

wwPDB X-ray Structure Validation Summary Report (i)

Sep 15, 2020 – 06:27 PM BST

PDB ID : 6ZY1

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 following versions of software and data (see references (1)) were used in the production of this report:

Mol Probity : 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)

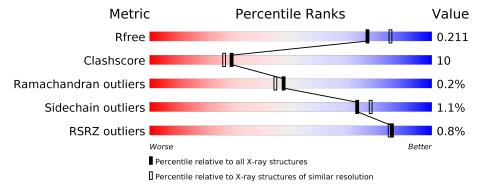
Validation Pipeline (wwPDB-VP) : 2.14.4

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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
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	83%	14%	·
1	В	725	81%	14%	-
1	С	725	77%	18%	

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	В	703	X	-	=	-
3	B12	С	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
1	Λ	700	Total	С	N	О	S	0	1	0
1	A	700	5336	3330	972	994	40	0	1	
1	В	606	Total	С	N	О	S	0	1	0
1	В	696	5280	3293	956	991	40	U		
1	С	605	Total	С	N	О	S	0	1	0
1		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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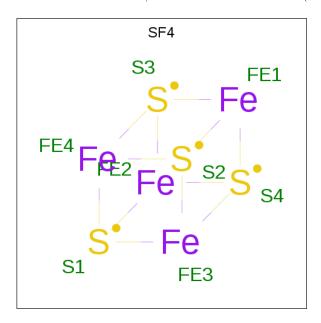
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	_	expression tag	UNP K2MB66
A	-3	ALA	_	expression tag	UNP K2MB66
A	-2	GLN	-	expression tag	UNP K2MB66
A	-1	ILE	_	expression tag	UNP K2MB66
A	0	SER	-	expression tag	UNP K2MB66
В	-26	MET	_	initiating methionine	UNP K2MB66
В	-25	VAL	-	expression tag	UNP K2MB66
В	-24	GLN	-	expression tag	UNP K2MB66
В	-23	THR	-	expression tag	UNP K2MB66
В	-22	SER	-	expression tag	UNP K2MB66
В	-21	PHE	-	expression tag	UNP K2MB66
В	-20	GLU	-	expression tag	UNP K2MB66
В	-19	HIS	_	expression tag	UNP K2MB66
В	-18	HIS	-	expression tag	UNP K2MB66
В	-17	HIS	-	expression tag	UNP K2MB66
В	-16	HIS	_	expression tag	UNP K2MB66
В	-15	HIS	-	expression tag	UNP K2MB66
В	-14	HIS	-	expression tag	UNP K2MB66
В	-13	SER	-	expression tag	UNP K2MB66
В	-12	ALA	-	expression tag	UNP K2MB66
В	-11	GLY	-	expression tag	UNP K2MB66
В	-10	GLU	=	expression tag	UNP K2MB66
В	-9	ASN	=	expression tag	UNP K2MB66
В	-8	LEU	_	expression tag	UNP K2MB66
В	-7	TYR	_	expression tag	UNP K2MB66
В	-6	PHE	-	expression tag	UNP K2MB66
В	-5	GLN	_	expression tag	UNP K2MB66
В	-4	GLY	_	expression tag	UNP K2MB66
В	-3	ALA	_	expression tag	UNP K2MB66
В	-2	GLN	ı	expression tag	UNP K2MB66
В	-1	ILE	ı	expression tag	UNP K2MB66
В	0	SER	-	expression tag	UNP K2MB66
С	-26	MET	-	initiating methionine	UNP K2MB66
С	-25	VAL		expression tag	UNP K2MB66
С	-24	GLN	-	expression tag	UNP K2MB66
С	-23	THR		expression tag	UNP K2MB66
С	-22	SER		expression tag	UNP K2MB66
С	-21	PHE		expression tag	UNP K2MB66
С	-20	GLU		expression tag	UNP K2MB66
С	-19	HIS		expression tag	UNP K2MB66
С	-18	HIS	-	expression tag	UNP K2MB66
С	-17	HIS		expression tag	UNP K2MB66



