Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 10:03 am GMT

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

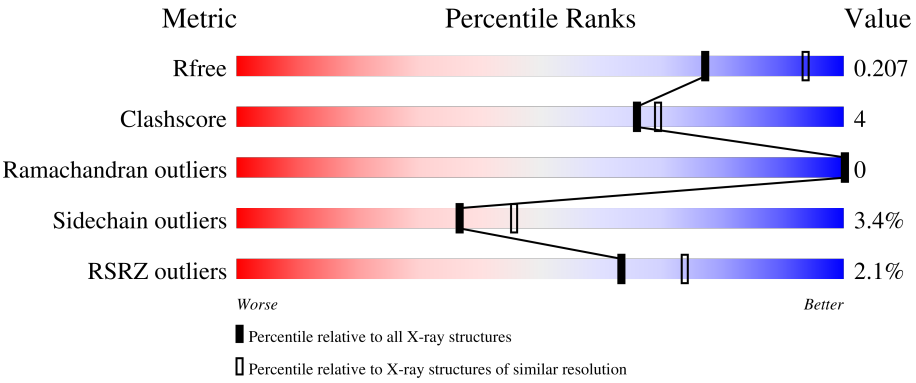
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.35 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 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	663	% 89% 10%
1	B	663	3% 88% 11%
1	C	663	89% 10%
1	D	663	5% 90% 8%
1	E	663	% 89% 10%

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Mol	Chain	Length	Quality of chain
1	F	663	2% 89% 9%
1	G	663	% 89% 10%
1	H	663	4% 88% 10%

2 Entry composition (i)

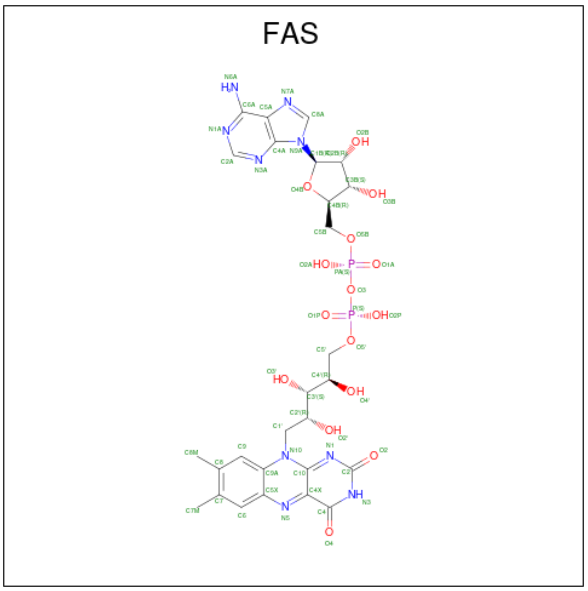
There are 9 unique types of molecules in this entry. The entry contains 44407 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

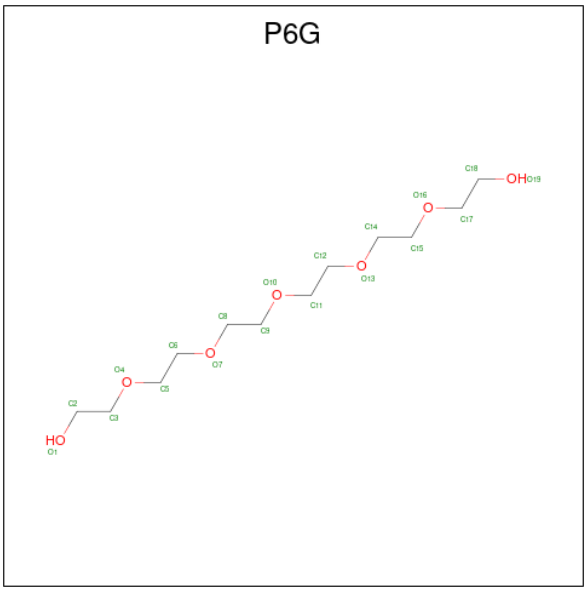
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	B	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	C	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	D	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	E	662	Total	C	N	O	S	0	1	0
			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: $C_{27}H_{33}N_9O_{15}P_2$).



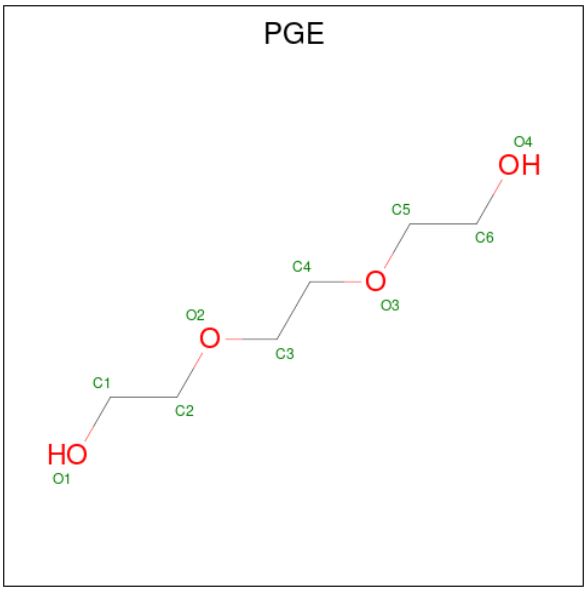
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	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: $C_{12}H_{26}O_7$).



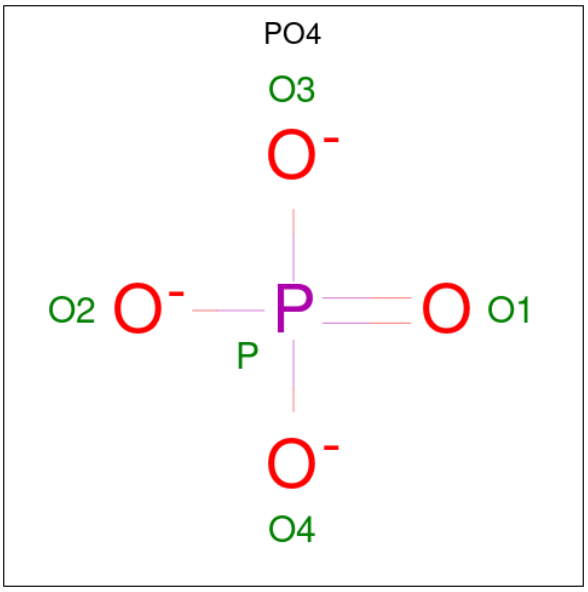
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 19 12 7	0	0
3	B	1	Total C O 19 12 7	0	0
3	B	1	Total C O 19 12 7	0	0
3	C	1	Total C O 19 12 7	0	0
3	C	1	Total C O 19 12 7	0	0
3	D	1	Total C O 19 12 7	0	0
3	E	1	Total C O 19 12 7	0	0
3	F	1	Total C O 19 12 7	0	0
3	F	1	Total C O 19 12 7	0	0

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



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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

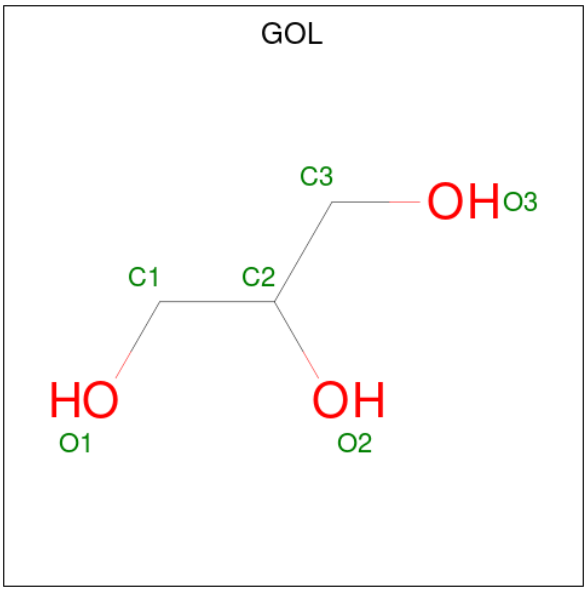


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	1
5	F	1	Total O P 5 4 1	0	0

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

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

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

- Molecule 9 is water.

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

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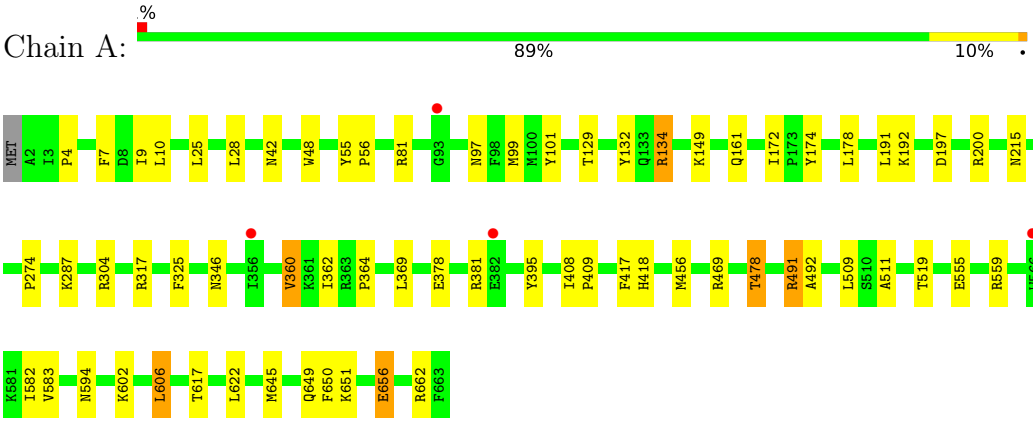
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	211	Total O 211 211	0	0
9	H	129	Total O 129 129	0	0

3 Residue-property plots

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.

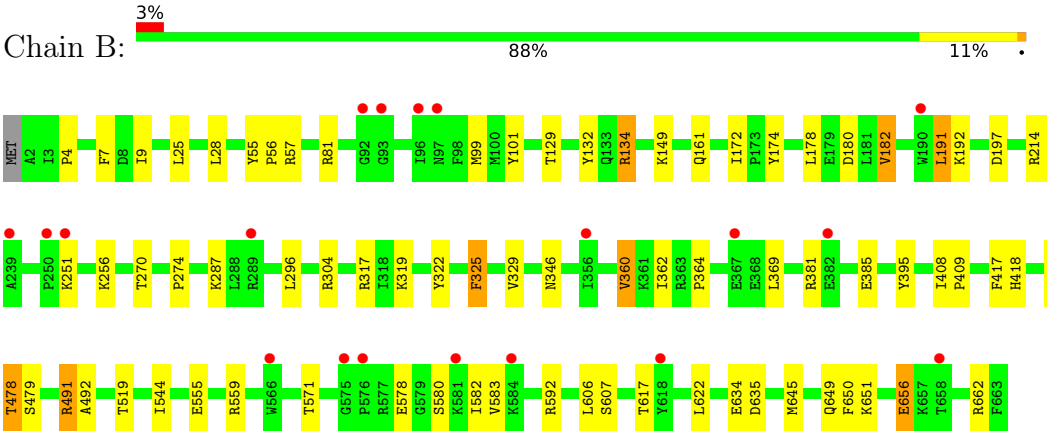
• Molecule 1: Alcohol oxidase 1

Chain A:



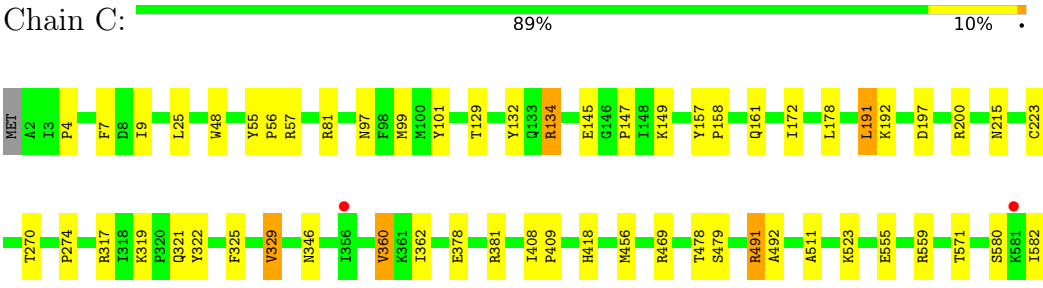
• Molecule 1: Alcohol oxidase 1

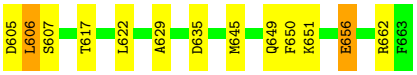
Chain B:



• Molecule 1: Alcohol oxidase 1

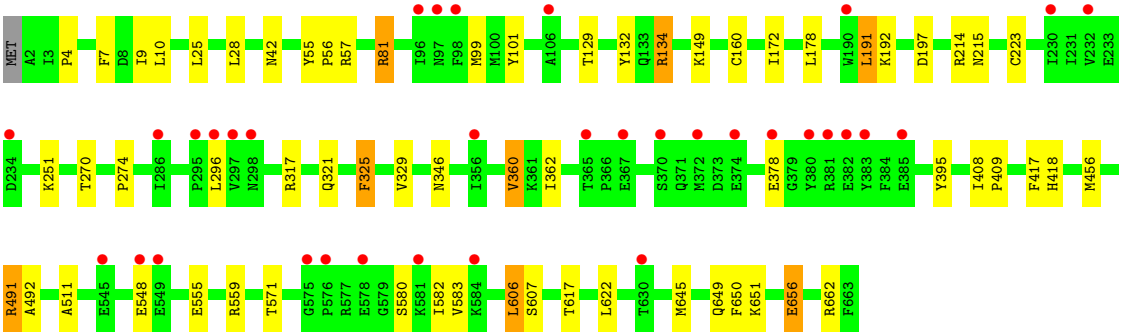
Chain C:





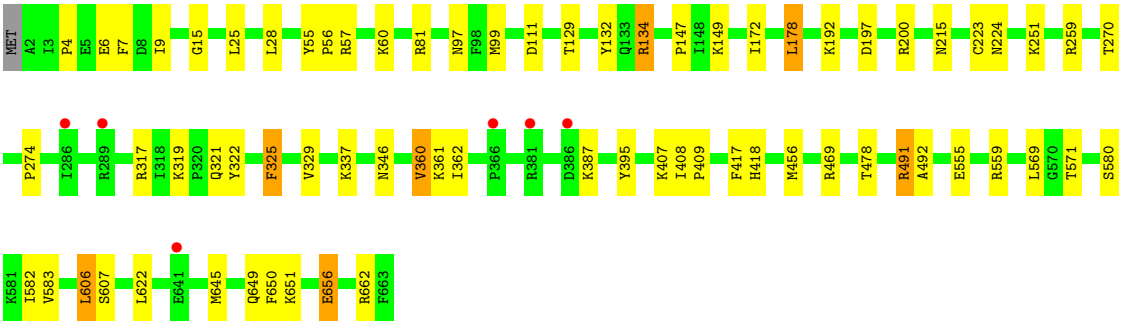
• Molecule 1: Alcohol oxidase 1

Chain D:



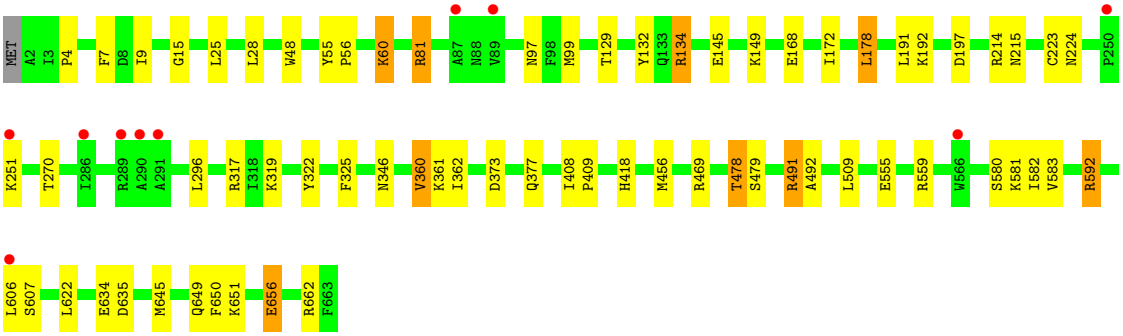
• Molecule 1: Alcohol oxidase 1

Chain E:



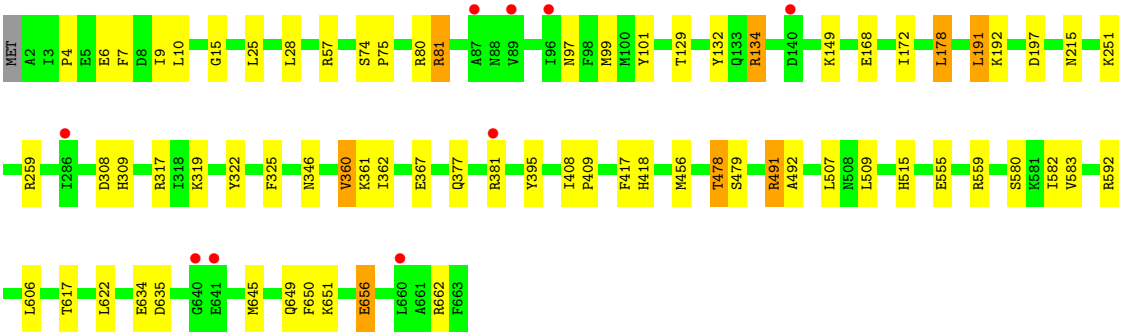
• Molecule 1: Alcohol oxidase 1

Chain F:

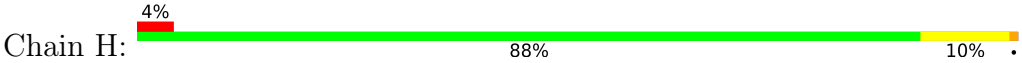


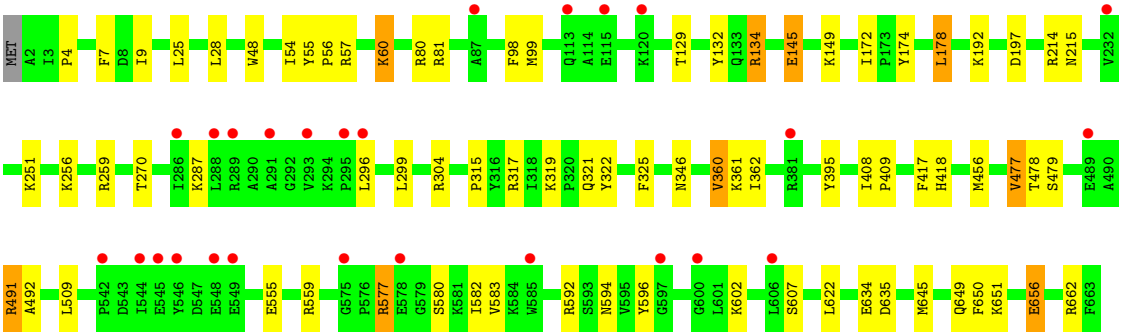
• Molecule 1: Alcohol oxidase 1

Chain G:



• Molecule 1: Alcohol oxidase 1





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P6G, FAS, PGE, GOL, PO4, CA, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	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

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.

