wwPDB X-ray Structure Validation Summary Report (i)

Sep 15, 2020 – 06:23 PM BST

PDB ID	:	6ZXX
Title	:	Catabolic reductive dehalogenase NpRdhA, N-terminally tagged.
Authors	:	Leys, D.; Halliwell, T.
Deposited on	:	2020-07-30
Resolution	:	1.99 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 (i) symbol.

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

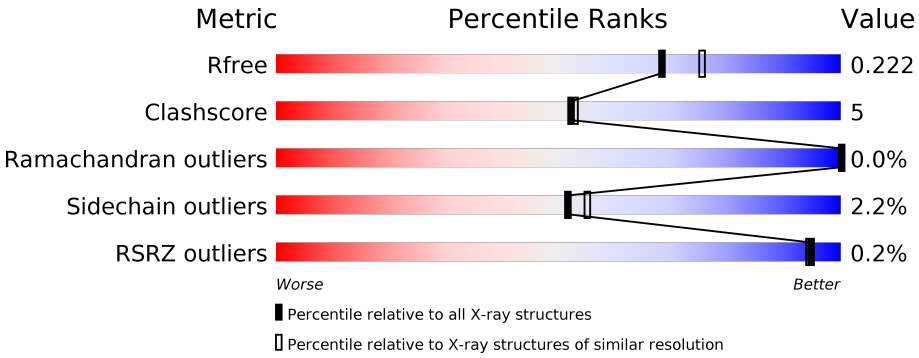
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4

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 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	725	87% 9%
1	B	725	86% 9%
1	C	725	% 85% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	B12	A	703	X	-	-	-
3	B12	B	703	X	-	-	-
3	B12	C	803	X	-	-	-
5	QSH	A	705[A]	-	-	X	-
5	QSH	B	705[A]	-	-	X	-
7	BR	A	707[A]	-	-	X	-
7	BR	B	707[A]	-	-	X	-
7	BR	C	807[A]	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16958 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 Oxidoreductase, NAD-binding/iron-sulfur cluster-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	700	Total	C	N	O	S	0	1	0
			5322	3320	976	986	40			
1	B	695	Total	C	N	O	S	0	3	0
			5312	3310	967	994	41			
1	C	696	Total	C	N	O	S	0	1	0
			5180	3238	942	960	40			

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	initiating methionine	UNP K2MB66
A	-25	VAL	-	expression tag	UNP K2MB66
A	-24	GLN	-	expression tag	UNP K2MB66
A	-23	THR	-	expression tag	UNP K2MB66
A	-22	SER	-	expression tag	UNP K2MB66
A	-21	PHE	-	expression tag	UNP K2MB66
A	-20	GLU	-	expression tag	UNP K2MB66
A	-19	HIS	-	expression tag	UNP K2MB66
A	-18	HIS	-	expression tag	UNP K2MB66
A	-17	HIS	-	expression tag	UNP K2MB66
A	-16	HIS	-	expression tag	UNP K2MB66
A	-15	HIS	-	expression tag	UNP K2MB66
A	-14	HIS	-	expression tag	UNP K2MB66
A	-13	SER	-	expression tag	UNP K2MB66
A	-12	ALA	-	expression tag	UNP K2MB66
A	-11	GLY	-	expression tag	UNP K2MB66
A	-10	GLU	-	expression tag	UNP K2MB66
A	-9	ASN	-	expression tag	UNP K2MB66
A	-8	LEU	-	expression tag	UNP K2MB66
A	-7	TYR	-	expression tag	UNP K2MB66
A	-6	PHE	-	expression tag	UNP K2MB66
A	-5	GLN	-	expression tag	UNP K2MB66

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP K2MB66
A	-3	ALA	-	expression tag	UNP K2MB66
A	-2	GLN	-	expression tag	UNP K2MB66
A	-1	ILE	-	expression tag	UNP K2MB66
A	0	SER	-	expression tag	UNP K2MB66
B	-26	MET	-	initiating methionine	UNP K2MB66
B	-25	VAL	-	expression tag	UNP K2MB66
B	-24	GLN	-	expression tag	UNP K2MB66
B	-23	THR	-	expression tag	UNP K2MB66
B	-22	SER	-	expression tag	UNP K2MB66
B	-21	PHE	-	expression tag	UNP K2MB66
B	-20	GLU	-	expression tag	UNP K2MB66
B	-19	HIS	-	expression tag	UNP K2MB66
B	-18	HIS	-	expression tag	UNP K2MB66
B	-17	HIS	-	expression tag	UNP K2MB66
B	-16	HIS	-	expression tag	UNP K2MB66
B	-15	HIS	-	expression tag	UNP K2MB66
B	-14	HIS	-	expression tag	UNP K2MB66
B	-13	SER	-	expression tag	UNP K2MB66
B	-12	ALA	-	expression tag	UNP K2MB66
B	-11	GLY	-	expression tag	UNP K2MB66
B	-10	GLU	-	expression tag	UNP K2MB66
B	-9	ASN	-	expression tag	UNP K2MB66
B	-8	LEU	-	expression tag	UNP K2MB66
B	-7	TYR	-	expression tag	UNP K2MB66
B	-6	PHE	-	expression tag	UNP K2MB66
B	-5	GLN	-	expression tag	UNP K2MB66
B	-4	GLY	-	expression tag	UNP K2MB66
B	-3	ALA	-	expression tag	UNP K2MB66
B	-2	GLN	-	expression tag	UNP K2MB66
B	-1	ILE	-	expression tag	UNP K2MB66
B	0	SER	-	expression tag	UNP K2MB66
C	-23	MET	-	initiating methionine	UNP K2MB66
C	-22	VAL	-	expression tag	UNP K2MB66
C	-21	GLN	-	expression tag	UNP K2MB66
C	-20	THR	-	expression tag	UNP K2MB66
C	-19	SER	-	expression tag	UNP K2MB66
C	-18	PHE	-	expression tag	UNP K2MB66
C	-17	GLU	-	expression tag	UNP K2MB66
C	-16	HIS	-	expression tag	UNP K2MB66
C	-15	HIS	-	expression tag	UNP K2MB66
C	-14	HIS	-	expression tag	UNP K2MB66

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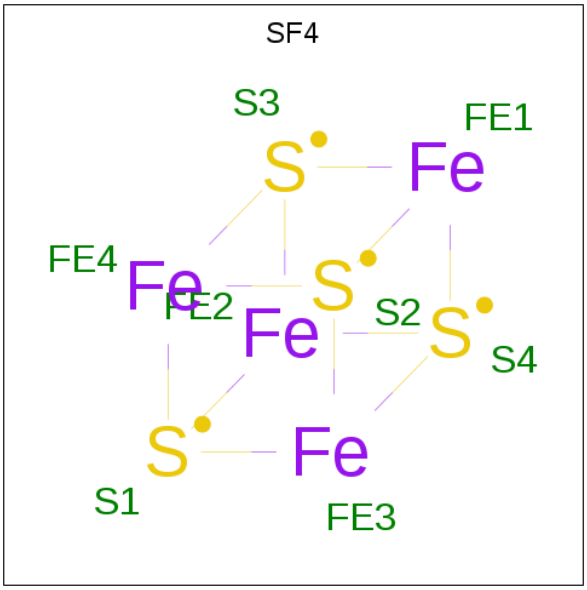
Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	HIS	-	expression tag	UNP K2MB66
C	-12	HIS	-	expression tag	UNP K2MB66
C	-11	HIS	-	expression tag	UNP K2MB66
C	-10	SER	-	expression tag	UNP K2MB66
C	-9	ALA	-	expression tag	UNP K2MB66
C	-8	GLY	-	expression tag	UNP K2MB66
C	-7	GLU	-	expression tag	UNP K2MB66
C	-6	ASN	-	expression tag	UNP K2MB66
C	-5	LEU	-	expression tag	UNP K2MB66
C	-4	TYR	-	expression tag	UNP K2MB66
C	-3	PHE	-	expression tag	UNP K2MB66
C	-2	GLN	-	expression tag	UNP K2MB66
C	-1	GLY	-	expression tag	UNP K2MB66
C	0	ALA	-	expression tag	UNP K2MB66
C	1	GLN	-	expression tag	UNP K2MB66
C	2	ILE	-	expression tag	UNP K2MB66
C	3	SER	-	expression tag	UNP K2MB66

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0

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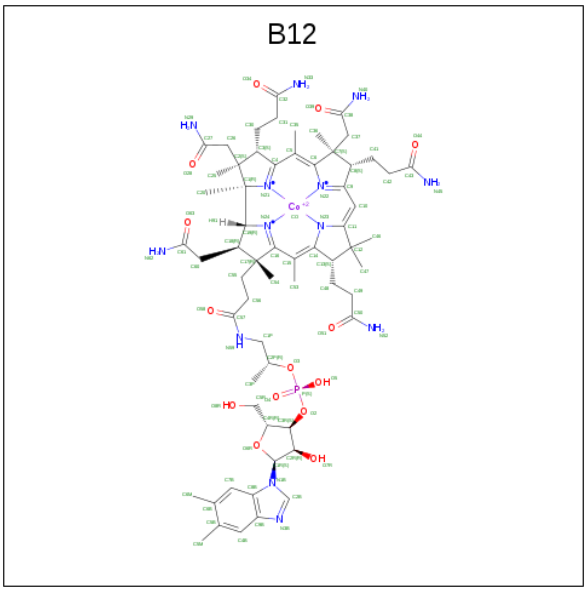
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$) (labeled as "Ligand of Interest" by author).

