wwPDB X-ray Structure Validation Summary Report (i)

Aug 26, 2026 – 05:51 am BST

PDB ID	:	6ZY1 / pdb_00006zy1
Title	:	Catabolic reductive dehalogenase NpRdhA, N-terminally tagged in complex with 3-bromo-4-hydroxybenzoic acid
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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

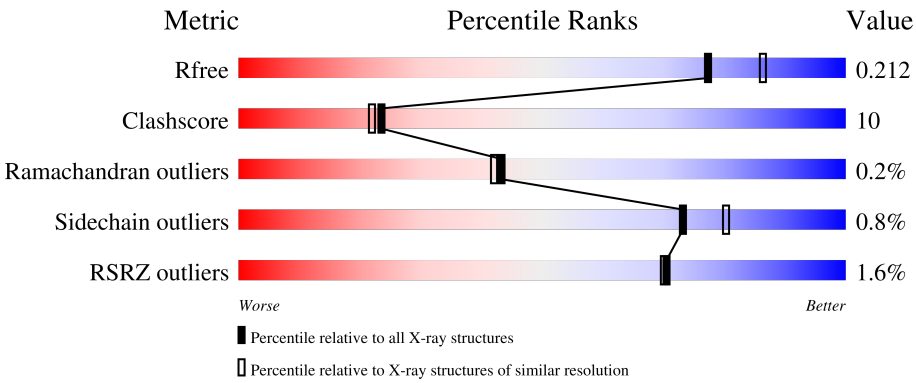
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	725	.% 82% 14% • •
1	B	725	2% 81% 15% •
1	C	725	2% 76% 19% • •

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	703	X	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17478 atoms, of which 36 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
			Total	C	N	O	S			
1	A	700	5336	3330	972	994	40	0	1	0
1	B	696	5280	3293	956	991	40	0	1	0
1	C	695	5238	3269	953	976	40	0	1	0

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	-26	MET	-	initiating methionine	UNP K2MB66
C	-25	VAL	-	expression tag	UNP K2MB66
C	-24	GLN	-	expression tag	UNP K2MB66
C	-23	THR	-	expression tag	UNP K2MB66
C	-22	SER	-	expression tag	UNP K2MB66
C	-21	PHE	-	expression tag	UNP K2MB66
C	-20	GLU	-	expression tag	UNP K2MB66
C	-19	HIS	-	expression tag	UNP K2MB66
C	-18	HIS	-	expression tag	UNP K2MB66
C	-17	HIS	-	expression tag	UNP K2MB66

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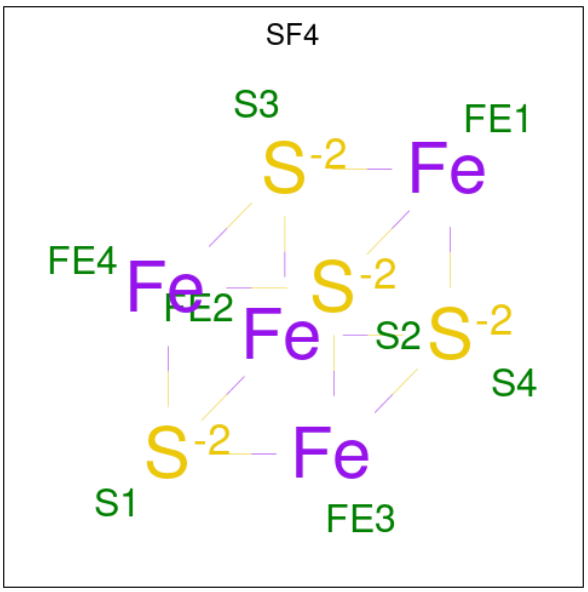
Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	HIS	-	expression tag	UNP K2MB66
C	-15	HIS	-	expression tag	UNP K2MB66
C	-14	HIS	-	expression tag	UNP K2MB66
C	-13	SER	-	expression tag	UNP K2MB66
C	-12	ALA	-	expression tag	UNP K2MB66
C	-11	GLY	-	expression tag	UNP K2MB66
C	-10	GLU	-	expression tag	UNP K2MB66
C	-9	ASN	-	expression tag	UNP K2MB66
C	-8	LEU	-	expression tag	UNP K2MB66
C	-7	TYR	-	expression tag	UNP K2MB66
C	-6	PHE	-	expression tag	UNP K2MB66
C	-5	GLN	-	expression tag	UNP K2MB66
C	-4	GLY	-	expression tag	UNP K2MB66
C	-3	ALA	-	expression tag	UNP K2MB66
C	-2	GLN	-	expression tag	UNP K2MB66
C	-1	ILE	-	expression tag	UNP K2MB66
C	0	SER	-	expression tag	UNP K2MB66

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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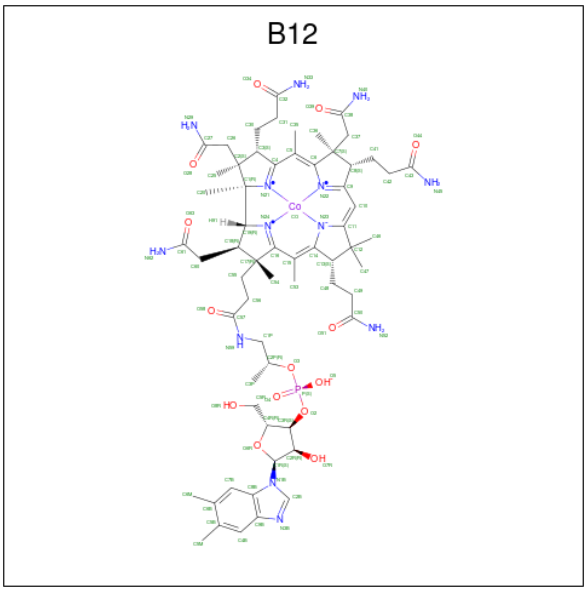
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	B	1	8	4	4	0	0
			Total	Fe	S		
2	C	1	8	4	4	0	0
			Total	Fe	S		
2	C	1	8	4	4	0	0

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

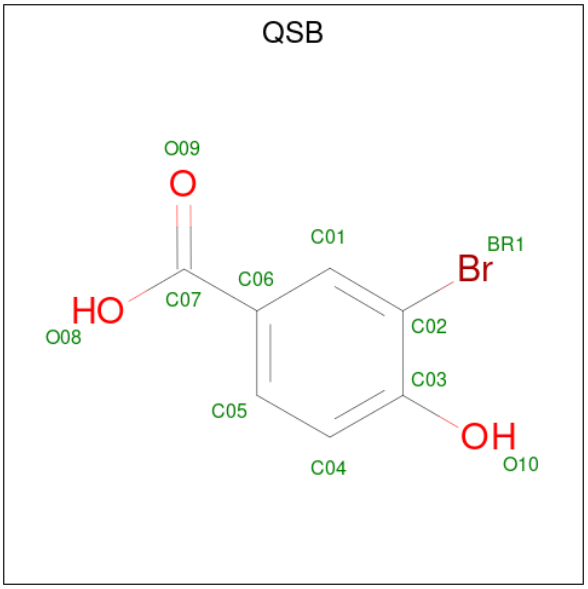


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Co	N	O	P		
3	A	1	91	62	1	13	14	1	0	0
			Total	C	Co	N	O	P		
3	B	1	91	62	1	13	14	1	0	0
			Total	C	Co	N	O	P		
3	C	1	91	62	1	13	14	1	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is 3 bromo 4 hydroxybenzoic acid (CCD ID: QSB) (formula: $C_7H_5BrO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	H	O		
5	A	1	45	3	21	12	9	0	1
5	B	1	45	3	21	12	9	0	1
5	C	1	45	3	21	12	9	0	1

- Molecule 6 is water.

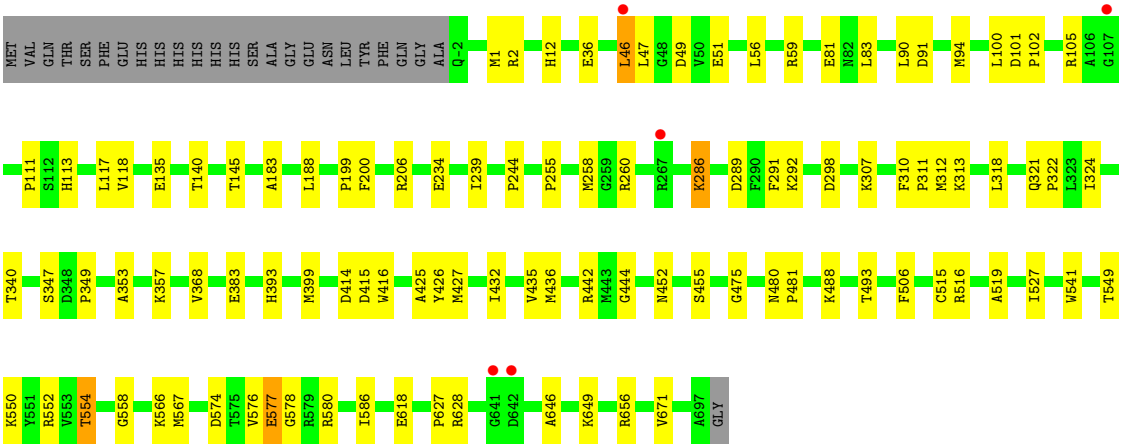
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	442	442	442	0	0
6	B	457	457	457	0	0
6	C	266	266	266	0	0

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.

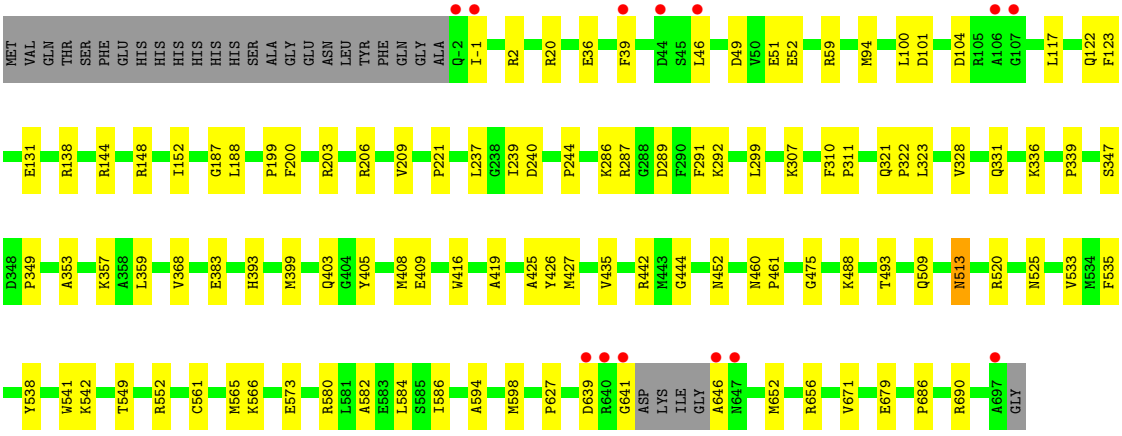
• Molecule 1: Oxidoreductase, NAD-binding/iron-sulfur cluster-binding protein

Chain A:



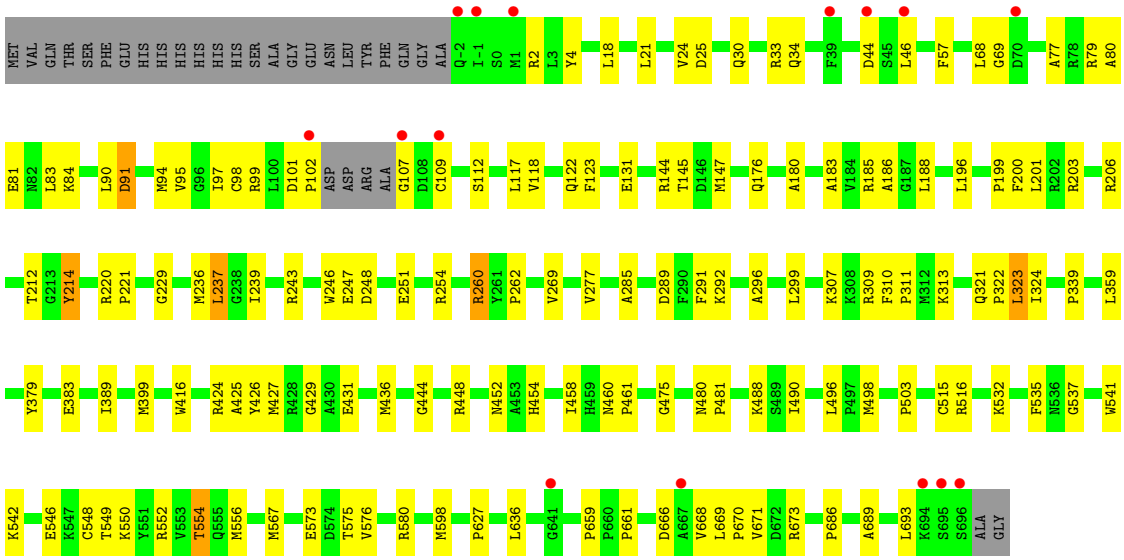
• Molecule 1: Oxidoreductase, NAD-binding/iron-sulfur cluster-binding protein

Chain B:



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

Chain C:


MET VAL GLN THR SER PHE GLU HIS HIS HIS HIS HIS HIS SER ALA GLY GLU ASN LEU TYR PHE GLN GLY ALA Q-2 I-1 S0 M1 R2 L3 Y4 L18 L21 V24 D25 Q30 R33 Q34 F39 D44 S45 L46 F57 L68 G69 D70 A77 R78 R79 A80
E81 N82 L83 K84 L90 D91 M94 V95 G96 I97 C98 R99 L100 D101 P102 ASP ASP ARG ALA G107 D108 C109 S112 L117 V118 Q122 F123 E131 R144 T145 D146 M147 Q176 A180 A183 V184 R185 A186 G187 L188 L196 P199 F200 L201 R202 R203 R206
T212 G213 Y214 R220 P221 G229 M236 L237 G238 I239 R243 W246 E247 D248 E251 R254 R260 Y261 P262 V269 V277 A285 D289 F290 F291 K292 A296 L299 K307 K308 R309 F310 P311 M312 K313 Q321 P322 L323 I324 P339 L359
Y379 E383 I389 M399 W416 R424 A425 Y426 M427 R428 G429 A430 E431 M436 G444 R448 N452 A453 H454 I458 H459 N460 P461 G475 N480 P481 K488 S489 I490 L496 P497 M498 P503 C515 R516 K532 F535 N536 G537 W541
K542 E546 K547 C548 T549 K550 Y551 R552 V553 T554 Q555 M556 M567 E573 D574 T575 V576 R580 M598 P627 L636 G641 P659 P660 P661 D666 A667 V668 L669 P670 V671 D672 R673 P686 A689 L693 K694 S695 S696 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	175.87Å 170.10Å 107.65Å 90.00° 98.35° 90.00°	Depositor
Resolution (Å)	106.00 – 1.99 106.00 – 1.99	Depositor EDS
% Data completeness (in resolution range)	94.0 (106.00-1.99) 52.8 (106.00-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.0	Depositor
R, R_{free}	0.177 , 0.211 0.178 , 0.212	Depositor DCC
R_{free} test set	2000 reflections (0.94%)	wwPDB-VP
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 35.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17478	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: B12, SF4, QSB, NA

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	0.17	0/5452	0.39	0/7382
1	B	0.17	0/5395	0.39	0/7311
1	C	0.15	0/5348	0.37	0/7248
All	All	0.16	0/16195	0.38	0/21941

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5336	0	5222	84	0
1	B	5280	0	5119	83	0
1	C	5238	0	5065	113	0
2	A	16	0	0	0	0
2	B	16	0	0	0	0
2	C	16	0	0	1	0
3	A	91	0	87	19	0
3	B	91	0	87	20	0
3	C	91	0	87	24	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	33	12	0	3	0
5	B	33	12	0	3	0
5	C	33	12	0	2	0
6	A	442	0	0	10	0
6	B	457	0	0	13	0
6	C	266	0	0	12	0
All	All	17442	36	15667	327	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 10.

The worst 5 of 327 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:255:PRO:HD2	1:A:258:MET:HE2	1.30	1.12
1:C:291:PHE:CD2	3:C:703:B12:H532	1.98	0.98
3:C:703:B12:H362	3:C:703:B12:H351	1.49	0.94
1:A:312:MET:HE3	1:A:318:LEU:HD23	1.47	0.94
1:C:277:VAL:HG11	1:C:693:LEU:HD11	1.49	0.94

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%)	685 (98%)	13 (2%)	1 (0%)	48 46
1	B	693/725 (96%)	675 (97%)	17 (2%)	1 (0%)	48 46
1	C	692/725 (95%)	668 (96%)	22 (3%)	2 (0%)	36 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2084/2175 (96%)	2028 (97%)	52 (2%)	4 (0%)	43 42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	214	TYR
1	A	46	LEU
1	C	91	ASP
1	B	-1	ILE

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	538/569 (95%)	534 (99%)	4 (1%)	76 82
1	B	529/569 (93%)	527 (100%)	2 (0%)	84 89
1	C	518/569 (91%)	512 (99%)	6 (1%)	63 70
All	All	1585/1707 (93%)	1573 (99%)	12 (1%)	73 80

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	131	GLU
1	C	237	LEU
1	C	554	THR
1	C	260	ARG
1	A	577	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	513	ASN
1	B	514	GLN

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Mol	Chain	Res	Type
1	C	257	HIS
1	C	82	ASN
1	A	513	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
2	SF4	B	702	1	0,12,12	-	-	-		
5	QSB	A	705[C]	-	11,11,11	1.18	1 (9%)	15,15,15	0.98	1 (6%)
3	B12	A	703	-	93,101,101	1.43	13 (13%)	146,166,166	2.50	39 (26%)
5	QSB	B	705[B]	-	11,11,11	1.19	2 (18%)	15,15,15	0.97	1 (6%)
2	SF4	B	701	1	0,12,12	-	-	-		
2	SF4	A	702	1	0,12,12	-	-	-		
2	SF4	C	701	1	0,12,12	-	-	-		
5	QSB	C	705[A]	-	11,11,11	1.19	2 (18%)	15,15,15	1.04	2 (13%)
2	SF4	A	701	1	0,12,12	-	-	-		
5	QSB	A	705[A]	-	11,11,11	1.19	1 (9%)	15,15,15	1.40	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	QSB	A	705[B]	-	11,11,11	1.22	1 (9%)	15,15,15	1.25	2 (13%)
3	B12	B	703	-	93,101,101	1.41	12 (12%)	146,166,166	2.50	37 (25%)
5	QSB	B	705[C]	-	11,11,11	1.20	2 (18%)	15,15,15	1.10	2 (13%)
5	QSB	C	705[C]	-	11,11,11	1.23	2 (18%)	15,15,15	1.06	1 (6%)
5	QSB	C	705[B]	-	11,11,11	1.24	1 (9%)	15,15,15	1.22	1 (6%)
3	B12	C	703	-	93,101,101	1.45	13 (13%)	146,166,166	2.42	37 (25%)
2	SF4	C	702	1	0,12,12	-	-	-		
5	QSB	B	705[A]	-	11,11,11	1.22	2 (18%)	15,15,15	1.19	1 (6%)

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
5	QSB	B	705[B]	-	-	4/4/4/4	0/1/1/1
5	QSB	A	705[C]	-	-	0/4/4/4	0/1/1/1
3	B12	A	703	-	1/1/36/38	16/56/223/223	0/3/11/11
5	QSB	C	705[A]	-	-	0/4/4/4	0/1/1/1
2	SF4	A	702	1	-	-	0/6/5/5
2	SF4	B	701	1	-	-	0/6/5/5
2	SF4	B	702	1	-	-	0/6/5/5
2	SF4	C	701	1	-	-	0/6/5/5
2	SF4	A	701	1	-	-	0/6/5/5
5	QSB	A	705[A]	-	-	0/4/4/4	0/1/1/1
5	QSB	A	705[B]	-	-	4/4/4/4	0/1/1/1
3	B12	B	703	-	1/1/36/38	10/56/223/223	0/3/11/11
5	QSB	B	705[C]	-	-	0/4/4/4	0/1/1/1
5	QSB	C	705[C]	-	-	4/4/4/4	0/1/1/1
2	SF4	C	702	1	-	-	0/6/5/5
3	B12	C	703	-	1/1/36/38	13/56/223/223	0/3/11/11
5	QSB	C	705[B]	-	-	4/4/4/4	0/1/1/1
5	QSB	B	705[A]	-	-	4/4/4/4	0/1/1/1

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	703	B12	C14-N23	5.85	1.42	1.35
3	A	703	B12	C14-N23	5.56	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	703	B12	C14-N23	5.36	1.41	1.35
3	A	703	B12	C8B-C9B	4.98	1.48	1.40
3	C	703	B12	C8B-C9B	4.93	1.48	1.40

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	703	B12	C20-C1-C19	-8.58	101.08	109.36
3	A	703	B12	C12-C11-C10	-8.47	112.34	123.37
3	C	703	B12	C47-C12-C46	8.16	123.14	109.35
3	B	703	B12	C12-C11-C10	-8.02	112.92	123.37
3	B	703	B12	C12-C11-N23	7.92	122.86	111.83

All (3) chirality outliers are listed below:

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

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	B12	C38-C37-C7-C6
3	A	703	B12	C38-C37-C7-C36
3	A	703	B12	C56-C57-N59-C1P
3	A	703	B12	O58-C57-N59-C1P
3	A	703	B12	N59-C1P-C2P-C3P

There are no ring outliers.

11 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	705[C]	QSB	1	0
3	A	703	B12	19	0
5	B	705[B]	QSB	1	0
2	C	701	SF4	1	0
5	C	705[A]	QSB	1	0
5	A	705[A]	QSB	1	0
5	A	705[B]	QSB	1	0
3	B	703	B12	20	0