All (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
1:C:346:ASN:O	1:C:662:ARG:NH2	2.25	0.70
1:C:592:ARG:NH2	1:C:635:ASP:OD1	2.25	0.69
1:E:346:ASN:O	1:E:662:ARG:NH2	2.26	0.68
1:E:649:GLN:NE2	1:E:651:LYS:HG2	2.08	0.68
1:F:215:ASN:OD1	1:H:656:GLU:HG3	1.93	0.68
1:H:346:ASN:O	1:H:662:ARG:NH2	2.25	0.68
1:B:346:ASN:O	1:B:662:ARG:NH2	2.27	0.68
1:G:346:ASN:O	1:G:662:ARG:NH2	2.26	0.68
1:A:346:ASN:O	1:A:662:ARG:NH2	2.26	0.68
3:C:703:P6G:H141	1:D:223:CYS:HB2	1.75	0.68
1:F:346:ASN:O	1:F:662:ARG:NH2	2.26	0.68
1:D:346:ASN:O	1:D:662:ARG:NH2	2.27	0.67
1:B:214:ARG:C	1:B:215:ASN:HD22	1.97	0.67
1:E:656:GLU:HG3	1:G:215:ASN:OD1	1.95	0.67
5:A:704[B]:PO4:O1	9:A:801:HOH:O	2.12	0.67
1:C:161:GLN:HE21	3:C:703:P6G:H52	1.59	0.67
1:G:656:GLU:HG3	1:H:215:ASN:OD1	1.96	0.66
1:A:215:ASN:OD1	1:B:656:GLU:HG3	1.97	0.65
1:E:215:ASN:OD1	1:F:656:GLU:HG3	1.98	0.64
1:C:147:PRO:HA	1:C:649:GLN:OE1	1.98	0.64
1:H:48:TRP:HH2	4:H:702:PGE:H3	1.62	0.64
1:C:656:GLU:HG3	1:D:215:ASN:OD1	1.97	0.63
1:B:592:ARG:NH2	1:B:635:ASP:OD1	2.32	0.63
1:E:569:LEU:HB3	1:E:606:LEU:HD23	1.81	0.62
1:F:223:CYS:H	3:F:703:P6G:H62	1.65	0.62
1:C:649:GLN:HE21	1:C:651:LYS:HG2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:GLU:OE1	1:A:381:ARG:NH1	2.32	0.62
1:E:147:PRO:HA	1:E:649:GLN:OE1	2.00	0.61
1:A:656:GLU:HG3	1:C:215:ASN:OD1	2.00	0.61
1:C:223:CYS:H	3:C:702:P6G:H82	1.65	0.61
1:B:606:LEU:HD21	1:B:617:THR:HB	1.84	0.60
1:A:28:LEU:HB2	1:A:645:MET:HE2	1.82	0.60
1:A:224:ASN:HB2	3:B:702:P6G:H21	1.85	0.59
1:F:478:THR:HG23	3:F:702:P6G:H31	1.83	0.59
1:F:360:VAL:HG13	1:F:362:ILE:HG23	1.86	0.58
1:E:28:LEU:HB2	1:E:645:MET:HE3	1.86	0.58
1:F:28:LEU:HB2	1:F:645:MET:HE3	1.86	0.57
1:H:360:VAL:HG13	1:H:362:ILE:HG23	1.87	0.56
1:C:161:GLN:HE21	3:C:703:P6G:H31	1.69	0.56
1:A:174:TYR:CG	3:C:702:P6G:H51	2.40	0.56
1:C:360:VAL:HG13	1:C:362:ILE:HG23	1.86	0.56
1:D:28:LEU:HB2	1:D:645:MET:HE3	1.86	0.56
1:E:360:VAL:HG13	1:E:362:ILE:HG23	1.86	0.56
1:A:101:TYR:HB3	1:A:191:LEU:HB3	1.87	0.56
1:C:48:TRP:HH2	4:C:704:PGE:H5	1.71	0.56
1:H:28:LEU:HB2	1:H:645:MET:HE3	1.88	0.56
1:A:360:VAL:HG13	1:A:362:ILE:HG23	1.88	0.56
1:D:360:VAL:HG13	1:D:362:ILE:HG23	1.88	0.56
3:C:703:P6G:C14	1:D:223:CYS:H	2.19	0.55
1:C:172:ILE:HG21	1:C:360:VAL:HG22	1.89	0.55
3:B:703:P6G:O19	1:G:478:THR:HG23	2.07	0.55
1:E:172:ILE:HG21	1:E:360:VAL:HG22	1.87	0.55
1:F:48:TRP:HH2	7:F:705:GOL:H2	1.71	0.55
1:G:360:VAL:HG13	1:G:362:ILE:HG23	1.87	0.55
1:H:594:ASN:OD1	1:H:602:LYS:NZ	2.37	0.55
1:G:172:ILE:HG21	1:G:360:VAL:HG22	1.88	0.54
1:H:315:PRO:HG2	1:H:477:VAL:CG1	2.37	0.54
1:B:360:VAL:HG13	1:B:362:ILE:HG23	1.88	0.54
1:D:172:ILE:HG21	1:D:360:VAL:HG22	1.90	0.54
1:H:592:ARG:NH2	1:H:635:ASP:OD1	2.41	0.54
1:H:172:ILE:HG21	1:H:360:VAL:HG22	1.89	0.54
1:A:172:ILE:HG21	1:A:360:VAL:HG22	1.90	0.53
1:C:582:ILE:HG13	1:C:583:VAL:HG23	1.89	0.53
1:H:315:PRO:HG2	1:H:477:VAL:HG11	1.89	0.53
1:B:172:ILE:HG21	1:B:360:VAL:HG22	1.89	0.53
1:F:197:ASP:O	1:F:662:ARG:NH1	2.42	0.53
1:H:197:ASP:O	1:H:662:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LEU:HB2	1:B:645:MET:HE3	1.91	0.53
1:G:606[A]:LEU:HD21	1:G:617:THR:HB	1.91	0.53
4:B:704:PGE:H5	1:G:507:LEU:HA	1.91	0.52
1:D:197:ASP:O	1:D:662:ARG:NH1	2.42	0.52
1:E:223:CYS:H	3:E:702:P6G:C14	2.22	0.52
1:E:649:GLN:HE21	1:E:651:LYS:HG2	1.72	0.52
1:F:172:ILE:HG21	1:F:360:VAL:HG22	1.89	0.52
1:G:28:LEU:HB2	1:G:645:MET:HE3	1.90	0.52
1:E:197:ASP:O	1:E:662:ARG:NH1	2.42	0.52
1:E:325:PHE:O	1:E:329[A]:VAL:HG22	2.09	0.52
1:F:223:CYS:N	3:F:703:P6G:H62	2.24	0.52
1:A:197:ASP:O	1:A:662:ARG:NH1	2.42	0.52
1:B:582:ILE:HG13	1:B:583:VAL:HG23	1.92	0.52
1:B:174:TYR:CD2	3:B:702:P6G:H51	2.45	0.51
1:C:408:ILE:HG12	1:C:409:PRO:HD2	1.92	0.51
1:G:592:ARG:NH2	1:G:635:ASP:OD1	2.43	0.51
1:D:329:VAL:HA	1:H:509:LEU:HD12	1.92	0.51
1:F:582:ILE:HG13	1:F:583:VAL:HG23	1.92	0.51
1:G:606[B]:LEU:HD11	1:G:617:THR:HB	1.91	0.51
1:E:337:LYS:NZ	9:E:805:HOH:O	2.43	0.51
1:B:329:VAL:HA	1:G:509:LEU:HD12	1.93	0.51
1:H:319:LYS:HB2	1:H:322:TYR:CD2	2.46	0.51
1:H:582:ILE:HG13	1:H:583:VAL:HG23	1.93	0.51
1:C:197:ASP:O	1:C:662:ARG:NH1	2.44	0.50
1:E:224:ASN:HD22	3:E:702:P6G:H172	1.77	0.50
1:H:408:ILE:HG12	1:H:409:PRO:HD2	1.93	0.50
1:E:582:ILE:HG13	1:E:583:VAL:HG23	1.92	0.50
1:F:48:TRP:CH2	7:F:705:GOL:H2	2.47	0.50
1:G:656:GLU:OE2	1:H:214:ARG:NH1	2.35	0.50
1:E:223:CYS:H	3:E:702:P6G:H141	1.77	0.50
1:B:408:ILE:HG12	1:B:409:PRO:HD2	1.93	0.50
1:D:649:GLN:NE2	1:D:651:LYS:HG2	2.27	0.50
1:B:364:PRO:HB2	1:B:369:LEU:HG	1.94	0.50
1:G:408:ILE:HG12	1:G:409:PRO:HD2	1.93	0.49
1:H:592:ARG:NH1	1:H:634:GLU:OE1	2.45	0.49
1:G:582:ILE:HG13	1:G:583:VAL:HG23	1.93	0.49
1:A:469:ARG:HD2	9:A:820:HOH:O	2.10	0.49
3:D:702:P6G:H111	1:H:479:SER:HA	1.94	0.49
1:E:319:LYS:HB2	1:E:322:TYR:CD2	2.47	0.49
1:D:408:ILE:HG12	1:D:409:PRO:HD2	1.94	0.49
1:H:649:GLN:NE2	1:H:651:LYS:HG2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:SER:HB3	3:B:703:P6G:H32	1.95	0.49
1:F:592:ARG:NH2	1:F:635:ASP:OD1	2.46	0.49
1:A:511:ALA:O	1:E:60:LYS:HE2	2.12	0.49
1:F:408:ILE:HG12	1:F:409:PRO:HD2	1.94	0.49
1:B:478:THR:HG23	3:B:703:P6G:H31	1.95	0.49
1:F:479:SER:HA	3:F:702:P6G:H82	1.94	0.49
1:G:197:ASP:O	1:G:662:ARG:NH1	2.46	0.49
1:A:132:TYR:CE2	1:A:134:ARG:HD2	2.48	0.48
1:F:649:GLN:NE2	1:F:651:LYS:HG2	2.28	0.48
1:C:469:ARG:HD2	9:C:837:HOH:O	2.12	0.48
1:C:629:ALA:HB1	1:C:645:MET:HE1	1.95	0.48
1:A:408:ILE:HG12	1:A:409:PRO:HD2	1.95	0.48
1:A:582:ILE:HG13	1:A:583:VAL:HG23	1.95	0.48
1:E:408:ILE:HG12	1:E:409:PRO:HD2	1.95	0.48
1:E:650:PHE:HB2	1:F:656:GLU:HA	1.95	0.48
1:F:319:LYS:HB2	1:F:322:TYR:CD2	2.48	0.48
3:F:703:P6G:H51	1:H:174:TYR:CG	2.48	0.48
1:A:48:TRP:HH2	4:A:703:PGE:H42	1.79	0.48
1:B:197:ASP:O	1:B:662:ARG:NH1	2.46	0.48
1:H:577:ARG:HG2	1:H:596:TYR:CZ	2.48	0.48
3:C:703:P6G:H142	1:D:223:CYS:H	1.77	0.48
1:C:511:ALA:O	1:F:60:LYS:HE2	2.14	0.48
1:E:555:GLU:O	1:E:559:ARG:HG3	2.14	0.48
1:B:650:PHE:HB2	1:D:656:GLU:HA	1.95	0.48
1:C:134:ARG:NH1	9:C:810:HOH:O	2.47	0.47
1:E:223:CYS:HB2	3:E:702:P6G:H141	1.94	0.47
1:F:469:ARG:HD2	9:F:806:HOH:O	2.14	0.47
1:D:101:TYR:HB3	1:D:191:LEU:HB3	1.96	0.47
1:B:592:ARG:NH1	1:B:634:GLU:OE1	2.46	0.47
1:G:129:THR:HG21	1:G:622:LEU:HD13	1.96	0.47
1:A:287:LYS:HE3	1:A:304:ARG:NH2	2.29	0.47
1:D:9:ILE:HG21	1:D:25:LEU:HD13	1.97	0.47
1:G:168:GLU:OE2	1:H:256:LYS:NZ	2.48	0.47
1:B:256:LYS:NZ	9:B:805:HOH:O	2.37	0.47
1:F:168:GLU:OE1	9:F:802:HOH:O	2.21	0.47
1:H:129:THR:HG21	1:H:622:LEU:HD13	1.96	0.47
1:B:319:LYS:HB2	1:B:322:TYR:CD2	2.50	0.47
1:D:129:THR:HG21	1:D:622:LEU:HD13	1.96	0.47
1:A:129:THR:HG21	1:A:622:LEU:HD13	1.97	0.47
1:B:129:THR:HG21	1:B:622:LEU:HD13	1.96	0.47
1:B:132:TYR:CE2	1:B:134:ARG:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:TYR:CE2	1:C:134:ARG:HD2	2.50	0.47
1:H:9:ILE:HG21	1:H:25:LEU:HD13	1.97	0.47
1:E:491:ARG:HD3	1:E:492:ALA:O	2.15	0.47
1:H:132:TYR:CE2	1:H:134:ARG:HD2	2.50	0.47
1:C:101:TYR:HB3	1:C:191:LEU:HB3	1.97	0.46
1:A:649:GLN:NE2	1:A:651:LYS:HG2	2.29	0.46
1:C:329:VAL:HA	1:F:509:LEU:HD12	1.97	0.46
1:D:555:GLU:O	1:D:559:ARG:HG3	2.16	0.46
1:E:97:ASN:HA	2:E:701:FAS:C6	2.45	0.46
1:G:491:ARG:HD3	1:G:492:ALA:O	2.15	0.46
1:B:649:GLN:NE2	1:B:651:LYS:HG2	2.30	0.46
1:C:606:LEU:HD21	1:C:617:THR:HB	1.98	0.46
1:B:555:GLU:O	1:B:559:ARG:HG3	2.14	0.46
1:E:319:LYS:HB2	1:E:322:TYR:HD2	1.80	0.46
1:G:9:ILE:HG21	1:G:25:LEU:HD13	1.97	0.46
1:H:491:ARG:HD3	1:H:492:ALA:O	2.16	0.46
1:F:9:ILE:HG21	1:F:25:LEU:HD13	1.97	0.46
1:A:4:PRO:HG2	1:A:7:PHE:CE2	2.51	0.46
1:G:555:GLU:O	1:G:559:ARG:HG3	2.16	0.46
1:H:577:ARG:HG2	1:H:596:TYR:CE1	2.51	0.46
1:A:555:GLU:O	1:A:559:ARG:HG3	2.16	0.46
1:B:9:ILE:HG21	1:B:25:LEU:HD13	1.97	0.46
1:C:9:ILE:HG21	1:C:25:LEU:HD13	1.98	0.46
1:D:99:MET:O	1:D:192:LYS:HA	2.16	0.46
1:A:42:ASN:HB2	3:B:702:P6G:H91	1.97	0.46
1:F:97:ASN:HA	2:F:701:FAS:C6	2.46	0.45
1:H:555:GLU:O	1:H:559:ARG:HG3	2.15	0.45
1:A:656:GLU:HA	1:C:650:PHE:HB2	1.98	0.45
9:D:898:HOH:O	1:H:80:ARG:HD2	2.16	0.45
1:E:200:ARG:NH1	9:E:810:HOH:O	2.49	0.45
1:H:99:MET:O	1:H:192:LYS:HA	2.17	0.45
1:A:161:GLN:HG2	3:C:702:P6G:H121	1.98	0.45
1:H:145:GLU:HG3	1:H:651:LYS:HD3	1.99	0.45
1:B:99:MET:O	1:B:192:LYS:HA	2.16	0.45
1:B:101:TYR:HB3	1:B:191:LEU:HB3	1.98	0.45
1:B:325:PHE:O	1:B:329:VAL:HG13	2.17	0.45
1:E:99:MET:O	1:E:192:LYS:HA	2.16	0.45
1:G:132:TYR:CE2	1:G:134:ARG:HD2	2.51	0.45
1:C:491:ARG:HD3	1:C:492:ALA:O	2.16	0.45
1:E:4:PRO:HG2	1:E:7:PHE:CE2	2.52	0.45
1:E:97:ASN:HB2	2:E:701:FAS:C4X	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:ASN:HB2	3:F:703:P6G:H22	1.98	0.45
1:G:97:ASN:HA	2:G:701:FAS:C6	2.47	0.45
1:A:99:MET:O	1:A:192:LYS:HA	2.17	0.45
1:B:4:PRO:HG2	1:B:7:PHE:CE2	2.52	0.45
1:B:270:THR:HA	1:B:607:SER:HB3	1.98	0.45
1:D:132:TYR:CE2	1:D:134:ARG:HD2	2.52	0.45
1:E:656:GLU:HA	1:G:650:PHE:HB2	1.98	0.45
1:B:319:LYS:HB2	1:B:322:TYR:HD2	1.82	0.45
1:C:129:THR:HG21	1:C:622:LEU:HD13	1.98	0.45
1:C:555:GLU:O	1:C:559:ARG:HG3	2.15	0.45
1:A:491:ARG:HD3	1:A:492:ALA:O	2.17	0.45
1:G:319:LYS:HB2	1:G:322:TYR:HD2	1.82	0.45
1:H:270:THR:HA	1:H:607:SER:HB3	1.99	0.45
1:F:555:GLU:O	1:F:559:ARG:HG3	2.17	0.45
1:A:9:ILE:HG21	1:A:25:LEU:HD13	1.99	0.44
1:C:270:THR:HA	1:C:607:SER:HB3	2.00	0.44
1:F:373:ASP:O	1:F:377:GLN:HG3	2.17	0.44
1:B:180:ASP:O	1:B:182:VAL:HG12	2.17	0.44
1:B:287:LYS:HE3	1:B:304:ARG:NH2	2.33	0.44
1:C:99:MET:O	1:C:192:LYS:HA	2.17	0.44
1:C:319:LYS:HB2	1:C:322:TYR:CD2	2.51	0.44
1:F:129:THR:HG21	1:F:622:LEU:HD13	1.99	0.44
9:B:958:HOH:O	1:G:80:ARG:HD2	2.17	0.44
1:F:4:PRO:HG2	1:F:7:PHE:CE2	2.53	0.44
1:G:649:GLN:NE2	1:G:651:LYS:HG2	2.31	0.44
1:A:48:TRP:CH2	4:A:703:PGE:H5	2.52	0.44
1:A:478:THR:HG21	1:A:519:THR:HG22	1.99	0.44
1:F:97:ASN:HB2	2:F:701:FAS:C4X	2.47	0.44
1:G:97:ASN:HB2	2:G:701:FAS:C4X	2.47	0.44
1:G:656:GLU:HA	1:H:650:PHE:HB2	2.00	0.44
3:B:703:P6G:H111	1:G:479:SER:HA	1.99	0.44
1:C:4:PRO:HG2	1:C:7:PHE:CE2	2.52	0.44
1:F:132:TYR:CE2	1:F:134:ARG:HD2	2.53	0.44
1:D:4:PRO:HG2	1:D:7:PHE:CE2	2.53	0.44
1:E:9:ILE:HG21	1:E:25:LEU:HD13	1.99	0.44
1:G:99:MET:O	1:G:192:LYS:HA	2.18	0.44
1:G:178:LEU:HD22	1:G:361:LYS:HD2	2.00	0.44
1:C:319:LYS:HB2	1:C:322:TYR:HD2	1.83	0.44
1:D:606:LEU:HD21	1:D:617:THR:HB	1.98	0.44
1:E:129:THR:HG21	1:E:622:LEU:HD13	1.99	0.44
1:C:223:CYS:N	3:C:702:P6G:H62	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:GLY:HA3	2:E:701:FAS:O5B	2.18	0.44
1:E:178:LEU:HD22	1:E:361:LYS:HD2	2.00	0.43
1:F:99:MET:O	1:F:192:LYS:HA	2.17	0.43
1:H:4:PRO:HG2	1:H:7:PHE:CE2	2.52	0.43
1:H:319:LYS:HB2	1:H:322:TYR:HD2	1.82	0.43
1:C:656:GLU:HA	1:D:650:PHE:HB2	2.00	0.43
1:F:491:ARG:HD3	1:F:492:ALA:O	2.17	0.43
1:E:132:TYR:CE2	1:E:134:ARG:HD2	2.53	0.43
1:G:592:ARG:NH1	1:G:634:GLU:OE1	2.46	0.43
1:A:606:LEU:HD21	1:A:617:THR:HB	2.00	0.43
1:B:161:GLN:HE21	3:B:702:P6G:H172	1.83	0.43
1:F:214:ARG:NH1	1:H:656:GLU:OE2	2.37	0.43
1:G:4:PRO:HG2	1:G:7:PHE:CE2	2.53	0.43
1:D:10:LEU:HD12	1:D:10:LEU:HA	1.89	0.43
1:D:582:ILE:HG13	1:D:583:VAL:HG23	2.01	0.43
1:A:274:PRO:HG3	1:A:571:THR:HB	2.01	0.43
1:C:97:ASN:HA	2:C:701:FAS:C6	2.48	0.43
1:D:160:CYS:HB3	9:D:896:HOH:O	2.18	0.43
1:D:511:ALA:O	1:H:60:LYS:HE2	2.18	0.43
1:E:111:ASP:OD2	1:E:387:LYS:NZ	2.51	0.43
1:A:55:TYR:CD1	1:A:56:PRO:HD3	2.54	0.43
1:C:161:GLN:NE2	3:C:703:P6G:H31	2.32	0.43
1:F:478:THR:HG23	3:F:702:P6G:O1	2.18	0.43
1:F:650:PHE:HB2	1:H:656:GLU:HA	2.00	0.43
1:C:223:CYS:H	3:C:702:P6G:H62	1.84	0.43
1:E:274:PRO:HG3	1:E:571:THR:HB	2.01	0.43
1:G:319:LYS:HB2	1:G:322:TYR:CD2	2.53	0.43
1:G:367:GLU:OE1	1:G:367:GLU:N	2.43	0.43
1:F:15:GLY:HA3	2:F:701:FAS:O5B	2.19	0.42
1:H:54:ILE:H	1:H:54:ILE:HG13	1.75	0.42
3:A:702:P6G:H172	1:E:407:LYS:O	2.18	0.42
1:C:378:GLU:OE1	1:C:381:ARG:NH1	2.52	0.42
1:C:605:ASP:HB2	2:C:701:FAS:O2P	2.19	0.42
1:D:325:PHE:O	1:D:329:VAL:HG22	2.19	0.42
1:A:650:PHE:HB2	1:B:656:GLU:HA	2.00	0.42
1:B:491:ARG:HD3	1:B:492:ALA:O	2.19	0.42
1:F:319:LYS:HB2	1:F:322:TYR:HD2	1.84	0.42
1:A:594:ASN:OD1	1:A:602:LYS:NZ	2.52	0.42
1:C:409:PRO:HD3	9:C:973:HOH:O	2.19	0.42
1:A:364:PRO:HB2	1:A:369:LEU:HG	2.00	0.42
1:B:381:ARG:HG2	1:B:385:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:259:ARG:HD2	9:H:875:HOH:O	2.19	0.42
1:B:478:THR:HG21	1:B:519:THR:HG22	2.00	0.42
1:C:55:TYR:CD1	1:C:56:PRO:HD3	2.55	0.42
1:D:55:TYR:CD1	1:D:56:PRO:HD3	2.54	0.42
1:H:287:LYS:HE3	1:H:304:ARG:NH2	2.35	0.42
1:B:55:TYR:CD1	1:B:56:PRO:HD3	2.54	0.42
1:E:270:THR:HA	1:E:607:SER:HB3	2.02	0.42
1:H:178:LEU:HD22	1:H:361:LYS:HD2	2.01	0.42
1:A:10:LEU:HD12	1:A:10:LEU:HA	1.88	0.41
1:A:97:ASN:HB2	2:A:701:FAS:C4X	2.50	0.41
1:C:200:ARG:HD2	9:C:804:HOH:O	2.19	0.41
1:D:270:THR:HA	1:D:607:SER:HB3	2.02	0.41
1:F:81:ARG:H	1:F:81:ARG:HG2	1.72	0.41
1:G:10:LEU:HD12	1:G:10:LEU:HA	1.91	0.41
1:A:223:CYS:H	3:B:702:P6G:C6	2.18	0.41
1:B:55:TYR:CG	1:B:56:PRO:HD3	2.55	0.41
1:D:55:TYR:CG	1:D:56:PRO:HD3	2.55	0.41
1:E:55:TYR:CD1	1:E:56:PRO:HD3	2.55	0.41
1:F:55:TYR:CD1	1:F:56:PRO:HD3	2.54	0.41
1:F:270:THR:HA	1:F:607:SER:HB3	2.01	0.41
1:C:161:GLN:NE2	3:C:703:P6G:H52	2.32	0.41
1:F:592:ARG:NH1	1:F:634:GLU:OE1	2.47	0.41
1:A:606:LEU:HD13	2:A:701:FAS:H5'2	2.02	0.41
1:C:157:TYR:HA	1:C:158:PRO:HD3	1.90	0.41
1:E:469:ARG:HD2	9:E:1036:HOH:O	2.20	0.41
1:F:178:LEU:HD22	1:F:361:LYS:HD2	2.01	0.41
1:F:581:LYS:HA	1:F:581:LYS:HD3	1.88	0.41
1:G:377:GLN:O	1:G:381:ARG:HG3	2.20	0.41
1:A:200:ARG:HD2	9:A:841:HOH:O	2.20	0.41
1:H:55:TYR:CD1	1:H:56:PRO:HD3	2.55	0.41
1:D:274:PRO:HG3	1:D:571:THR:HB	2.02	0.41
1:B:468:ARG:NE	1:B:544:ILE:HD11	2.35	0.41
1:C:274:PRO:HG3	1:C:571:THR:HB	2.02	0.41
1:D:491:ARG:HD3	1:D:492:ALA:O	2.19	0.41
1:G:6:GLU:HG3	1:G:259:ARG:HB2	2.03	0.41
1:A:395:TYR:HA	1:A:417:PHE:O	2.21	0.41
1:B:274:PRO:HG3	1:B:571:THR:HB	2.03	0.41
1:C:55:TYR:CG	1:C:56:PRO:HD3	2.55	0.41
1:G:81:ARG:H	1:G:81:ARG:HG2	1.70	0.41
1:G:101:TYR:HB3	1:G:191:LEU:HB3	2.01	0.41
1:H:299:LEU:HD23	1:H:299:LEU:HA	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:395:TYR:HA	1:G:417:PHE:O	2.21	0.41
1:E:55:TYR:CG	1:E:56:PRO:HD3	2.56	0.40
1:G:15:GLY:HA3	2:G:701:FAS:O5B	2.21	0.40
1:G:74:SER:HA	1:G:75:PRO:HD3	1.94	0.40
1:G:308:ASP:OD1	1:G:309:HIS:N	2.54	0.40
1:A:509:LEU:HD12	1:E:329[A]:VAL:HA	2.02	0.40
2:D:701:FAS:H51A	9:D:851:HOH:O	2.20	0.40
1:E:395:TYR:HA	1:E:417:PHE:O	2.22	0.40
1:A:55:TYR:CG	1:A:56:PRO:HD3	2.57	0.40
1:D:81:ARG:H	1:D:81:ARG:HG2	1.71	0.40
1:E:6:GLU:HG3	1:E:259:ARG:HB2	2.02	0.40
1:H:98:PHE:HB2	2:H:701:FAS:O4	2.21	0.40
1:H:395:TYR:HA	1:H:417:PHE:O	2.21	0.40
1:C:656:GLU:OE2	1:D:214:ARG:NH1	2.38	0.40
1:D:395:TYR:HA	1:D:417:PHE:O	2.21	0.40
1:B:395:TYR:HA	1:B:417:PHE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	660/663 (100%)	638 (97%)	22 (3%)	0	100	100
All	All	5282/5304 (100%)	5102 (97%)	180 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ARG
1	A	134	ARG
1	A	149	LYS
1	A	178	LEU
1	A	251	LYS
1	A	317	ARG
1	A	325	PHE
1	A	360	VAL
1	A	418	HIS
1	A	456	MET