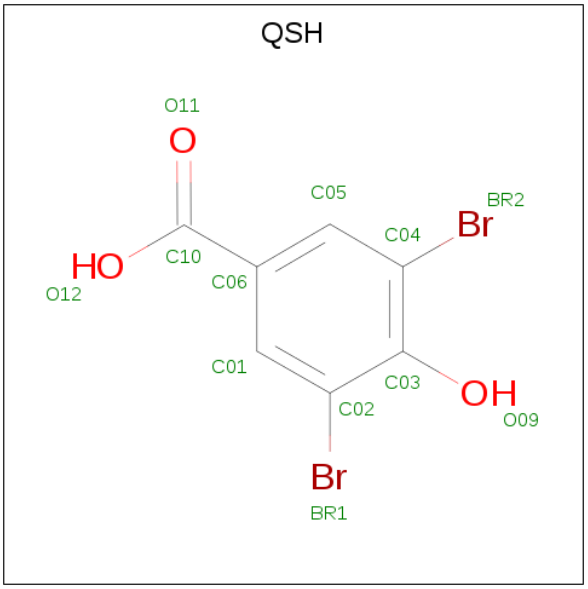


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Co N O P 91 62 1 13 14 1	0	0
3	B	1	Total C Co N O P 91 62 1 13 14 1	0	0
3	C	1	Total C Co N O P 91 62 1 13 14 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

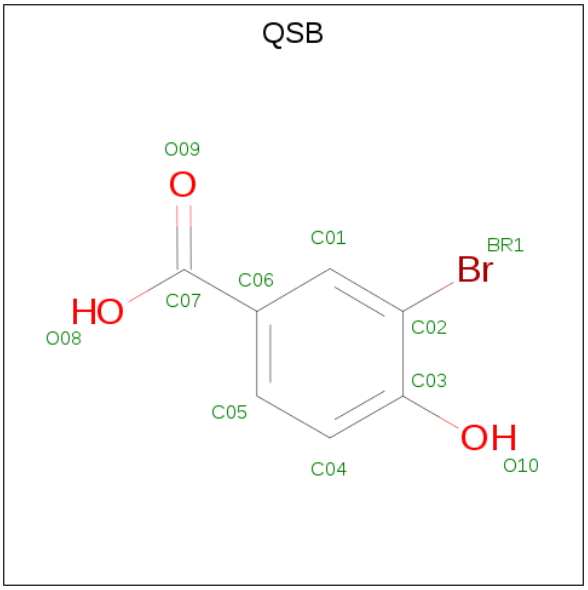
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0

- Molecule 5 is 3,5-bis(bromanyl)-4-oxidanyl-benzoic acid (three-letter code: QSH) (formula: $C_7H_4Br_2O_3$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Br	C	O	0	1
			12	2	7	3		
5	B	1	Total	Br	C	O	0	1
			12	2	7	3		
5	C	1	Total	Br	C	O	0	1
			12	2	7	3		

- Molecule 6 is 3 bromo 4 hydroxybenzoic acid (three-letter code: QSB) (formula: $C_7H_5BrO_3$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Br C O 11 1 7 3	0	1
6	B	1	Total Br C O 11 1 7 3	0	1
6	C	1	Total Br C O 11 1 7 3	0	1

- Molecule 7 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Br 1 1	0	1
7	A	1	Total Br 1 1	0	1
7	C	1	Total Br 1 1	0	1

- Molecule 8 is water.

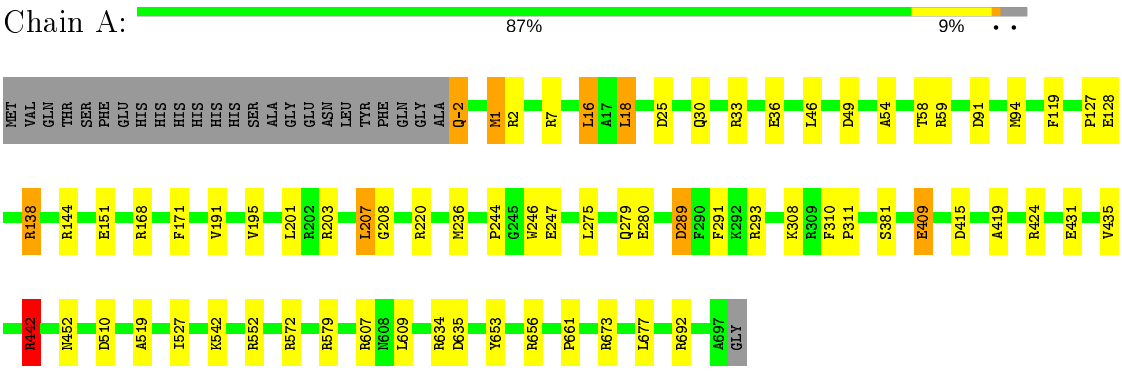
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	314	Total O 314 314	0	6
8	B	304	Total O 304 304	0	0
8	C	130	Total O 130 130	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

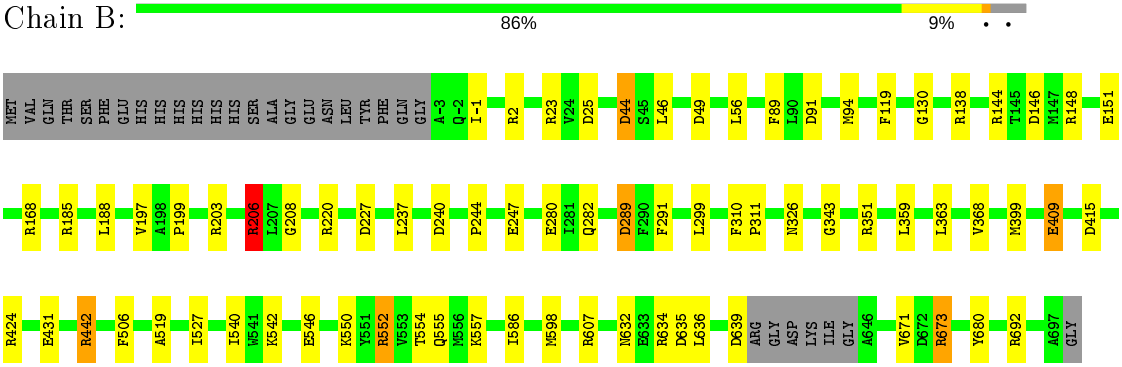
- Molecule 1: Oxidoreductase, NAD-binding/iron-sulfur cluster-binding protein

Chain A:



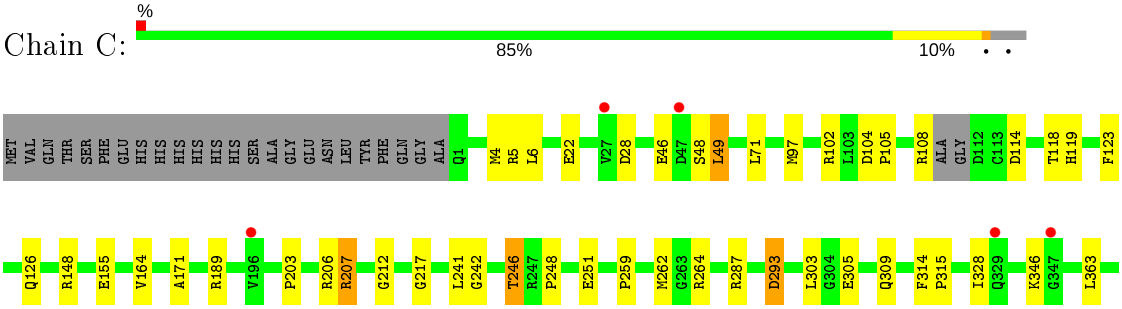
- Molecule 1: Oxidoreductase, NAD-binding/iron-sulfur cluster-binding protein

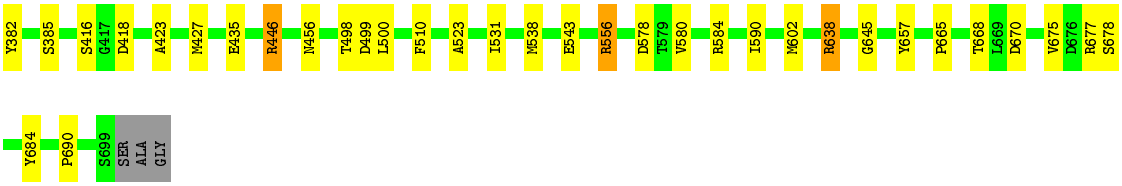
Chain B:



- Molecule 1: Oxidoreductase, NAD-binding/iron-sulfur cluster-binding protein

Chain C:




Y382
S385
S416
G417
D418
A423
M427
E435
R446
N456
T498
D499
L500
F510
A523
I531
M538
E543
R556
D578
T579
V580
R584
I590
M602
R638
G645
Y657
P665
T668
L669
D670
V675
D676
R677
S678
Y684
P690
S699
SER
ALA
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	180.18Å 170.39Å 107.96Å 90.00° 99.16° 90.00°	Depositor
Resolution (Å)	106.58 – 1.99 123.05 – 1.99	Depositor EDS
% Data completeness (in resolution range)	94.5 (106.58-1.99) 46.5 (123.05-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.182 , 0.218 0.188 , 0.222	Depositor DCC
R_{free} test set	5033 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16958	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: QSB, NA, SF4, QSH, B12, BR

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	0.72	1/5434 (0.0%)	0.90	9/7358 (0.1%)
1	B	0.70	0/5424	0.88	11/7346 (0.1%)
1	C	0.64	0/5290	0.84	8/7178 (0.1%)
All	All	0.69	1/16148 (0.0%)	0.87	28/21882 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	-2	GLN	C-N	9.06	1.54	1.34

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	227	ASP	CB-CG-OD1	8.02	125.52	118.30
1	A	7	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	C	207	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	C	556	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	138	ARG	NE-CZ-NH1	6.43	123.51	120.30

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	5322	0	5204	45	0
1	B	5312	0	5164	43	0
1	C	5180	0	4969	51	0
2	A	16	0	0	0	0
2	B	16	0	0	0	0
2	C	16	0	0	0	0
3	A	91	0	87	14	0
3	B	91	0	87	12	0
3	C	91	0	87	7	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	12	0	0	4	0
5	B	12	0	0	5	0
5	C	12	0	0	3	0
6	A	11	0	0	3	0
6	B	11	0	0	2	0
6	C	11	0	0	2	0
7	A	1	0	0	2	0
7	B	1	0	0	2	0
7	C	1	0	0	2	0
8	A	314	0	0	9	0
8	B	304	0	0	4	0
8	C	130	0	0	1	0
All	All	16958	0	15598	174	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 5.

