	635 (96%)	25 (4%)	0	100	100
1	C	660/663 (100%)	638 (97%)	22 (3%)	0	100	100
1	D	660/663 (100%)	638 (97%)	22 (3%)	0	100	100
1	E	661/663 (100%)	639 (97%)	22 (3%)	0	100	100
1	F	660/663 (100%)	638 (97%)	22 (3%)	0	100	100
1	G	661/663 (100%)	639 (97%)	22 (3%)	0	100	100
1	H	660/663 (100%)	638 (97%)	22 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5282/5304 (100%)	5102 (97%)	180 (3%)	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	560/561 (100%)	545 (97%)	15 (3%)	44	55
1	B	560/561 (100%)	541 (97%)	19 (3%)	37	46
1	C	560/561 (100%)	538 (96%)	22 (4%)	32	40
1	D	560/561 (100%)	540 (96%)	20 (4%)	35	43
1	E	561/561 (100%)	544 (97%)	17 (3%)	41	50
1	F	560/561 (100%)	540 (96%)	20 (4%)	35	43
1	G	561/561 (100%)	544 (97%)	17 (3%)	41	50
1	H	560/561 (100%)	539 (96%)	21 (4%)	33	41
All	All	4482/4488 (100%)	4331 (97%)	151 (3%)	37	46

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	378	GLU
1	E	325	PHE
1	H	317	ARG
1	D	456	MET
1	E	57	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	215	ASN
1	F	556	ASN

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Mol	Chain	Res	Type
1	G	321	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 9 are monoatomic - leaving 30 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$
7	GOL	C	705[B]	6	5,5,5	0.37	0	5,5,5	0.29	0
2	FAS	F	701	-	51,58,58	1.88	6 (11%)	60,89,89	2.07	12 (20%)
2	FAS	D	701	-	51,58,58	1.85	6 (11%)	60,89,89	1.99	10 (16%)
2	FAS	A	701	-	51,58,58	1.89	6 (11%)	60,89,89	1.99	12 (20%)
3	P6G	D	702	-	18,18,18	0.47	0	17,17,17	0.30	0
3	P6G	E	702	-	18,18,18	0.48	0	17,17,17	0.40	0
4	PGE	B	704	-	9,9,9	0.32	0	8,8,8	0.29	0
5	PO4	F	704	-	4,4,4	0.80	0	6,6,6	0.38	0
3	P6G	F	703	-	18,18,18	0.46	0	17,17,17	0.38	0
2	FAS	C	701	-	51,58,58	1.85	6 (11%)	60,89,89	1.97	11 (18%)
4	PGE	G	703	-	9,9,9	0.33	0	8,8,8	0.25	0
3	P6G	F	702	-	18,18,18	0.45	0	17,17,17	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	P6G	C	703	-	18,18,18	0.50	0	17,17,17	0.47	0
4	PGE	G	702	-	9,9,9	0.33	0	8,8,8	0.22	0
2	FAS	E	701	-	51,58,58	1.92	6 (11%)	60,89,89	1.94	11 (18%)
4	PGE	E	703	-	9,9,9	0.37	0	8,8,8	0.23	0
2	FAS	H	701	-	51,58,58	1.89	5 (9%)	60,89,89	2.00	12 (20%)
3	P6G	C	702	-	18,18,18	0.45	0	17,17,17	0.42	0
4	PGE	B	705	-	9,9,9	0.32	0	8,8,8	0.28	0
3	P6G	A	702	-	18,18,18	0.46	0	17,17,17	0.38	0
3	P6G	B	703	-	18,18,18	0.44	0	17,17,17	0.51	0
4	PGE	D	703	-	9,9,9	0.32	0	8,8,8	0.29	0
7	GOL	F	705	-	5,5,5	0.36	0	5,5,5	0.27	0
4	PGE	A	703	-	9,9,9	0.31	0	8,8,8	0.34	0
4	PGE	C	704	-	9,9,9	0.37	0	8,8,8	0.21	0
2	FAS	B	701	-	51,58,58	1.86	6 (11%)	60,89,89	2.04	12 (20%)
5	PO4	A	704[B]	-	4,4,4	1.02	0	6,6,6	0.57	0
4	PGE	H	702	-	9,9,9	0.32	0	8,8,8	0.25	0
2	FAS	G	701	-	51,58,58	1.85	5 (9%)	60,89,89	2.03	13 (21%)
3	P6G	B	702	-	18,18,18	0.48	0	17,17,17	0.37	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
7	GOL	C	705[B]	6	-	2/4/4/4	-
2	FAS	F	701	-	-	3/30/50/50	0/6/6/6
2	FAS	D	701	-	-	3/30/50/50	0/6/6/6
2	FAS	A	701	-	-	3/30/50/50	0/6/6/6
3	P6G	D	702	-	-	1/16/16/16	-
3	P6G	E	702	-	-	7/16/16/16	-
4	PGE	B	704	-	-	6/7/7/7	-
3	P6G	F	703	-	-	3/16/16/16	-
2	FAS	C	701	-	-	3/30/50/50	0/6/6/6
4	PGE	G	703	-	-	5/7/7/7	-
3	P6G	F	702	-	-	5/16/16/16	-
3	P6G	C	703	-	-	8/16/16/16	-
4	PGE	G	702	-	-	4/7/7/7	-
2	FAS	E	701	-	-	2/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	E	703	-	-	2/7/7/7	-
2	FAS	H	701	-	-	3/30/50/50	0/6/6/6
3	P6G	C	702	-	-	3/16/16/16	-
4	PGE	B	705	-	-	5/7/7/7	-
3	P6G	A	702	-	-	2/16/16/16	-
3	P6G	B	703	-	-	5/16/16/16	-
4	PGE	D	703	-	-	5/7/7/7	-
7	GOL	F	705	-	-	0/4/4/4	-
4	PGE	A	703	-	-	5/7/7/7	-
4	PGE	C	704	-	-	5/7/7/7	-
2	FAS	B	701	-	-	4/30/50/50	0/6/6/6
4	PGE	H	702	-	-	3/7/7/7	-
2	FAS	G	701	-	-	1/30/50/50	0/6/6/6
3	P6G	B	702	-	-	4/16/16/16	-

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	701	FAS	C4X-C10	10.00	1.48	1.38
2	H	701	FAS	C4X-C10	9.92	1.48	1.38
2	F	701	FAS	C4X-C10	9.80	1.48	1.38
2	A	701	FAS	C4X-C10	9.79	1.48	1.38
2	C	701	FAS	C4X-C10	9.62	1.48	1.38

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	701	FAS	C4-N3-C2	9.19	122.90	115.14
2	H	701	FAS	C4-N3-C2	8.81	122.58	115.14
2	B	701	FAS	C4-N3-C2	8.66	122.45	115.14
2	A	701	FAS	C4-N3-C2	8.62	122.42	115.14
2	D	701	FAS	C4-N3-C2	8.56	122.37	115.14

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	705[B]	GOL	O1-C1-C2-C3
2	D	701	FAS	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	D	701	FAS	C3B-C4B-C5B-O5B
2	C	701	FAS	O4B-C4B-C5B-O5B
2	B	701	FAS	O4B-C4B-C5B-O5B

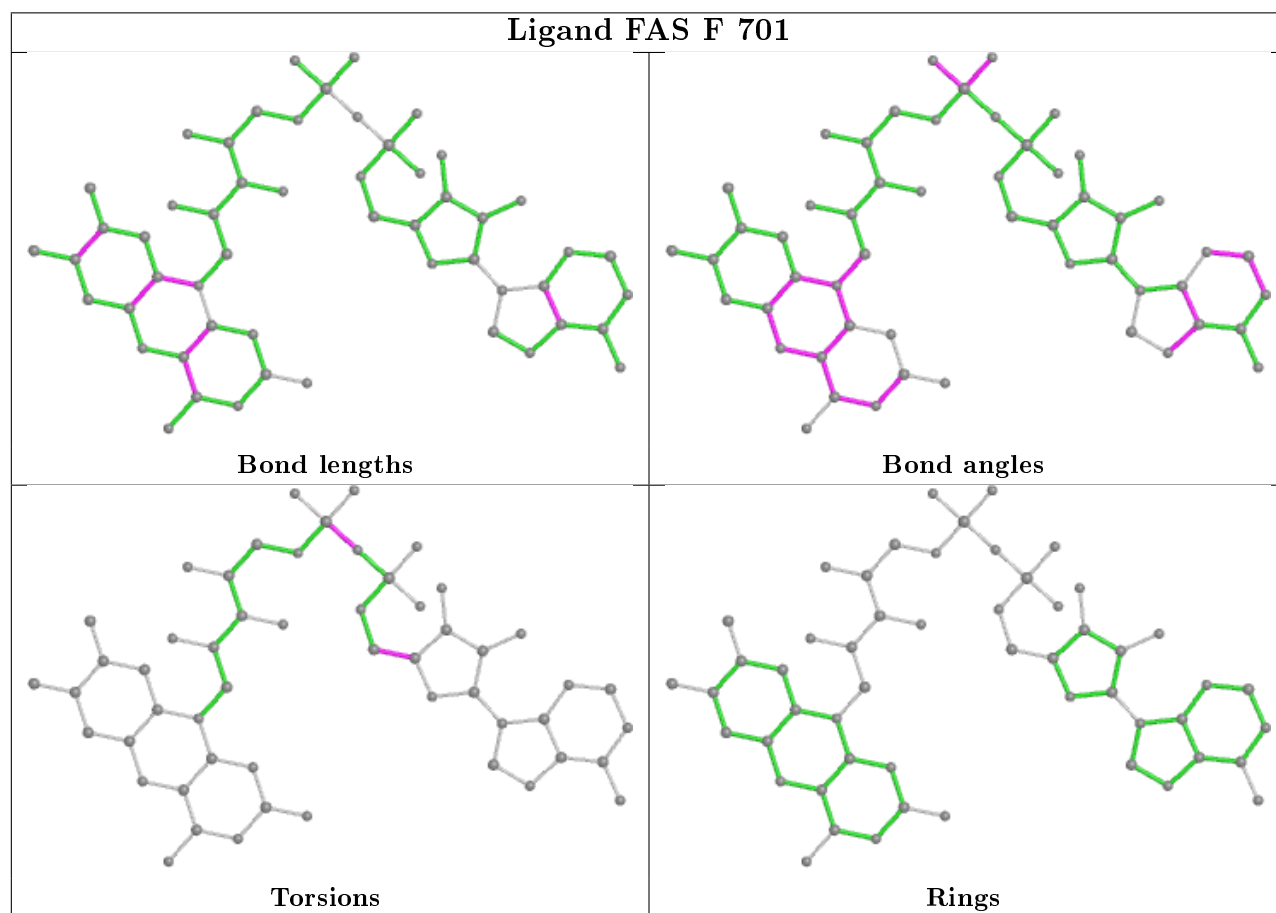
There are no ring outliers.