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Mol	Chain	Res	Type
1	A	478	THR
1	A	491	ARG
1	A	580	SER
1	A	606	LEU
1	A	656	GLU
1	B	57	ARG
1	B	81	ARG
1	B	134	ARG
1	B	149	LYS
1	B	178	LEU
1	B	182	VAL
1	B	191	LEU
1	B	251	LYS
1	B	296	LEU
1	B	317	ARG
1	B	325	PHE
1	B	360	VAL
1	B	418	HIS
1	B	456	MET
1	B	478	THR
1	B	491	ARG
1	B	578	GLU
1	B	580	SER
1	B	656	GLU
1	C	57	ARG
1	C	81	ARG
1	C	134	ARG
1	C	145	GLU
1	C	149	LYS
1	C	178	LEU
1	C	191	LEU
1	C	251	LYS
1	C	317	ARG
1	C	321	GLN
1	C	325	PHE
1	C	329	VAL
1	C	360	VAL
1	C	418	HIS
1	C	456	MET
1	C	478	THR
1	C	491	ARG
1	C	523	LYS

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Mol	Chain	Res	Type
1	C	580	SER
1	C	592	ARG
1	C	606	LEU
1	C	656	GLU
1	D	57	ARG
1	D	81	ARG
1	D	134	ARG
1	D	149	LYS
1	D	178	LEU
1	D	191	LEU
1	D	251	LYS
1	D	296	LEU
1	D	317	ARG
1	D	321	GLN
1	D	325	PHE
1	D	360	VAL
1	D	378	GLU
1	D	418	HIS
1	D	456	MET
1	D	491	ARG
1	D	548	GLU
1	D	580	SER
1	D	606	LEU
1	D	656	GLU
1	E	57	ARG
1	E	81	ARG
1	E	134	ARG
1	E	149	LYS
1	E	178	LEU
1	E	251	LYS
1	E	317	ARG
1	E	321	GLN
1	E	325	PHE
1	E	360	VAL
1	E	418	HIS
1	E	456	MET
1	E	478	THR
1	E	491	ARG
1	E	580	SER
1	E	606	LEU
1	E	656	GLU
1	F	60	LYS

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Mol	Chain	Res	Type
1	F	81	ARG
1	F	134	ARG
1	F	145	GLU
1	F	149	LYS
1	F	178	LEU
1	F	191	LEU
1	F	251	LYS
1	F	296	LEU
1	F	317	ARG
1	F	325	PHE
1	F	360	VAL
1	F	418	HIS
1	F	456	MET
1	F	478	THR
1	F	491	ARG
1	F	580	SER
1	F	592	ARG
1	F	606	LEU
1	F	656	GLU
1	G	57	ARG
1	G	81	ARG
1	G	134	ARG
1	G	149	LYS
1	G	178	LEU
1	G	191	LEU
1	G	251	LYS
1	G	317	ARG
1	G	325	PHE
1	G	360	VAL
1	G	418	HIS
1	G	456	MET
1	G	478	THR
1	G	491	ARG
1	G	515	HIS
1	G	580	SER
1	G	656	GLU
1	H	57	ARG
1	H	60	LYS
1	H	81	ARG
1	H	134	ARG
1	H	145	GLU
1	H	149	LYS

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Mol	Chain	Res	Type
1	H	178	LEU
1	H	251	LYS
1	H	296	LEU
1	H	317	ARG
1	H	321	GLN
1	H	325	PHE
1	H	360	VAL
1	H	418	HIS
1	H	456	MET
1	H	477	VAL
1	H	478	THR
1	H	491	ARG
1	H	577	ARG
1	H	580	SER
1	H	656	GLU

Sometimes 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
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 monosaccharides 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	$\#\|Z\| > 2$
3	P6G	E	702	-	18,18,18	0.48	0	17,17,17	0.40	0
4	PGE	E	703	-	9,9,9	0.37	0	8,8,8	0.23	0
3	P6G	A	702	-	18,18,18	0.46	0	17,17,17	0.38	0
2	FAS	F	701	-	53,58,58	1.25	5 (9%)	68,89,89	1.35	11 (16%)
4	PGE	G	703	-	9,9,9	0.33	0	8,8,8	0.25	0
3	P6G	D	702	-	18,18,18	0.47	0	17,17,17	0.30	0
3	P6G	F	702	-	18,18,18	0.45	0	17,17,17	0.45	0
2	FAS	D	701	-	53,58,58	1.26	5 (9%)	68,89,89	1.34	11 (16%)
7	GOL	C	705[B]	6	5,5,5	0.37	0	5,5,5	0.29	0
3	P6G	F	703	-	18,18,18	0.46	0	17,17,17	0.38	0
2	FAS	C	701	-	53,58,58	1.25	5 (9%)	68,89,89	1.35	11 (16%)
4	PGE	C	704	-	9,9,9	0.37	0	8,8,8	0.21	0
2	FAS	B	701	-	53,58,58	1.28	5 (9%)	68,89,89	1.34	9 (13%)
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
4	PGE	A	703	-	9,9,9	0.31	0	8,8,8	0.34	0
2	FAS	H	701	-	53,58,58	1.28	5 (9%)	68,89,89	1.34	10 (14%)
5	PO4	F	704	-	4,4,4	0.80	0	6,6,6	0.38	0
4	PGE	B	705	-	9,9,9	0.32	0	8,8,8	0.28	0
7	GOL	F	705	-	5,5,5	0.36	0	5,5,5	0.27	0
4	PGE	D	703	-	9,9,9	0.32	0	8,8,8	0.29	0
4	PGE	B	704	-	9,9,9	0.32	0	8,8,8	0.29	0
2	FAS	G	701	-	53,58,58	1.26	5 (9%)	68,89,89	1.37	9 (13%)
3	P6G	B	703	-	18,18,18	0.44	0	17,17,17	0.51	0
3	P6G	C	702	-	18,18,18	0.45	0	17,17,17	0.42	0
5	PO4	A	704[B]	-	4,4,4	1.02	0	6,6,6	0.57	0
3	P6G	B	702	-	18,18,18	0.48	0	17,17,17	0.37	0
2	FAS	E	701	-	53,58,58	1.32	6 (11%)	68,89,89	1.32	10 (14%)
4	PGE	H	702	-	9,9,9	0.32	0	8,8,8	0.25	0
2	FAS	A	701	-	53,58,58	1.31	5 (9%)	68,89,89	1.35	10 (14%)

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	P6G	E	702	-	-	7/16/16/16	-
4	PGE	E	703	-	-	2/7/7/7	-
3	P6G	A	702	-	-	2/16/16/16	-
2	FAS	F	701	-	-	3/30/50/50	0/6/6/6
4	PGE	G	703	-	-	5/7/7/7	-
3	P6G	D	702	-	-	1/16/16/16	-
3	P6G	F	702	-	-	5/16/16/16	-
2	FAS	D	701	-	-	3/30/50/50	0/6/6/6
7	GOL	C	705[B]	6	-	2/4/4/4	-
3	P6G	F	703	-	-	3/16/16/16	-
2	FAS	C	701	-	-	3/30/50/50	0/6/6/6
4	PGE	C	704	-	-	5/7/7/7	-
2	FAS	B	701	-	-	4/30/50/50	0/6/6/6
3	P6G	C	703	-	-	8/16/16/16	-
4	PGE	G	702	-	-	4/7/7/7	-
4	PGE	A	703	-	-	5/7/7/7	-
2	FAS	H	701	-	-	3/30/50/50	0/6/6/6
4	PGE	B	705	-	-	5/7/7/7	-
7	GOL	F	705	-	-	0/4/4/4	-
4	PGE	D	703	-	-	5/7/7/7	-
4	PGE	B	704	-	-	6/7/7/7	-
2	FAS	G	701	-	-	1/30/50/50	0/6/6/6
3	P6G	B	703	-	-	5/16/16/16	-
3	P6G	C	702	-	-	3/16/16/16	-
3	P6G	B	702	-	-	4/16/16/16	-
2	FAS	E	701	-	-	2/30/50/50	0/6/6/6
4	PGE	H	702	-	-	3/7/7/7	-
2	FAS	A	701	-	-	3/30/50/50	0/6/6/6

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	FAS	C9A-C5X	5.04	1.49	1.41
2	E	701	FAS	C9A-C5X	4.86	1.49	1.41
2	C	701	FAS	C9A-C5X	4.81	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FAS	C9A-C5X	4.81	1.49	1.41
2	H	701	FAS	C9A-C5X	4.78	1.49	1.41
2	D	701	FAS	C9A-C5X	4.77	1.49	1.41
2	F	701	FAS	C9A-C5X	4.77	1.49	1.41
2	G	701	FAS	C9A-C5X	4.66	1.49	1.41
2	E	701	FAS	C8-C7	3.41	1.49	1.40
2	H	701	FAS	C8-C7	3.26	1.49	1.40
2	B	701	FAS	C8-C7	3.24	1.49	1.40
2	F	701	FAS	C8-C7	3.19	1.48	1.40
2	A	701	FAS	C8-C7	3.16	1.48	1.40
2	D	701	FAS	C8-C7	3.12	1.48	1.40
2	C	701	FAS	C8-C7	3.09	1.48	1.40
2	G	701	FAS	C8-C7	3.08	1.48	1.40
2	C	701	FAS	C4X-N5	2.80	1.36	1.30
2	E	701	FAS	C4-N3	-2.78	1.33	1.38
2	B	701	FAS	C4X-N5	2.76	1.36	1.30
2	D	701	FAS	C4X-N5	2.72	1.36	1.30
2	A	701	FAS	C4-N3	-2.72	1.33	1.38
2	F	701	FAS	C4X-N5	2.72	1.36	1.30
2	H	701	FAS	C4X-N5	2.68	1.36	1.30
2	E	701	FAS	C4X-N5	2.63	1.35	1.30
2	G	701	FAS	C4X-N5	2.60	1.35	1.30
2	A	701	FAS	C4X-N5	2.59	1.35	1.30
2	B	701	FAS	C5A-C4A	2.56	1.47	1.40
2	A	701	FAS	C5A-C4A	2.52	1.47	1.40
2	F	701	FAS	C5A-C4A	2.50	1.47	1.40
2	E	701	FAS	C5A-C4A	2.48	1.47	1.40
2	G	701	FAS	C5A-C4A	2.48	1.47	1.40
2	B	701	FAS	C4-N3	-2.46	1.34	1.38
2	H	701	FAS	C5A-C4A	2.43	1.47	1.40
2	H	701	FAS	C4-N3	-2.43	1.34	1.38
2	G	701	FAS	C4-N3	-2.41	1.34	1.38
2	C	701	FAS	C5A-C4A	2.38	1.47	1.40
2	D	701	FAS	C5A-C4A	2.34	1.47	1.40
2	D	701	FAS	C4-N3	-2.30	1.34	1.38
2	F	701	FAS	C4-N3	-2.17	1.34	1.38
2	C	701	FAS	C4-N3	-2.16	1.34	1.38
2	E	701	FAS	C10-N10	2.04	1.41	1.37