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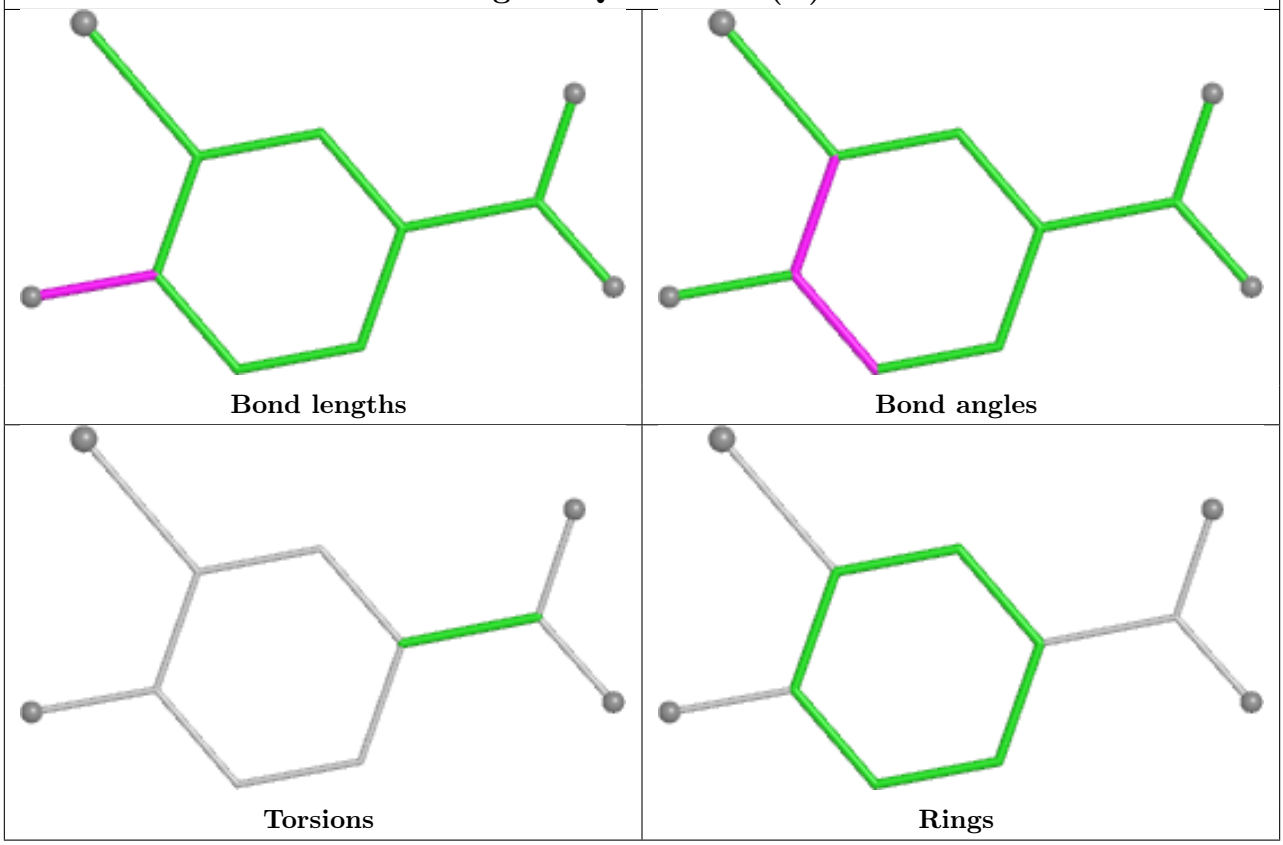
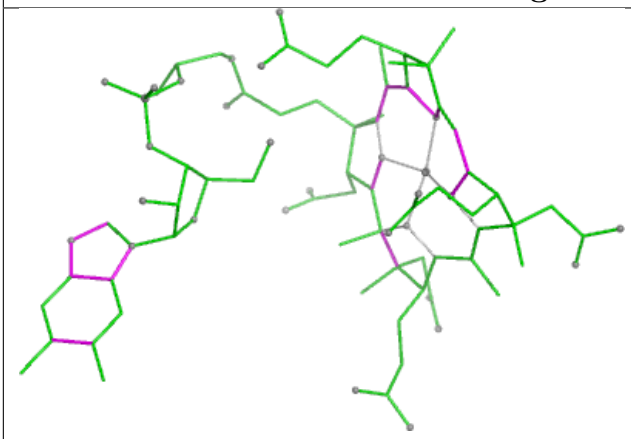
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	705[B]	QSB	1	0
3	C	703	B12	24	0
5	B	705[A]	QSB	2	0

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.

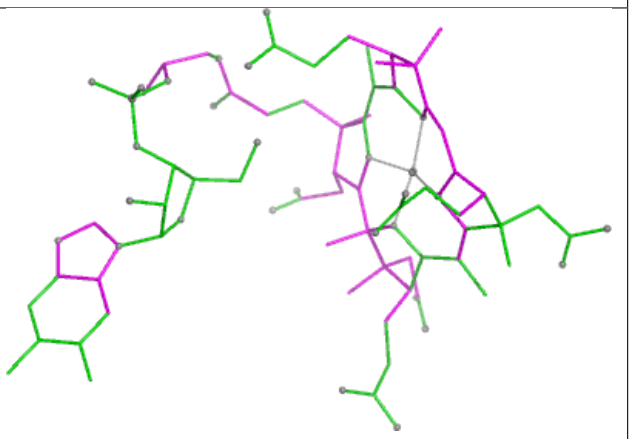
Ligand QSB A 705 (C)



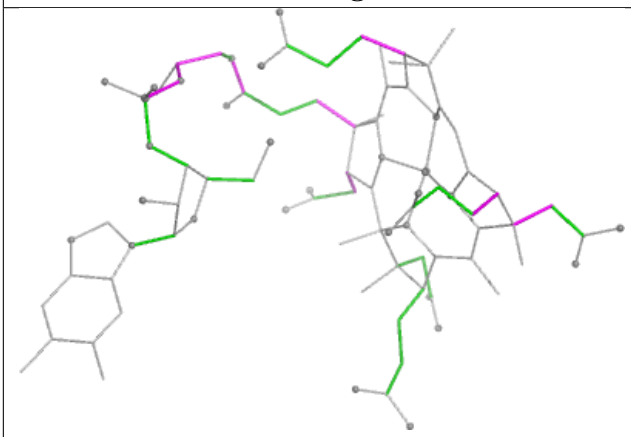
Ligand B12 A 703



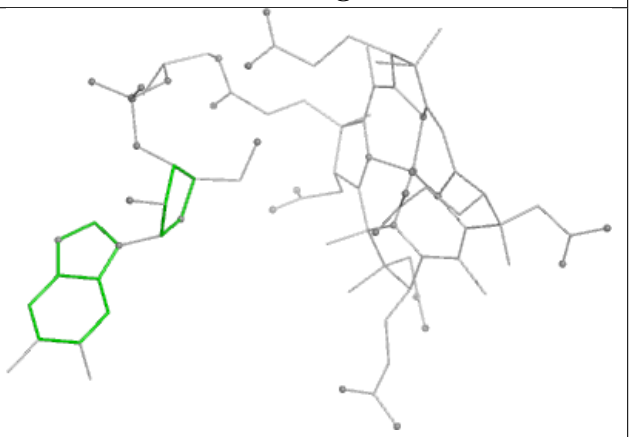
Bond lengths



Bond angles

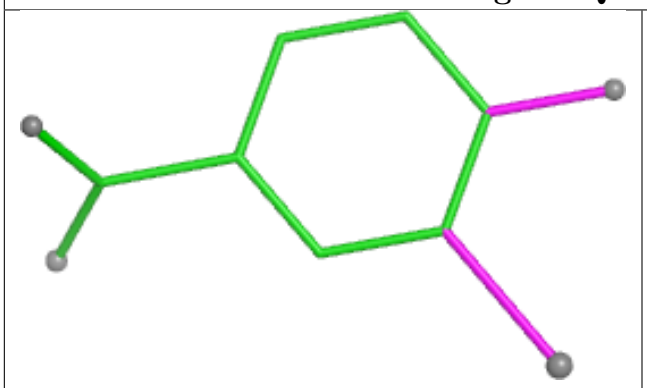


Torsions

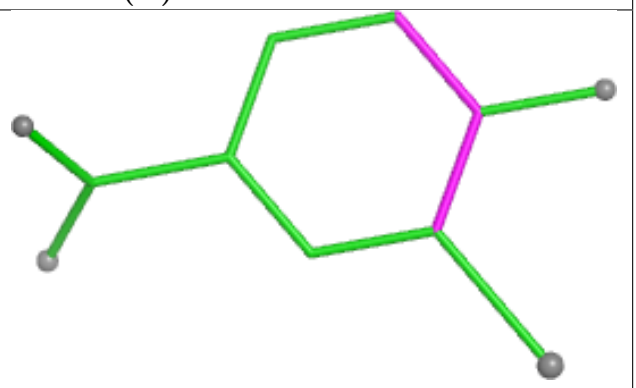


Rings

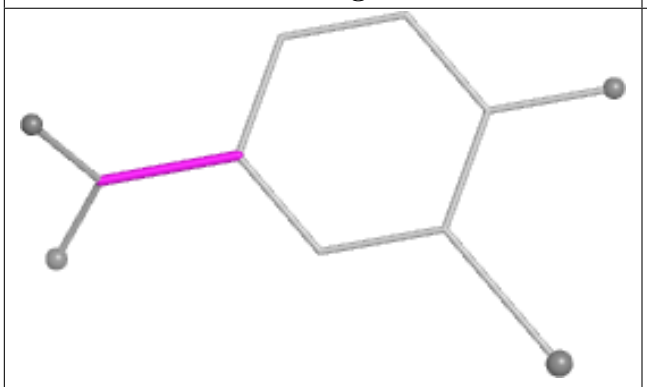
Ligand QSB B 705 (B)



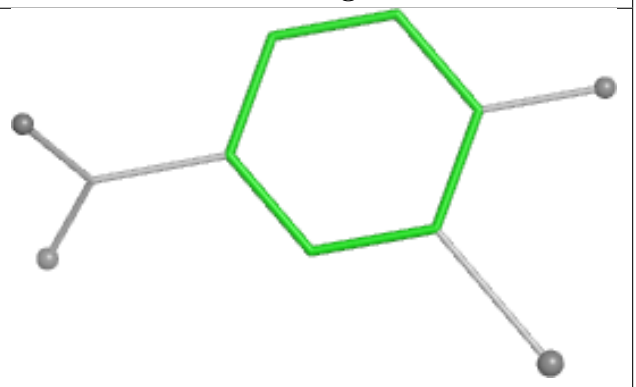
Bond lengths



Bond angles

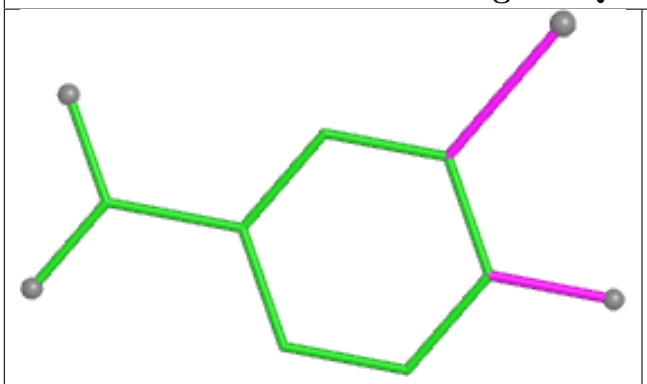


Torsions

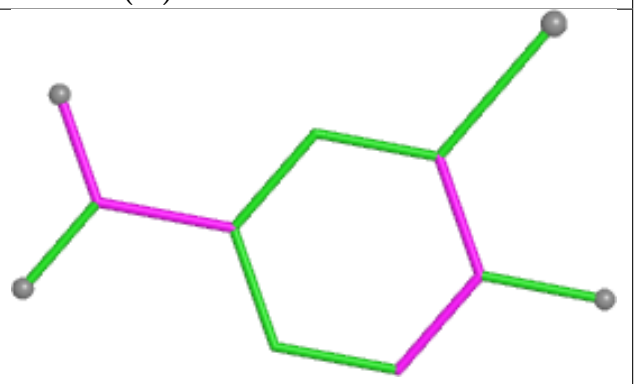


Rings

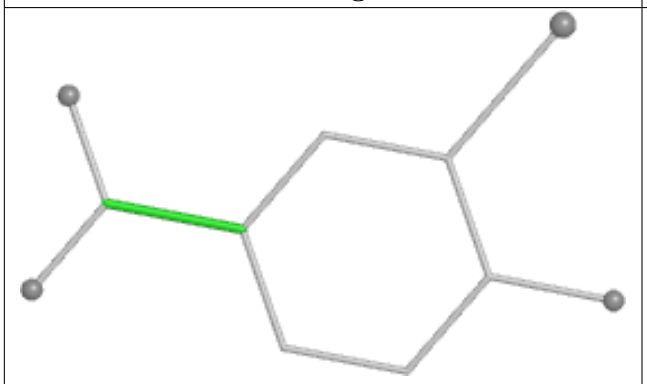
Ligand QSB C 705 (A)