23 monomers are involved in 61 short contacts:

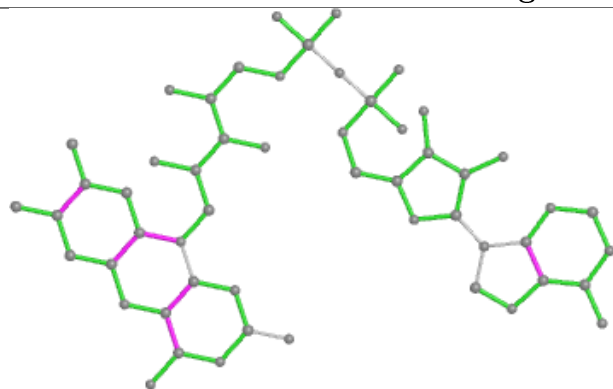
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	701	FAS	3	0
2	D	701	FAS	1	0
2	A	701	FAS	2	0
3	D	702	P6G	1	0
3	E	702	P6G	4	0
4	B	704	PGE	1	0
5	F	704	PO4	1	0
3	F	703	P6G	4	0
2	C	701	FAS	2	0
3	F	702	P6G	4	0
3	C	703	P6G	8	0
2	E	701	FAS	3	0
2	H	701	FAS	1	0
3	C	702	P6G	5	0
3	A	702	P6G	1	0
3	B	703	P6G	4	0
7	F	705	GOL	2	0
4	A	703	PGE	2	0
4	C	704	PGE	1	0
5	A	704[B]	PO4	1	0
4	H	702	PGE	1	0
2	G	701	FAS	3	0
3	B	702	P6G	6	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.

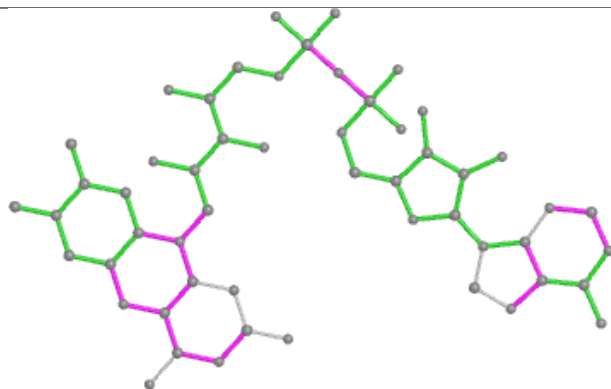
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