All (81) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	FAS	C4-C4X-N5	3.74	123.56	118.23
2	F	701	FAS	C4-C4X-N5	3.74	123.56	118.23
2	D	701	FAS	C4-C4X-N5	3.68	123.47	118.23
2	G	701	FAS	C4-C4X-N5	3.65	123.43	118.23
2	C	701	FAS	C4-C4X-N5	3.57	123.31	118.23
2	D	701	FAS	N3A-C2A-N1A	-3.35	123.44	128.68
2	G	701	FAS	N3A-C2A-N1A	-3.30	123.52	128.68
2	A	701	FAS	C4A-C5A-N7A	-3.30	105.96	109.40
2	H	701	FAS	C4-C4X-N5	3.29	122.92	118.23
2	F	701	FAS	N3A-C2A-N1A	-3.29	123.54	128.68
2	E	701	FAS	N3A-C2A-N1A	-3.27	123.56	128.68
2	A	701	FAS	C4-C4X-N5	3.25	122.85	118.23
2	H	701	FAS	N3A-C2A-N1A	-3.25	123.61	128.68
2	E	701	FAS	C4-C4X-N5	3.12	122.67	118.23
2	B	701	FAS	N3A-C2A-N1A	-3.04	123.92	128.68
2	G	701	FAS	C4A-C5A-N7A	-3.01	106.27	109.40
2	C	701	FAS	C4A-C5A-N7A	-2.96	106.31	109.40
2	A	701	FAS	N3A-C2A-N1A	-2.96	124.05	128.68
2	B	701	FAS	C9A-C5X-N5	-2.96	119.22	122.43
2	H	701	FAS	C4A-C5A-N7A	-2.91	106.37	109.40
2	C	701	FAS	N3A-C2A-N1A	-2.87	124.20	128.68
2	G	701	FAS	C9A-C5X-N5	-2.85	119.33	122.43
2	F	701	FAS	C4A-C5A-N7A	-2.83	106.45	109.40
2	B	701	FAS	P-O3-PA	-2.83	123.13	132.83
2	B	701	FAS	C4A-C5A-N7A	-2.80	106.48	109.40
2	E	701	FAS	C4X-C10-N1	-2.73	118.40	124.73
2	D	701	FAS	C9A-C5X-N5	-2.70	119.50	122.43
2	C	701	FAS	C9A-C5X-N5	-2.65	119.56	122.43
2	D	701	FAS	C4A-C5A-N7A	-2.61	106.68	109.40
2	C	701	FAS	O2-C2-N1	-2.60	117.51	121.83
2	E	701	FAS	C4A-C5A-N7A	-2.58	106.70	109.40
2	F	701	FAS	C9A-N10-C10	-2.56	116.78	120.77
2	D	701	FAS	P-O3-PA	-2.55	124.07	132.83
2	A	701	FAS	C9A-C5X-N5	-2.53	119.68	122.43
2	A	701	FAS	C4X-C10-N1	-2.53	118.86	124.73
2	H	701	FAS	C1'-C2'-C3'	-2.48	102.87	109.79
2	E	701	FAS	P-O3-PA	-2.46	124.38	132.83
2	H	701	FAS	C9A-C5X-N5	-2.44	119.78	122.43
2	A	701	FAS	P-O3-PA	-2.43	124.48	132.83
2	H	701	FAS	C4X-C10-N1	-2.43	119.09	124.73
2	F	701	FAS	C9A-C5X-N5	-2.42	119.81	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	701	FAS	C9A-N10-C10	-2.40	117.02	120.77
2	H	701	FAS	P-O3-PA	-2.39	124.61	132.83
2	F	701	FAS	C4X-C10-N1	-2.39	119.19	124.73
2	F	701	FAS	C10-N1-C2	2.37	121.65	116.90
2	D	701	FAS	C4X-C10-N1	-2.33	119.31	124.73
2	H	701	FAS	C9A-N10-C10	-2.29	117.19	120.77
2	C	701	FAS	O4-C4-C4X	-2.25	120.64	126.60
2	C	701	FAS	C9A-N10-C10	-2.25	117.27	120.77
2	G	701	FAS	C4X-C10-N1	-2.24	119.53	124.73
2	B	701	FAS	C4X-C10-N1	-2.23	119.55	124.73
2	C	701	FAS	C4X-C10-N1	-2.22	119.58	124.73
2	B	701	FAS	C9A-N10-C10	-2.20	117.34	120.77
2	D	701	FAS	O2-C2-N1	-2.19	118.20	121.83
2	D	701	FAS	C10-C4X-N5	-2.15	120.30	124.86
2	A	701	FAS	O2P-P-O1P	2.14	122.82	112.24
2	G	701	FAS	C9A-N10-C10	-2.13	117.44	120.77
2	E	701	FAS	C2A-N1A-C6A	2.13	122.40	118.75
2	A	701	FAS	C9A-N10-C10	-2.13	117.45	120.77
2	D	701	FAS	C9A-N10-C10	-2.13	117.45	120.77
2	B	701	FAS	C4X-C4-N3	2.12	118.58	113.19
2	A	701	FAS	C10-N1-C2	2.12	121.13	116.90
2	A	701	FAS	C4X-C4-N3	2.11	118.56	113.19
2	D	701	FAS	C10-N1-C2	2.11	121.11	116.90
2	C	701	FAS	P-O3-PA	-2.10	125.62	132.83
2	C	701	FAS	C10-C4X-N5	-2.09	120.42	124.86
2	G	701	FAS	P-O3-PA	-2.09	125.67	132.83
2	F	701	FAS	C4X-C4-N3	2.08	118.47	113.19
2	E	701	FAS	C4X-C4-N3	2.06	118.41	113.19
2	D	701	FAS	O4-C4-C4X	-2.05	121.16	126.60
2	G	701	FAS	C10-C4X-N5	-2.05	120.50	124.86
2	H	701	FAS	O4-C4-C4X	-2.04	121.18	126.60
2	G	701	FAS	C4X-C4-N3	2.03	118.36	113.19
2	E	701	FAS	C10-N1-C2	2.03	120.97	116.90
2	F	701	FAS	C10-C4X-N5	-2.03	120.54	124.86
2	E	701	FAS	N3-C2-N1	2.03	123.37	119.38
2	C	701	FAS	C4X-C4-N3	2.02	118.33	113.19
2	F	701	FAS	O4-C4-C4X	-2.02	121.25	126.60
2	H	701	FAS	C10-N1-C2	2.01	120.93	116.90
2	F	701	FAS	O2P-P-O1P	2.01	122.19	112.24
2	B	701	FAS	C10-C4X-N5	-2.01	120.58	124.86

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	701	FAS	O4B-C4B-C5B-O5B
7	C	705[B]	GOL	O1-C1-C2-C3
2	B	701	FAS	O4B-C4B-C5B-O5B
2	B	701	FAS	C3B-C4B-C5B-O5B
2	C	701	FAS	O4B-C4B-C5B-O5B
2	D	701	FAS	C3B-C4B-C5B-O5B
3	C	702	P6G	O13-C14-C15-O16
3	C	703	P6G	O4-C5-C6-O7
3	C	703	P6G	O7-C8-C9-O10
3	B	702	P6G	O10-C11-C12-O13
4	A	703	PGE	O2-C3-C4-O3
3	E	702	P6G	O10-C11-C12-O13
4	C	704	PGE	O2-C3-C4-O3
4	B	704	PGE	O3-C5-C6-O4
3	E	702	P6G	O7-C8-C9-O10
7	C	705[B]	GOL	O1-C1-C2-O2
3	A	702	P6G	O16-C17-C18-O19
4	B	705	PGE	O3-C5-C6-O4
4	B	704	PGE	O2-C3-C4-O3
3	E	702	P6G	O1-C2-C3-O4
4	C	704	PGE	O1-C1-C2-O2
4	D	703	PGE	O3-C5-C6-O4
4	G	703	PGE	O3-C5-C6-O4
4	A	703	PGE	O1-C1-C2-O2
4	C	704	PGE	O3-C5-C6-O4
4	G	703	PGE	O2-C3-C4-O3
2	C	701	FAS	C3B-C4B-C5B-O5B
3	F	702	P6G	O7-C8-C9-O10
3	B	703	P6G	O1-C2-C3-O4
3	C	703	P6G	O16-C17-C18-O19
3	F	702	P6G	O1-C2-C3-O4
2	H	701	FAS	O4B-C4B-C5B-O5B
3	F	703	P6G	O7-C8-C9-O10
4	G	702	PGE	O1-C1-C2-O2
2	F	701	FAS	O4B-C4B-C5B-O5B
4	D	703	PGE	C1-C2-O2-C3
3	F	702	P6G	C6-C5-O4-C3
2	A	701	FAS	PA-O3-P-O5'
2	D	701	FAS	PA-O3-P-O5'
2	E	701	FAS	PA-O3-P-O5'
2	F	701	FAS	PA-O3-P-O5'
2	H	701	FAS	PA-O3-P-O5'

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Mol	Chain	Res	Type	Atoms
2	A	701	FAS	O4B-C4B-C5B-O5B
4	B	705	PGE	O1-C1-C2-O2
4	G	702	PGE	C1-C2-O2-C3
3	C	702	P6G	C8-C9-O10-C11
4	E	703	PGE	C1-C2-O2-C3
3	C	703	P6G	C5-C6-O7-C8
3	E	702	P6G	C18-C17-O16-C15
3	F	702	P6G	C9-C8-O7-C6
3	E	702	P6G	C11-C12-O13-C14
3	B	702	P6G	C12-C11-O10-C9
3	C	703	P6G	C15-C14-O13-C12
4	A	703	PGE	C6-C5-O3-C4
4	G	702	PGE	C6-C5-O3-C4
3	E	702	P6G	C14-C15-O16-C17
4	D	703	PGE	C3-C4-O3-C5
3	B	703	P6G	C9-C8-O7-C6
3	B	703	P6G	C6-C5-O4-C3
4	B	704	PGE	C1-C2-O2-C3
4	G	703	PGE	C1-C2-O2-C3
4	G	702	PGE	C3-C4-O3-C5
4	B	704	PGE	C4-C3-O2-C2
3	F	703	P6G	C8-C9-O10-C11
4	G	703	PGE	C3-C4-O3-C5
4	A	703	PGE	C3-C4-O3-C5
3	E	702	P6G	O13-C14-C15-O16
3	D	702	P6G	C9-C8-O7-C6
3	B	703	P6G	C5-C6-O7-C8
3	A	702	P6G	C18-C17-O16-C15
3	B	703	P6G	C2-C3-O4-C5
3	C	703	P6G	O1-C2-C3-O4
4	B	704	PGE	O1-C1-C2-O2
4	B	704	PGE	C3-C4-O3-C5
4	C	704	PGE	C3-C4-O3-C5
4	B	705	PGE	O2-C3-C4-O3
4	G	703	PGE	O1-C1-C2-O2
3	B	702	P6G	O7-C8-C9-O10
3	C	702	P6G	O4-C5-C6-O7
2	E	701	FAS	O4B-C4B-C5B-O5B
2	H	701	FAS	C3B-C4B-C5B-O5B
2	G	701	FAS	O4B-C4B-C5B-O5B
3	C	703	P6G	O13-C14-C15-O16
4	C	704	PGE	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
4	H	702	PGE	C4-C3-O2-C2
3	C	703	P6G	C9-C8-O7-C6
3	B	702	P6G	C5-C6-O7-C8
4	B	705	PGE	C6-C5-O3-C4
2	B	701	FAS	O2'-C2'-C3'-O3'
2	B	701	FAS	PA-O3-P-O5'
4	H	702	PGE	C1-C2-O2-C3
2	F	701	FAS	C3B-C4B-C5B-O5B
4	A	703	PGE	C4-C3-O2-C2
4	B	705	PGE	C3-C4-O3-C5
4	D	703	PGE	C6-C5-O3-C4
2	A	701	FAS	C3B-C4B-C5B-O5B
4	E	703	PGE	O1-C1-C2-O2
3	F	702	P6G	O4-C5-C6-O7
4	D	703	PGE	O2-C3-C4-O3
2	C	701	FAS	N10-C1'-C2'-O2'
4	H	702	PGE	O2-C3-C4-O3
3	F	703	P6G	C9-C8-O7-C6

There are no ring outliers.

23 monomers are involved in 61 short contacts:

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

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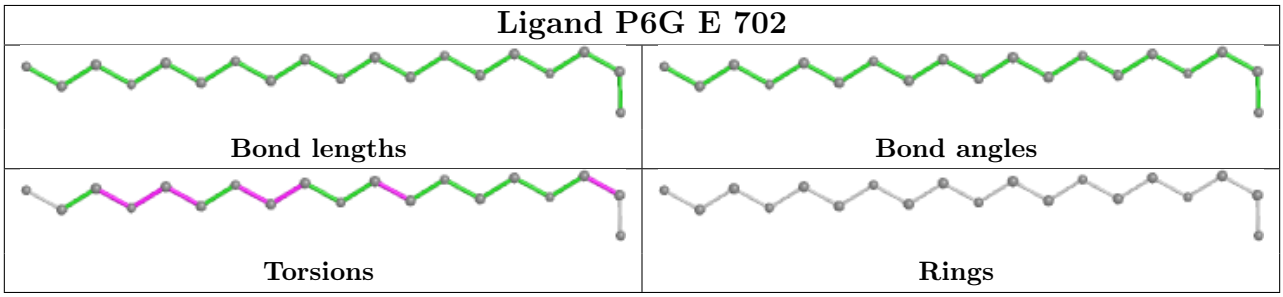
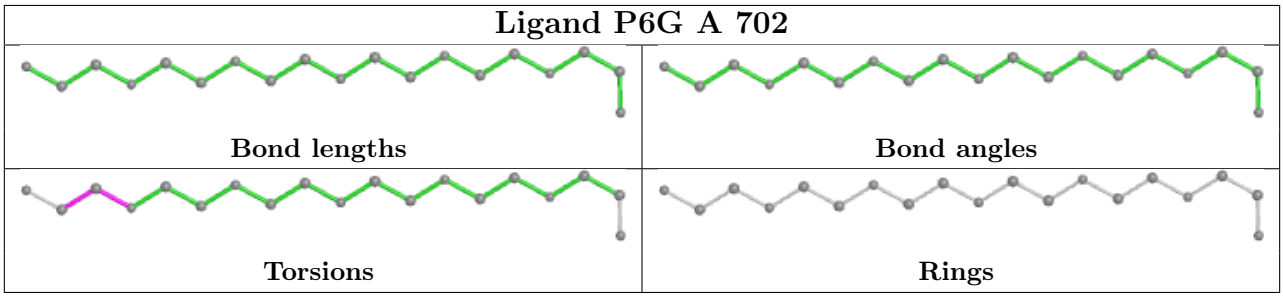
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	P6G	6	0
2	E	701	FAS	3	0
4	H	702	PGE	1	0
2	A	701	FAS	2	0

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 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.





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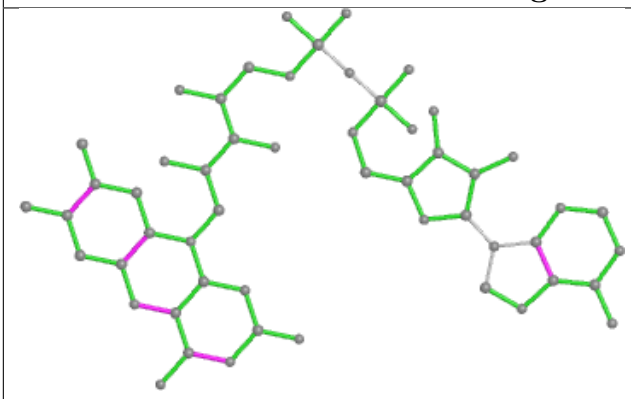
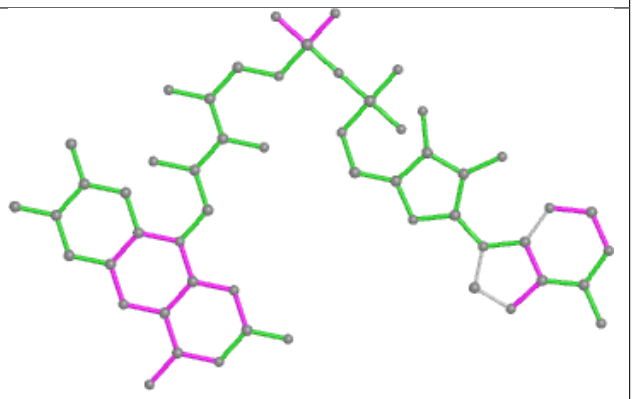
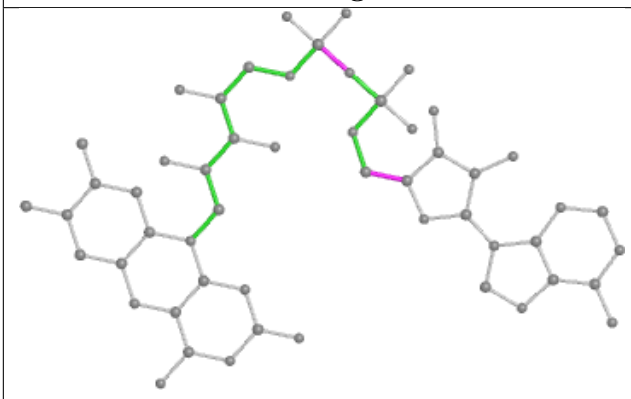