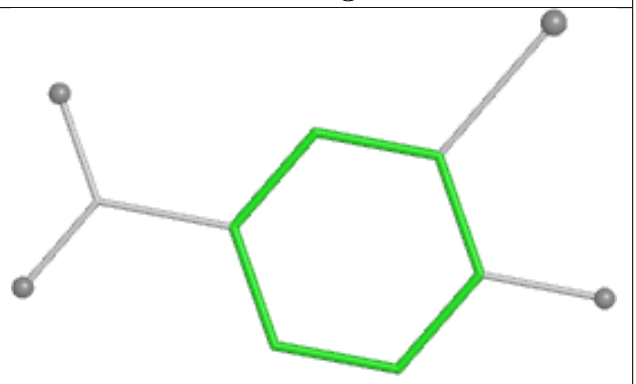
Bond lengths



Bond angles

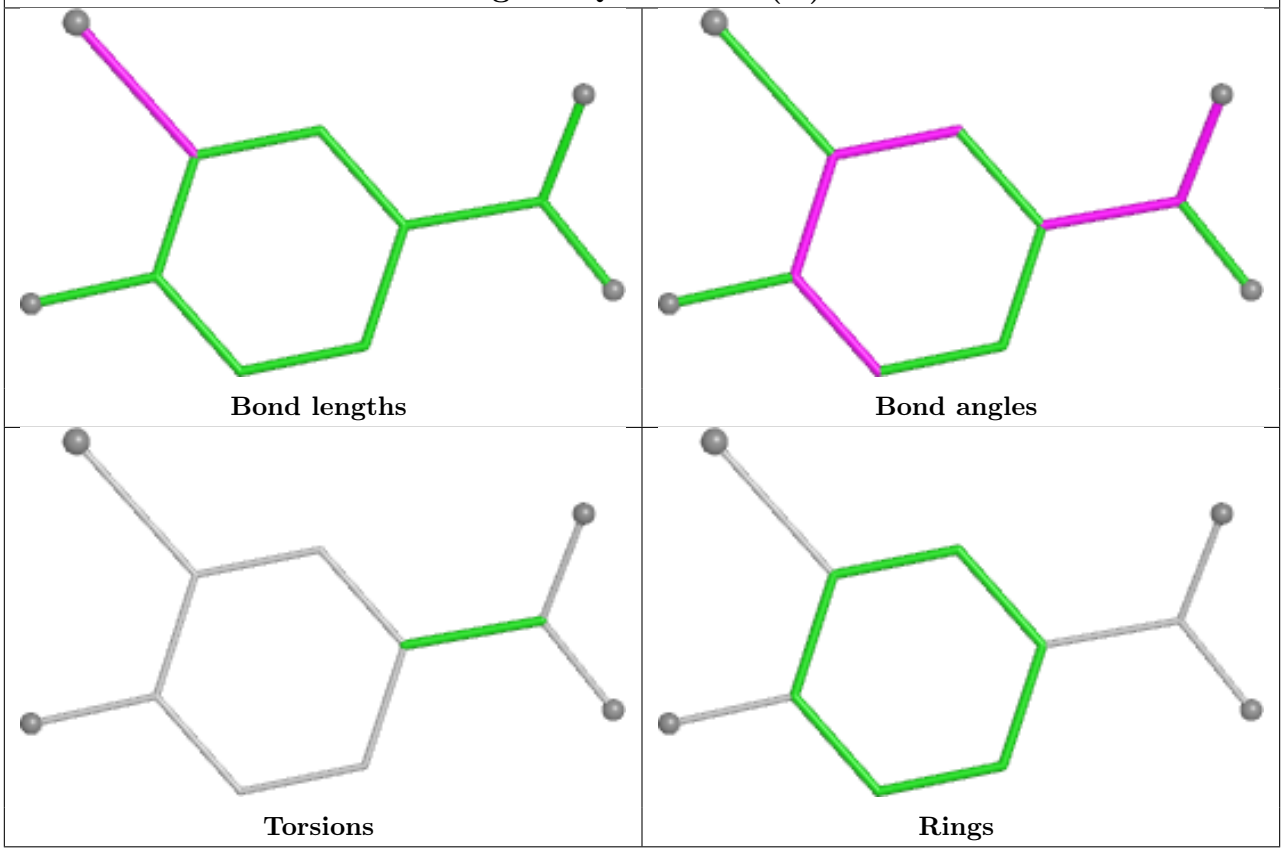


Torsions

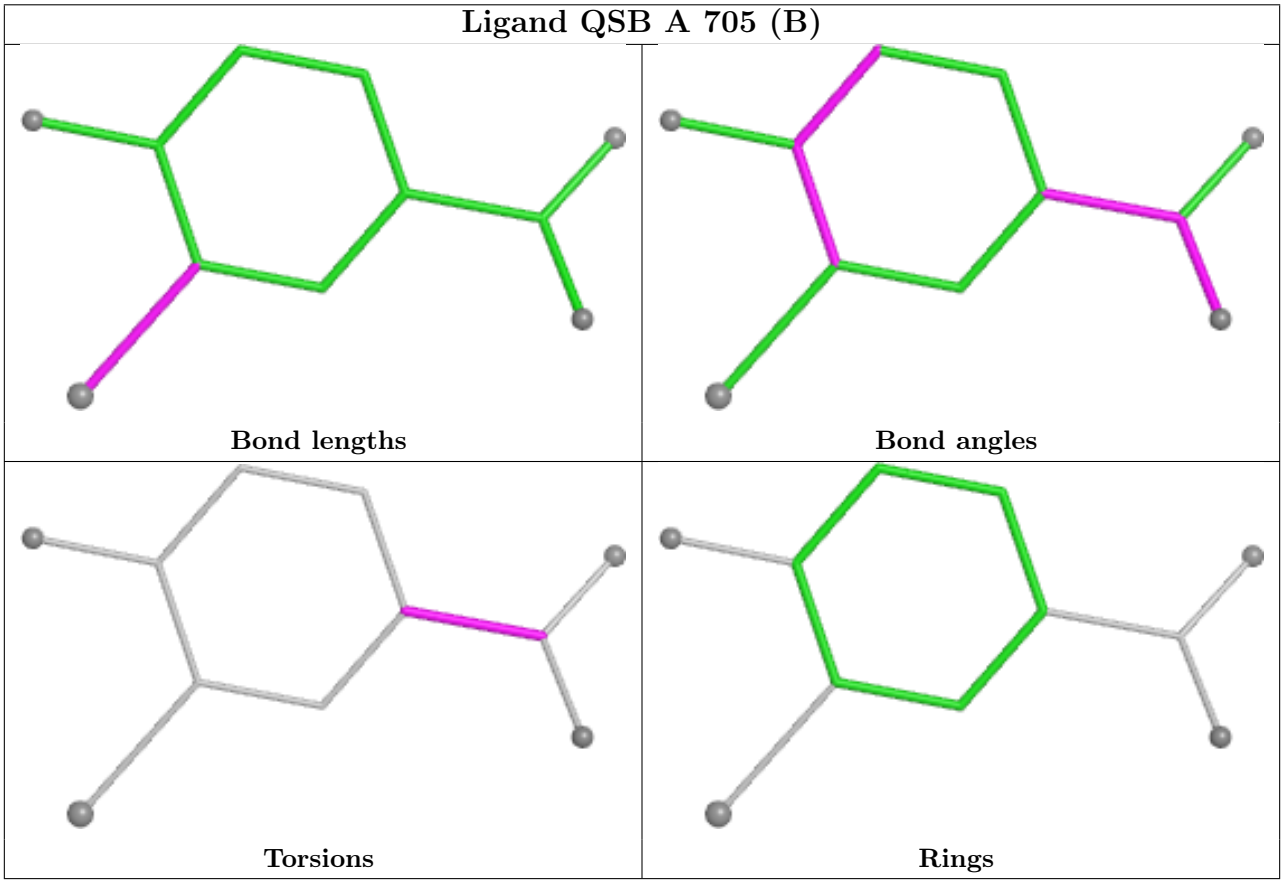


Rings

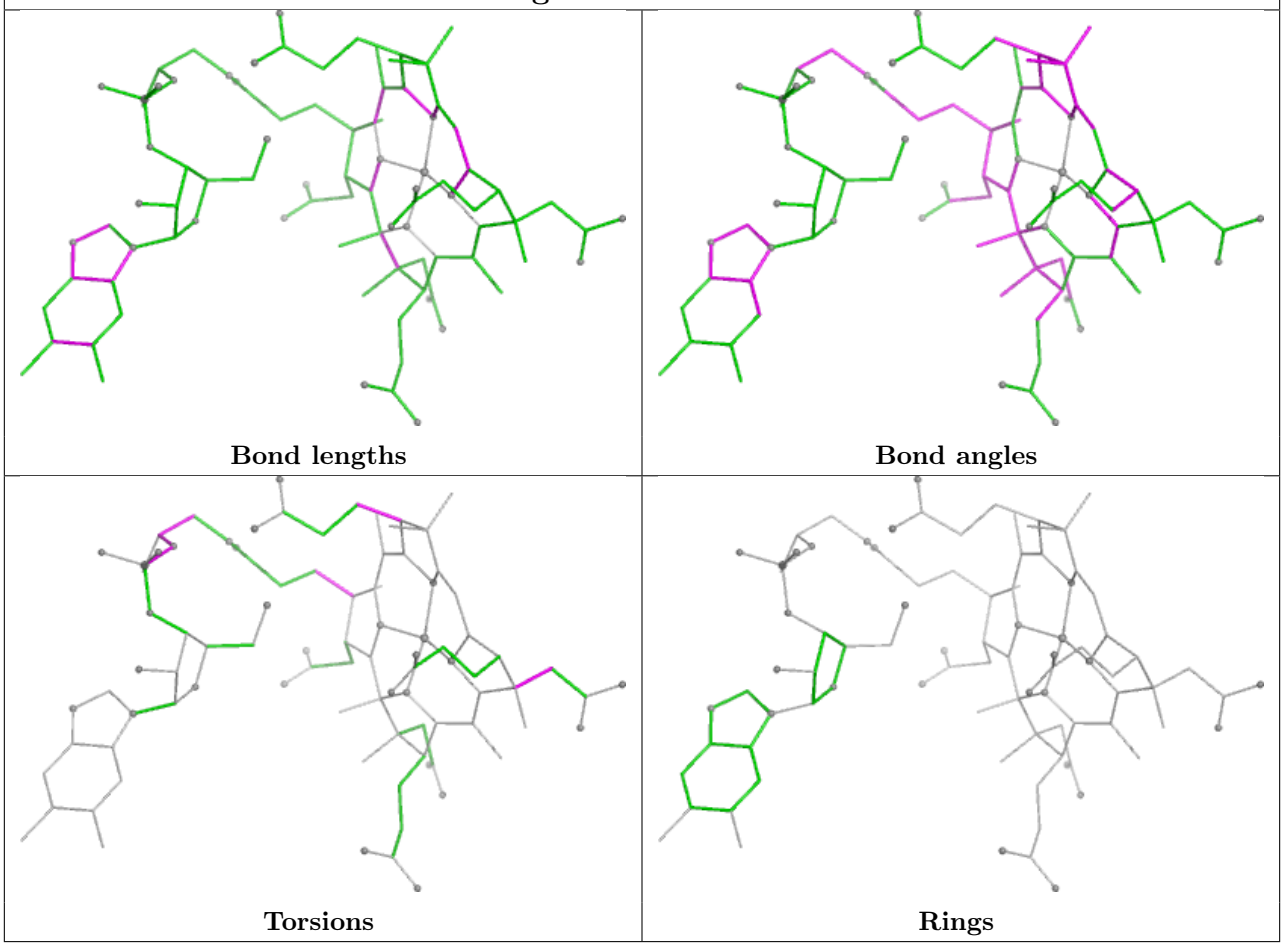
Ligand QSB A 705 (A)



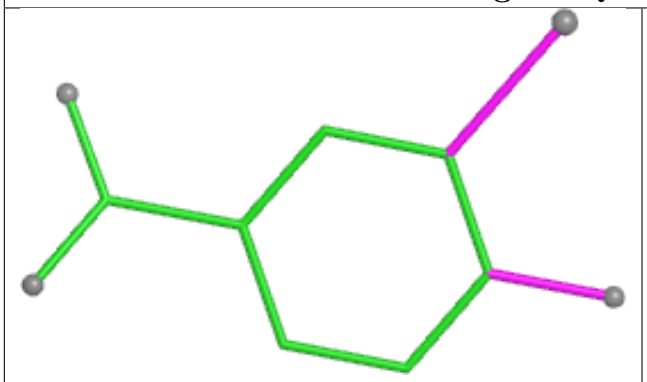
Ligand QSB A 705 (B)