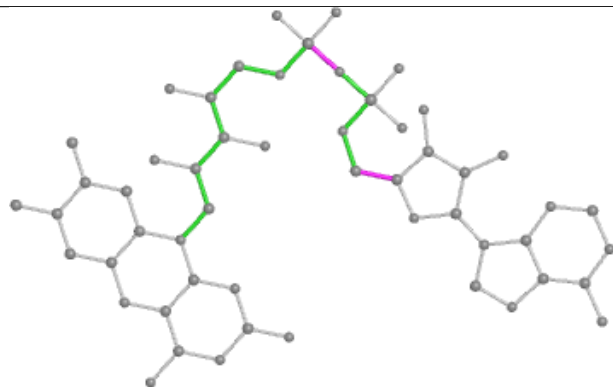
Ligand FAS D 701



Bond lengths



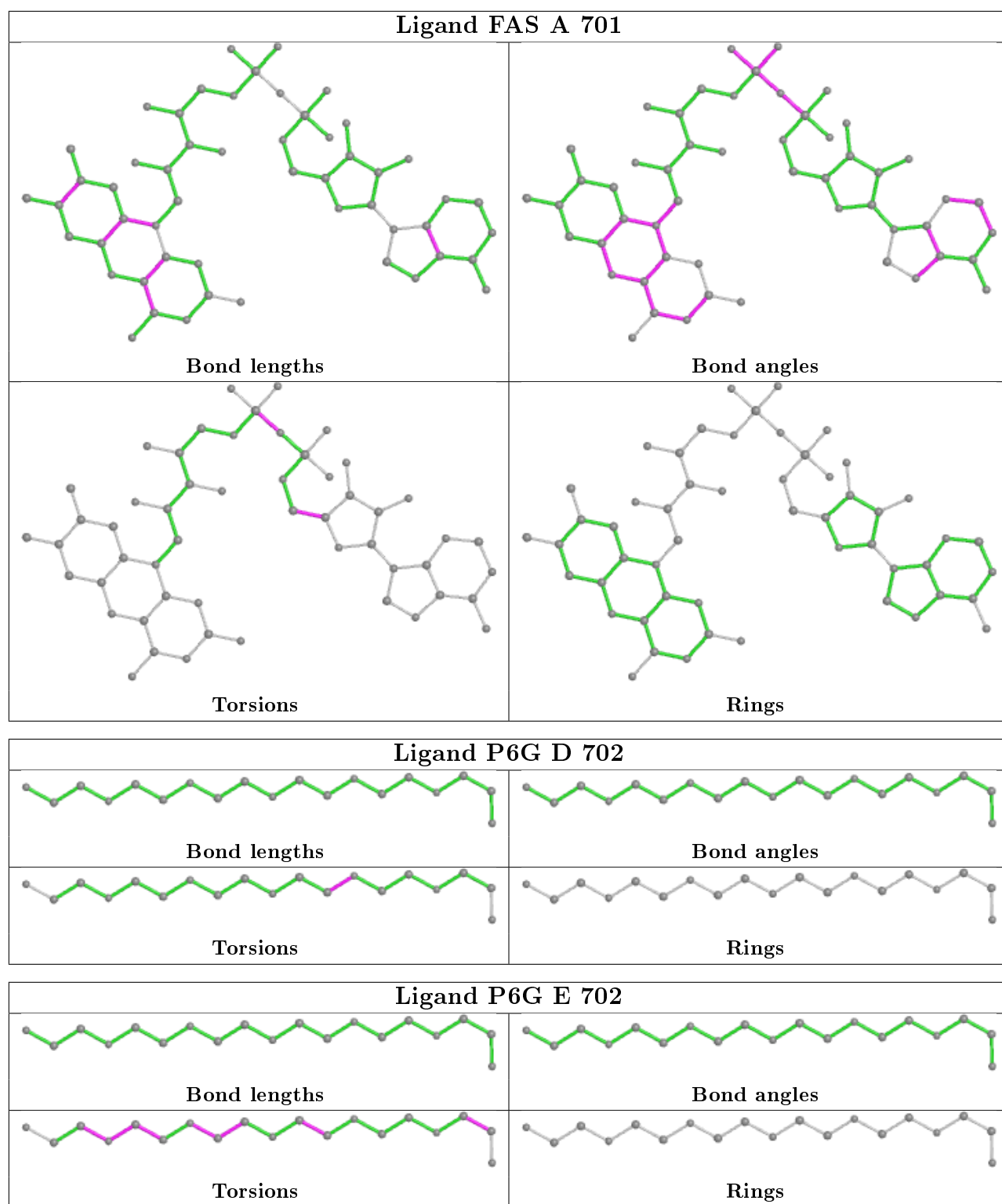
Bond angles

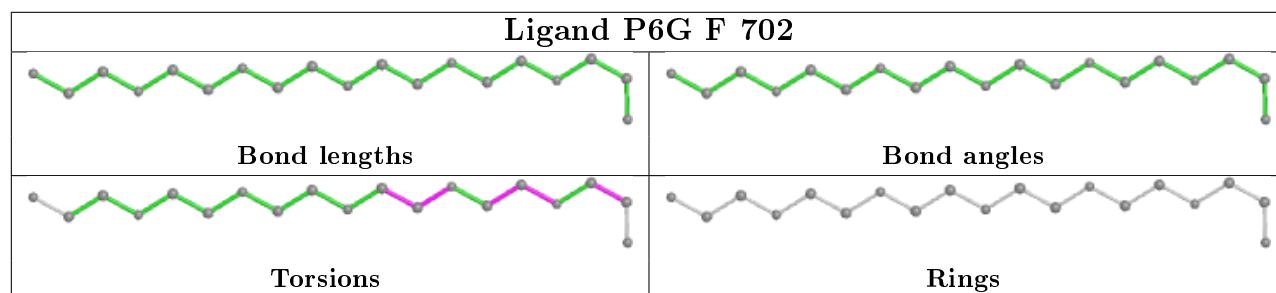
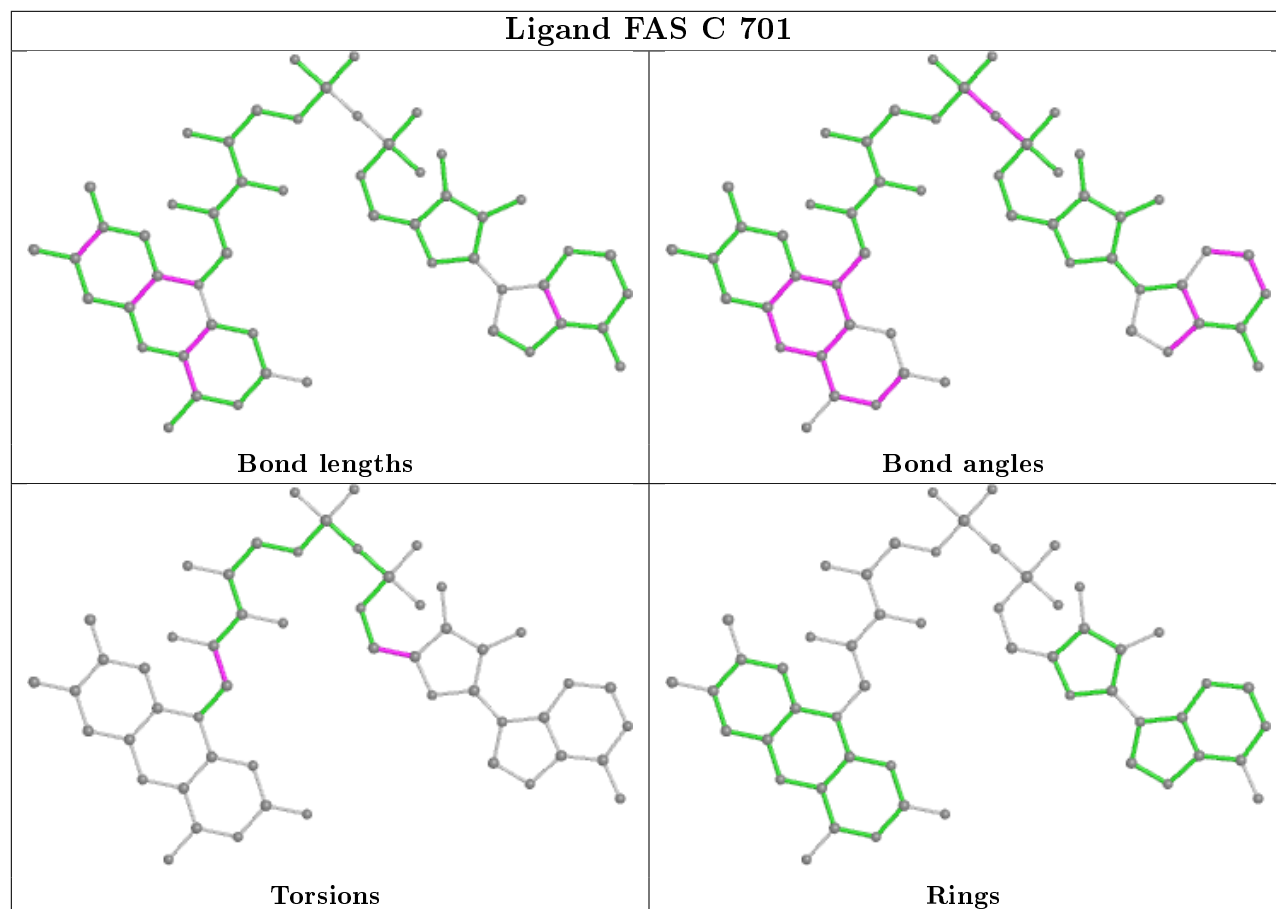
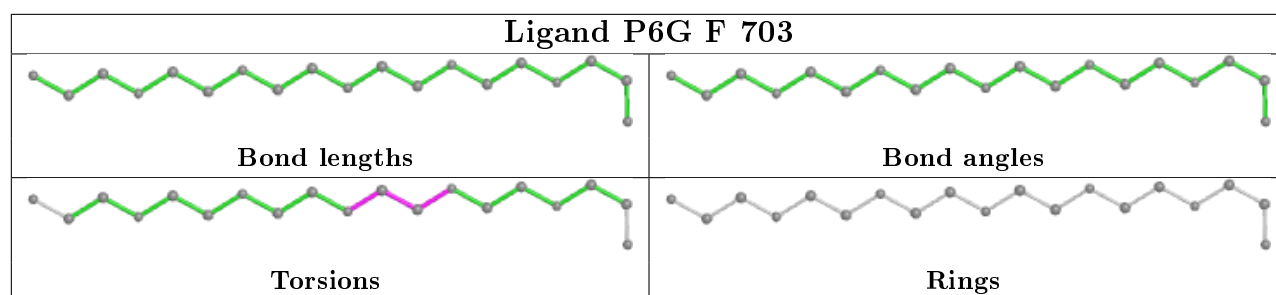


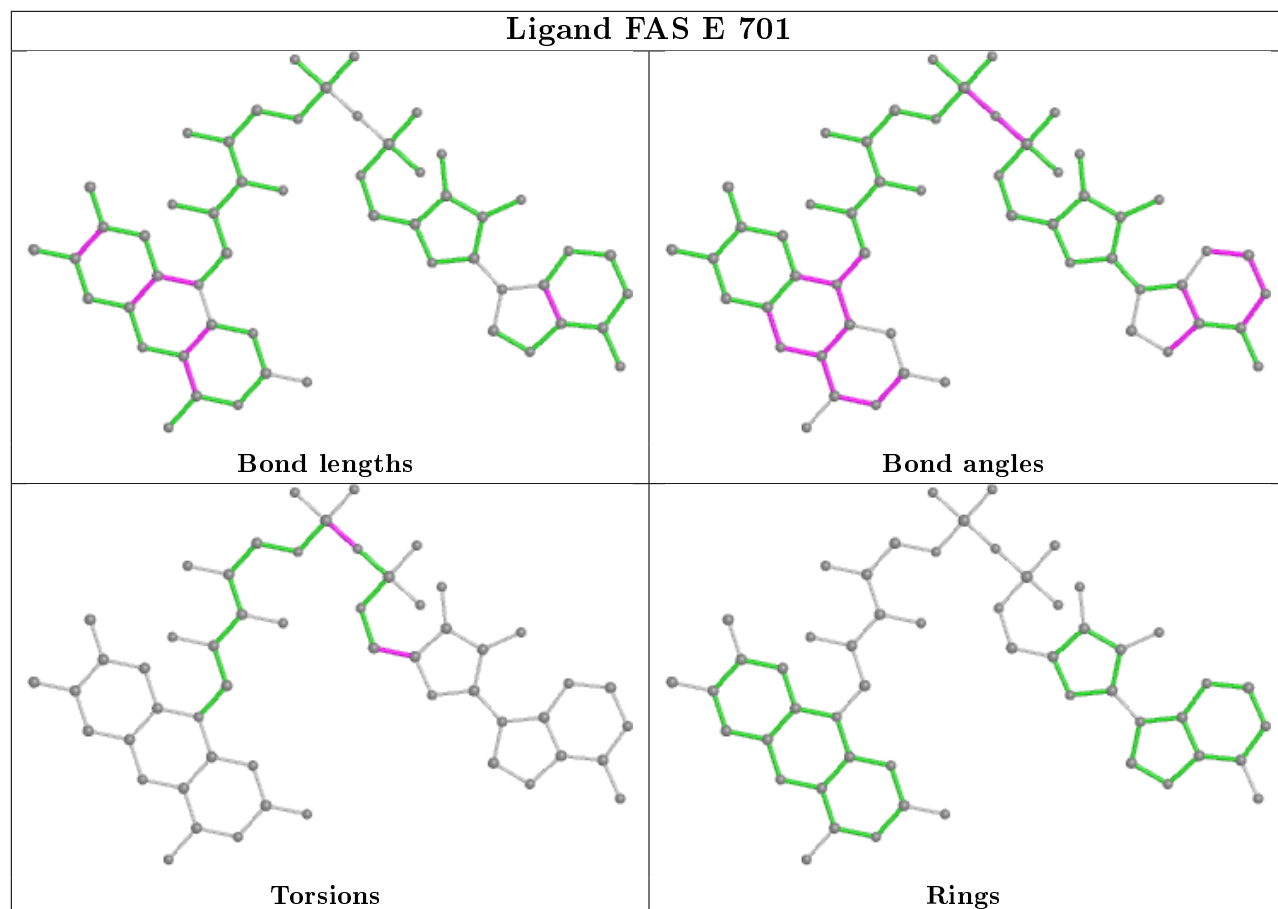
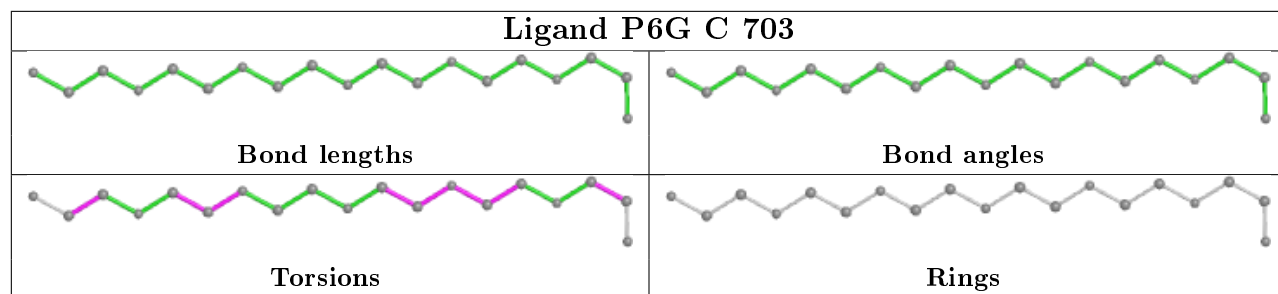
Torsions