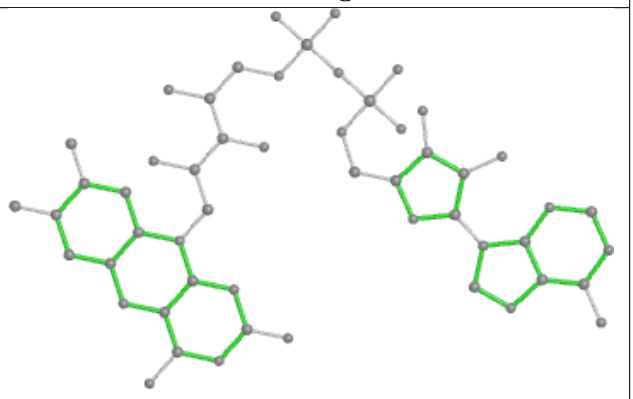
Bond lengths



Bond angles

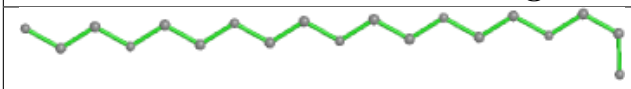


Torsions

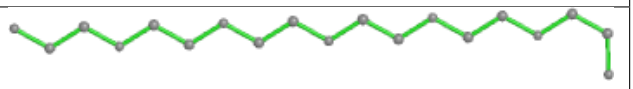


Rings

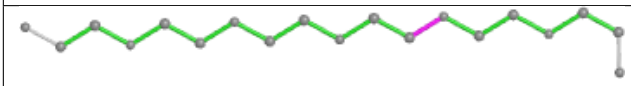
Ligand P6G D 702



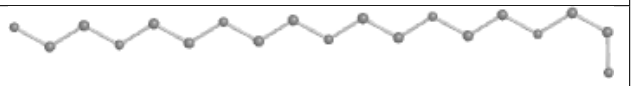
Bond lengths



Bond angles

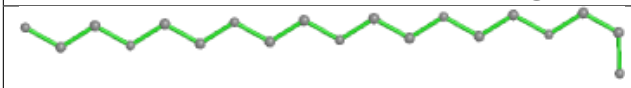


Torsions

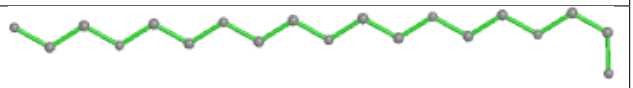


Rings

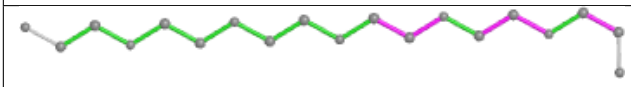
Ligand P6G F 702



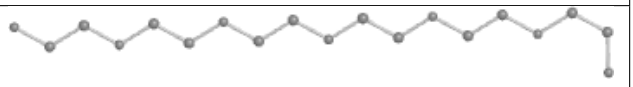
Bond lengths



Bond angles

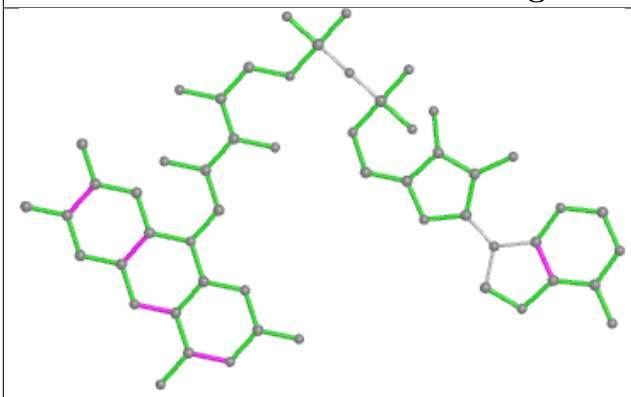


Torsions

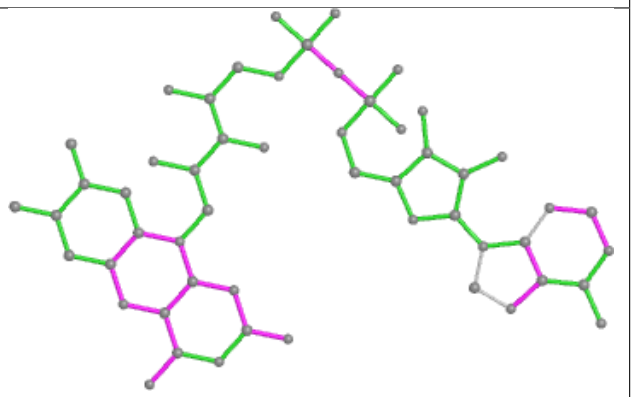


Rings

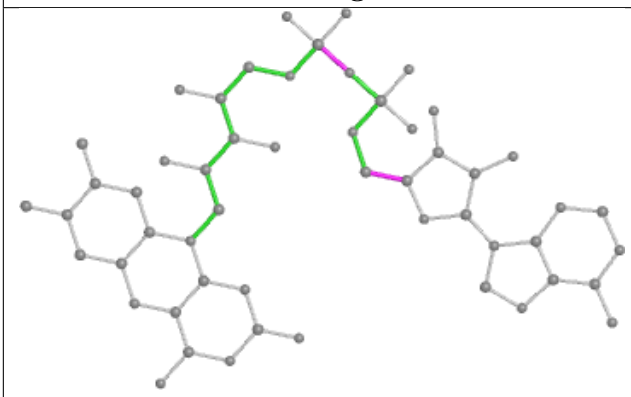
Ligand FAS D 701



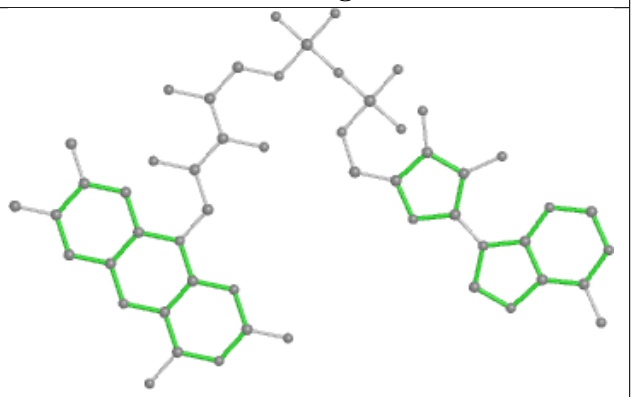
Bond lengths



Bond angles

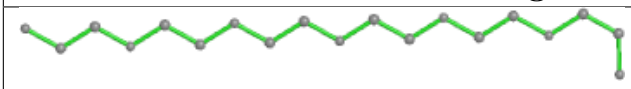


Torsions

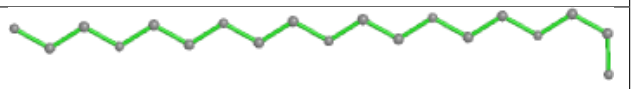


Rings

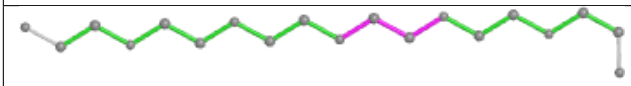
Ligand P6G F 703



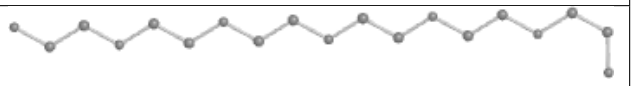
Bond lengths



Bond angles

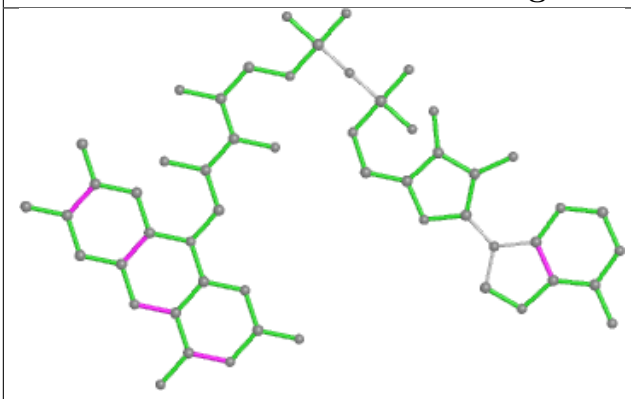


Torsions

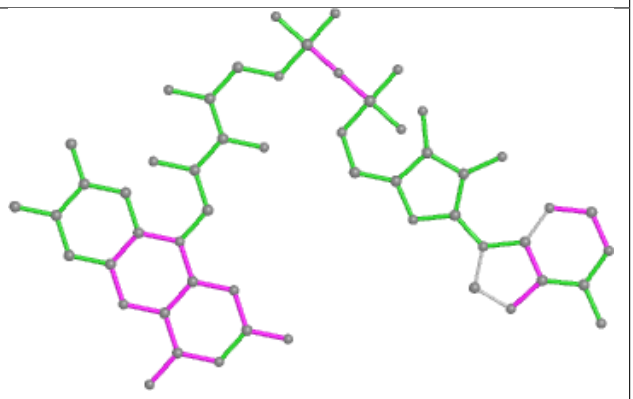


Rings

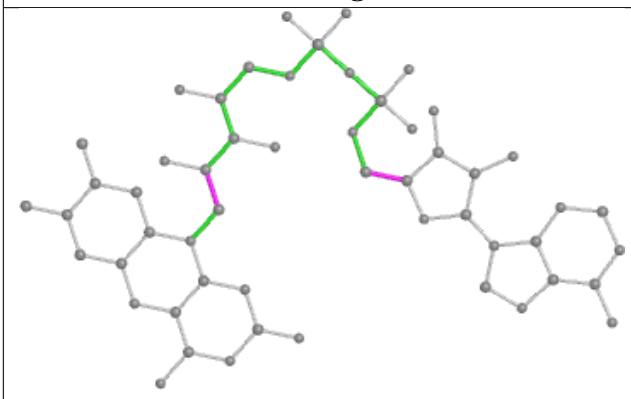
Ligand FAS C 701



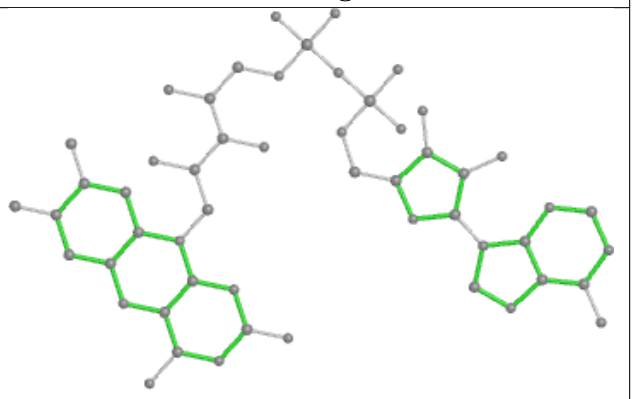
Bond lengths



Bond angles

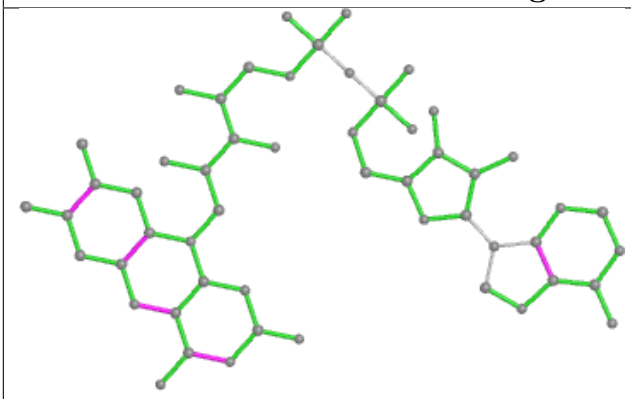


Torsions

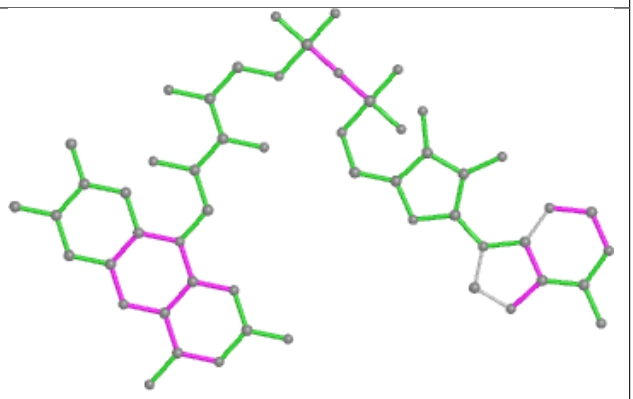


Rings

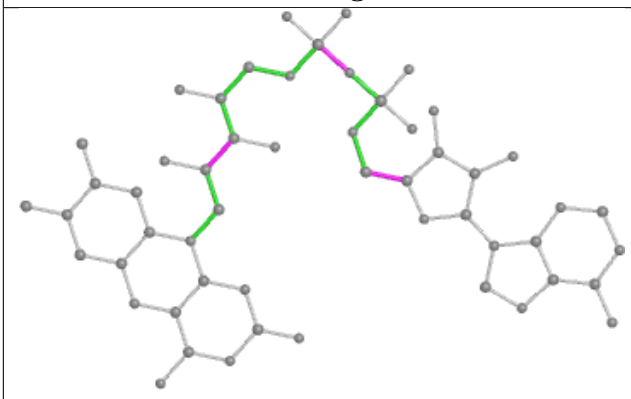
Ligand FAS B 701



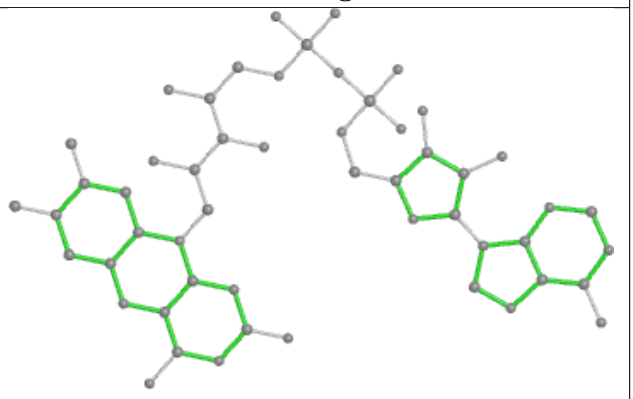
Bond lengths



Bond angles

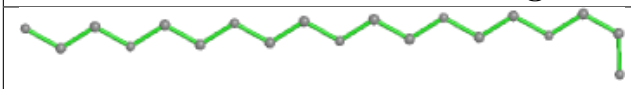


Torsions

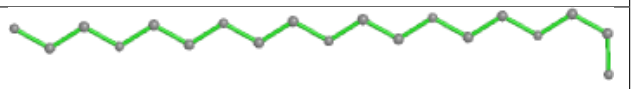


Rings

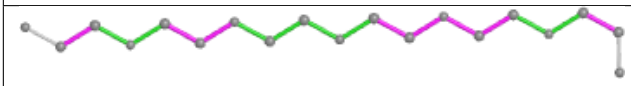
Ligand P6G C 703



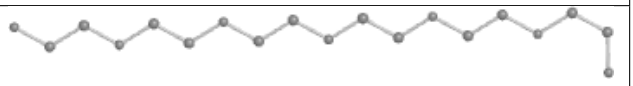
Bond lengths



Bond angles

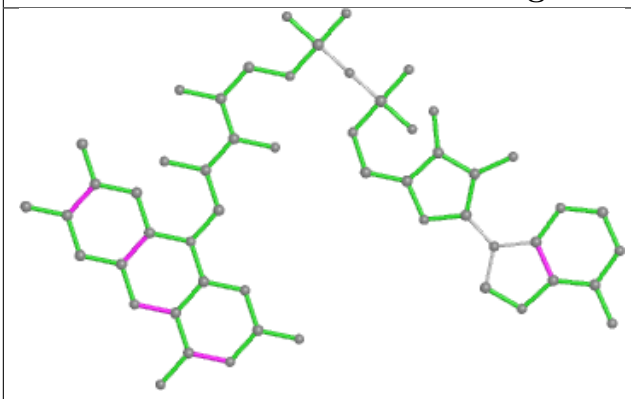


Torsions

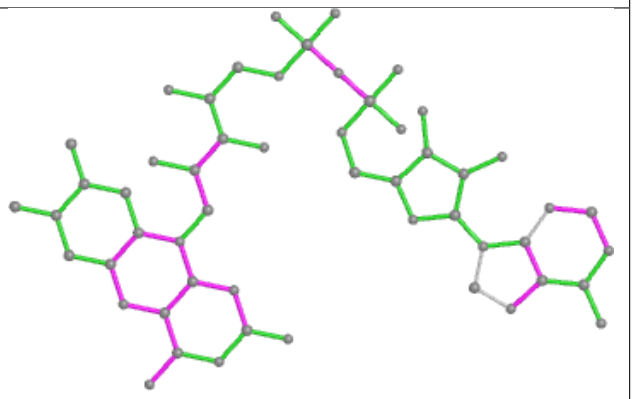


Rings

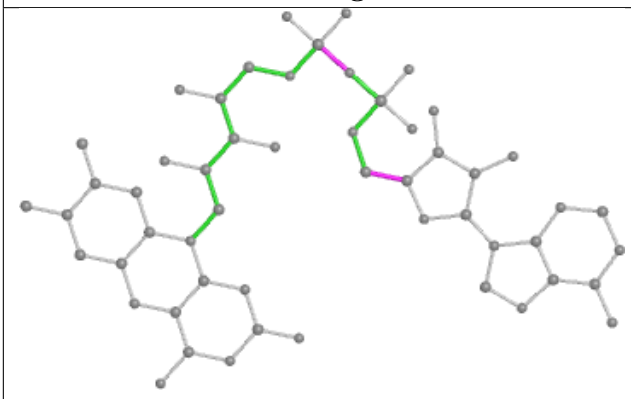
Ligand FAS H 701



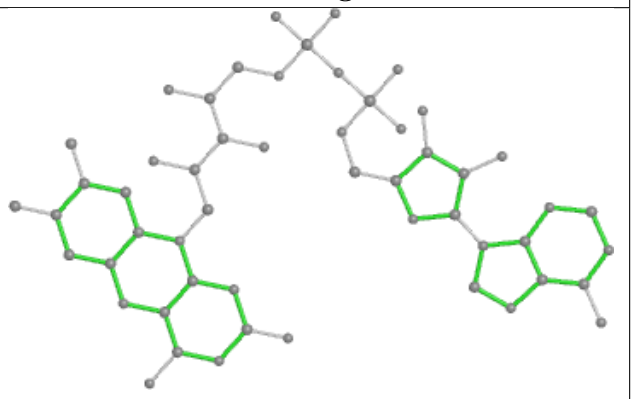
Bond lengths



Bond angles

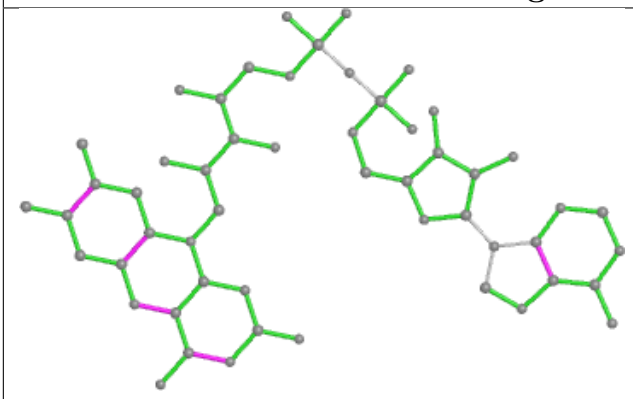


Torsions

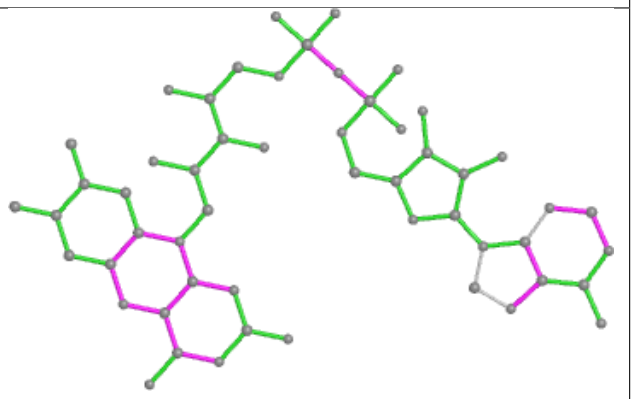


Rings

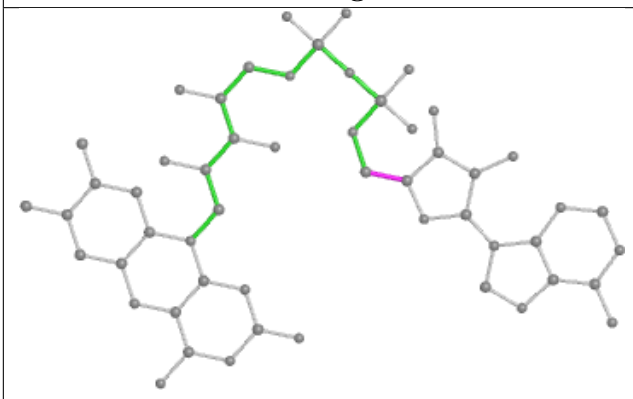
Ligand FAS G 701



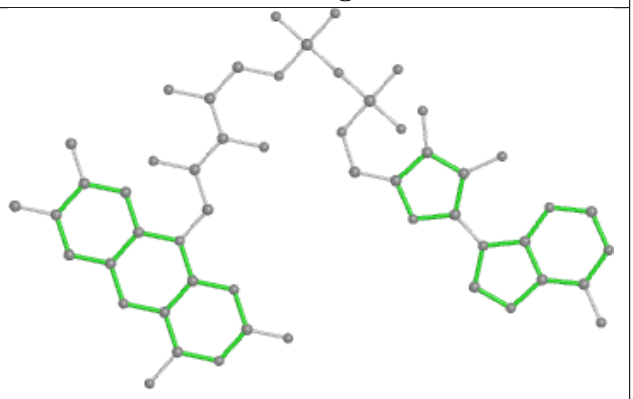
Bond lengths



Bond angles

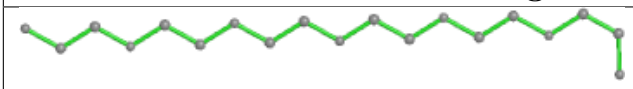


Torsions

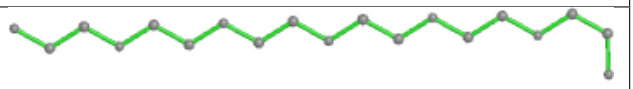


Rings

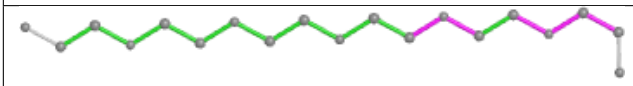
Ligand P6G B 703



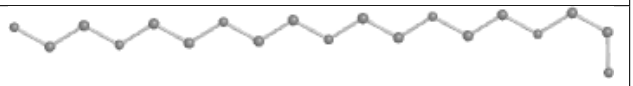
Bond lengths



Bond angles

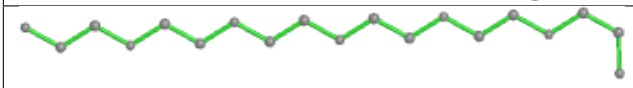


Torsions

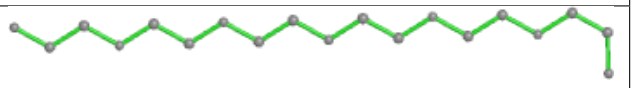


Rings

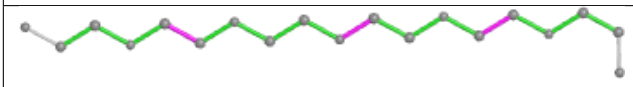
Ligand P6G C 702



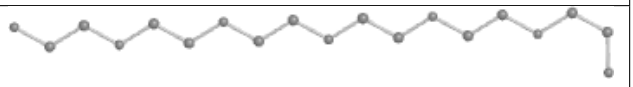
Bond lengths



Bond angles

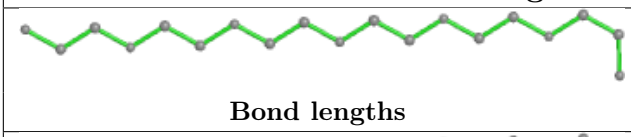


Torsions

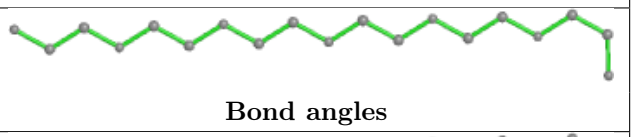


Rings

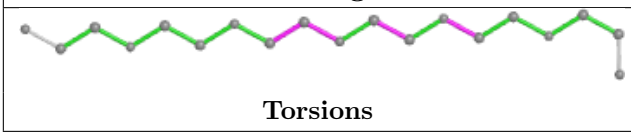
Ligand P6G B 702



Bond lengths



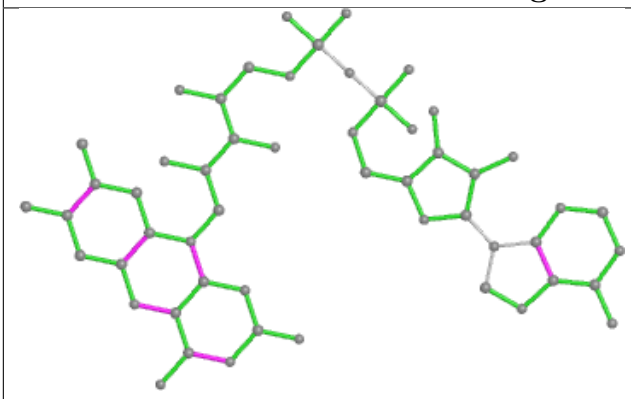
Bond angles



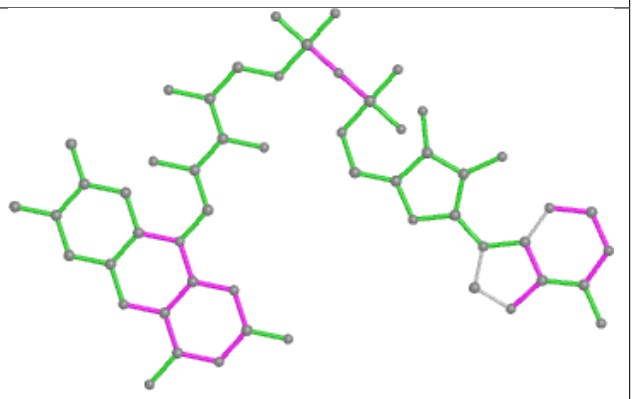
Torsions

Rings

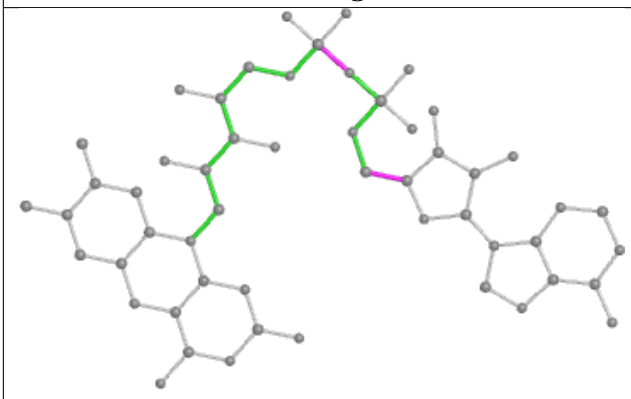
Ligand FAS E 701



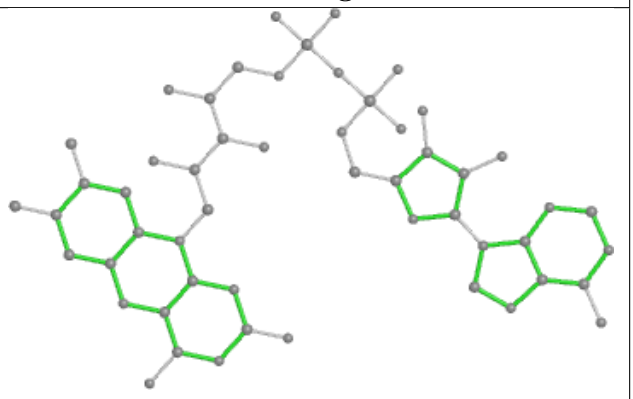
Bond lengths



Bond angles

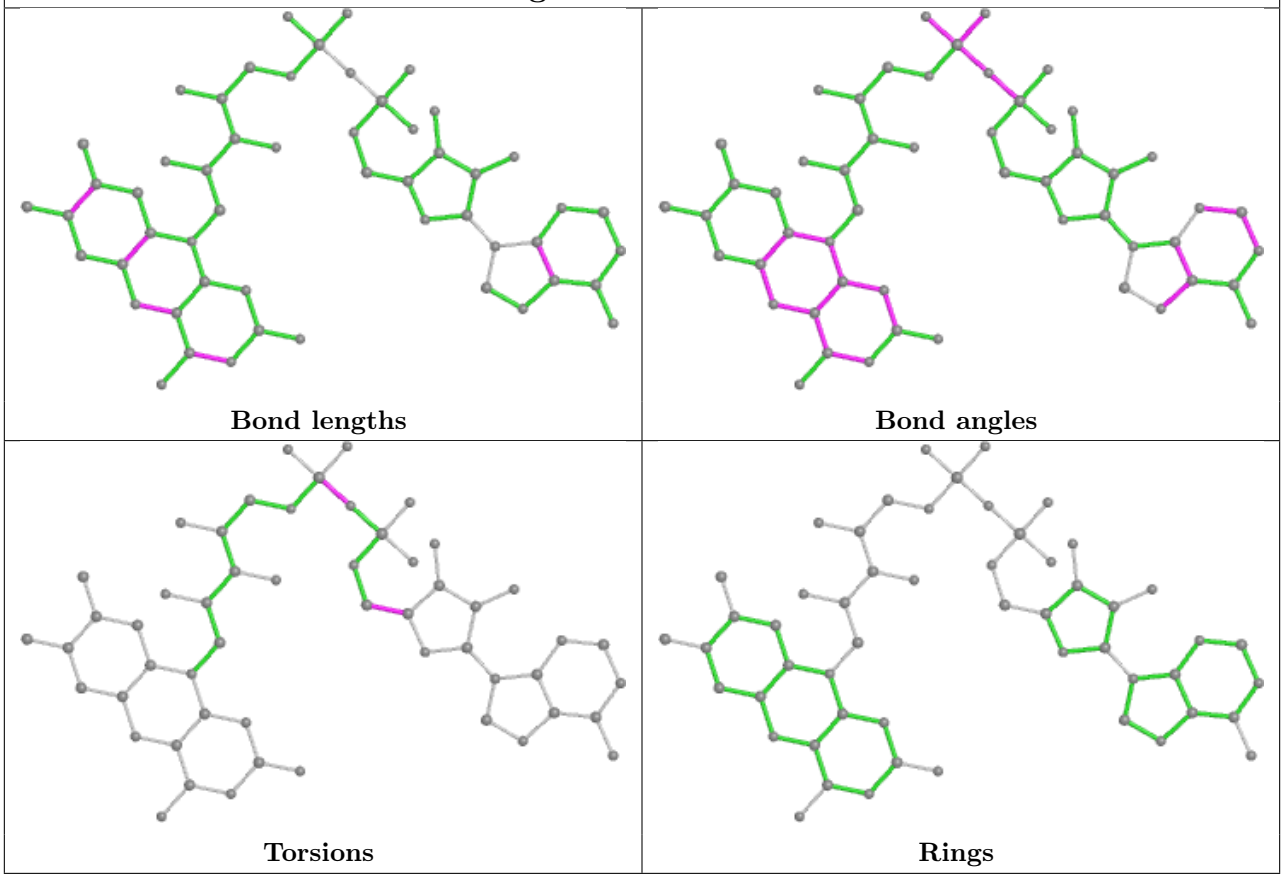


Torsions



Rings

Ligand FAS A 701



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	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

All (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
1	E	641	GLU	3.3
1	B	575	GLY	3.2
1	H	296	LEU	3.2
1	G	87	ALA	3.1
1	D	378	GLU	3.1
1	H	113	GLN	2.9
1	F	291	ALA	2.9
1	D	365	THR	2.9
1	D	581	LYS	2.9
1	H	381	ARG	2.9