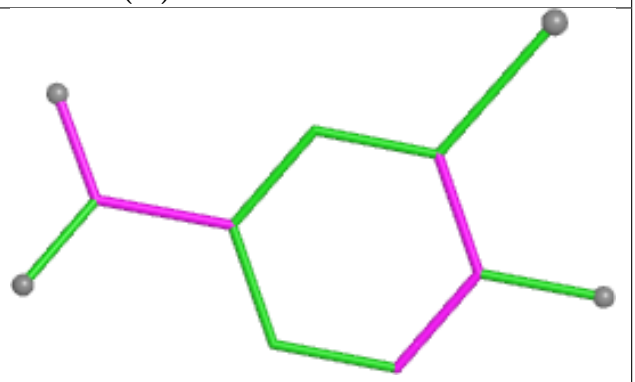
Ligand B12 B 703



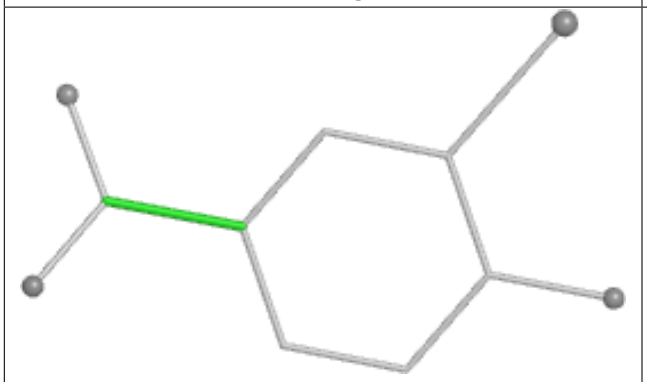
Ligand QSB B 705 (C)



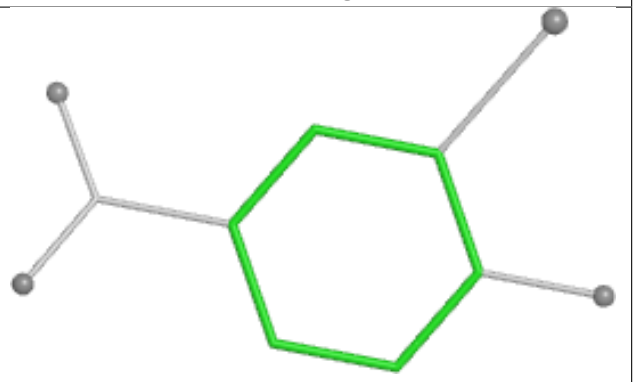
Bond lengths



Bond angles

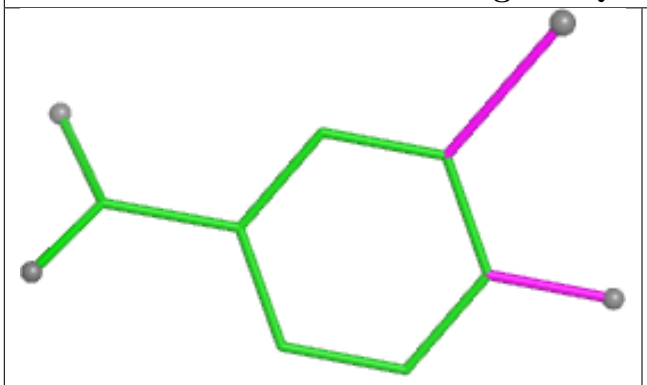


Torsions

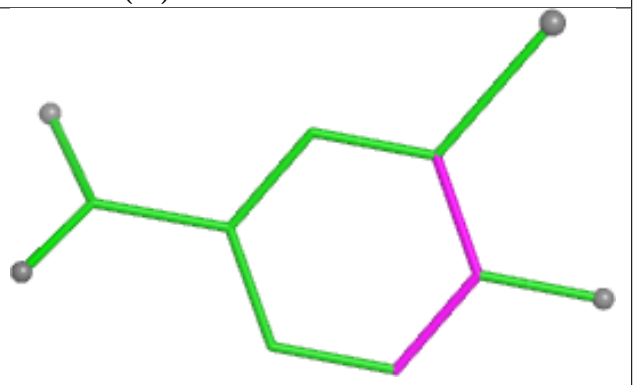


Rings

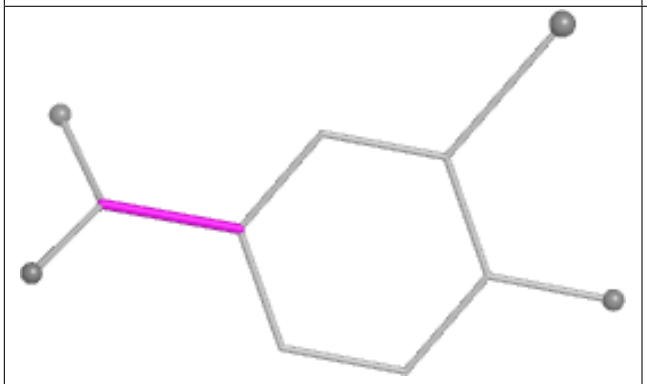
Ligand QSB C 705 (C)



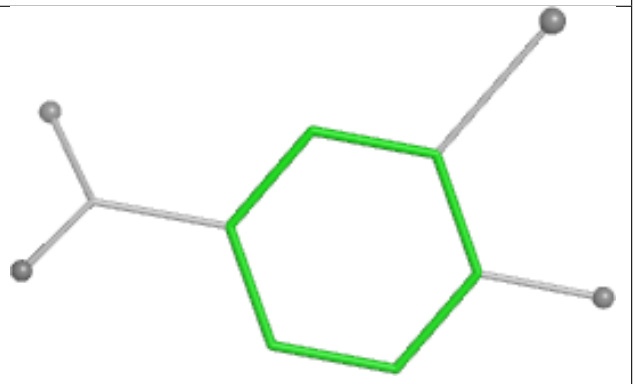
Bond lengths



Bond angles

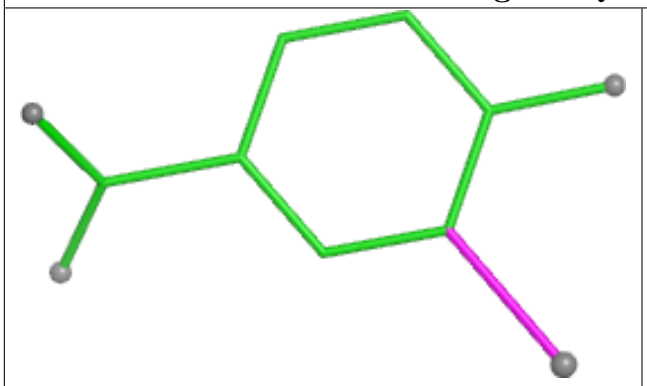


Torsions

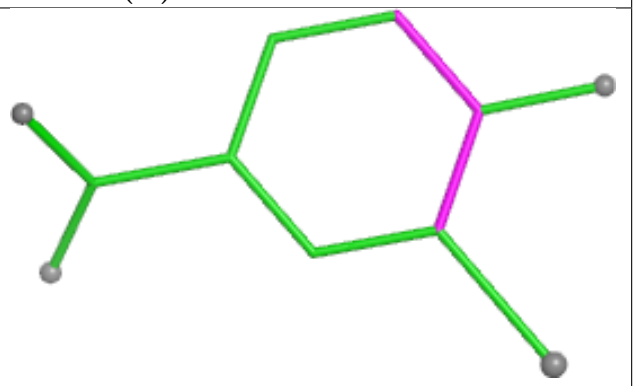


Rings

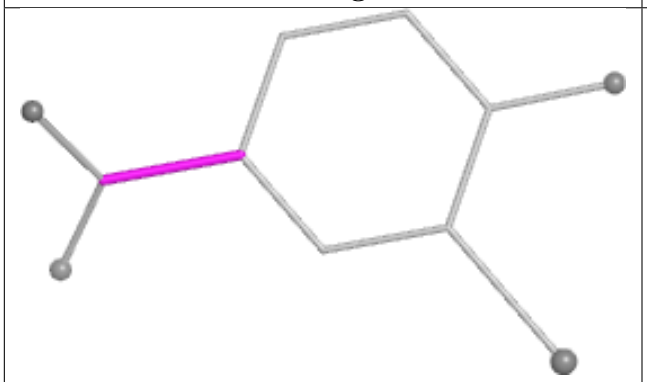
Ligand QSB C 705 (B)