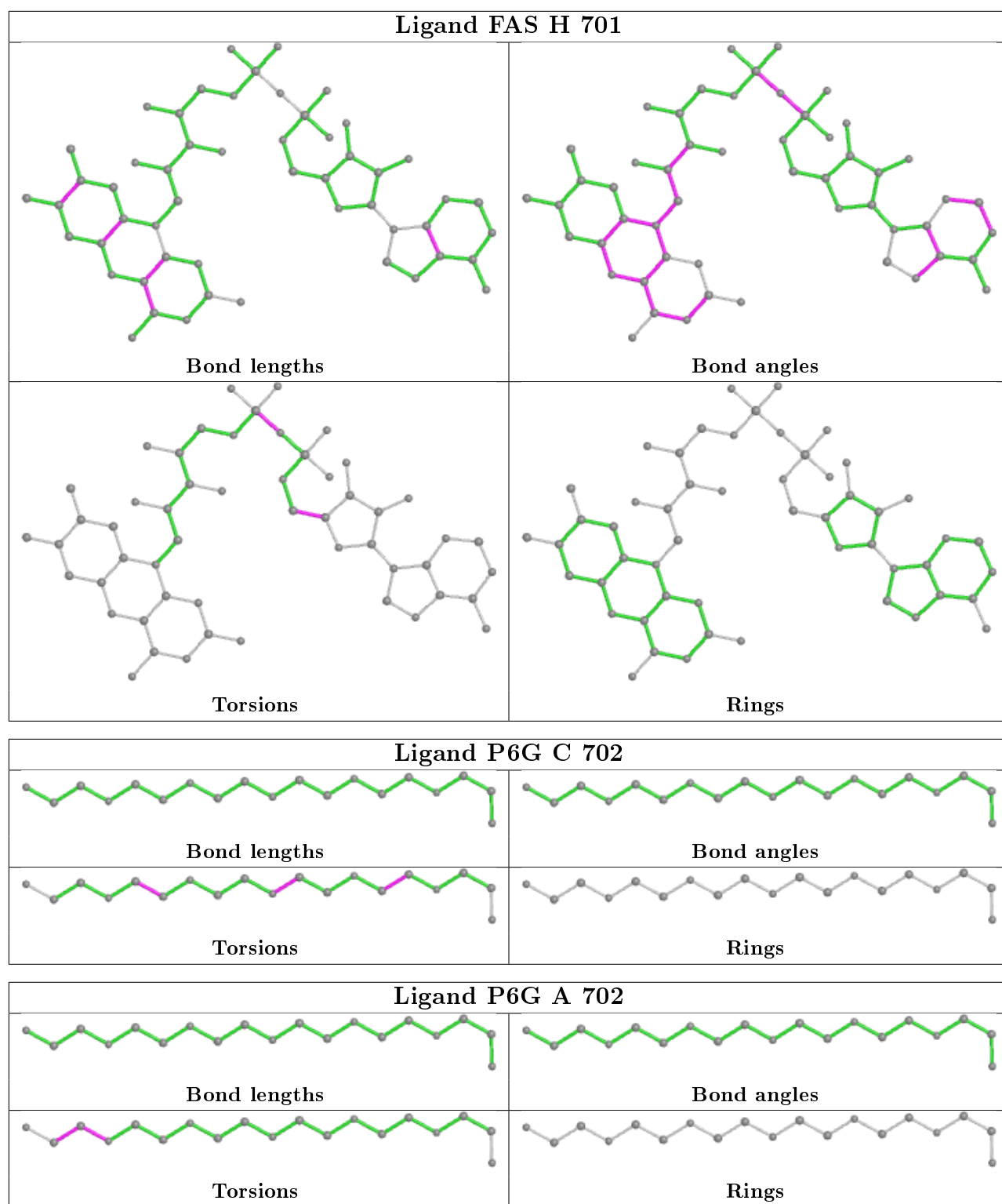


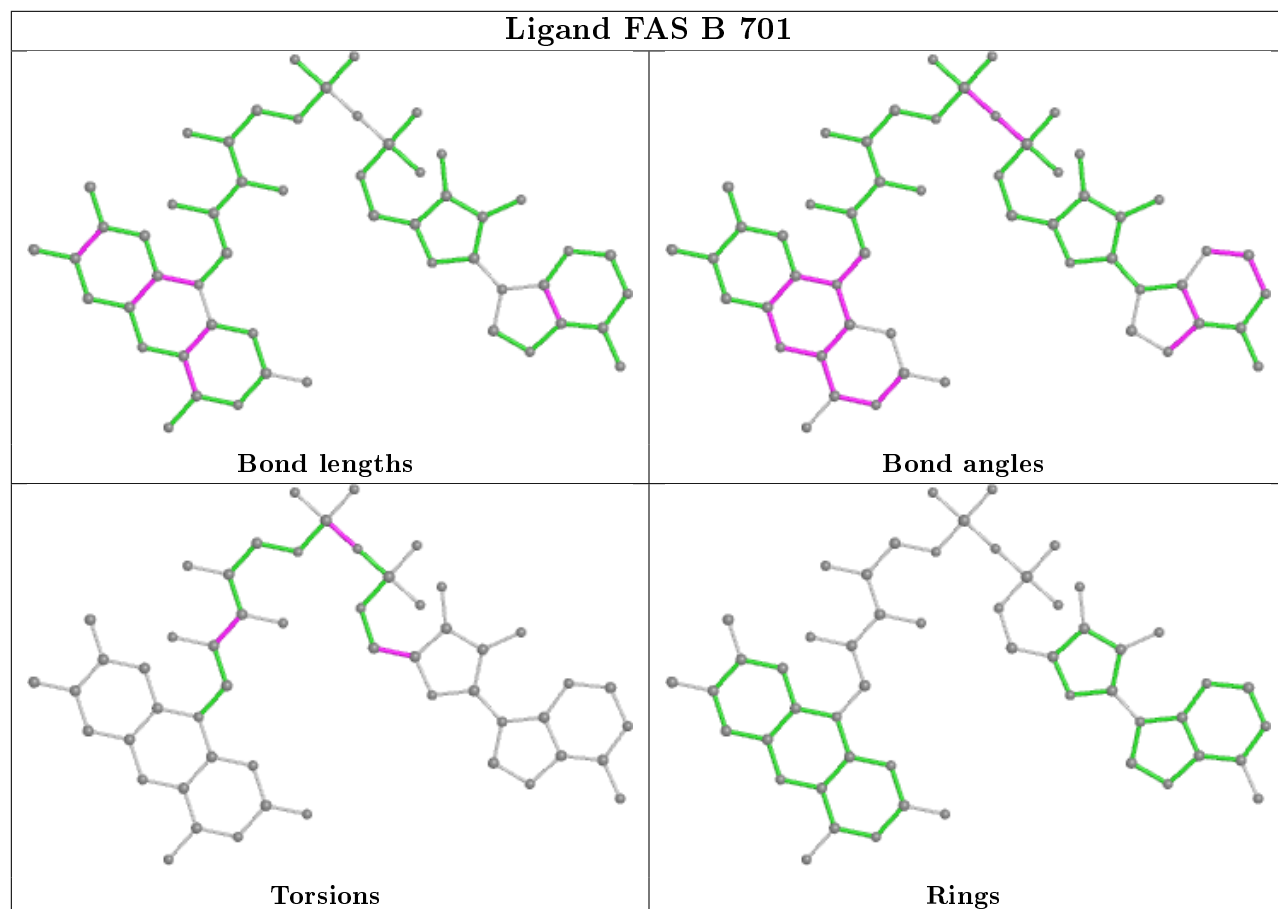
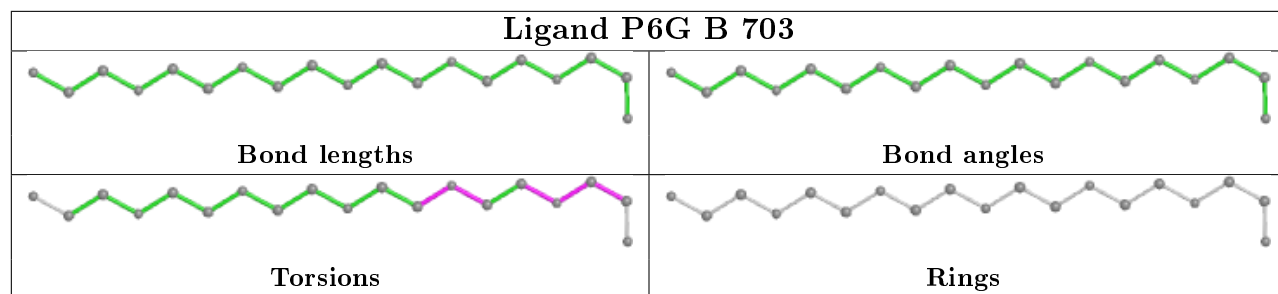
Rings