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

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



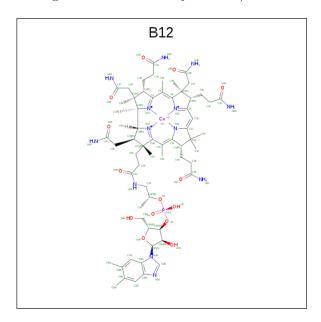
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
2	A	1	Total Fe S	0	0	
			Total Fe S			
$\frac{2}{}$	A	1	8 4 4	0	0	
2	В	1	Total Fe S	0	0	
_		_	8 4 4			



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total Fe S 8 4 4	0	0
2	С	1	Total Fe S 8 4 4	0	0
2	С	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).



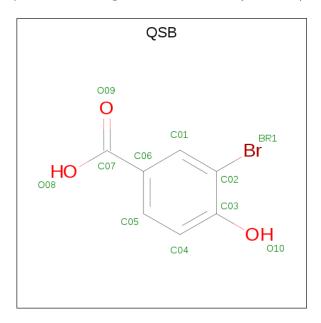
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 91		Co 1			P 1	0	0
3	В	1	Total 91	_	Co 1	- '	O 14	P 1	0	0
3	С	1	Total 91		Co 1		O 14	P 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0
4	С	1	Total Na 1 1	0	0



• Molecule 5 is 3 bromo 4 hydroxybenzoic acid (three-letter code: QSB) (formula: C₇H₅BrO₃) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	Br	С	Η	О	0	1
0	A		45	3	21	12	9	0	
5	D	1	Total	Br	С	Н	О	0	1
)	5 B	1	45	3	21	12	9	0	
5	5 C	C 1	Total	Br	С	Н	О	0	1
)			45	3	21	12	9	0	1

• Molecule 6 is water.

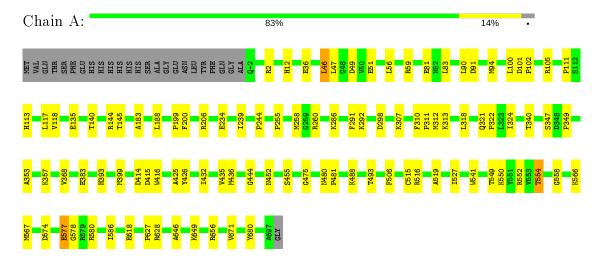
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	442	Total O 442 442	0	0
6	В	457	Total O 457 457	0	0
6	С	266	Total O 266 266	0	0



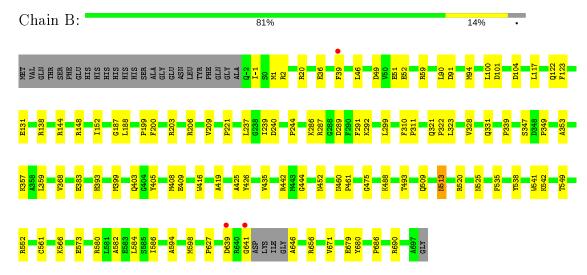
3 Residue-property plots (i)

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



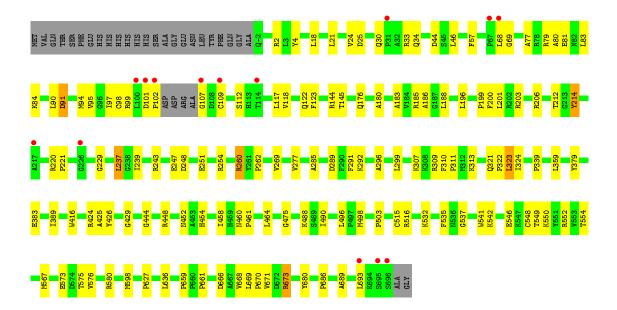
• Molecule 1: Oxidoreductase, NAD-binding/iron-sulfur cluster-binding protein



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

Chain C: 77% 18% . .