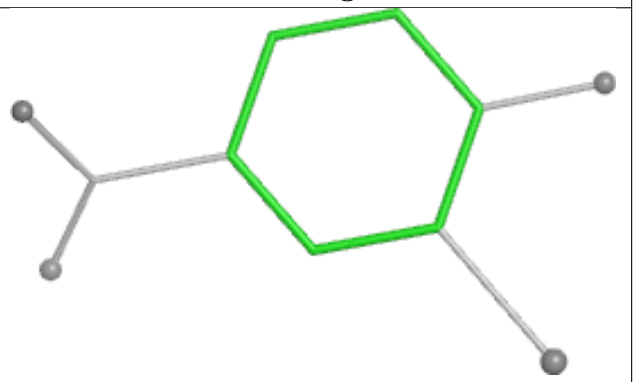
Bond lengths



Bond angles

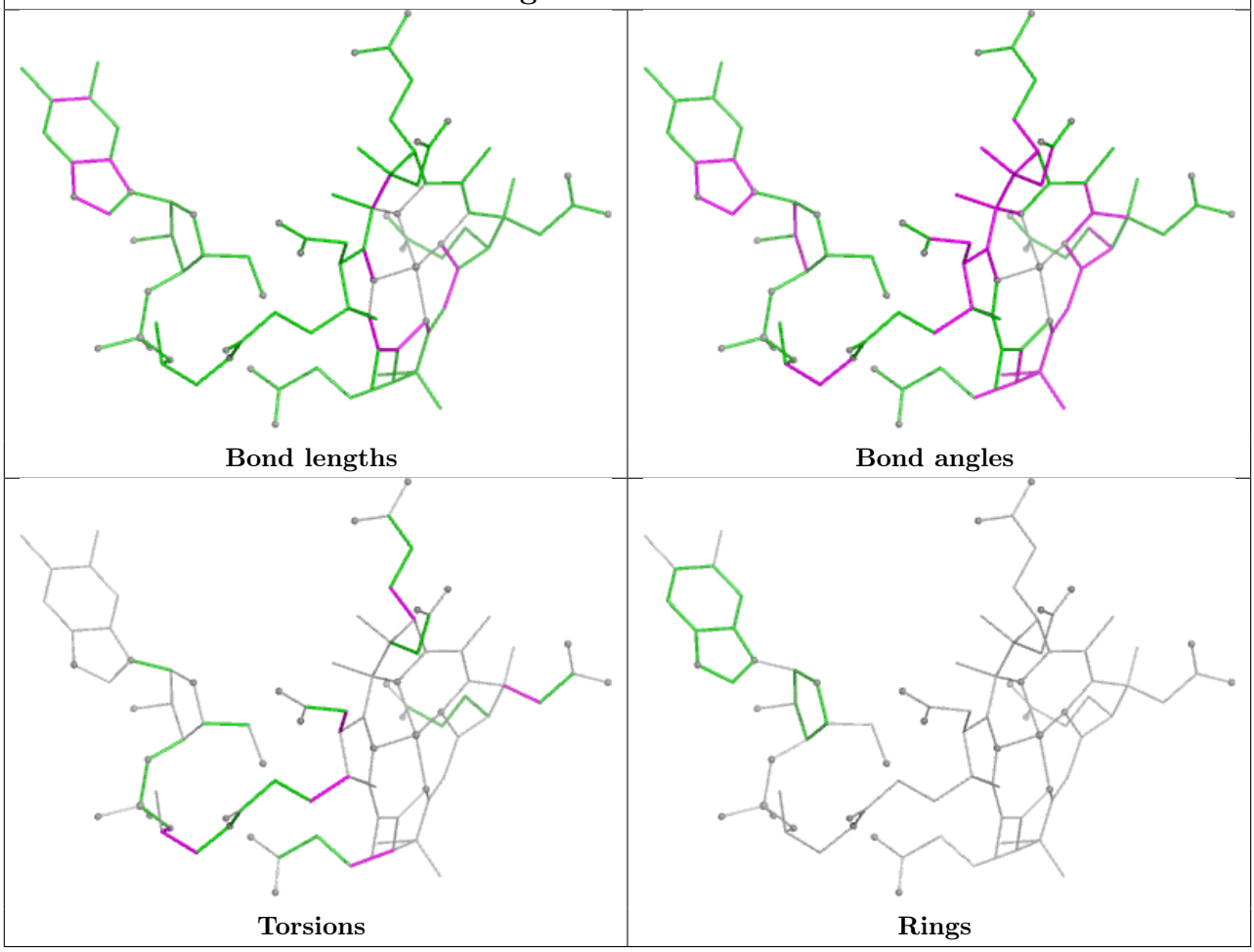


Torsions

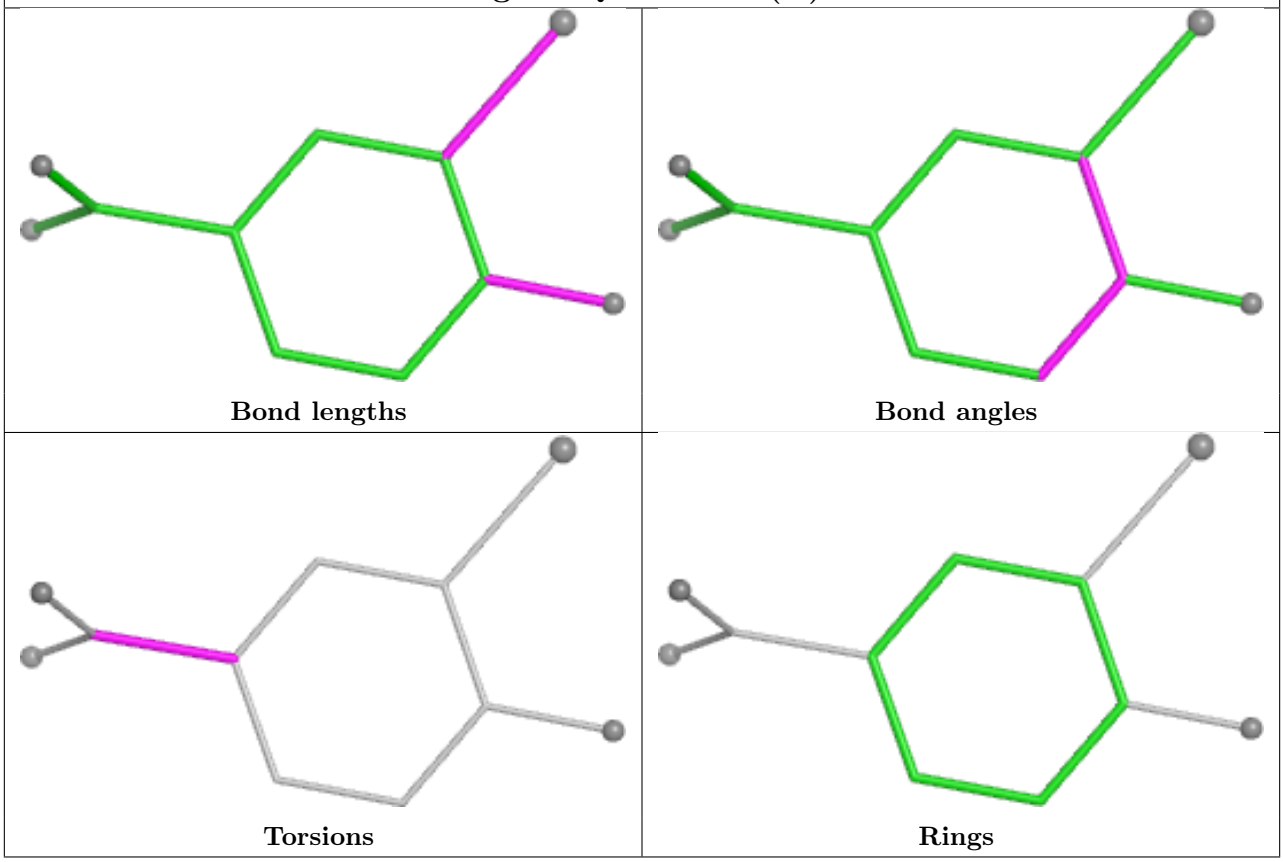


Rings

Ligand B12 C 703



Ligand QSB B 705 (A)



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	700/725 (96%)	-0.40	5 (0%)	84	84	10, 19, 32, 48	1 (0%)
1	B	696/725 (96%)	-0.36	13 (1%)	66	66	11, 20, 35, 57	1 (0%)
1	C	695/725 (95%)	0.14	15 (2%)	62	61	12, 28, 42, 62	1 (0%)
All	All	2091/2175 (96%)	-0.21	33 (1%)	70	70	10, 22, 39, 62	3 (0%)

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	-2	GLN	5.2
1	C	102	PRO	4.8
1	C	696	SER	4.2
1	B	-1	ILE	3.6
1	B	647	ASN	3.4

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

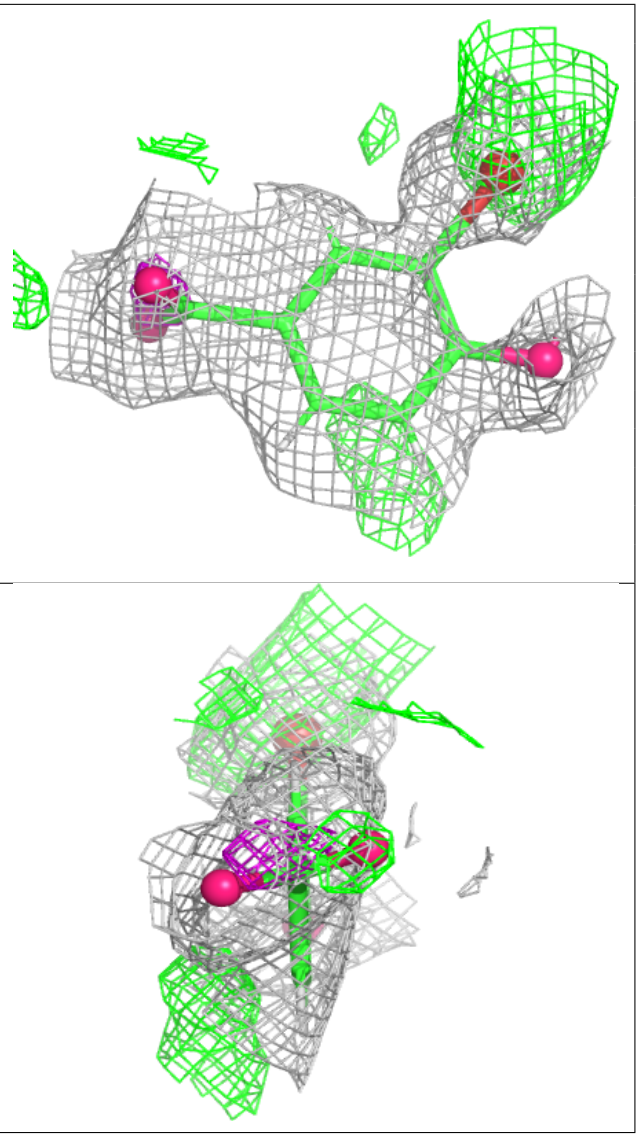
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	QSB	B	705[A]	11/11	0.78	0.20	19,22,27,27	15
5	QSB	B	705[B]	11/11	0.78	0.20	18,22,27,27	15
5	QSB	B	705[C]	11/11	0.78	0.20	21,23,28,28	15
5	QSB	C	705[A]	11/11	0.86	0.17	23,28,34,34	15
5	QSB	C	705[B]	11/11	0.86	0.17	23,28,34,34	15
5	QSB	C	705[C]	11/11	0.86	0.17	27,28,35,35	15
4	NA	A	704	1/1	0.88	0.07	25,25,25,25	0
5	QSB	A	705[B]	11/11	0.90	0.17	16,20,25,25	15
5	QSB	A	705[C]	11/11	0.90	0.17	17,20,25,25	15
4	NA	B	704	1/1	0.90	0.07	34,34,34,34	0
5	QSB	A	705[A]	11/11	0.90	0.17	20,21,26,27	15
4	NA	C	704	1/1	0.92	0.08	32,32,32,32	0
3	B12	C	703	91/91	0.96	0.07	14,22,26,29	0
3	B12	B	703	91/91	0.97	0.06	7,15,19,22	0
3	B12	A	703	91/91	0.97	0.07	7,14,19,27	0
2	SF4	B	702	8/8	0.99	0.02	16,18,20,21	0
2	SF4	C	701	8/8	0.99	0.02	17,19,20,21	0
2	SF4	C	702	8/8	0.99	0.02	17,18,21,21	0
2	SF4	A	701	8/8	0.99	0.02	11,14,14,15	0
2	SF4	A	702	8/8	0.99	0.02	10,12,17,18	0
2	SF4	B	701	8/8	0.99	0.02	12,15,17,18	0

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

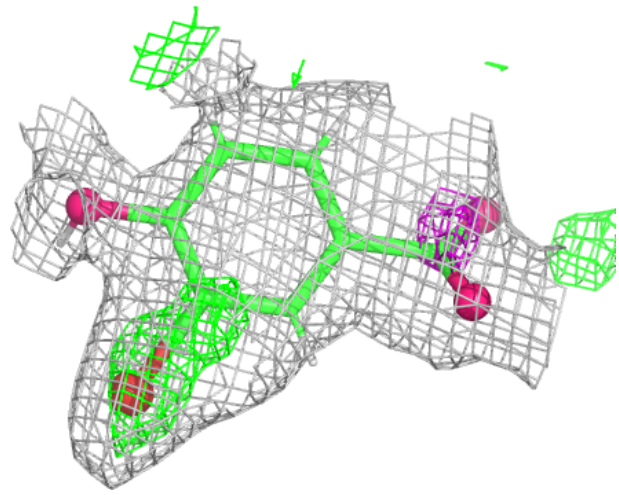
Electron density around QSB B 705 (A):

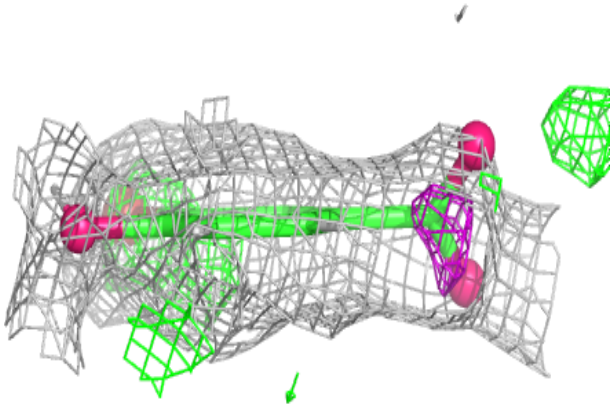
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

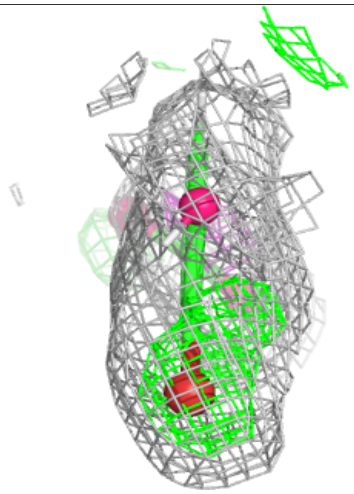


Electron density around QSB B 705 (B):