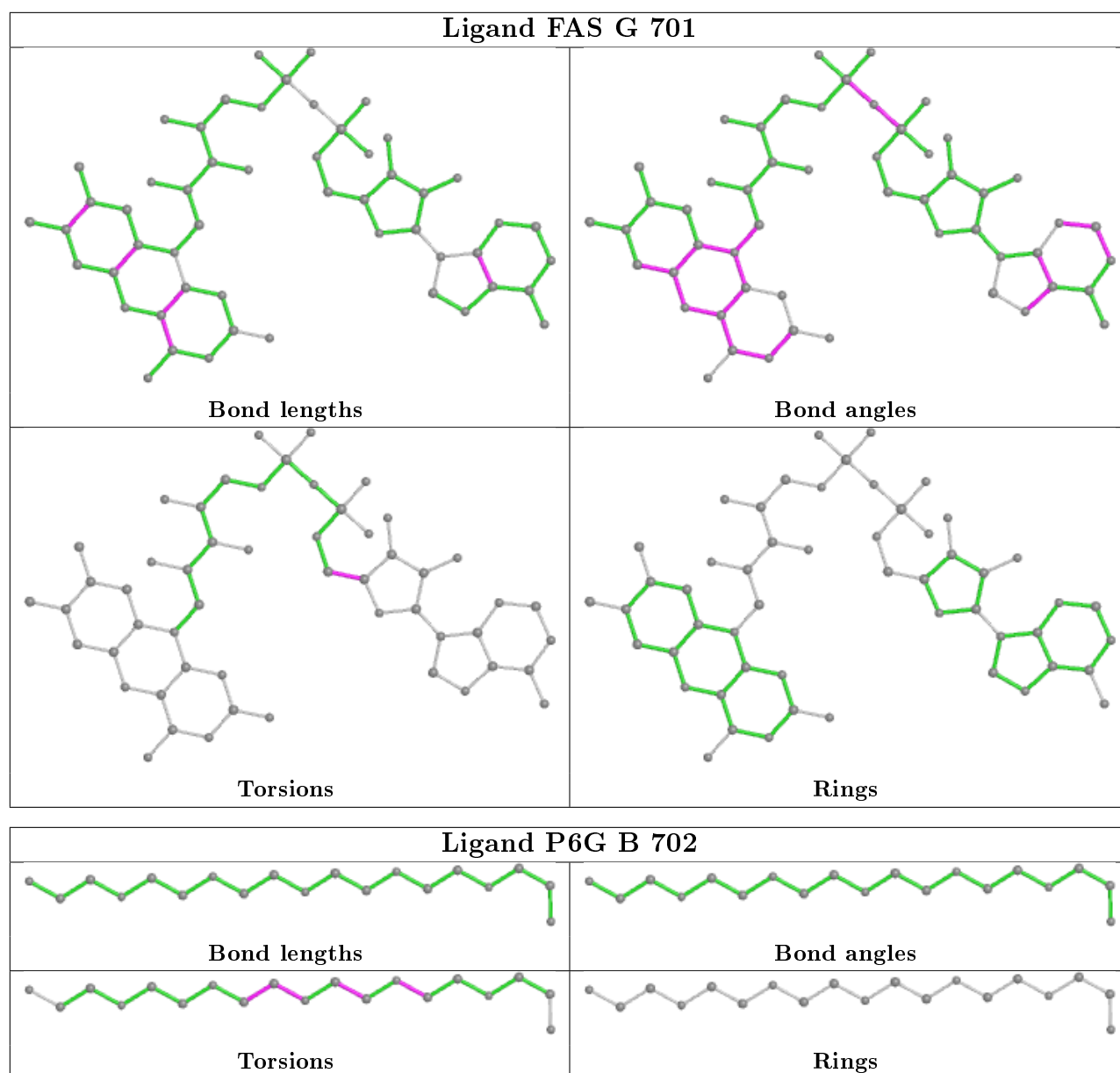












5.7 Other polymers [i](#)

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	662/663 (99%)	-0.21	4 (0%) 89 93	20, 34, 55, 70	0
1	B	662/663 (99%)	0.09	20 (3%) 50 61	25, 45, 73, 100	0
1	C	662/663 (99%)	-0.21	3 (0%) 91 95	22, 35, 53, 70	0
1	D	662/663 (99%)	0.20	34 (5%) 28 40	30, 52, 76, 102	0
1	E	662/663 (99%)	-0.25	6 (0%) 84 90	21, 34, 54, 91	0
1	F	662/663 (99%)	-0.12	10 (1%) 73 81	22, 41, 66, 86	0
1	G	662/663 (99%)	-0.05	9 (1%) 75 83	26, 44, 63, 87	0
1	H	662/663 (99%)	0.27	26 (3%) 39 52	34, 57, 86, 113	0
All	All	5296/5304 (99%)	-0.03	112 (2%) 63 74	20, 42, 70, 113	0

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	597	GLY	4.0
1	H	293	VAL	3.3
1	D	296	LEU	3.3
1	H	291	ALA	3.3
1	D	96	ILE	3.3

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
7	GOL	F	705	6/6	0.68	0.19	59,61,61,61	0
4	PGE	C	704	10/10	0.76	0.21	53,61,65,65	0
3	P6G	B	702	19/19	0.76	0.38	67,68,79,79	0
3	P6G	E	702	19/19	0.78	0.32	67,69,74,74	0
6	CA	G	704	1/1	0.79	0.22	103,103,103,103	0
3	P6G	C	703	19/19	0.80	0.29	67,75,77,77	0
3	P6G	F	703	19/19	0.80	0.31	71,74,75,76	0
4	PGE	G	703	10/10	0.81	0.39	69,69,71,71	0
6	CA	D	704	1/1	0.82	0.11	97,97,97,97	0
4	PGE	B	704	10/10	0.82	0.17	65,67,70,71	0
6	CA	E	704	1/1	0.84	0.12	98,98,98,98	0
4	PGE	D	703	10/10	0.84	0.17	64,67,70,70	0
4	PGE	E	703	10/10	0.86	0.18	50,54,58,58	0
4	PGE	G	702	10/10	0.86	0.34	56,59,59,60	0
3	P6G	C	702	19/19	0.87	0.31	64,67,71,71	0
4	PGE	H	702	10/10	0.87	0.15	67,68,69,69	0
6	CA	F	706	1/1	0.87	0.13	89,89,89,89	0
7	GOL	C	705[B]	6/6	0.90	0.14	48,50,51,51	6
4	PGE	A	703	10/10	0.90	0.15	55,56,61,61	0
5	PO4	F	704	5/5	0.90	0.16	46,50,51,52	0
6	CA	C	708	1/1	0.91	0.15	97,97,97,97	0
8	CL	C	706	1/1	0.91	0.07	84,84,84,84	0
4	PGE	B	705	10/10	0.92	0.14	54,55,57,58	0
3	P6G	F	702	19/19	0.94	0.14	36,38,41,42	0
3	P6G	B	703	19/19	0.94	0.15	42,47,52,52	0
3	P6G	D	702	19/19	0.94	0.14	49,52,55,56	0
2	FAS	B	701	53/53	0.95	0.19	40,43,52,52	0
6	CA	C	707	1/1	0.95	0.16	76,76,76,76	0
2	FAS	D	701	53/53	0.95	0.19	41,45,49,50	0
2	FAS	H	701	53/53	0.95	0.18	45,48,58,59	0
6	CA	A	705	1/1	0.96	0.12	64,64,64,64	0
3	P6G	A	702	19/19	0.96	0.13	29,34,37,37	0
2	FAS	A	701	53/53	0.97	0.17	28,30,35,37	0
2	FAS	G	701	53/53	0.97	0.19	31,33,36,37	0
2	FAS	F	701	53/53	0.97	0.19	36,40,45,48	0
2	FAS	C	701	53/53	0.98	0.17	25,28,30,35	0
2	FAS	E	701	53/53	0.98	0.19	28,29,32,34	0

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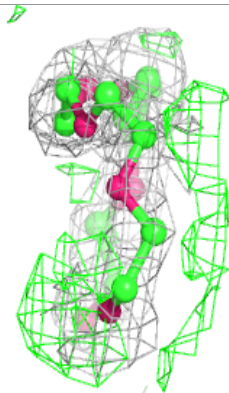
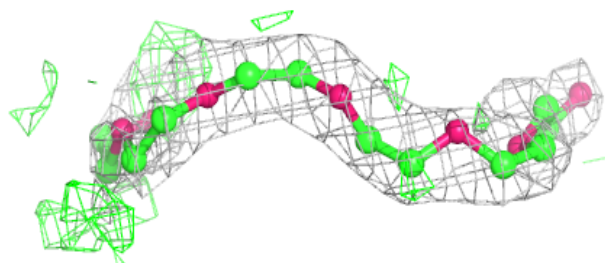
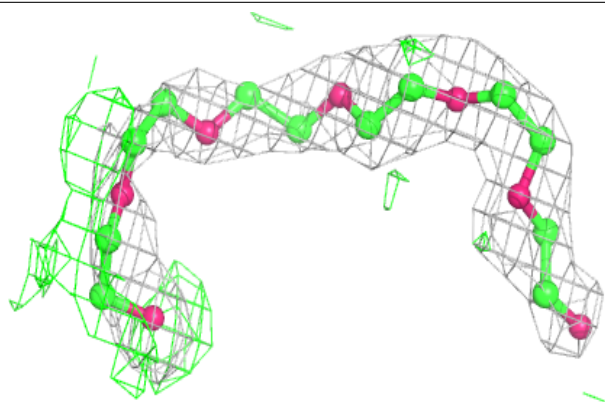
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CA	B	706	1/1	0.98	0.14	76,76,76,76	0
5	PO4	A	704[B]	5/5	0.98	0.16	39,41,43,44	5

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.