The worst 5 of 174 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ARG:NH1	1:B:431:GLU:OE1	1.90	1.03
5:C:805[A]:QSH:BR2	7:C:807[A]:BR:BR	1.03	1.03
5:A:705[A]:QSH:C04	7:A:707[A]:BR:BR	2.65	0.98
5:B:705[A]:QSH:BR2	7:B:707[A]:BR:BR	0.94	0.94
1:A:127:PRO:O	1:A:138:ARG:NH2	2.03	0.92

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	699/725 (96%)	686 (98%)	13 (2%)	0	100 100
1	B	694/725 (96%)	681 (98%)	13 (2%)	0	100 100
1	C	693/725 (96%)	679 (98%)	13 (2%)	1 (0%)	51 49
All	All	2086/2175 (96%)	2046 (98%)	39 (2%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	645	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	533/569 (94%)	519 (97%)	14 (3%)	46 48
1	B	534/569 (94%)	523 (98%)	11 (2%)	53 57
1	C	504/569 (89%)	494 (98%)	10 (2%)	55 58
All	All	1571/1707 (92%)	1536 (98%)	35 (2%)	52 55

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	185	ARG
1	B	409	GLU

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Mol	Chain	Res	Type
1	C	293	ASP
1	B	197	VAL
1	B	206	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	421	GLN
1	B	555	GLN
1	B	647	ASN
1	C	33	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 6 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	QSB	A	706[A]	5	9,11,11	0.95	1 (11%)	12,15,15	2.17	4 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SF4	A	701	1	0,12,12	0.00	-	-		
2	SF4	A	702	1	0,12,12	0.00	-	-		
6	QSB	C	806[A]	5	9,11,11	1.12	1 (11%)	12,15,15	1.89	3 (25%)
2	SF4	C	802	1	0,12,12	0.00	-	-		
2	SF4	C	801	1	0,12,12	0.00	-	-		
5	QSH	B	705[A]	6	10,12,12	0.76	0	14,17,17	2.00	4 (28%)
2	SF4	B	702	1	0,12,12	0.00	-	-		
5	QSH	C	805[A]	6	10,12,12	1.07	0	14,17,17	1.36	2 (14%)
3	B12	C	803	-	80,101,101	1.01	5 (6%)	101,166,166	2.21	19 (18%)
5	QSH	A	705[A]	6	10,12,12	1.29	1 (10%)	14,17,17	1.97	6 (42%)
6	QSB	B	706[A]	5	9,11,11	0.42	0	12,15,15	1.72	4 (33%)
3	B12	B	703	-	80,101,101	1.16	6 (7%)	101,166,166	2.18	20 (19%)
2	SF4	B	701	1	0,12,12	0.00	-	-		
3	B12	A	703	-	80,101,101	1.29	9 (11%)	101,166,166	2.63	22 (21%)

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
6	QSB	A	706[A]	5	-	0/0/4/4	0/1/1/1
2	SF4	A	701	1	-	-	0/6/5/5
3	B12	B	703	-	1/1/36/38	6/51/223/223	0/3/11/11
2	SF4	B	702	1	-	-	0/6/5/5
2	SF4	C	802	1	-	-	0/6/5/5
3	B12	C	803	-	1/1/36/38	5/51/223/223	0/3/11/11
2	SF4	C	801	1	-	-	0/6/5/5
5	QSH	B	705[A]	6	-	0/0/4/4	0/1/1/1
6	QSB	C	806[A]	5	-	0/0/4/4	0/1/1/1
5	QSH	C	805[A]	6	-	0/0/4/4	0/1/1/1
3	B12	A	703	-	1/1/36/38	7/51/223/223	0/3/11/11
6	QSB	B	706[A]	5	-	0/0/4/4	0/1/1/1
2	SF4	A	702	1	-	-	0/6/5/5
2	SF4	B	701	1	-	-	0/6/5/5
5	QSH	A	705[A]	6	-	0/0/4/4	0/1/1/1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	B12	O6R-C1R	4.41	1.47	1.41
3	B	703	B12	C11-C10	-4.32	1.33	1.40
3	A	703	B12	C8B-C9B	3.90	1.48	1.40
3	B	703	B12	C8B-C9B	3.84	1.48	1.40
5	A	705[A]	QSH	C06-C10	3.78	1.51	1.47

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	703	B12	C20-C1-C19	-15.29	94.62	109.36
3	C	803	B12	C20-C1-C19	-11.65	98.13	109.36
3	B	703	B12	C1-C19-N24	11.33	118.99	106.24
3	B	703	B12	C20-C1-C19	-9.37	100.33	109.36
3	C	803	B12	C1-C19-N24	8.64	115.96	106.24

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	803	B12	C19
3	B	703	B12	C19
3	A	703	B12	C19

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	803	B12	C1P-C2P-O3-P
3	C	803	B12	C3P-C2P-O3-P
3	B	703	B12	C38-C37-C7-C36
3	B	703	B12	C1P-C2P-O3-P
3	B	703	B12	C3P-C2P-O3-P

There are no ring outliers.

9 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	706[A]	QSB	3	0
6	C	806[A]	QSB	2	0
5	B	705[A]	QSH	5	0
5	C	805[A]	QSH	3	0
3	C	803	B12	7	0
5	A	705[A]	QSH	4	0
6	B	706[A]	QSB	2	0

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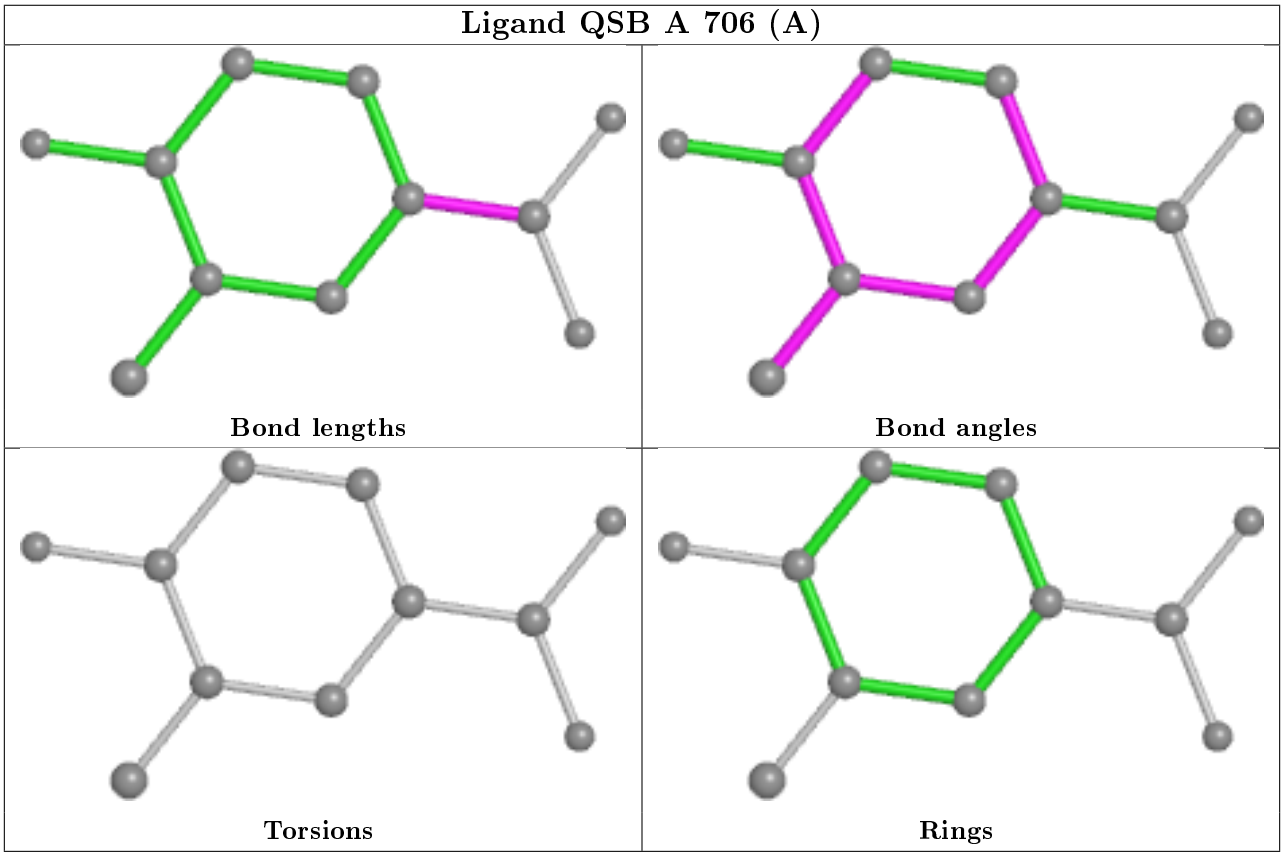
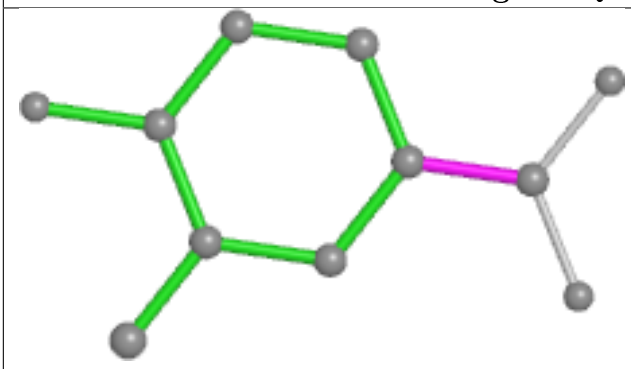
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	703	B12	12	0
3	A	703	B12	14	0

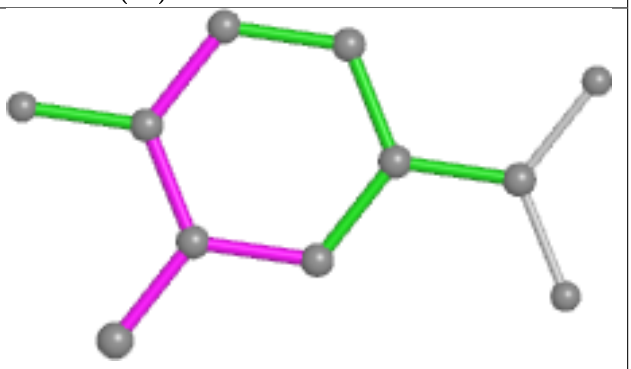
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



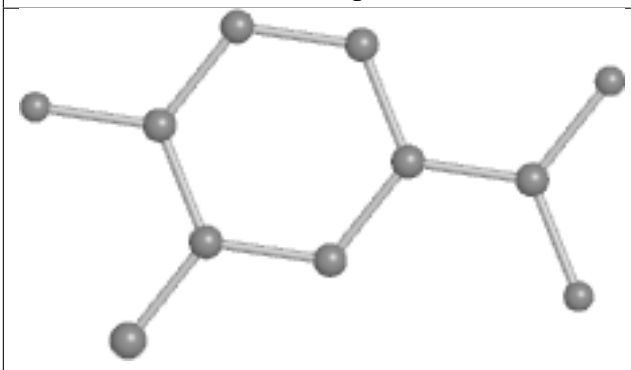
Ligand QSB C 806 (A)