1	D	232	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	230	ILE	2.8
1	G	89	VAL	2.8
1	H	288	LEU	2.7
1	F	286	ILE	2.7
1	B	96	ILE	2.7
1	D	548	GLU	2.7
1	H	489	GLU	2.7
1	F	87	ALA	2.7
1	H	575	GLY	2.6
1	H	289	ARG	2.6
1	D	382	GLU	2.6
1	H	545	GLU	2.6
1	B	584	LYS	2.6
1	B	190	TRP	2.6
1	H	600	GLY	2.6
1	B	356	ILE	2.6
1	H	546	TYR	2.6
1	H	286	ILE	2.6
1	D	298	ASN	2.5
1	D	374	GLU	2.5
1	D	549	GLU	2.5
1	D	584	LYS	2.5
1	G	140	ASP	2.5
1	D	356	ILE	2.5
1	H	232	VAL	2.4
1	D	106	ALA	2.4
1	B	97	ASN	2.4
1	D	381	ARG	2.4
1	F	89	VAL	2.4
1	D	385	GLU	2.4
1	D	545	GLU	2.4
1	D	578	GLU	2.4
1	G	641	GLU	2.4
1	A	356	ILE	2.4
1	D	230	ILE	2.4
1	B	289	ARG	2.4
1	D	576	PRO	2.4
1	D	190	TRP	2.3
1	D	370	SER	2.3
1	H	585	TRP	2.3
1	B	93	GLY	2.3
1	H	120	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	380	TYR	2.3
1	B	367	GLU	2.3
1	G	96	ILE	2.3
1	B	239	ALA	2.3
1	H	606	LEU	2.3
1	D	97	ASN	2.3
1	B	251	LYS	2.3
1	D	367	GLU	2.2
1	E	286	ILE	2.2
1	B	618	TYR	2.2
1	E	289	ARG	2.2
1	B	576	PRO	2.2
1	G	381	ARG	2.2
1	D	286	ILE	2.2
1	A	382	GLU	2.2
1	B	250	PRO	2.2
1	D	295	PRO	2.2
1	G	640	GLY	2.2
1	C	356	ILE	2.2
1	F	606	LEU	2.2
1	H	544	ILE	2.2
1	B	382	GLU	2.2
1	C	581	LYS	2.1
1	H	549	GLU	2.1
1	F	289	ARG	2.1
1	F	566	TRP	2.1
1	H	548	GLU	2.1
1	D	297	VAL	2.1
1	D	98	PHE	2.1
1	A	93	GLY	2.1
1	H	578	GLU	2.1
1	H	542	PRO	2.1
1	G	660	LEU	2.1
1	A	566	TRP	2.1
1	F	290	ALA	2.1
1	H	87	ALA	2.1
1	D	234	ASP	2.1
1	E	381	ARG	2.1
1	B	92	GLY	2.1
1	B	566	TRP	2.1
1	C	232	VAL	2.1
1	D	575	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	383	TYR	2.1
1	H	115	GLU	2.0
1	E	386	ASP	2.0
1	F	251	LYS	2.0
1	E	366	PRO	2.0
1	B	658	THR	2.0
1	F	250	PRO	2.0
1	H	295	PRO	2.0
1	B	581	LYS	2.0
1	G	286	ILE	2.0
1	D	372	MET	2.0
1	D	630	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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	F	703	19/19	0.80	0.31	71,74,75,76	0
3	P6G	C	703	19/19	0.80	0.29	67,75,77,77	0
4	PGE	G	703	10/10	0.81	0.39	69,69,71,71	0
4	PGE	B	704	10/10	0.82	0.17	65,67,70,71	0
6	CA	D	704	1/1	0.82	0.11	97,97,97,97	0
4	PGE	D	703	10/10	0.84	0.17	64,67,70,70	0

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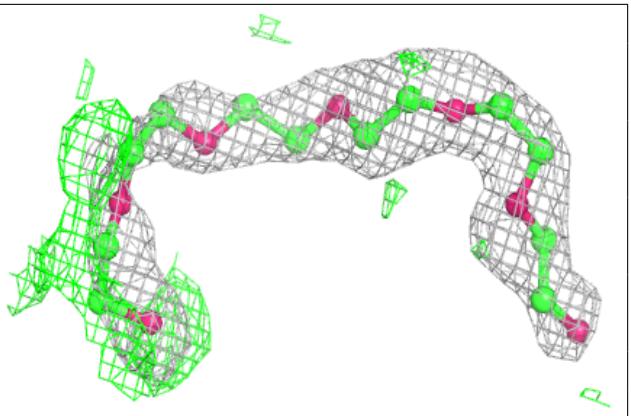
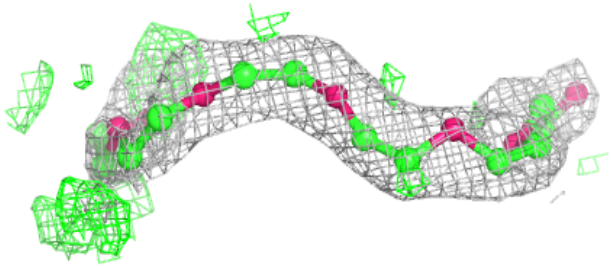
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CA	E	704	1/1	0.84	0.12	98,98,98,98	0
4	PGE	G	702	10/10	0.86	0.34	56,59,59,60	0
4	PGE	E	703	10/10	0.86	0.18	50,54,58,58	0
6	CA	F	706	1/1	0.87	0.13	89,89,89,89	0
3	P6G	C	702	19/19	0.87	0.31	64,67,71,71	0
4	PGE	H	702	10/10	0.87	0.15	67,68,69,69	0
5	PO4	F	704	5/5	0.90	0.16	46,50,51,52	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
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	B	703	19/19	0.94	0.15	42,47,52,52	0
3	P6G	F	702	19/19	0.94	0.14	36,38,41,42	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
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	C	707	1/1	0.95	0.16	76,76,76,76	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	F	701	53/53	0.97	0.19	36,40,45,48	0
2	FAS	G	701	53/53	0.97	0.19	31,33,36,37	0
2	FAS	E	701	53/53	0.98	0.19	28,29,32,34	0
2	FAS	C	701	53/53	0.98	0.17	25,28,30,35	0
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

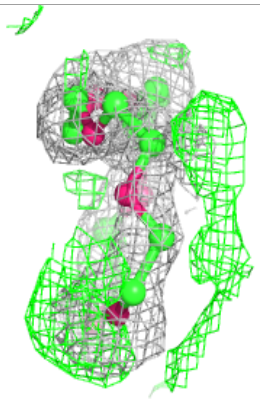
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

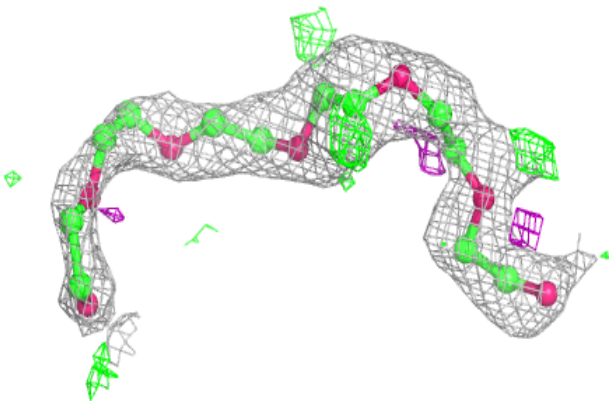


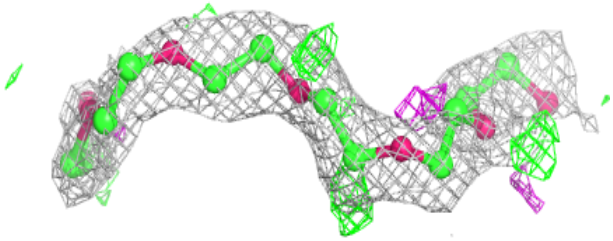


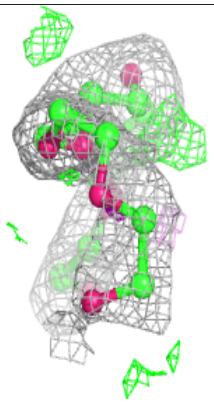


Electron density around P6G E 702:

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

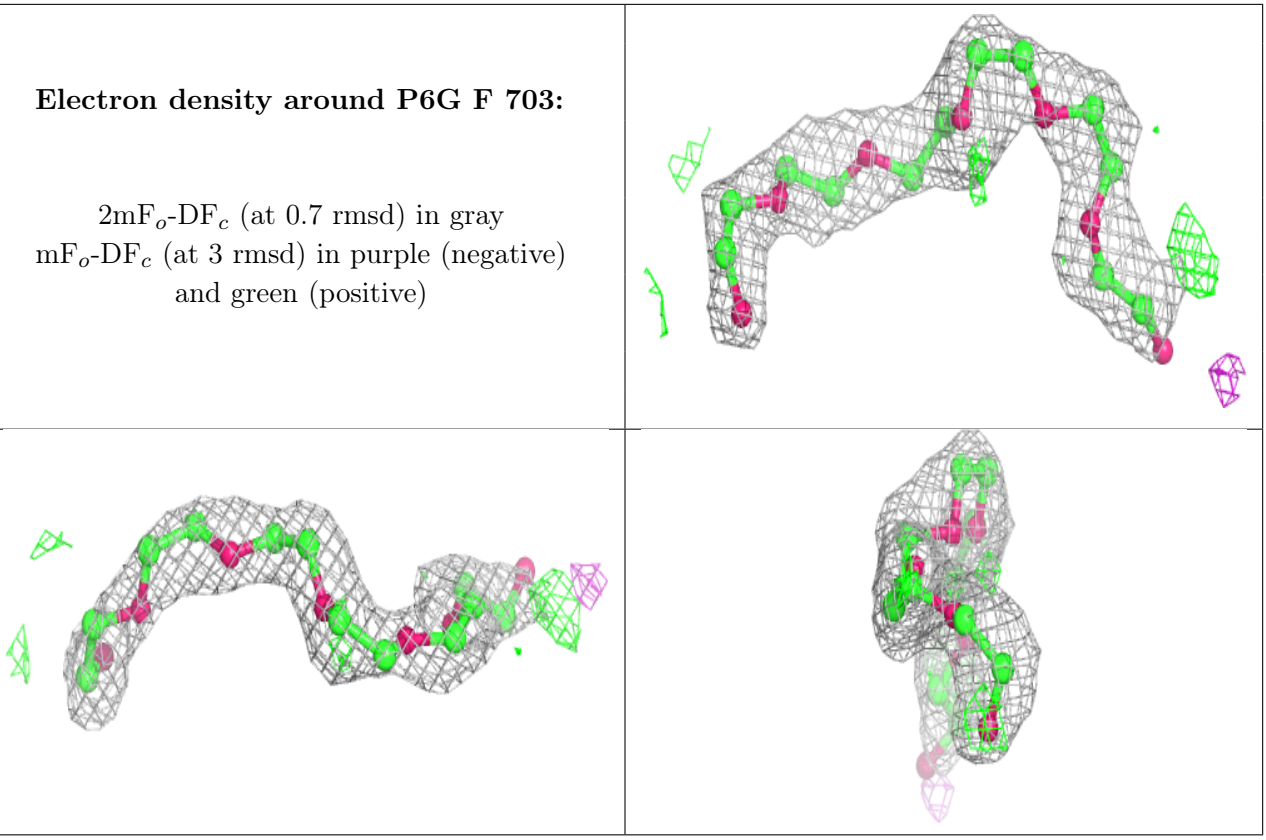






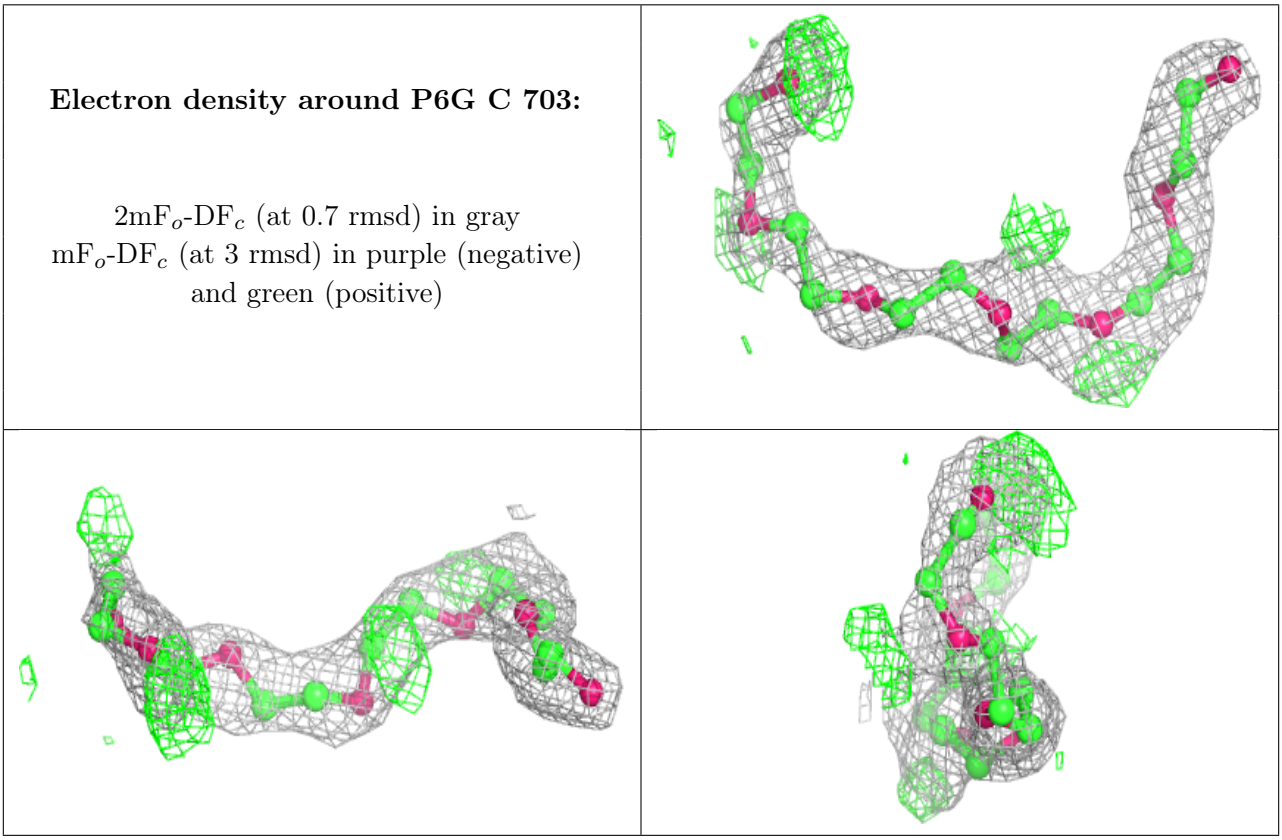
Electron density around P6G F 703:

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



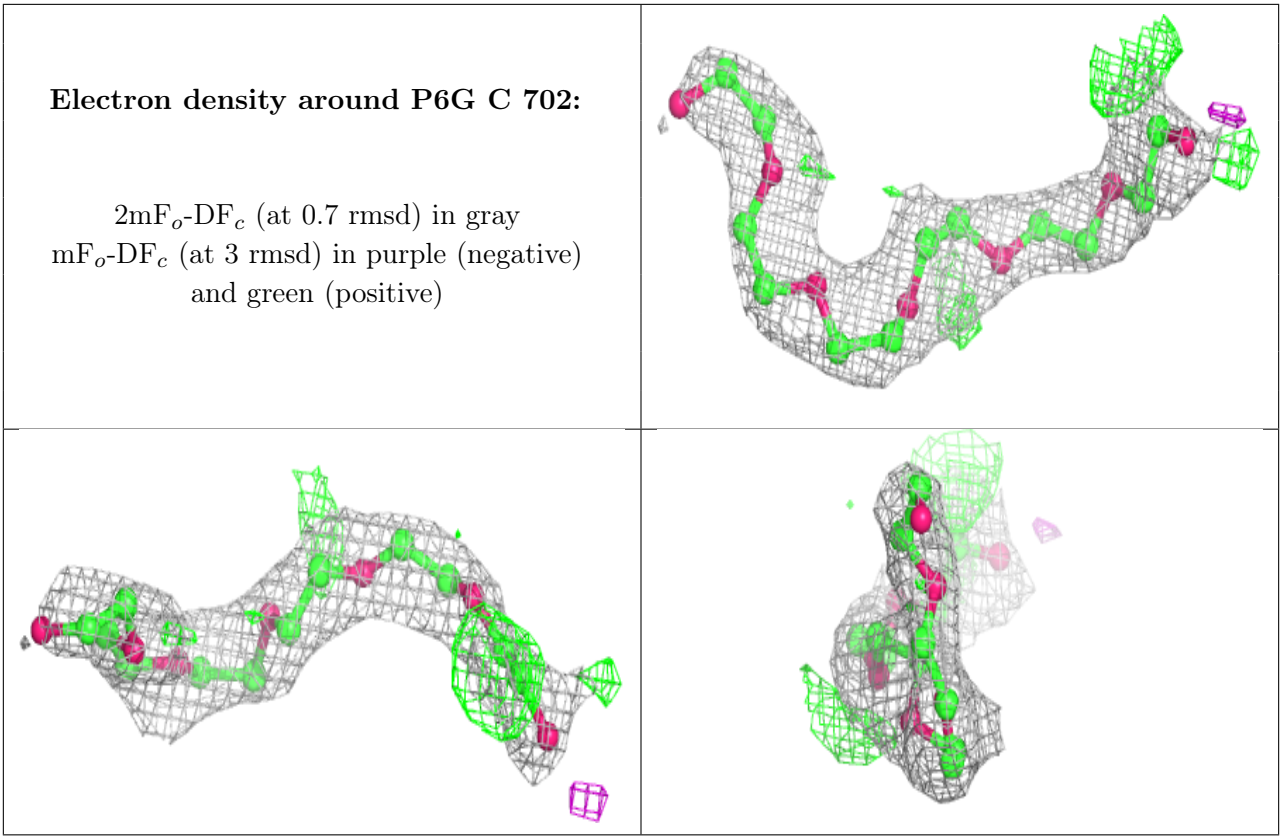
Electron density around P6G C 703:

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



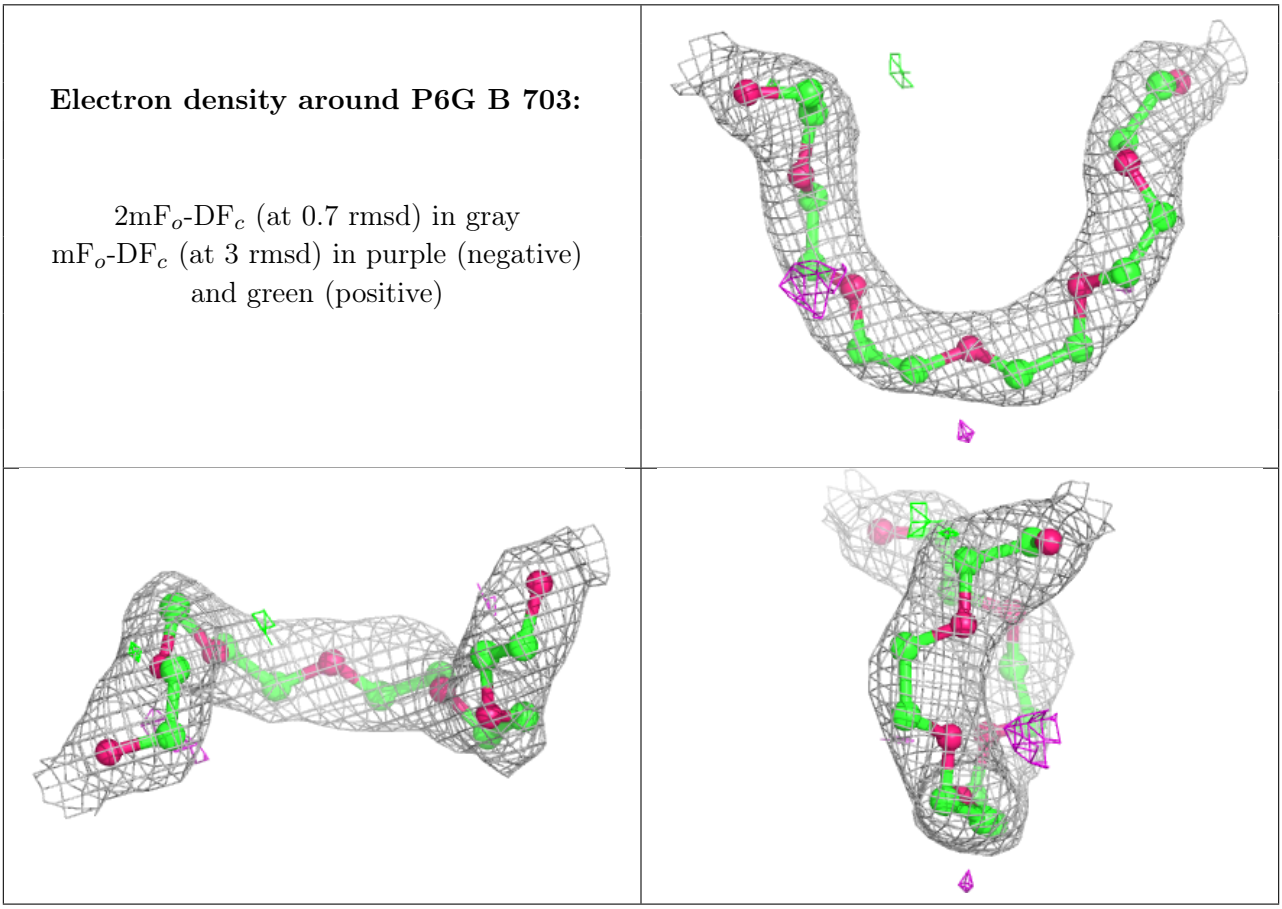
Electron density around P6G C 702:

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



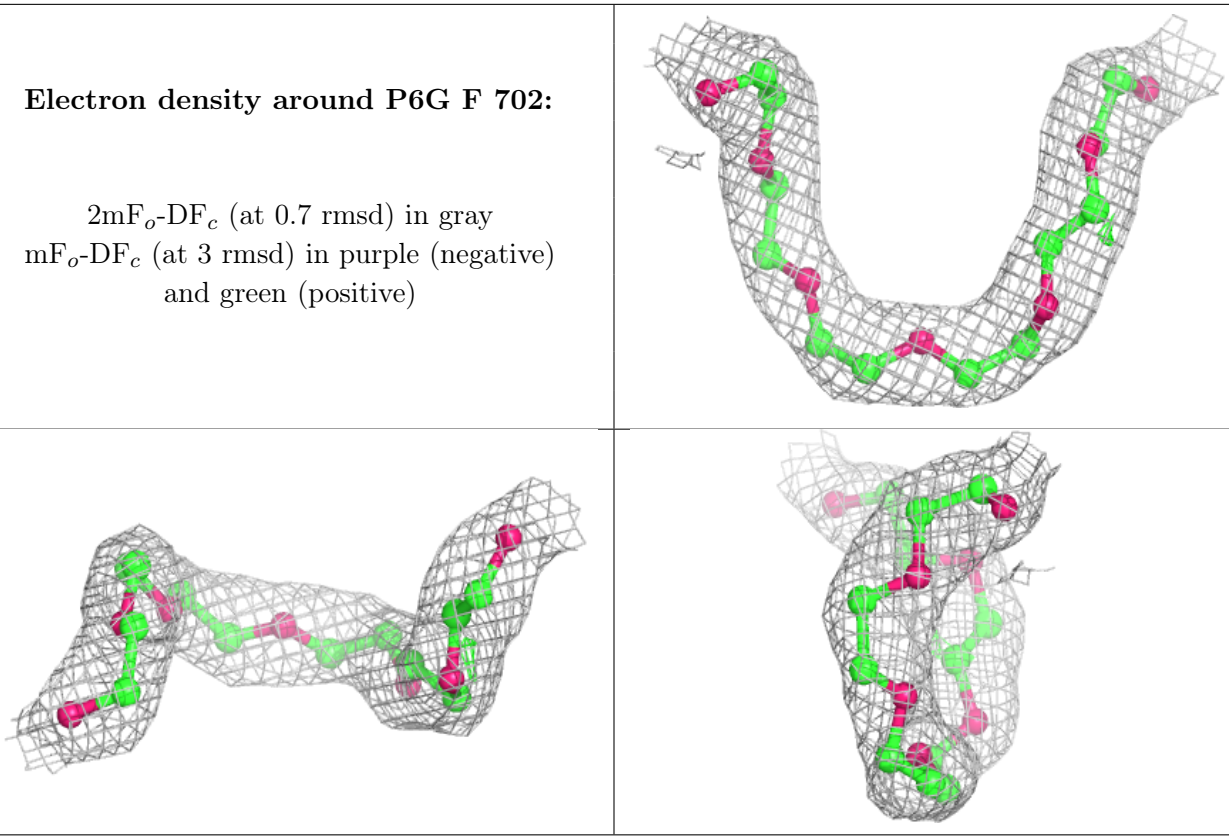
Electron density around P6G B 703:

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



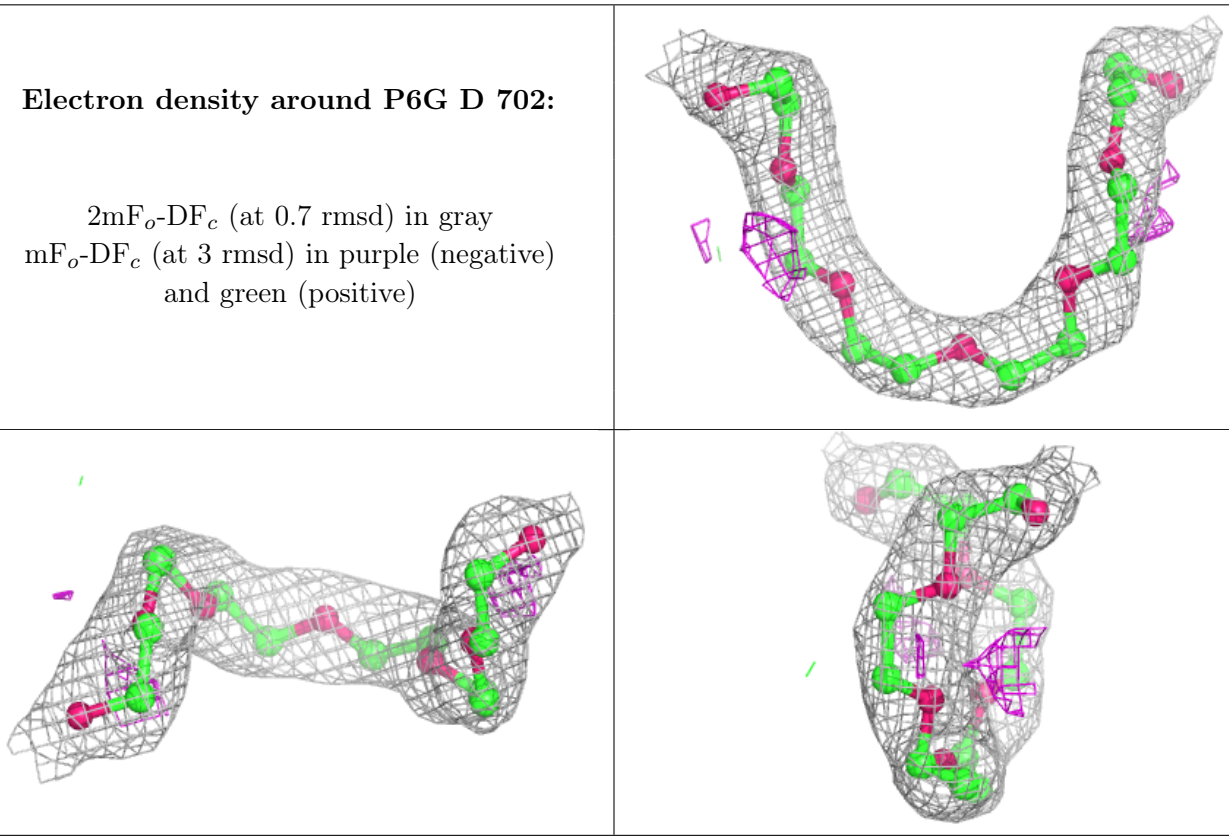
Electron density around P6G F 702:

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



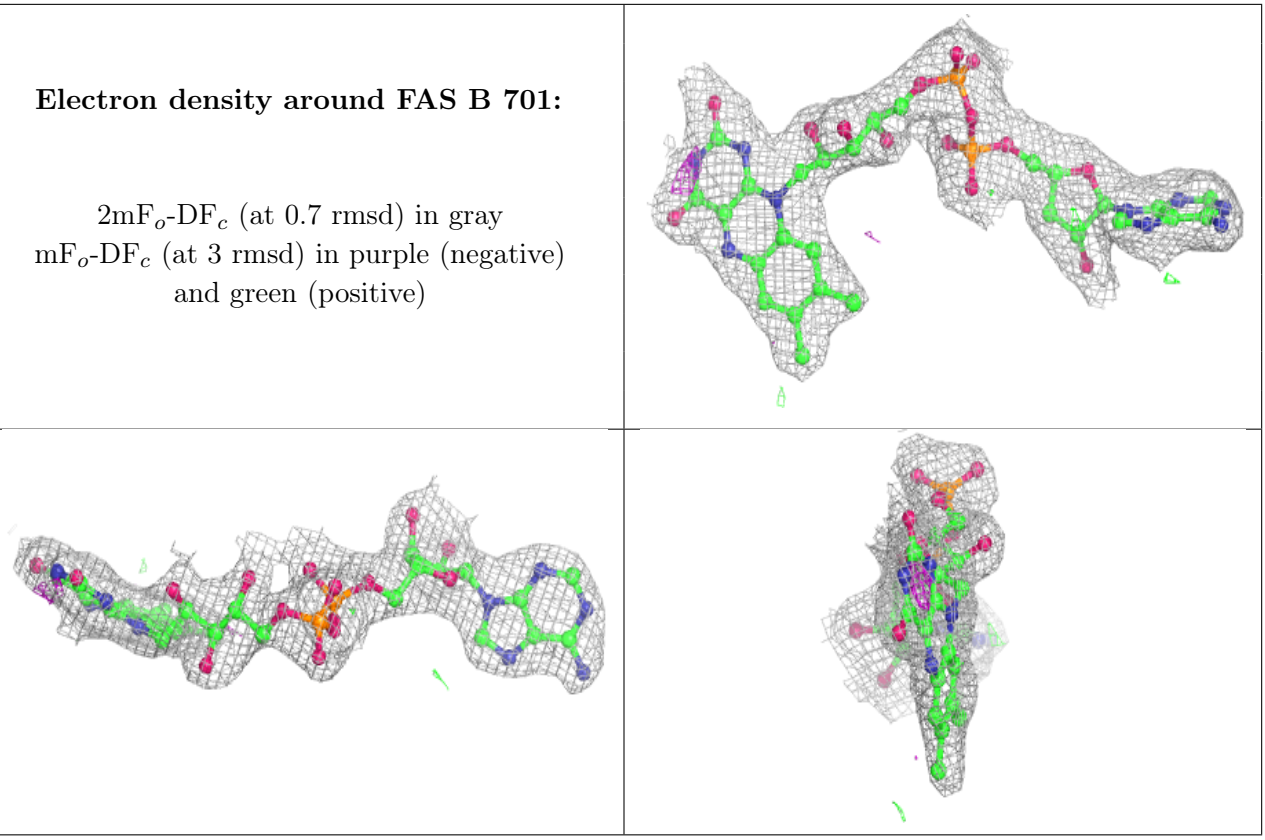
Electron density around P6G D 702:

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



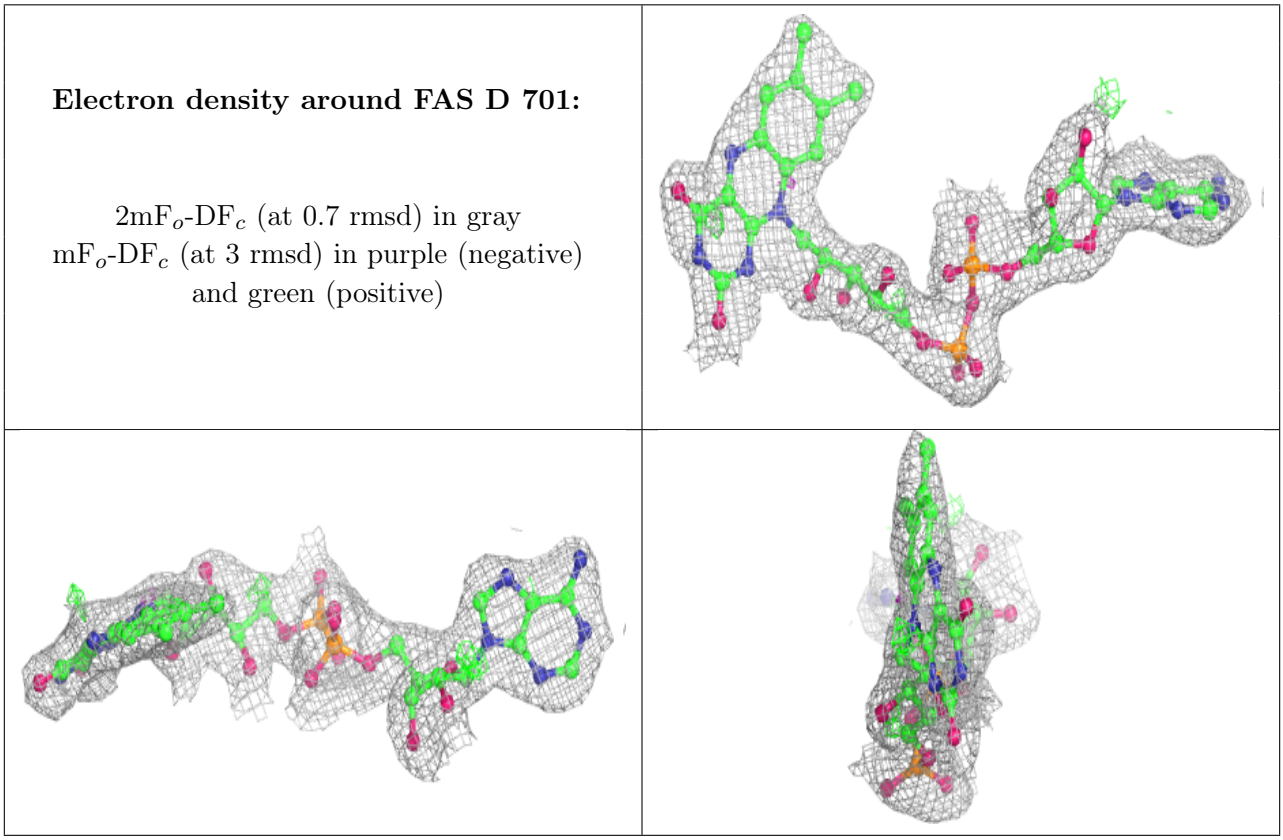
Electron density around FAS B 701:

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



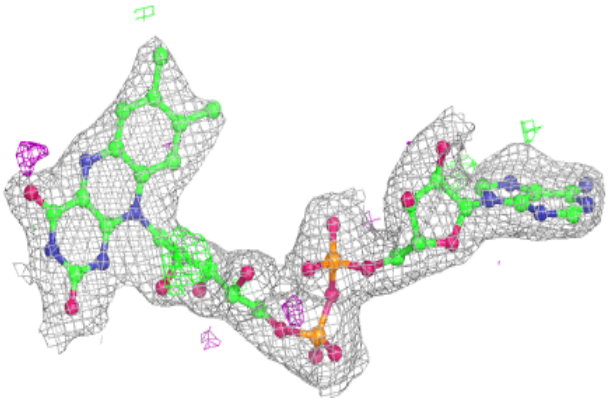
Electron density around FAS D 701:

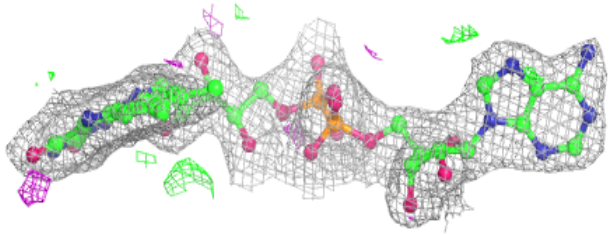
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

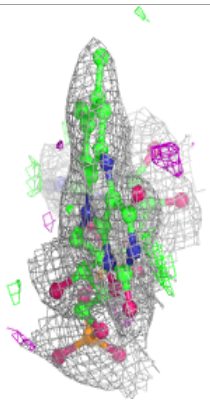


Electron density around FAS H 701:

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

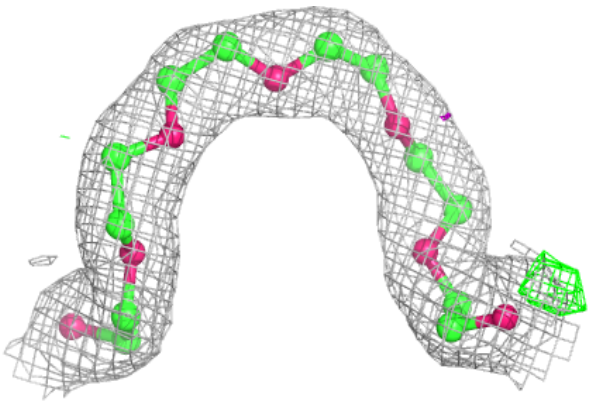


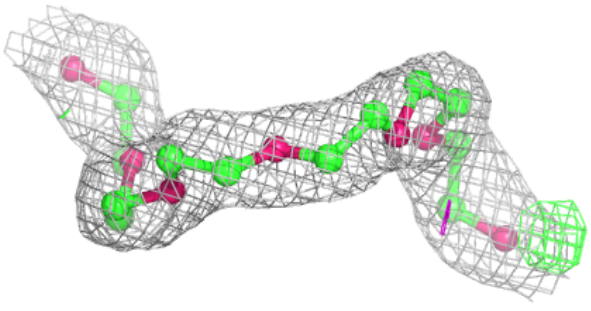


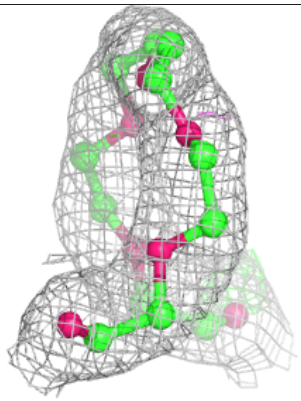


Electron density around P6G A 702:

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

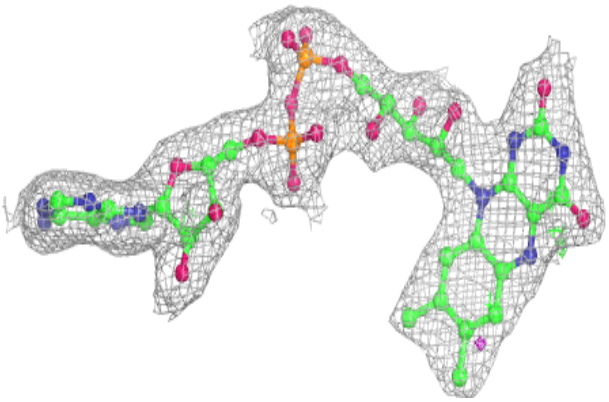


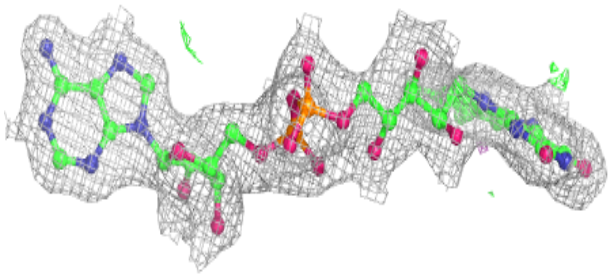


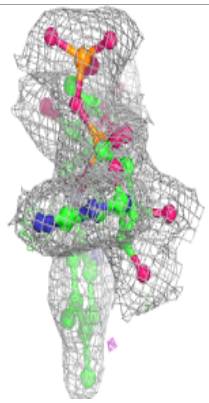


Electron density around FAS A 701:

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

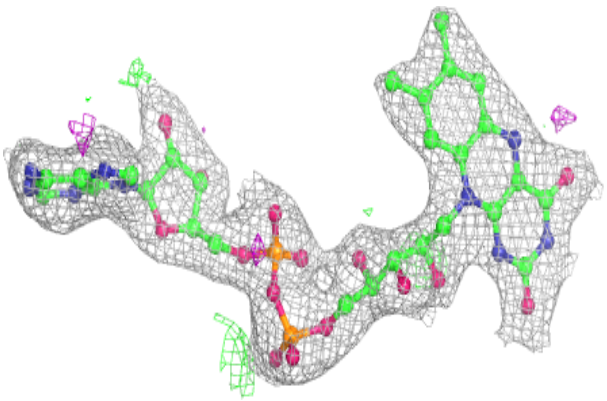


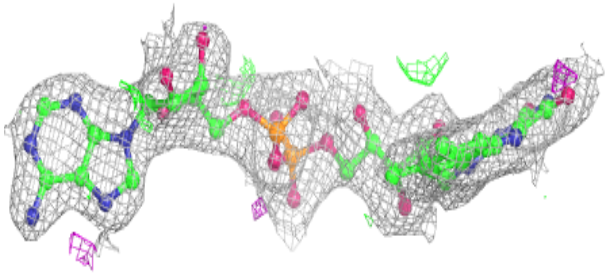


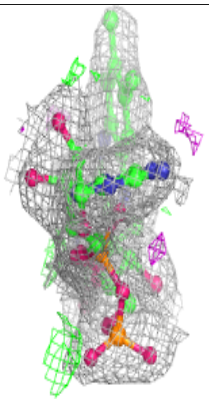


Electron density around FAS F 701:

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

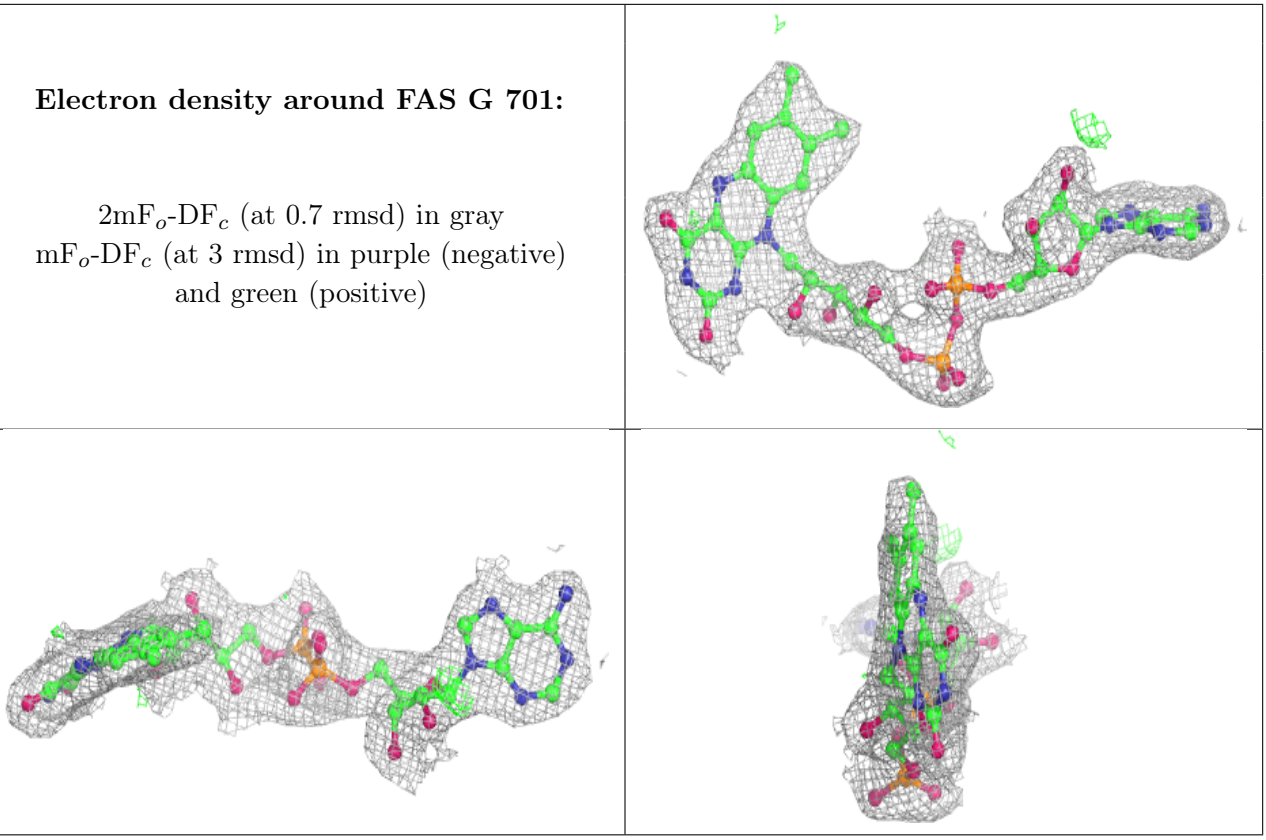






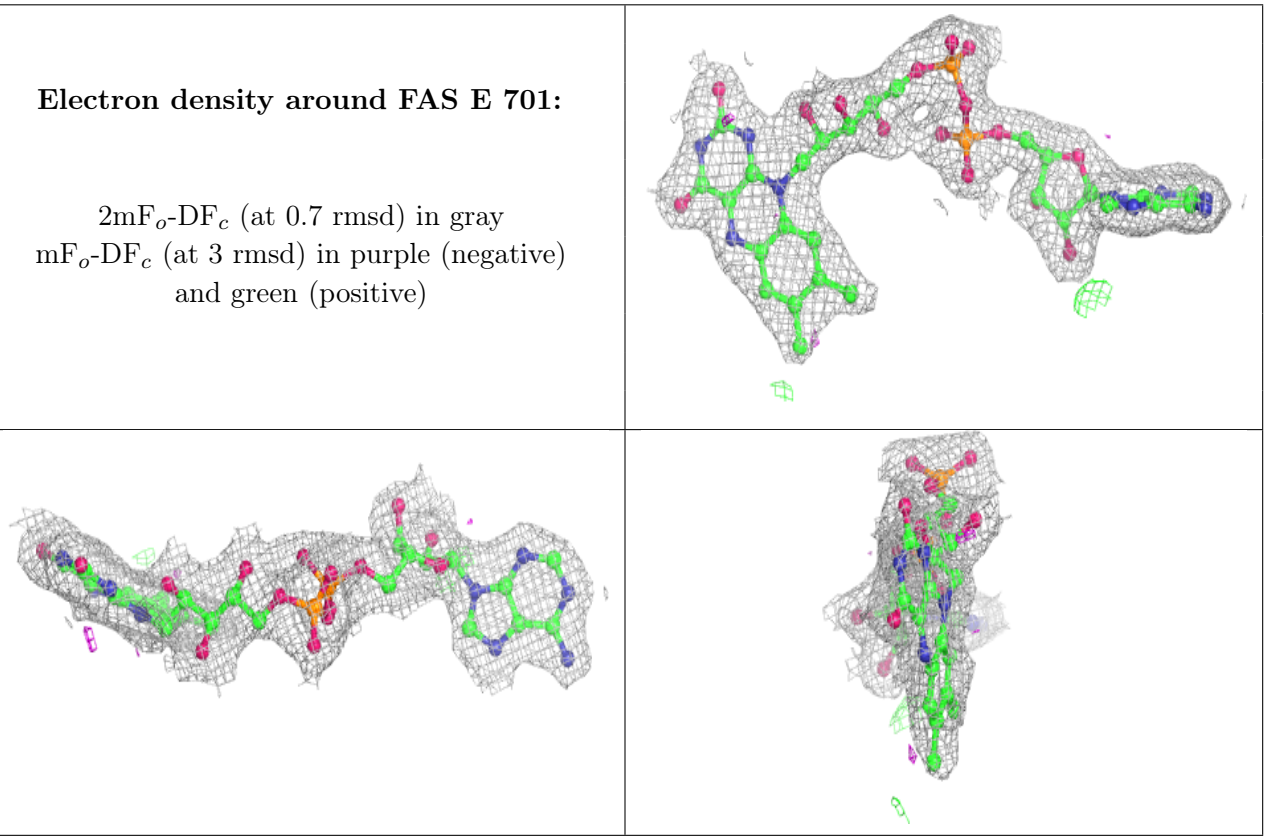
Electron density around FAS G 701:

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



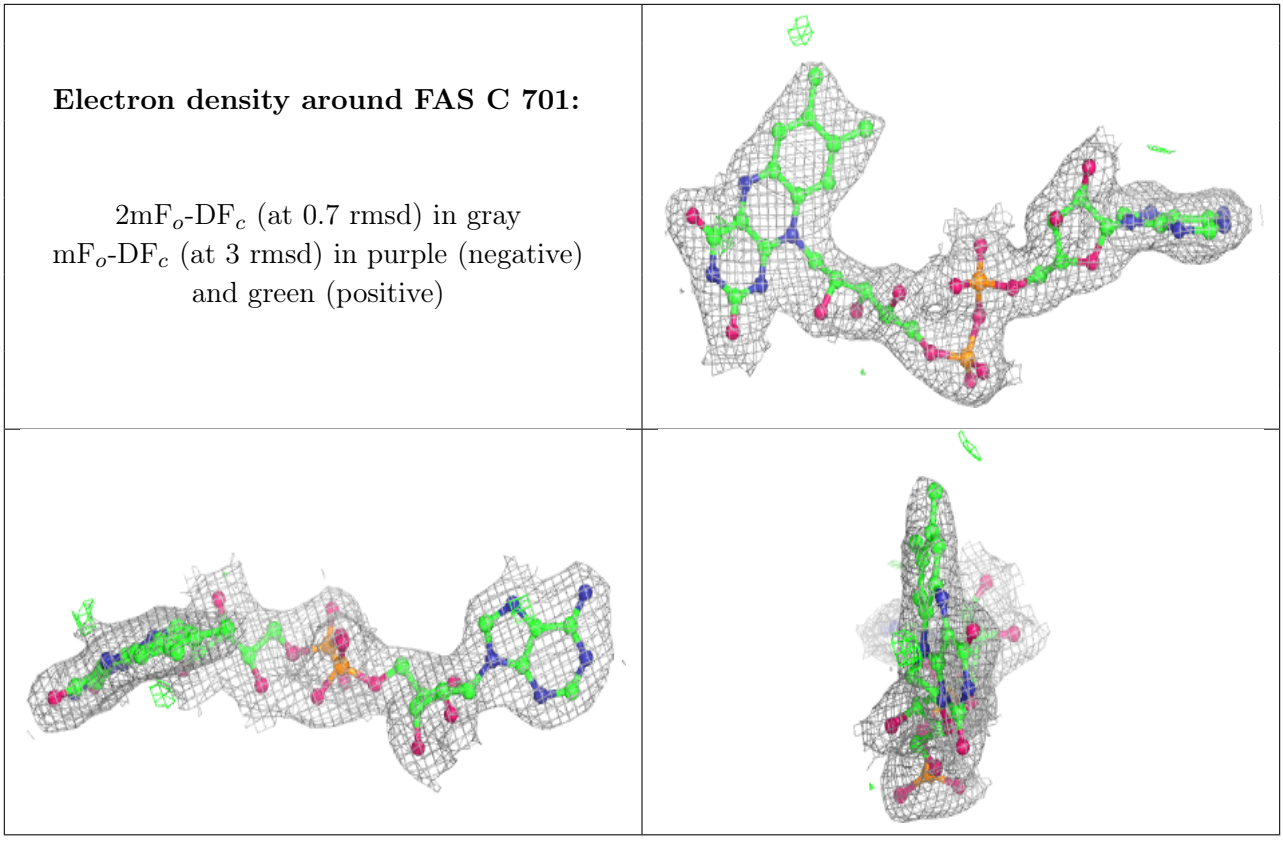
Electron density around FAS E 701:

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



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)



6.5 Other polymers (i)

There are no such residues in this entry.