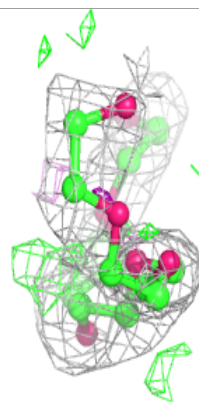
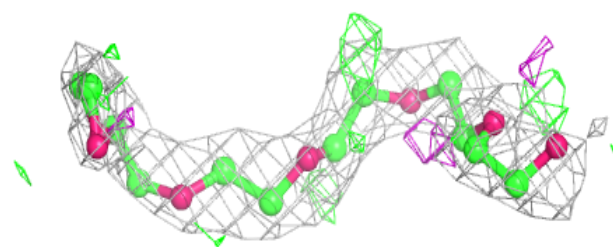
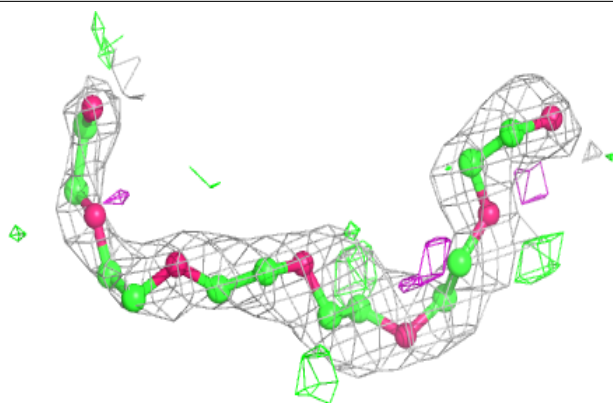
Electron density around P6G B 702:

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

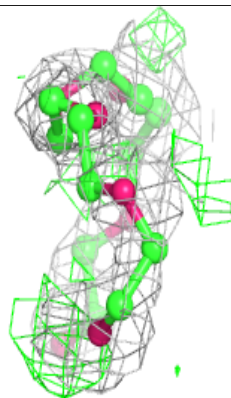
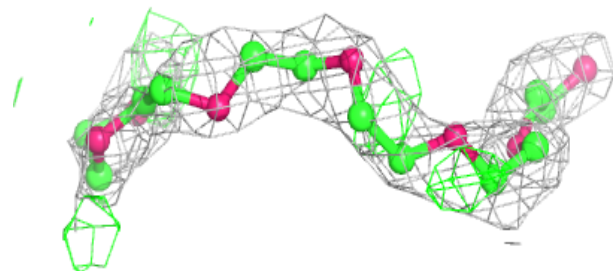
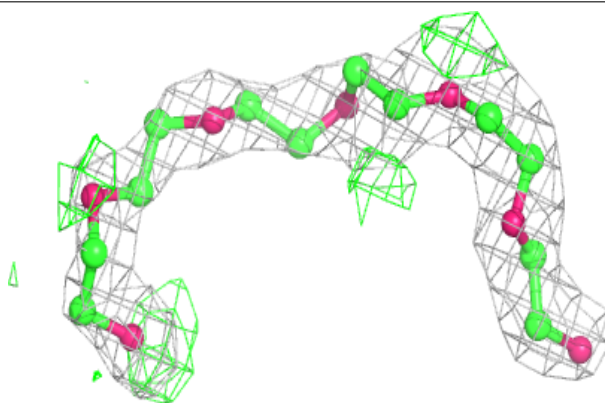


Electron density around P6G E 702:

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

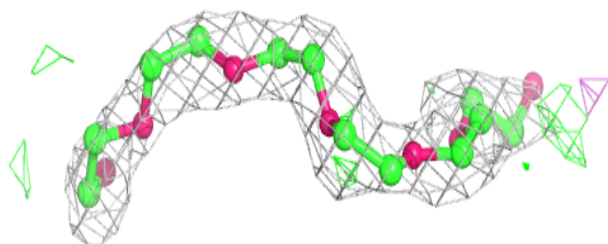
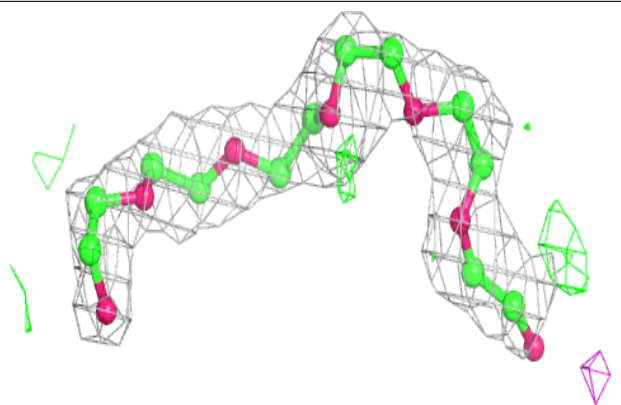
**Electron density around P6G C 703:**

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

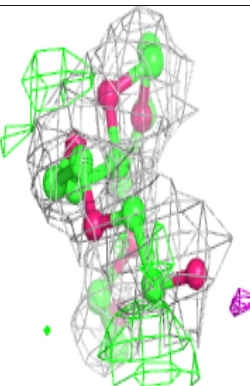
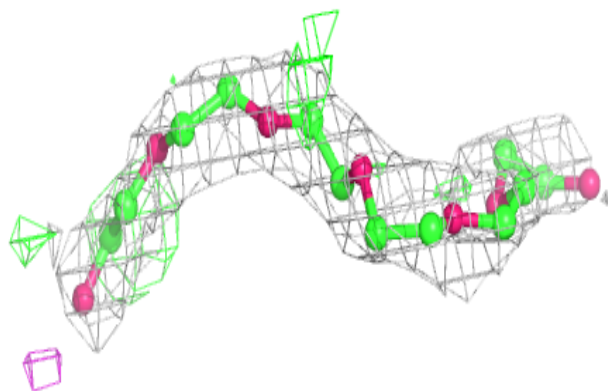
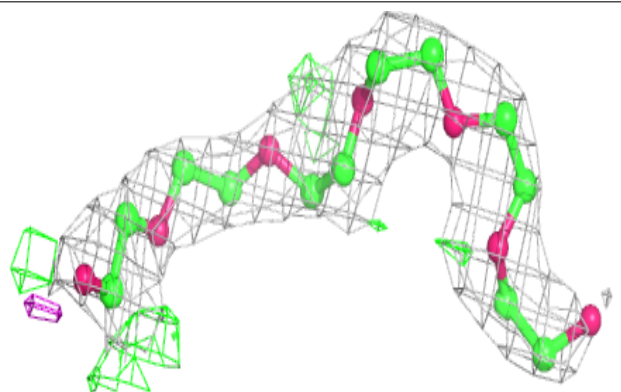


Electron density around P6G F 703:

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

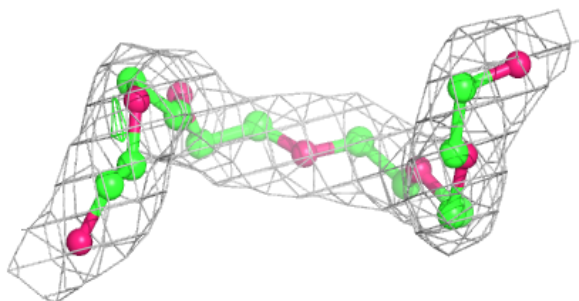
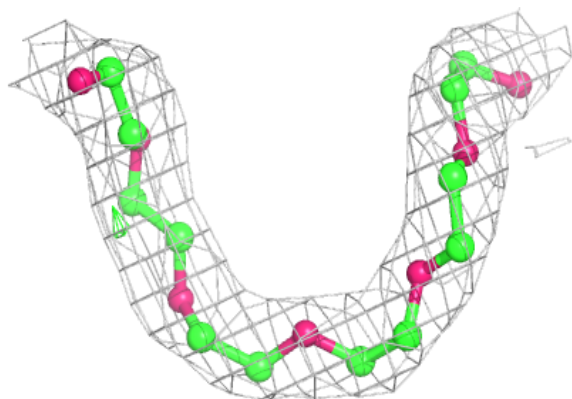
**Electron density around P6G C 702:**