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	175.87Å 170.10Å 107.65Å	Depositor
a, b, c, α , β , γ	90.00° 98.35° 90.00°	Depositor
Resolution (Å)	106.00 - 1.99	Depositor
Resolution (A)	106.51 - 1.99	EDS
% Data completeness	94.0 (106.00-1.99)	Depositor
(in resolution range)	52.8 (106.51-1.99)	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
P. P.	0.177 , 0.211	Depositor
R, R_{free}	0.176 , 0.211	DCC
R_{free} test set	2000 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 37.2	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	0.94	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.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: QSB, SF4, B12, 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	Bond lengths		Bond angles	
Moi Chain		RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.28	0/5452	0.48	0/7382	
1	В	0.27	0/5395	0.47	0/7311	
1	С	0.27	0/5348	0.46	0/7248	
All	All	0.27	0/16195	0.47	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	78	0
1	В	5280	0	5119	76	0
1	С	5238	0	5065	107	0
2	A	16	0	0	0	0
2	В	16	0	0	0	0
2	С	16	0	0	1	0
3	A	91	0	87	19	0
3	В	91	0	87	20	0
3	С	91	0	87	25	0
4	A	1	0	0	0	0



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I'antimuad	t_{mom}	mromanne	naaa
Continued		DICUIUU	Du/uc
	J	1	I J

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	В	1	0	0	0	0
4	С	1	0	0	0	0
5	A	33	12	0	3	0
5	В	33	12	0	3	0
5	С	33	12	0	2	0
6	A	442	0	0	10	0
6	В	457	0	0	12	0
6	С	266	0	0	12	0
All	All	17442	36	15667	308	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 308 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance} \ (ext{\AA}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:A:312:MET:HE1	1:A:321:GLN:HB2	1.40	1.03
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:C:277:VAL:HG11	1:C:693:LEU:HD11	1.49	0.94
3:B:703:B12:H351	3:B:703:B12:H362	1.49	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	${f Analysed}$	Favoured	Allowed	Outliers	Perce	ntiles
1	A	699/725~(96%)	685 (98%)	13 (2%)	1 (0%)	51	49
1	В	$693/725 \; (96\%)$	675 (97%)	17 (2%)	1 (0%)	51	49
1	С	$692/725 \; (95\%)$	668 (96%)	22 (3%)	2 (0%)	41	37



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	$2084/2175 \ (96\%)$	2028 (97%)	52 (2%)	4 (0%)	47 44

All (4) Ramachandran outliers are listed below:

Mol	Chain	${f Res}$	Type
1	С	214	TYR
1	A	46	LEU
1	С	91	ASP
1	В	-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	$538/569 \; (95\%)$	533 (99%)	5 (1%)	78 83
1	В	529/569~(93%)	524 (99%)	5 (1%)	78 83
1	С	518/569 (91%)	511 (99%)	7 (1%)	67 72
All	All	1585/1707 (93%)	1568 (99%)	17 (1%)	73 78

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	144	ARG
1	В	513	ASN
1	С	260	ARG
1	В	59	ARG
1	С	323	LEU