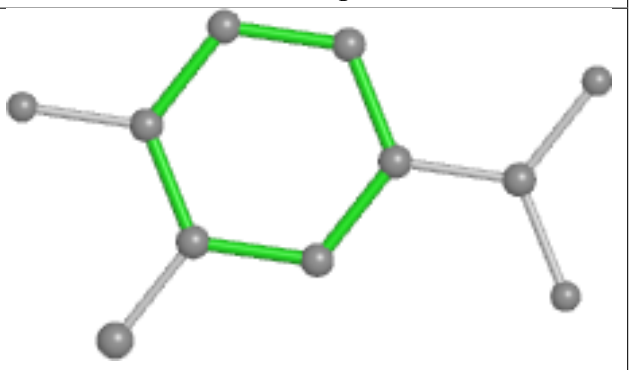
Bond lengths



Bond angles

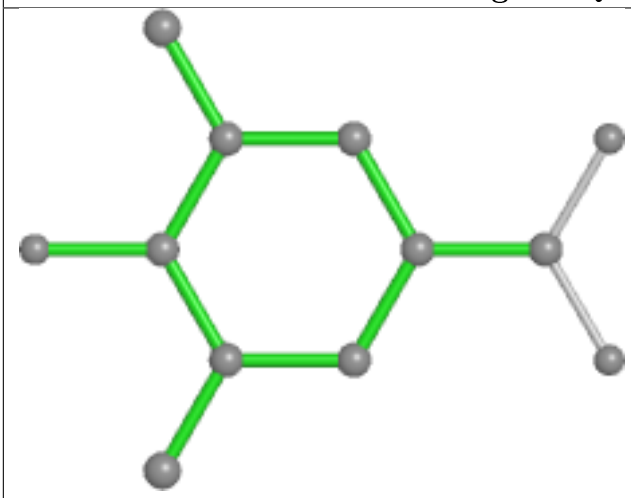


Torsions

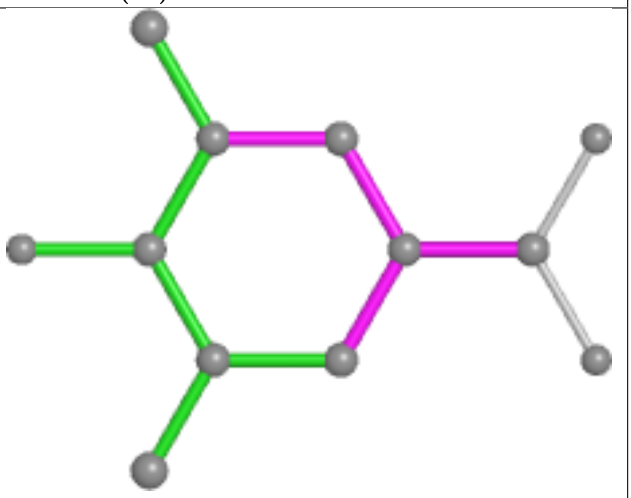


Rings

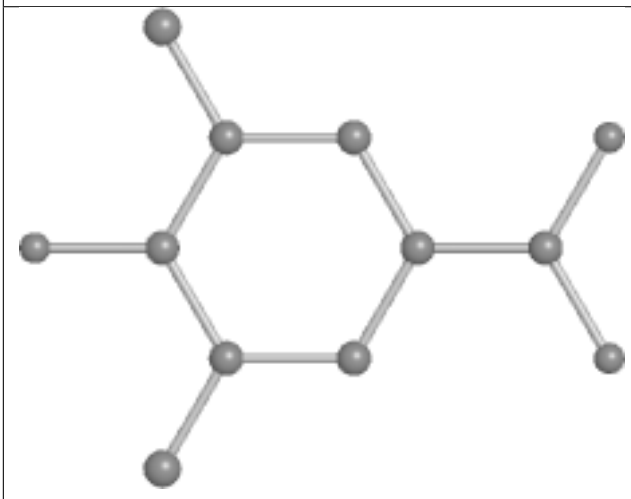
Ligand QSH B 705 (A)



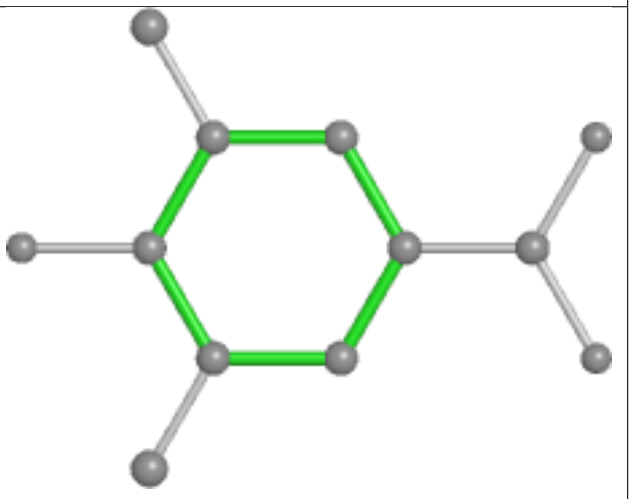
Bond lengths



Bond angles

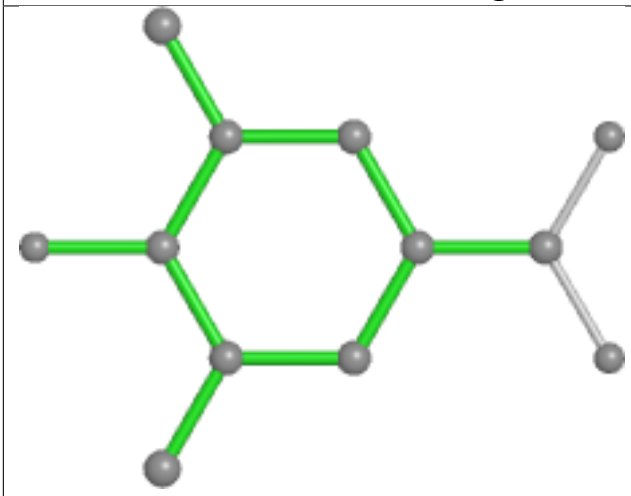


Torsions

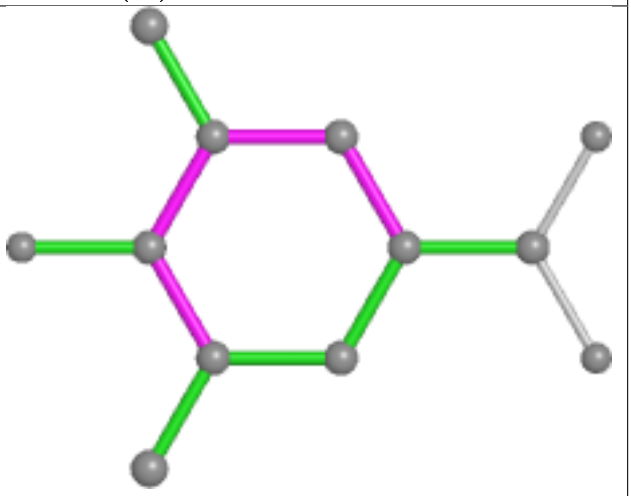


Rings

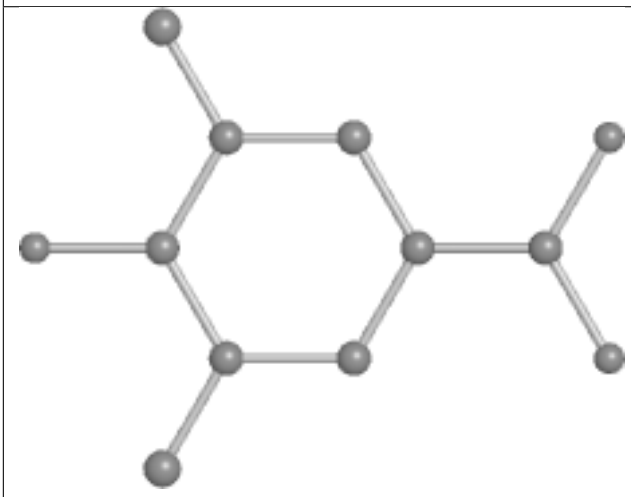
Ligand QSH C 805 (A)