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

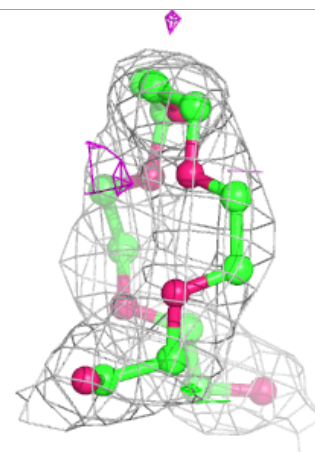
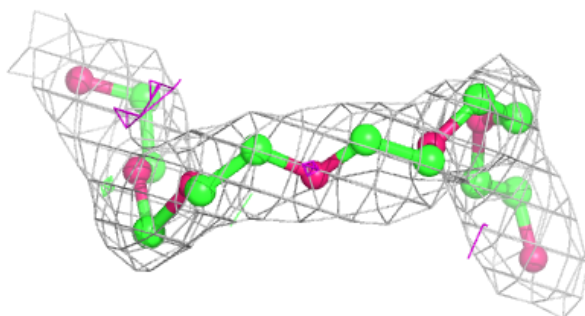
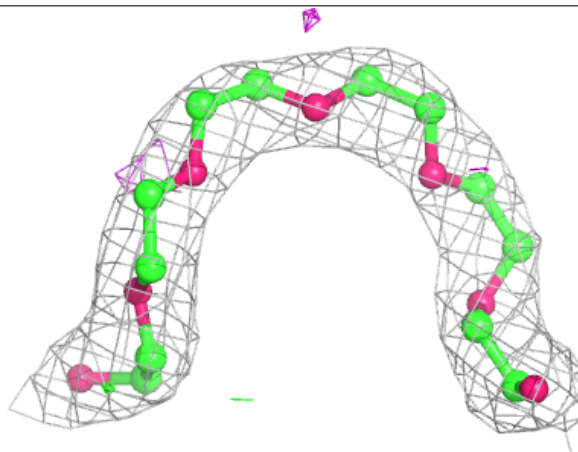


Electron density around P6G F 702:

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

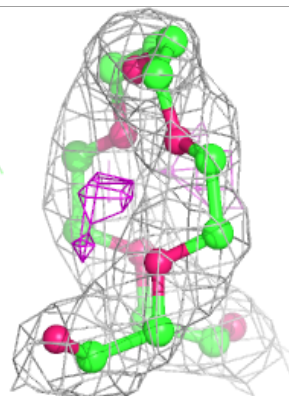
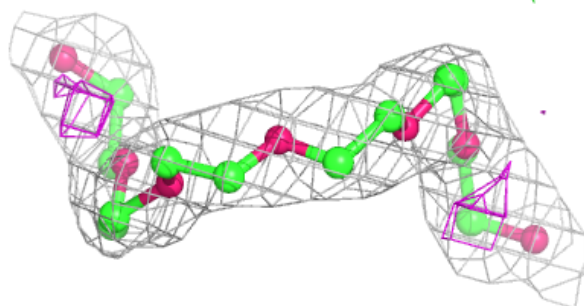
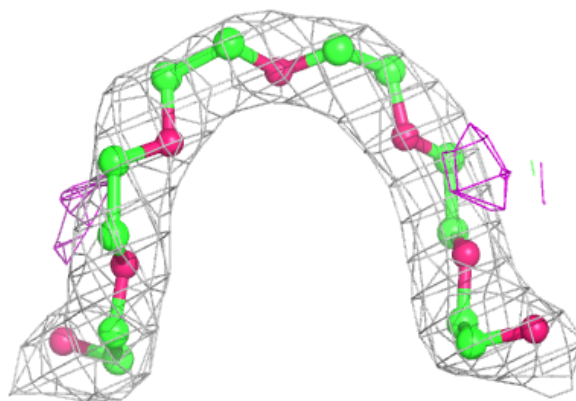
**Electron density around P6G B 703:**

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

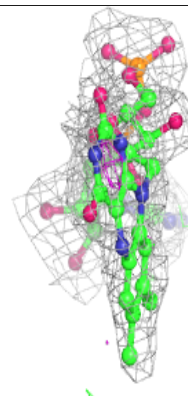
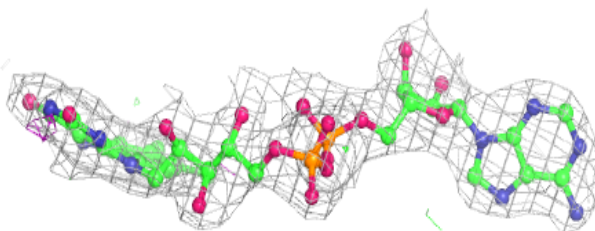
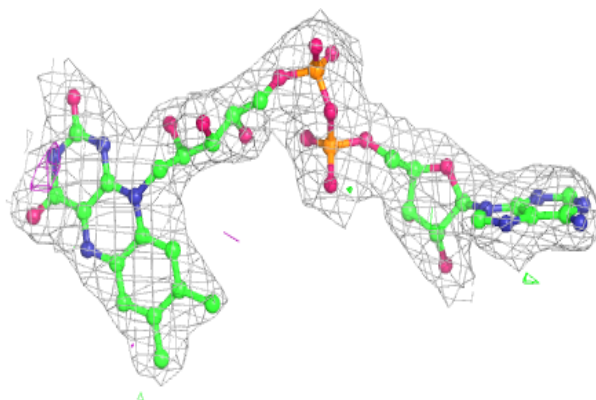


Electron density around P6G D 702:

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

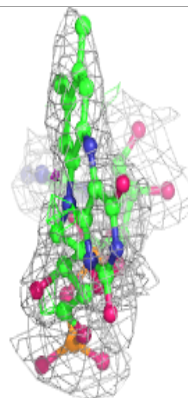
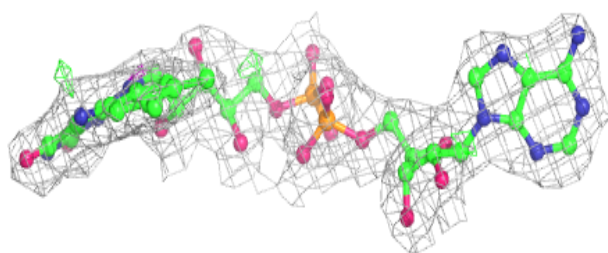
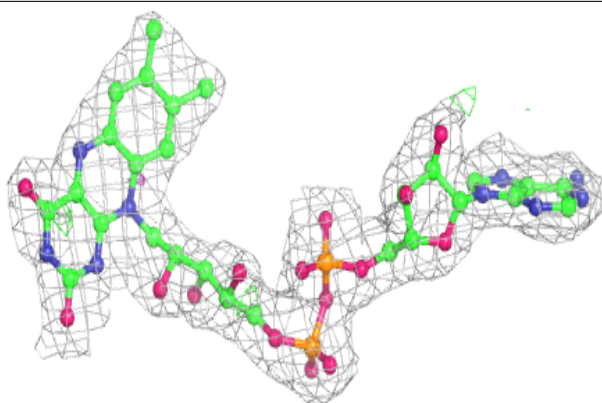
**Electron density around FAS B 701:**

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

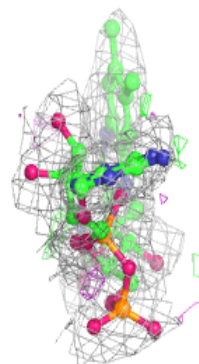
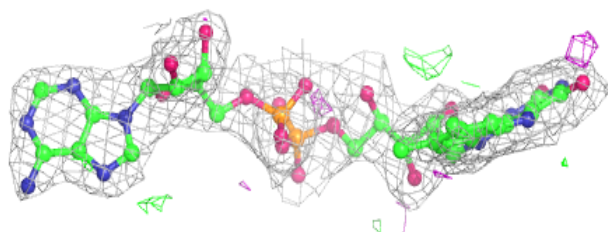
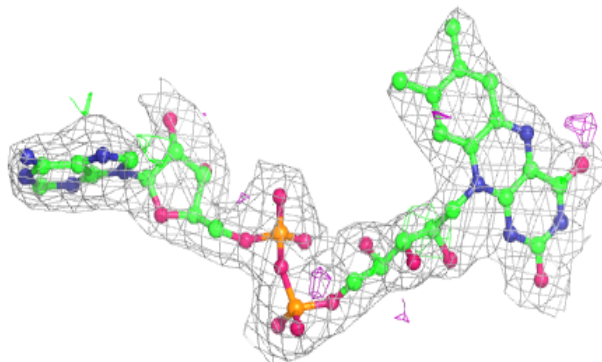


Electron density around FAS D 701:

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

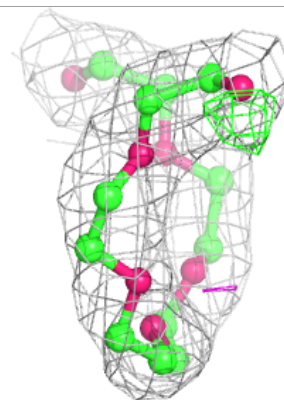
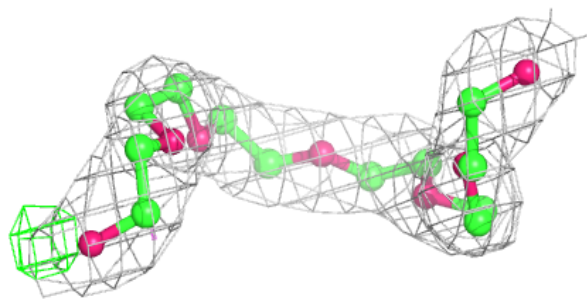
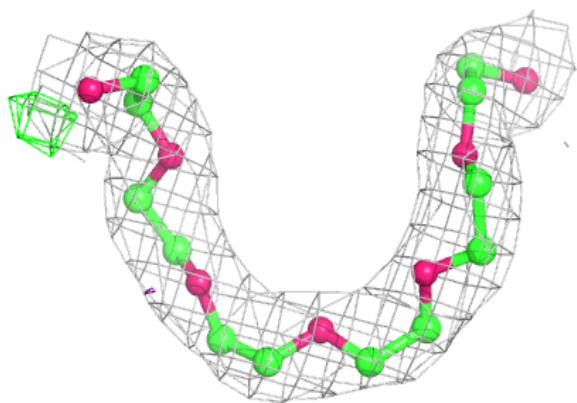
**Electron density around FAS H 701:**

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

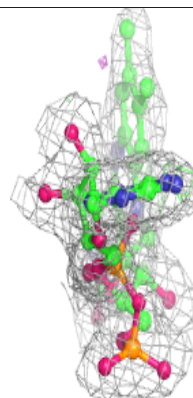
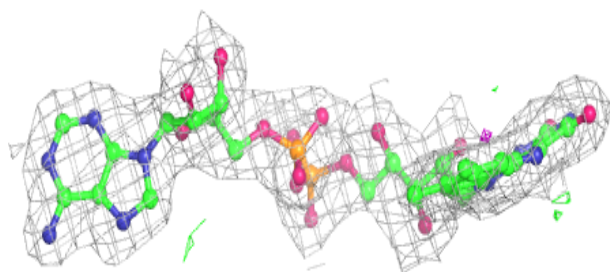
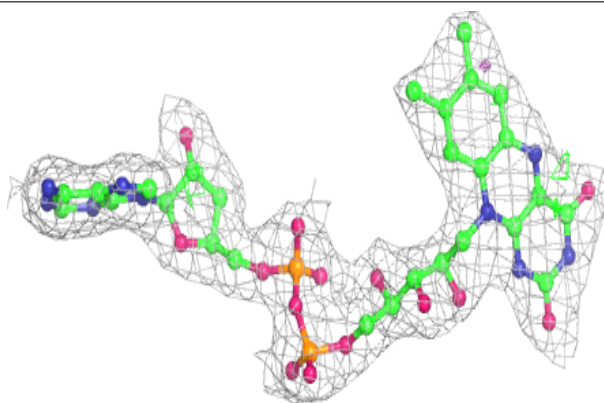


Electron density around P6G A 702:

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

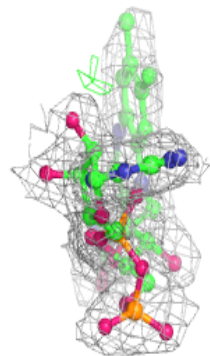
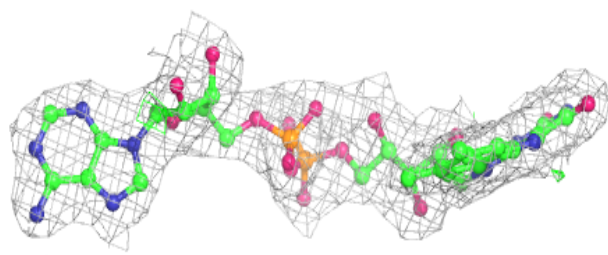
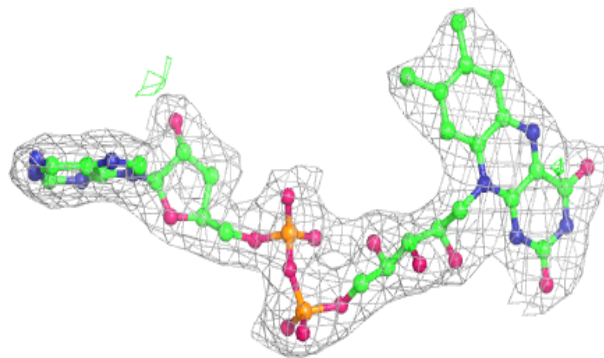
**Electron density around FAS A 701:**

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

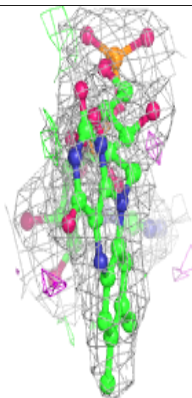
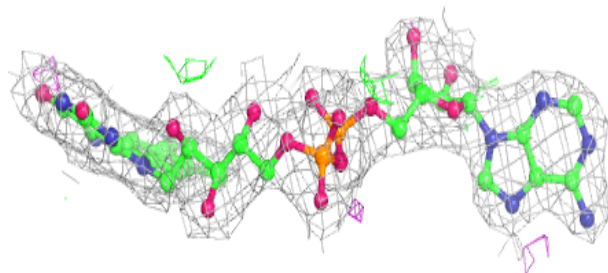
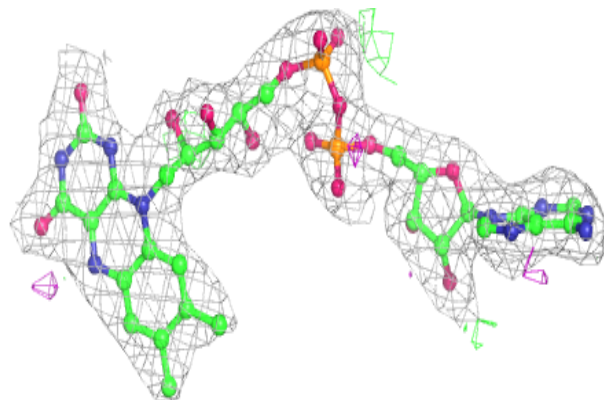


Electron density around FAS G 701:

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

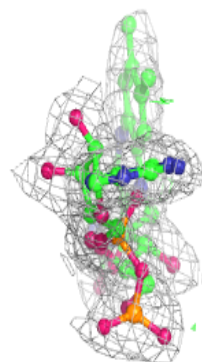
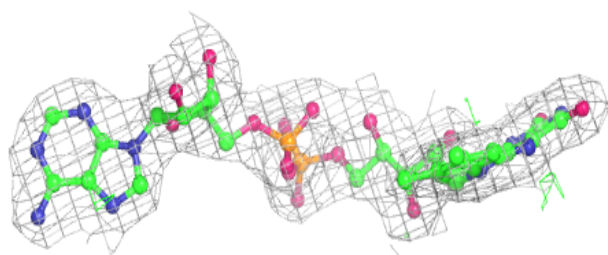
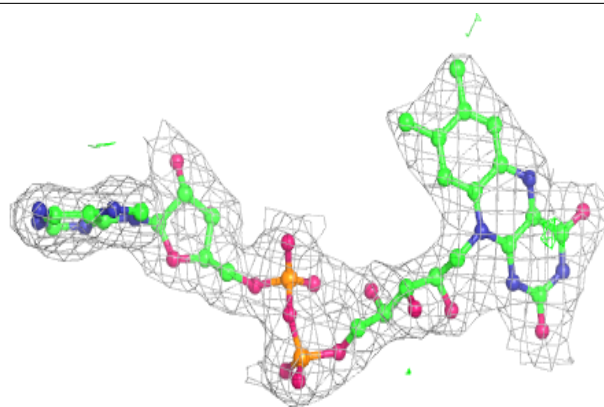
**Electron density around FAS F 701:**

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

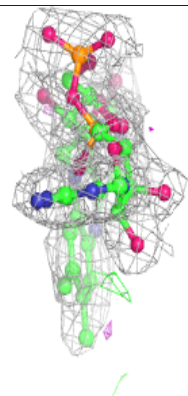
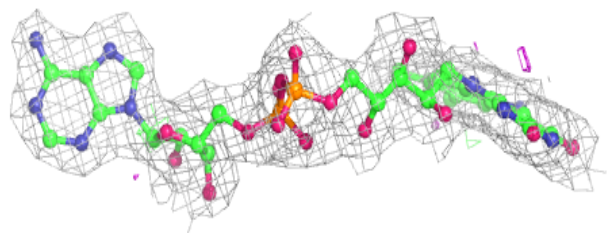
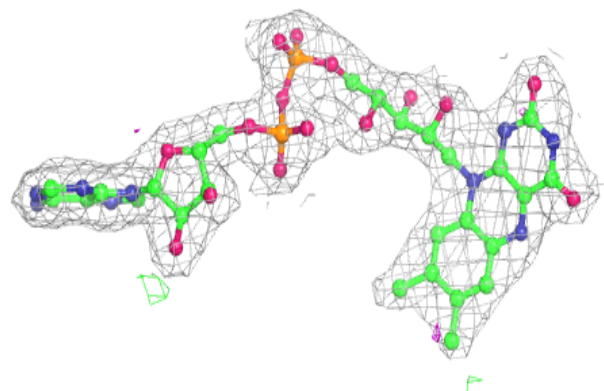


Electron density around FAS C 701:

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

**Electron density around FAS E 701:**

$2mF_o-DF_c$ (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.