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

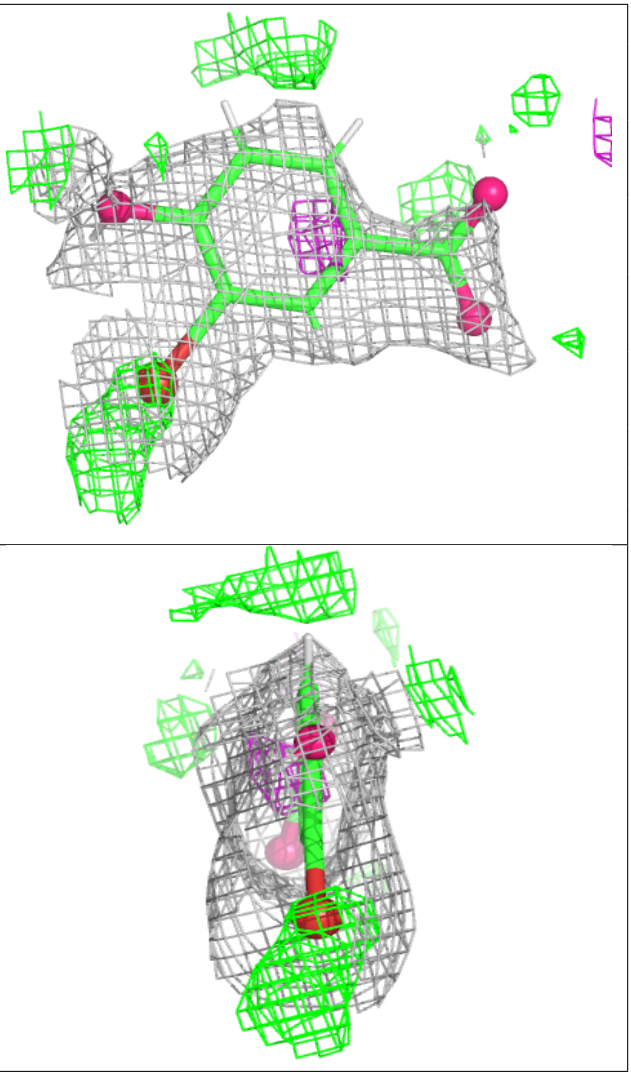






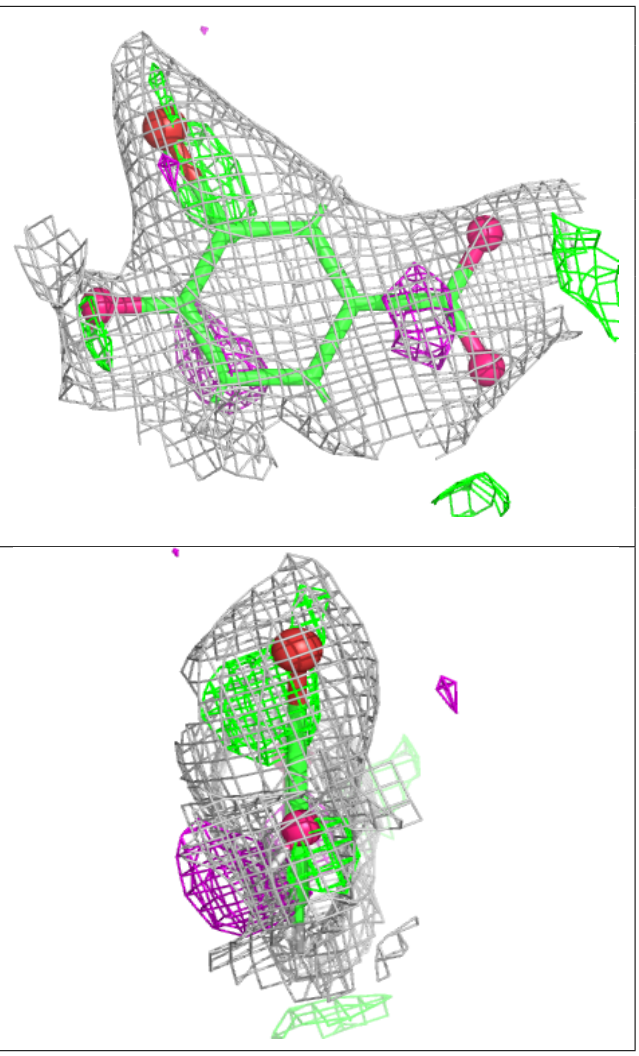
Electron density around QSB B 705 (C):

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



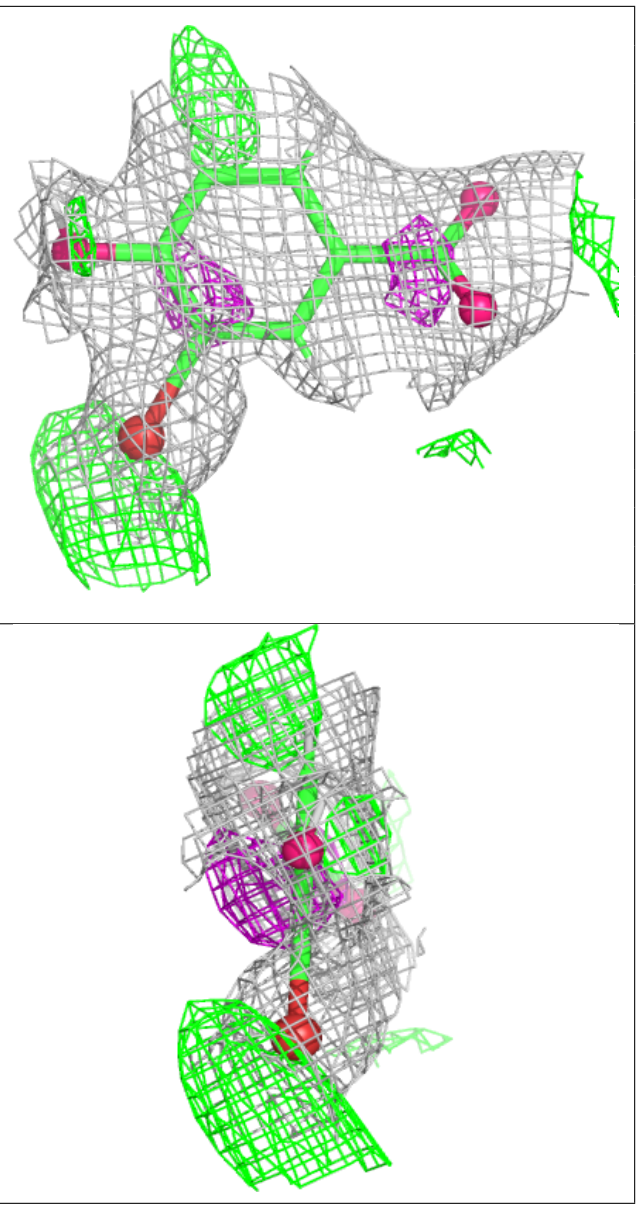
Electron density around QSB C 705 (A):

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



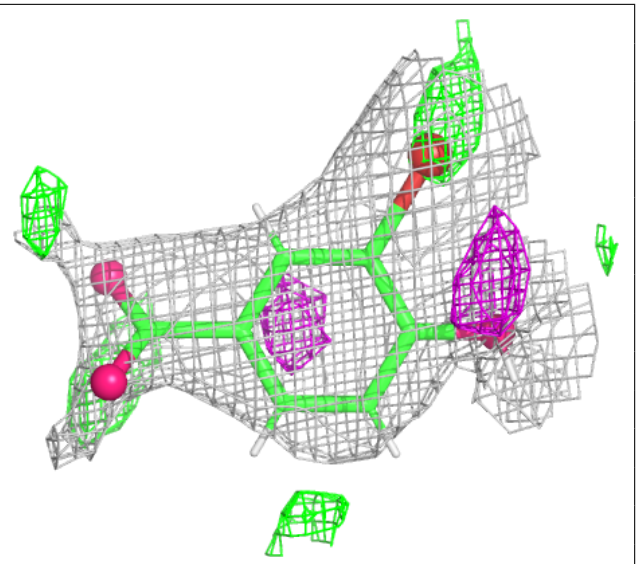
Electron density around QSB C 705 (B):

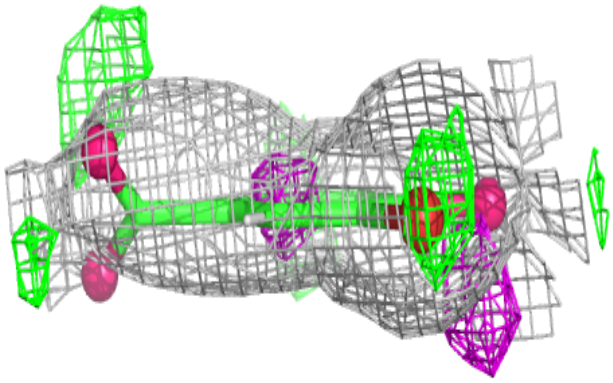
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

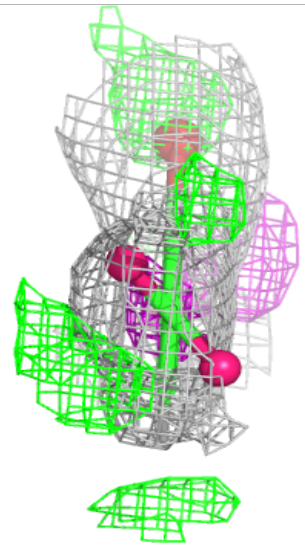


Electron density around QSB C 705 (C):

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

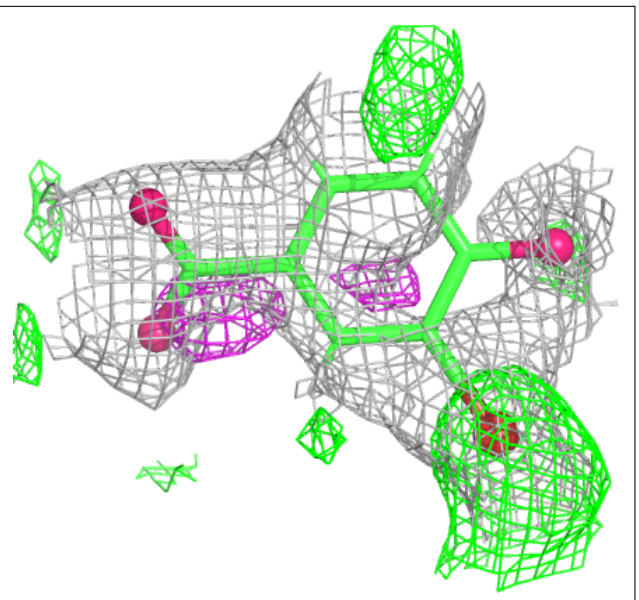


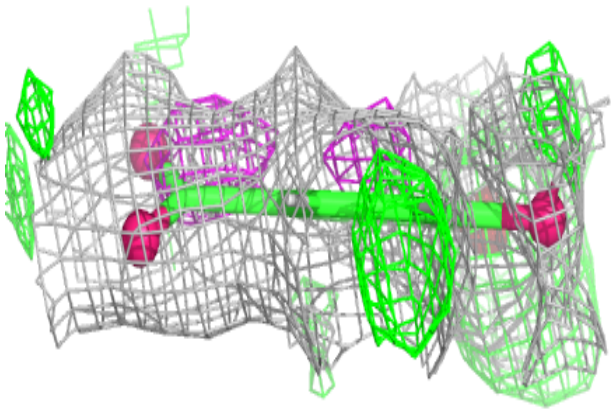


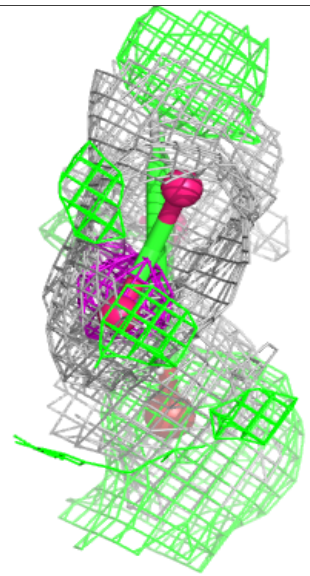


Electron density around QSB A 705 (B):