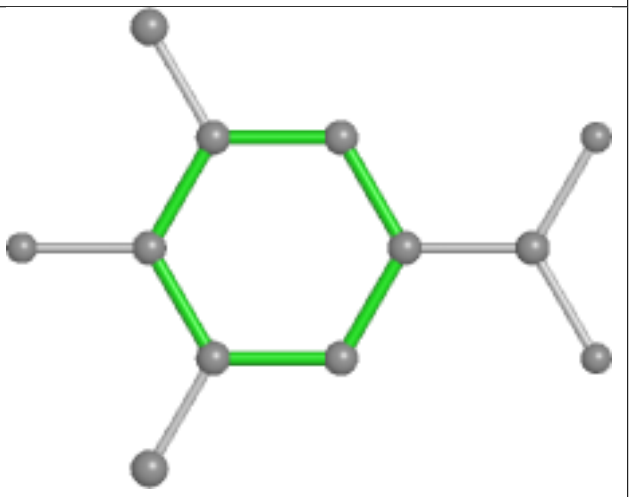
Bond lengths



Bond angles

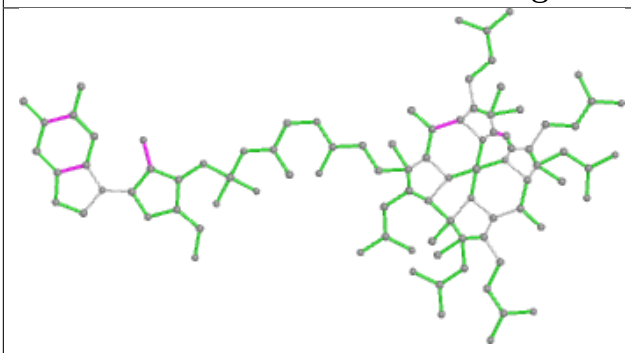


Torsions

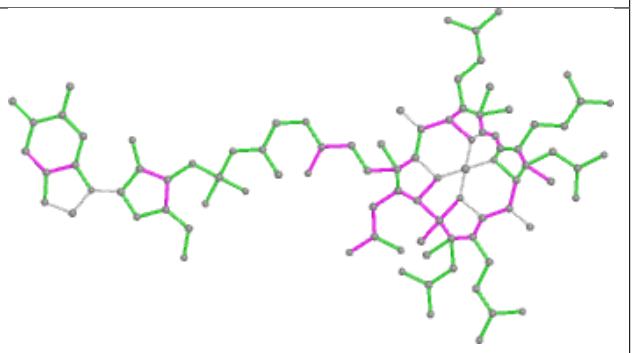


Rings

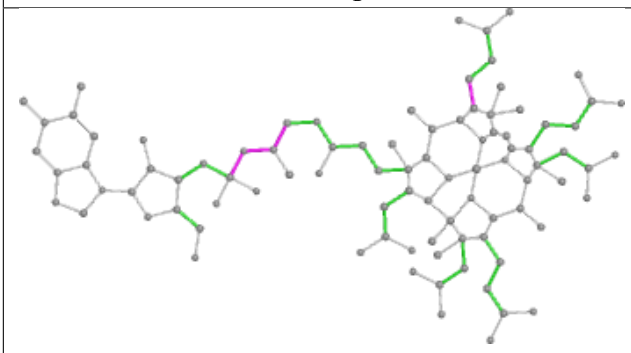
Ligand B12 C 803



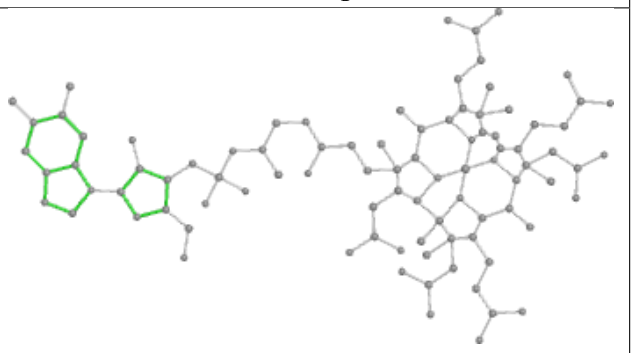
Bond lengths



Bond angles

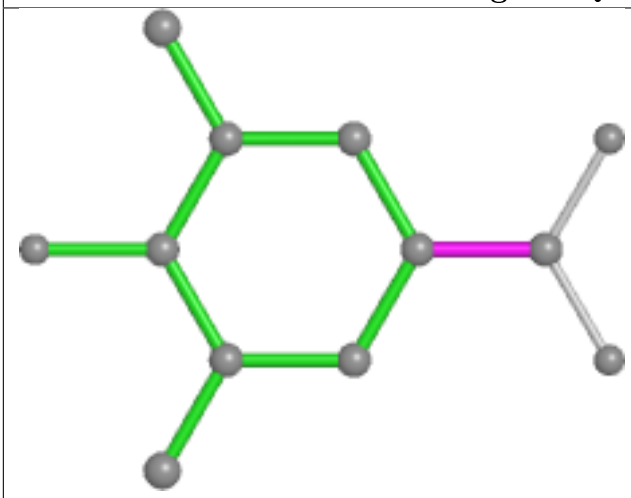


Torsions

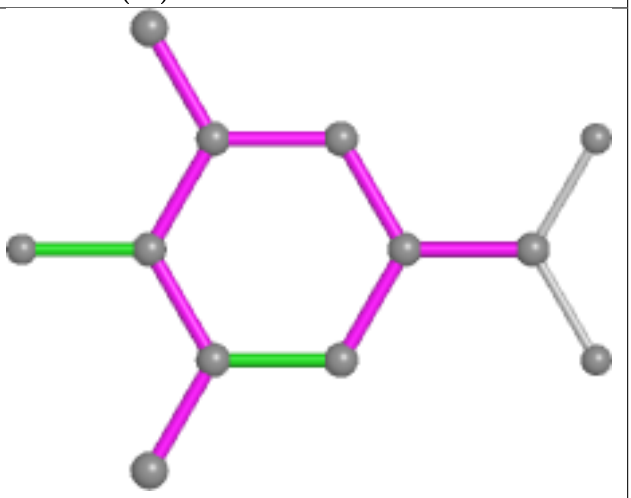


Rings

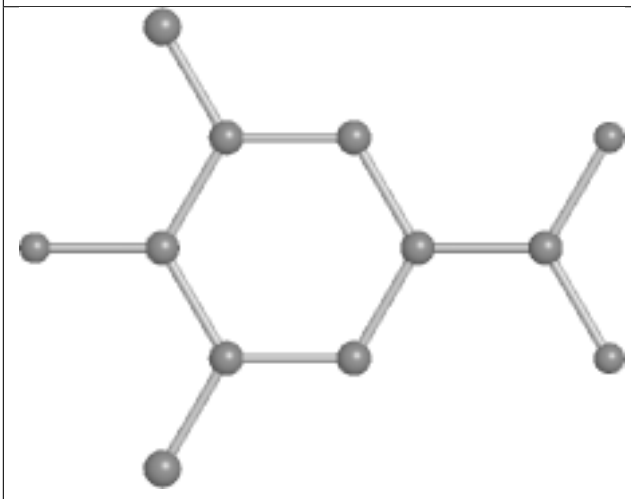
Ligand QSH A 705 (A)



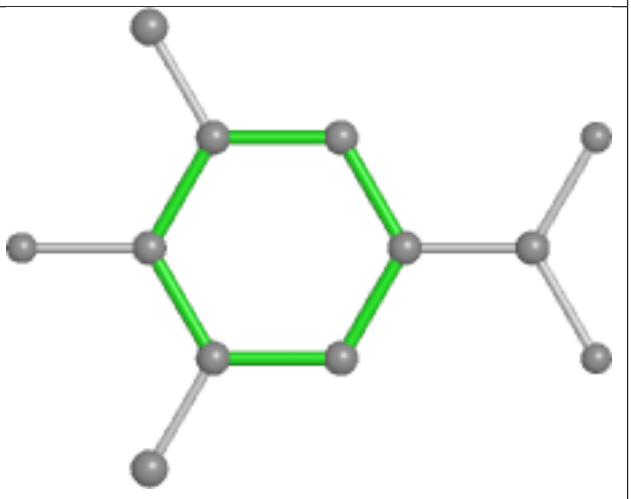
Bond lengths



Bond angles

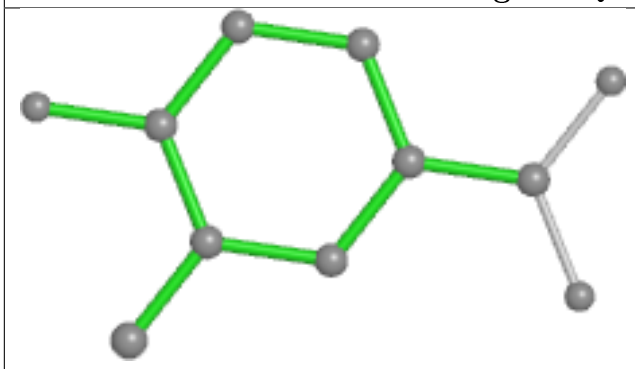


Torsions

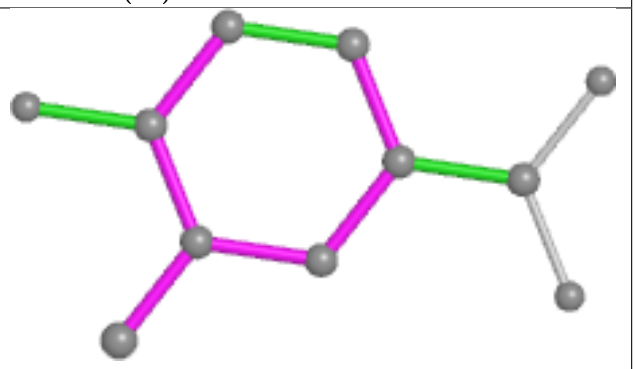


Rings

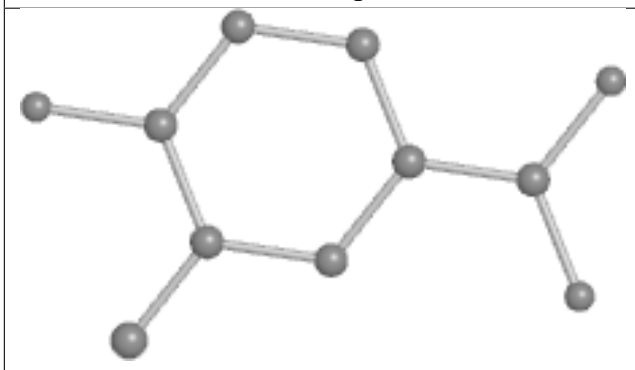
Ligand QSB B 706 (A)



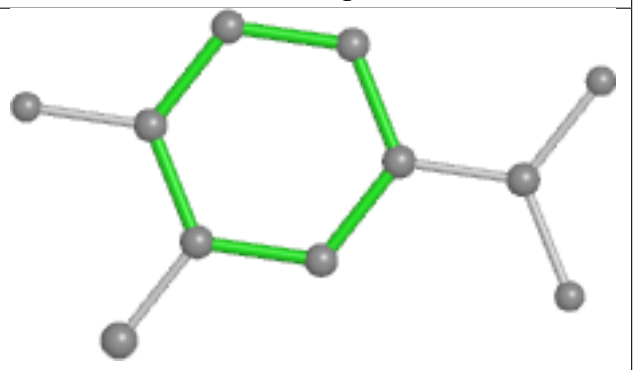
Bond lengths



Bond angles

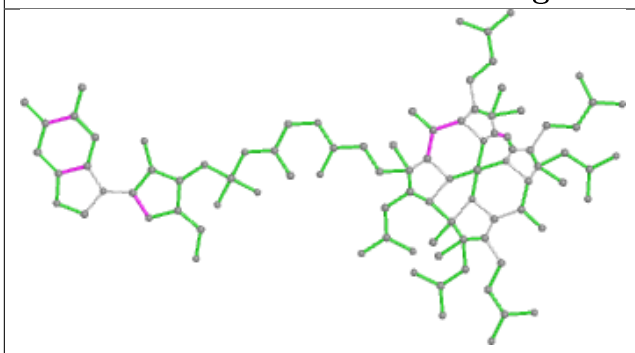


Torsions

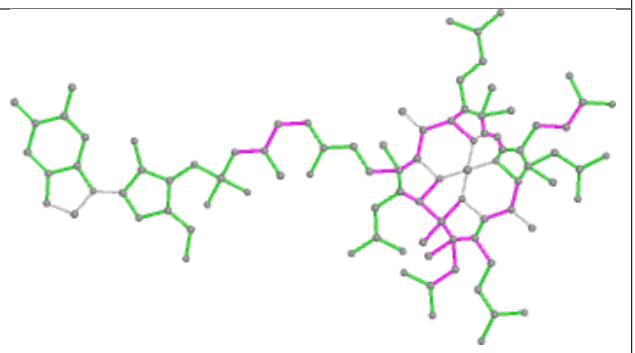


Rings

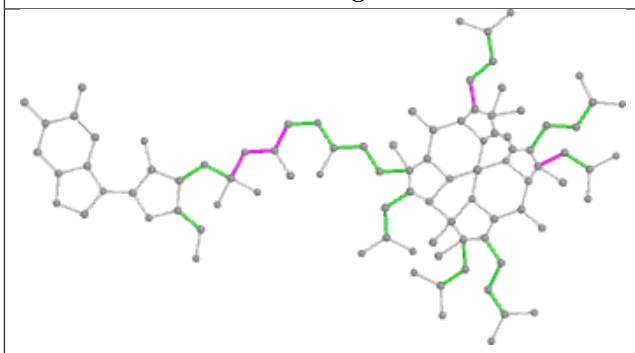
Ligand B12 B 703



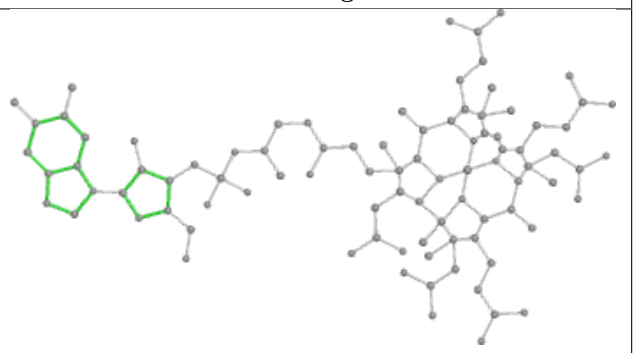
Bond lengths



Bond angles

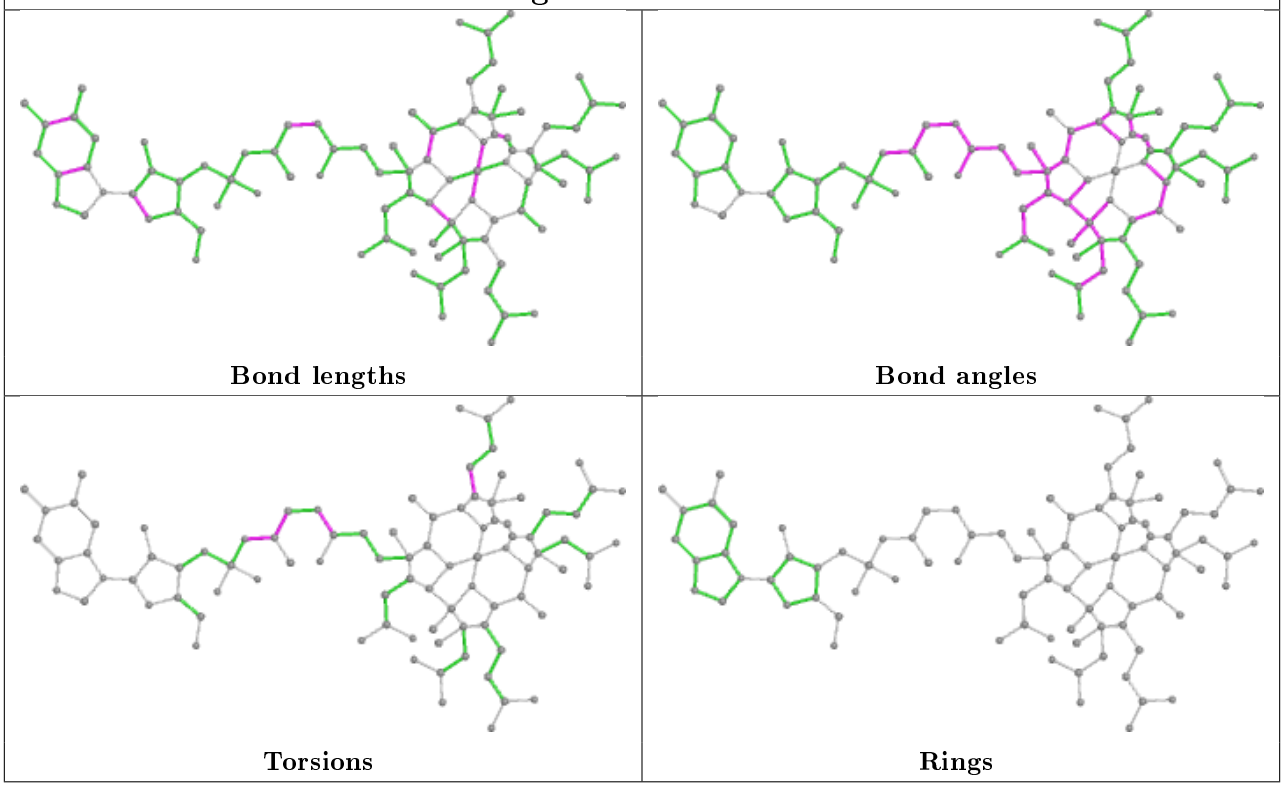


Torsions



Rings

Ligand B12 A 703



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	700/725 (96%)	-0.14	0	100	100	13, 23, 42, 70	0
1	B	695/725 (95%)	-0.16	0	100	100	16, 25, 44, 78	0
1	C	696/725 (96%)	0.09	5 (0%)	87	87	21, 42, 66, 100	0
All	All	2091/2175 (96%)	-0.07	5 (0%)	95	94	13, 28, 58, 100	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	347	GLY	3.3
1	C	47	ASP	3.0
1	C	27	VAL	2.9
1	C	196	VAL	2.4
1	C	329	GLN	2.3

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 monosaccharides in this entry.

6.4 Ligands

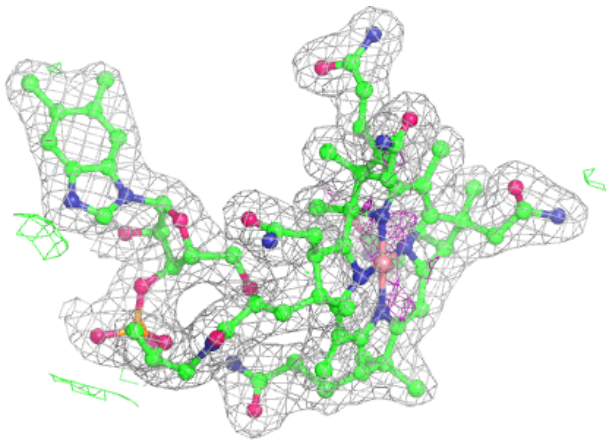
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

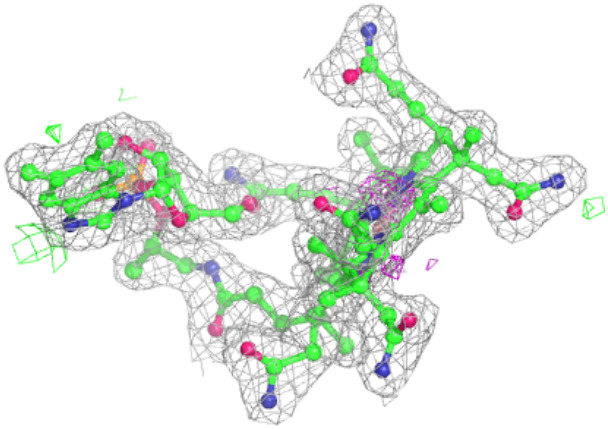
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NA	C	804	1/1	0.87	0.09	55,55,55,55	0
4	NA	B	704	1/1	0.96	0.08	44,44,44,44	0
3	B12	C	803	91/91	0.97	0.11	19,27,30,31	0
6	QSB	C	806[A]	11/11	0.98	0.13	28,31,34,36	11
3	B12	B	703	91/91	0.98	0.10	15,18,22,25	0
3	B12	A	703	91/91	0.98	0.10	12,15,20,21	0
6	QSB	B	706[A]	11/11	0.98	0.11	23,25,28,29	11
5	QSH	C	805[A]	12/12	0.98	0.12	24,27,29,30	12
5	QSH	B	705[A]	12/12	0.98	0.11	20,22,24,26	12
2	SF4	B	702	8/8	0.99	0.10	21,24,26,26	0
2	SF4	C	801	8/8	0.99	0.10	21,24,24,27	0
2	SF4	A	702	8/8	0.99	0.11	15,16,17,18	0
6	QSB	A	706[A]	11/11	0.99	0.11	19,20,22,24	11
2	SF4	A	701	8/8	0.99	0.11	15,16,17,17	0
2	SF4	B	701	8/8	0.99	0.10	19,20,22,22	0
4	NA	A	704	1/1	0.99	0.09	35,35,35,35	0
2	SF4	C	802	8/8	0.99	0.10	24,25,28,30	0
5	QSH	A	705[A]	12/12	0.99	0.12	20,20,23,23	12
7	BR	A	707[A]	1/1	1.00	0.11	21,21,21,21	1
7	BR	B	707[A]	1/1	1.00	0.10	23,23,23,23	1
7	BR	C	807[A]	1/1	1.00	0.07	28,28,28,28	1

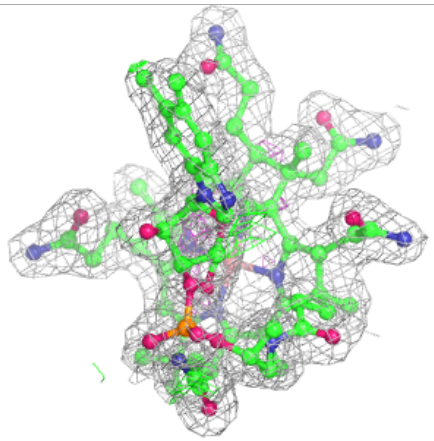
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B12 C 803:

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

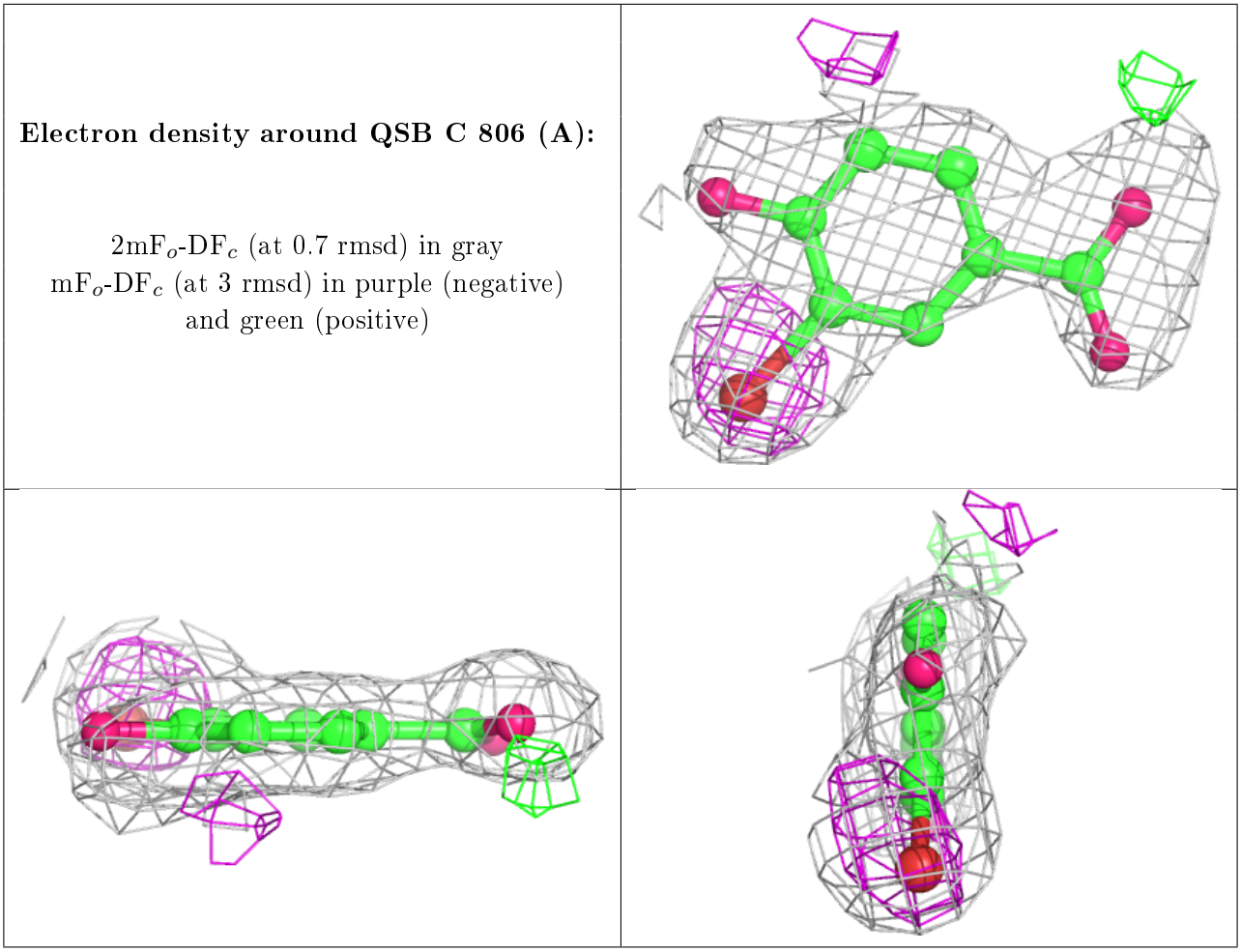






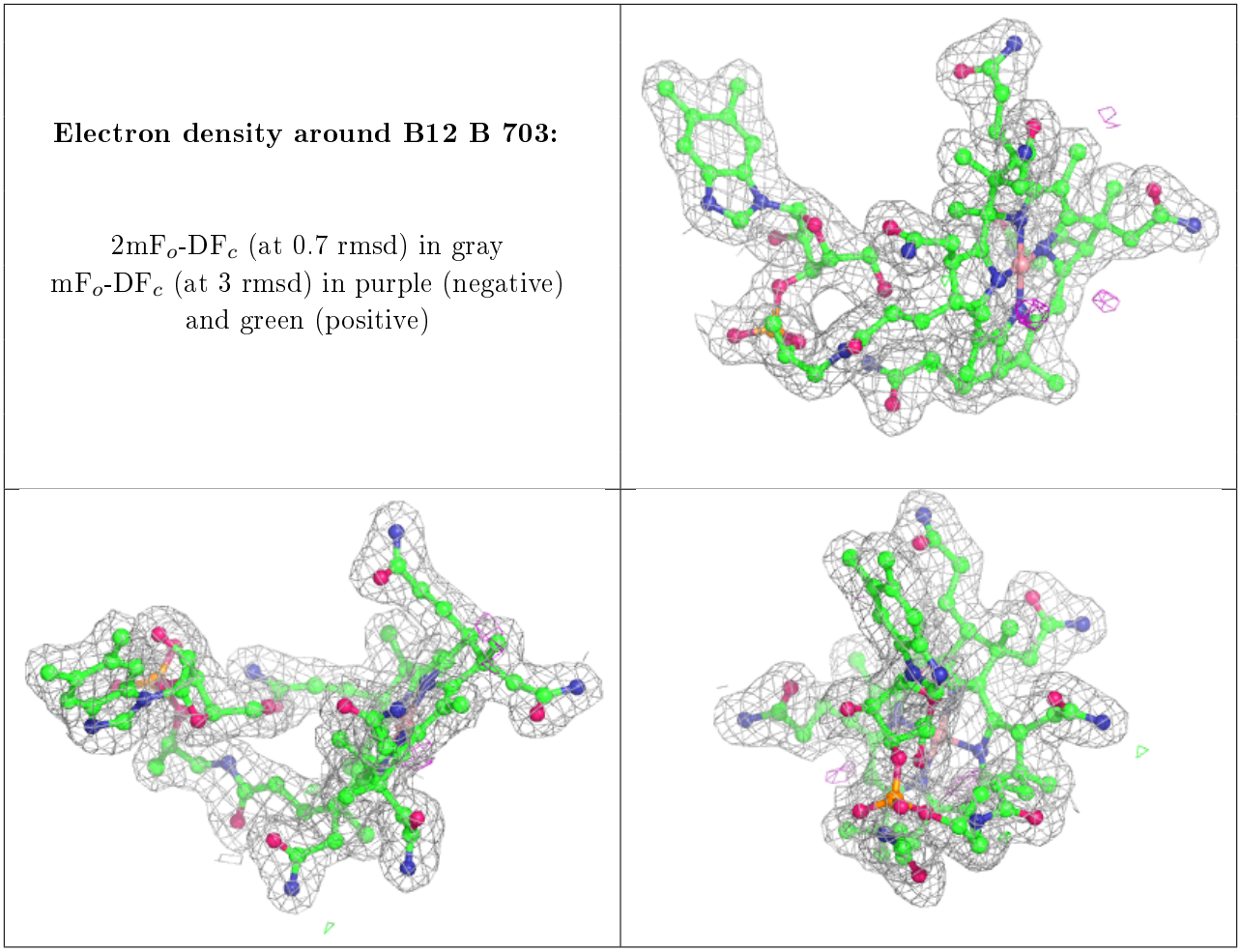
Electron density around QSB C 806 (A):

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



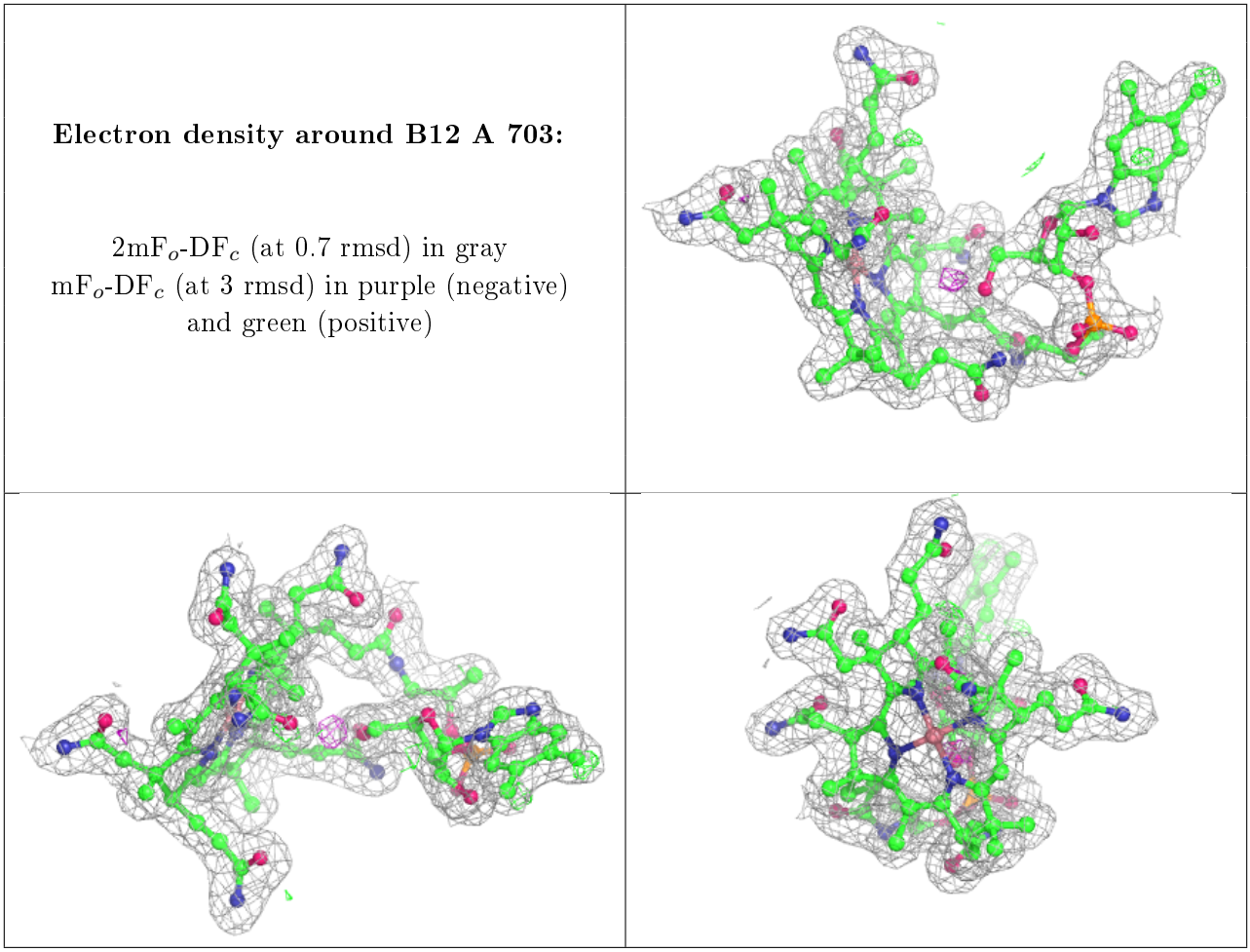
Electron density around B12 B 703:

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



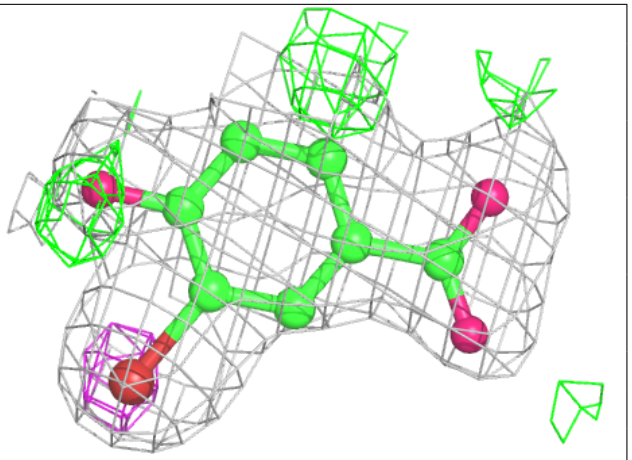
Electron density around B12 A 703:

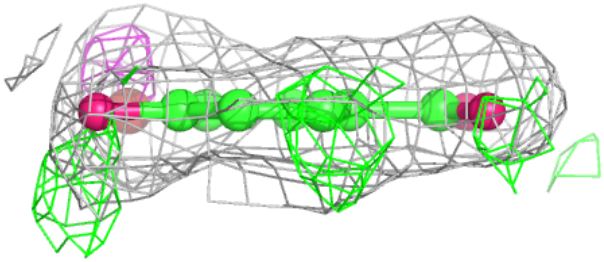
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

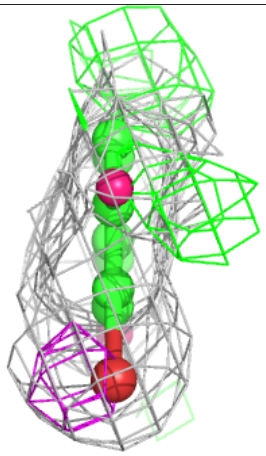


Electron density around QSB B 706 (A):

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

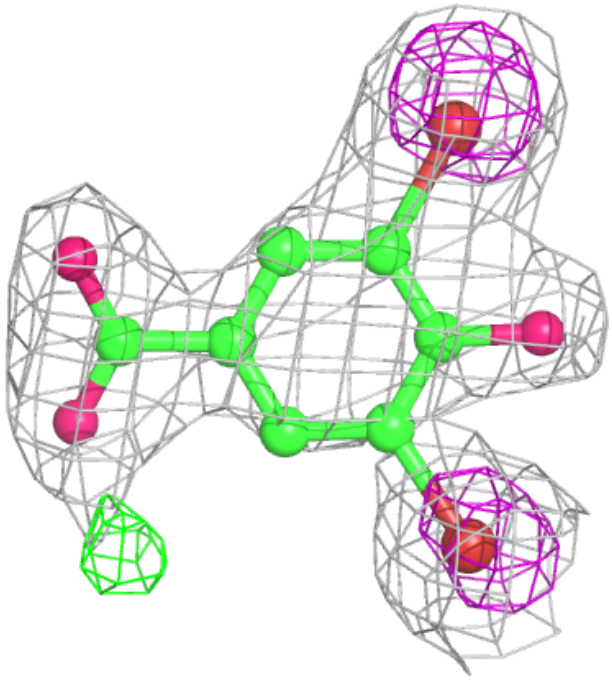


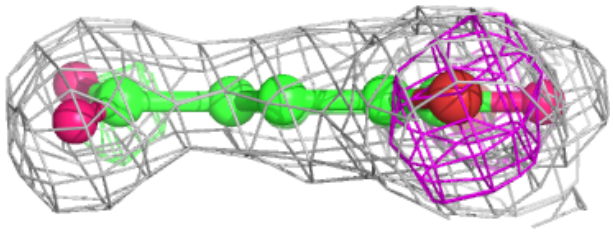


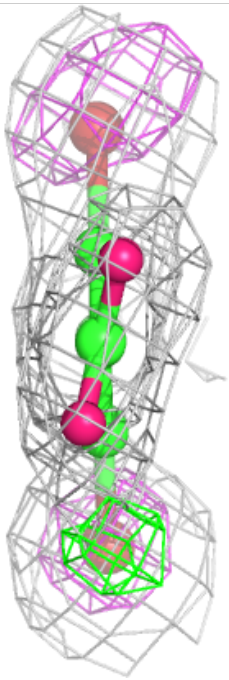


Electron density around QSH C 805 (A):

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

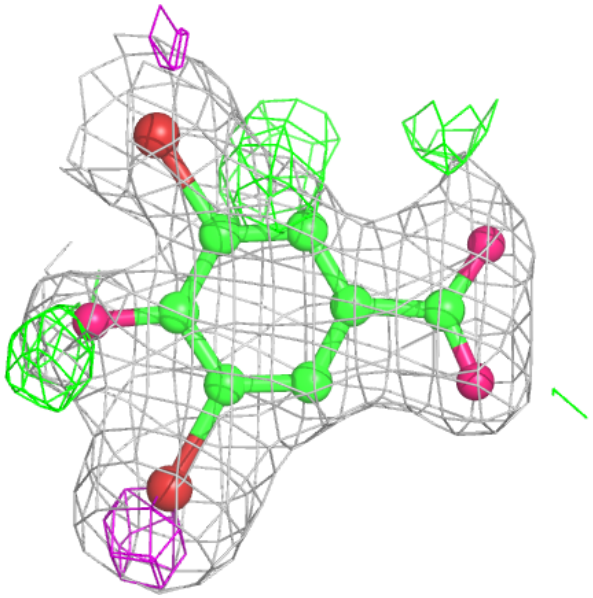


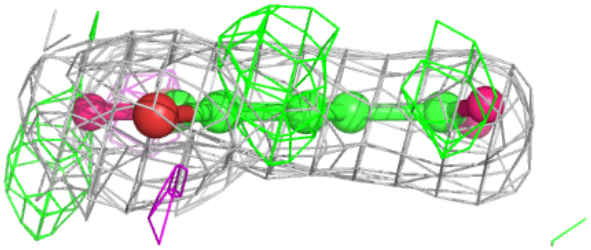


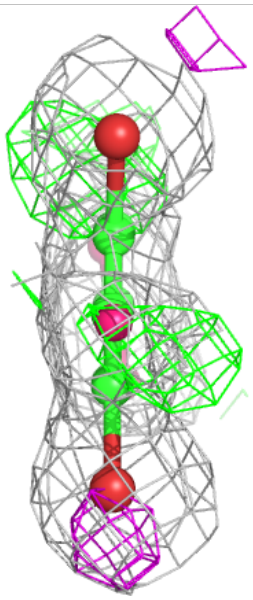


Electron density around QSH B 705 (A):

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

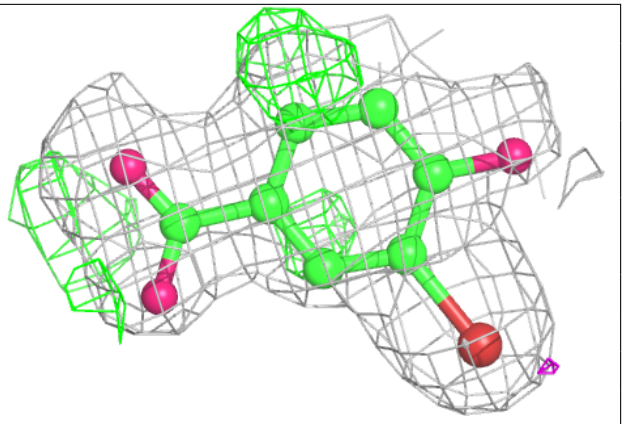


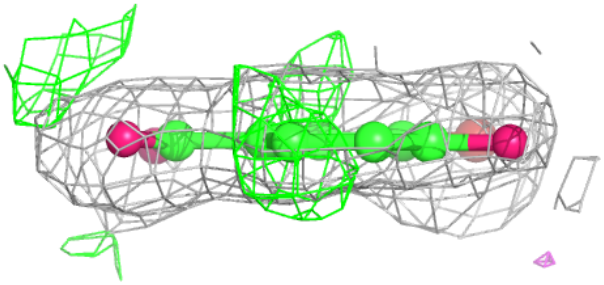


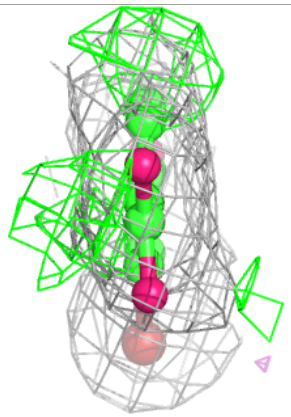


Electron density around QSB A 706 (A):

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

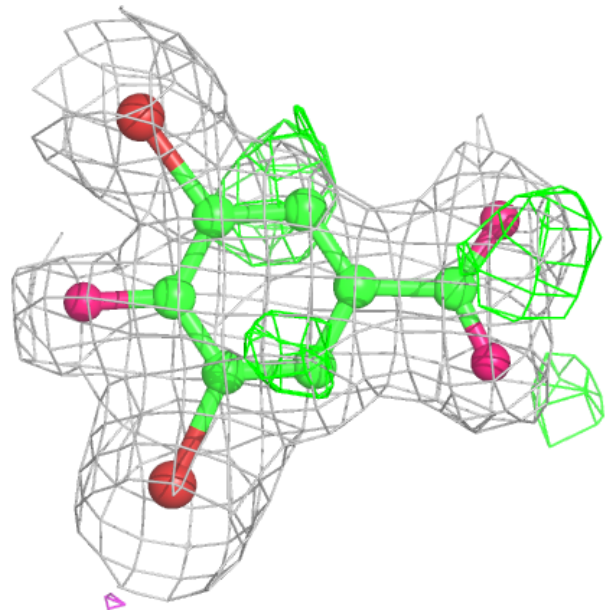


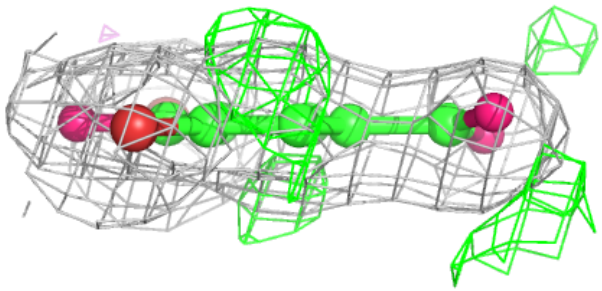


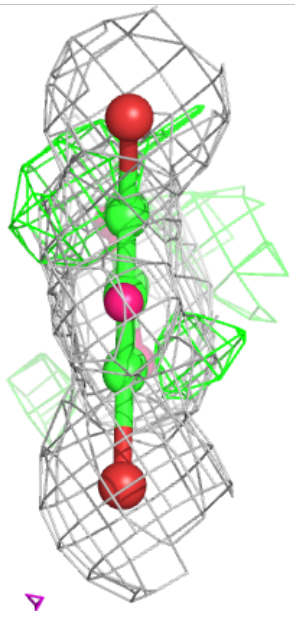


Electron density around QSH A 705 (A):

$2mF_o$-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

There are no such residues in this entry.