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

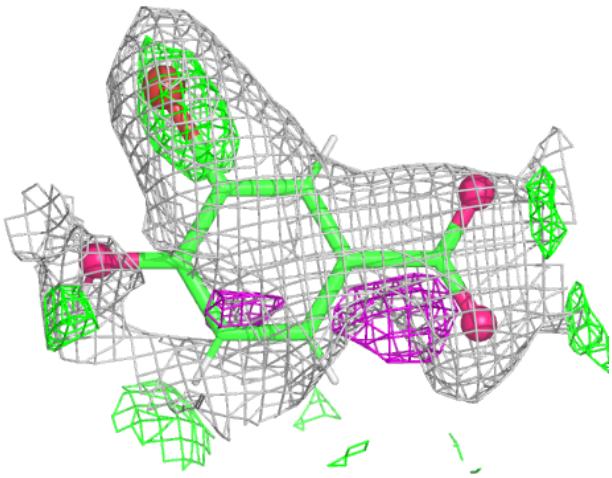


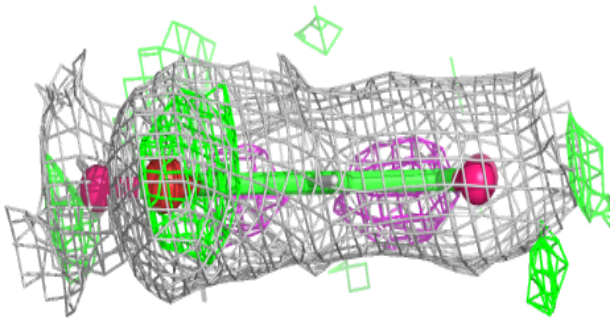


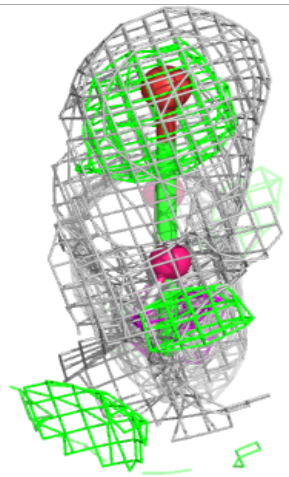


Electron density around QSB A 705 (C):

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

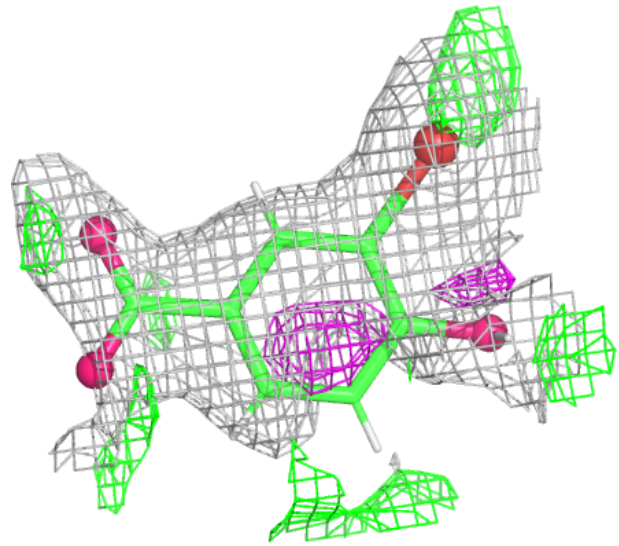


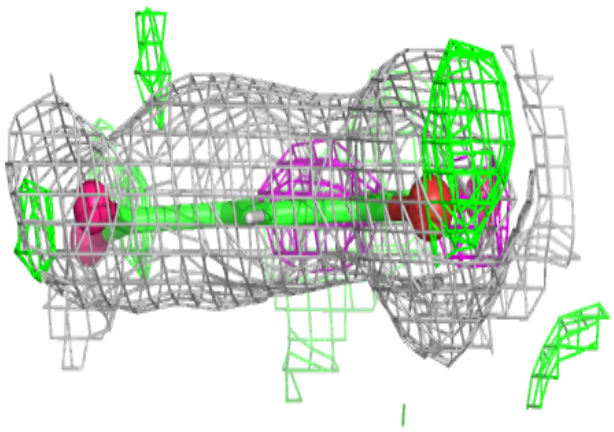


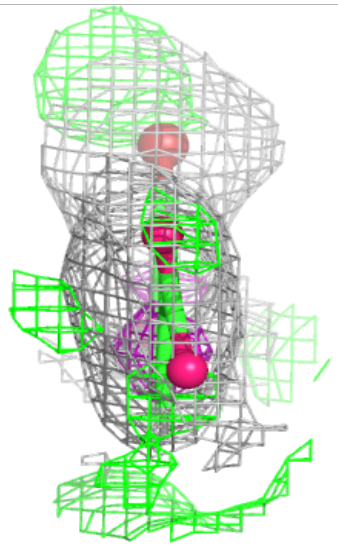


Electron density around QSB A 705 (A):

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

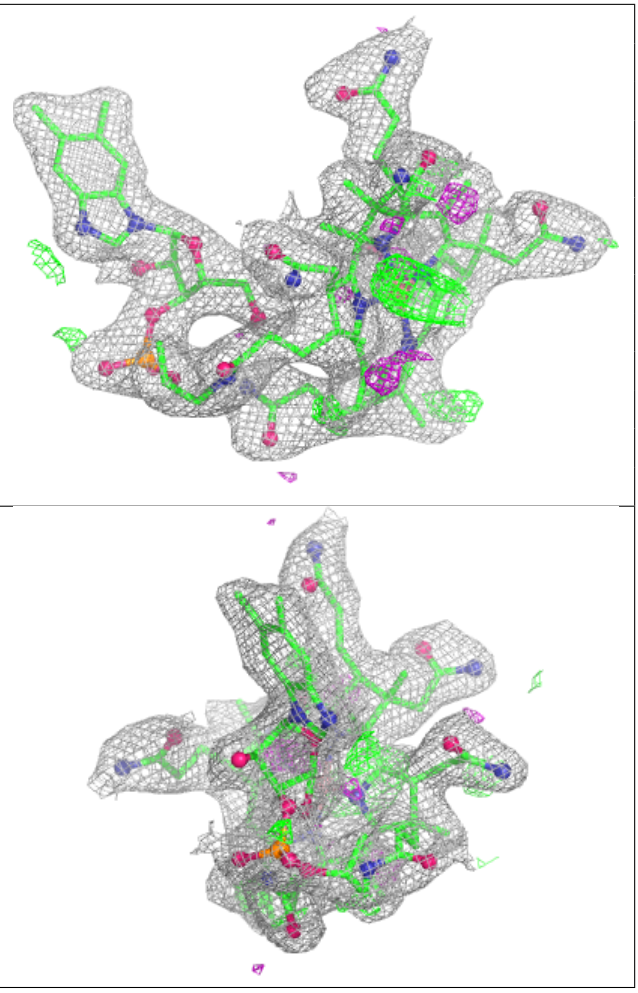






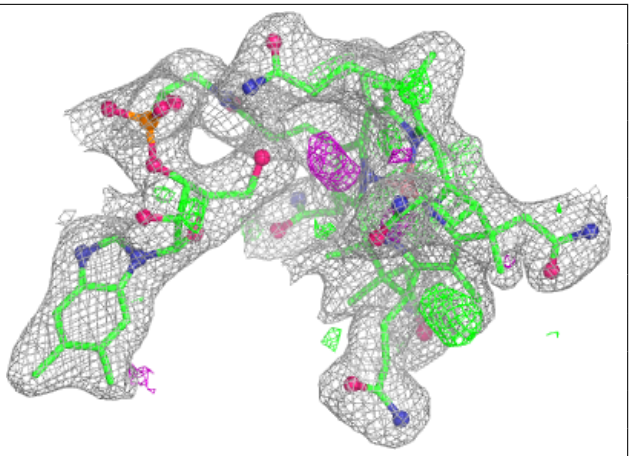
Electron density around B12 C 703:

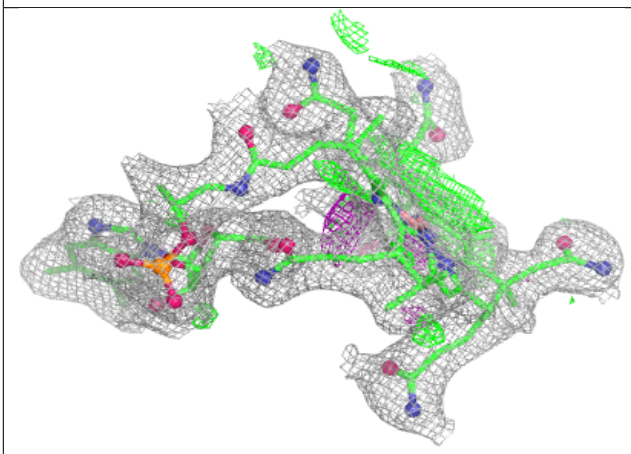
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

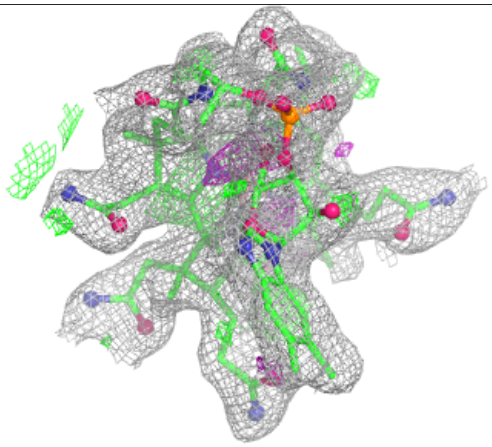


Electron density around B12 B 703:

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

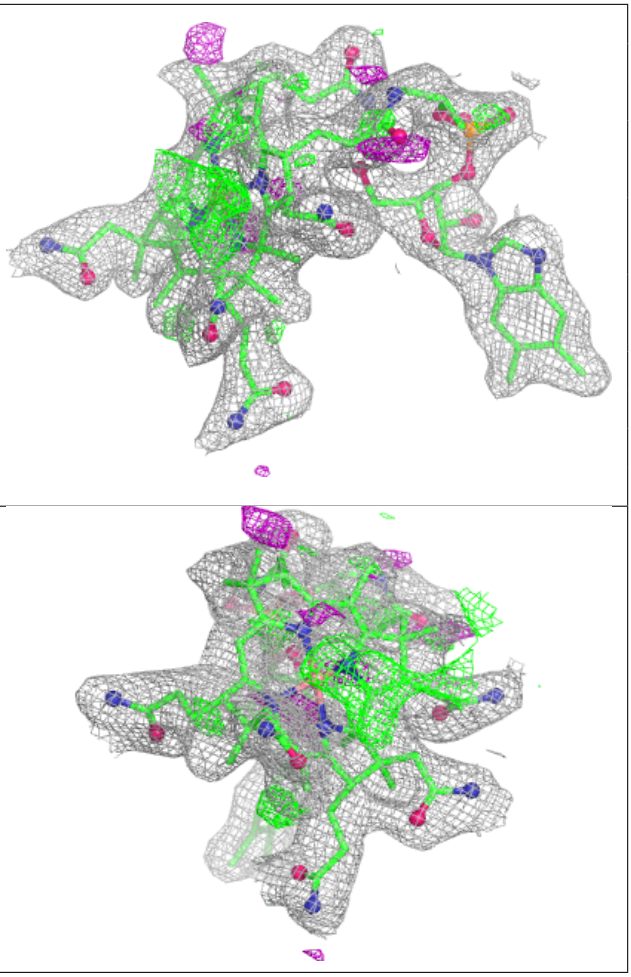






Electron density around B12 A 703:

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



6.5 Other polymers (i)

There are no such residues in this entry.