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

Mol	Chain	Res	Type
1	В	403	GLN
1	В	514	GLN
1	С	122	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 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	${ m Res}$	Link	Boı	nd lengt		Bo	nd angle	es
14101	Туре		1005	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	QSB	В	705[C]	-	9,11,11	2.25	3 (33%)	12,15,15	1.09	1 (8%)
3	B12	A	703	-	80,101,101	1.15	6 (7%)	101,166,166	2.25	24 (23%)
3	B12	С	703	-	80,101,101	1.14	6 (7%)	101,166,166	2.10	22 (21%)
2	SF4	В	701	1	0,12,12	0.00	-	-		
2	SF4	A	701	1	0,12,12	0.00	-	-		
2	SF4	С	701	1	0,12,12	0.00	-	-		
5	QSB	В	705[A]	-	9,11,11	2.29	3 (33%)	12,15,15	1.22	1 (8%)
5	QSB	A	705[A]	-	9,11,11	2.16	2 (22%)	12,15,15	1.42	2 (16%)
2	SF4	A	702	1	0,12,12	0.00	-	-		
5	QSB	С	705[A]	-	9,11,11	2.26	3 (33%)	12,15,15	0.99	1 (8%)
5	QSB	A	705[B]	-	9,11,11	2.32	2 (22%)	12,15,15	1.21	1 (8%)
5	QSB	A	705[C]	-	9,11,11	2.25	2 (22%)	12,15,15	0.94	1 (8%)
2	SF4	С	702	1	0,12,12	0.00	-	-		
3	B12	В	703	-	80,101,101	1.16	7 (8%)	101,166,166	2.25	22 (21%)
5	QSB	В	705[B]	_	9,11,11	2.25	3 (33%)	12,15,15	0.96	1 (8%)



Mal	Mol Type Chain Res		Link	Bond lengths			Bond angles			
MIOI	Type	Chain	nes	LINK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	QSB	С	705[B]	-	9,11,11	2.34	2 (22%)	12,15,15	1.18	1 (8%)
5	QSB	С	705[C]	-	9,11,11	2.32	3 (33%)	12,15,15	1.03	1 (8%)
2	SF4	В	702	1	0,12,12	0.00	_	_		

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
2	SF4	В	701	1	-	-	0/6/5/5
3	B12	A	703	-	1/1/36/38	15/51/223/223	0/3/11/11
3	B12	С	703	-	1/1/36/38	12/51/223/223	0/3/11/11
5	QSB	В	705[C]	-	-	0/0/4/4	0/1/1/1
2	SF4	A	701	1	·	-	0/6/5/5
5	QSB	В	705[B]	_	ı	0/0/4/4	0/1/1/1
5	QSB	В	705[A]	_	·	0/0/4/4	0/1/1/1
5	QSB	A	705[A]	-	-	0/0/4/4	0/1/1/1
3	B12	В	703	_	1/1/36/38	9/51/223/223	$ \ 0/3/11/11 \ $
5	QSB	С	705[A]	_	-	0/0/4/4	0/1/1/1
5	QSB	A	705[B]	_	-	0/0/4/4	0/1/1/1
5	QSB	A	705[C]	_	-	0/0/4/4	0/1/1/1
2	SF4	С	702	1	·	-	0/6/5/5
2	SF4	A	702	1	1	-	0/6/5/5
2	SF4	С	701	1		<u>-</u>	0/6/5/5
5	QSB	С	705[C]	_	-	0/0/4/4	0/1/1/1
5	QSB	С	705[B]	_		0/0/4/4	0/1/1/1
2	SF4	В	702	1	-	-	0/6/5/5

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\mathbf{Ideal}(\mathbf{\AA})$
5	С	705[B]	QSB	C06-C07	6.28	1.53	1.47
5	A	705[B]	QSB	C06-C07	6.26	1.53	1.47
5	С	705[C]	QSB	C06-C07	6.24	1.53	1.47
5	В	705[A]	QSB	C06-C07	6.11	1.53	1.47
5	A	705[C]	QSB	C06-C07	6.07	1.53	1.47

The worst 5 of 78 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	В	703	B12	C20-C1-C19	-8.58	101.08	109.36
3	С	703	B12	C1-C19-N24	7.75	114.96	106.24
3	В	703	B12	C1-C19-N24	7.60	114.79	106.24
3	A	703	B12	C1-C19-N24	7.45	114.62	106.24
3	A	703	B12	C20-C1-C19	-7.29	102.33	109.36

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	703	B12	C19
3	С	703	B12	C19
3	В	703	B12	C19

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	B12	C38-C37-C7-C36
3	A	703	B12	C42-C41-C8-C9
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.

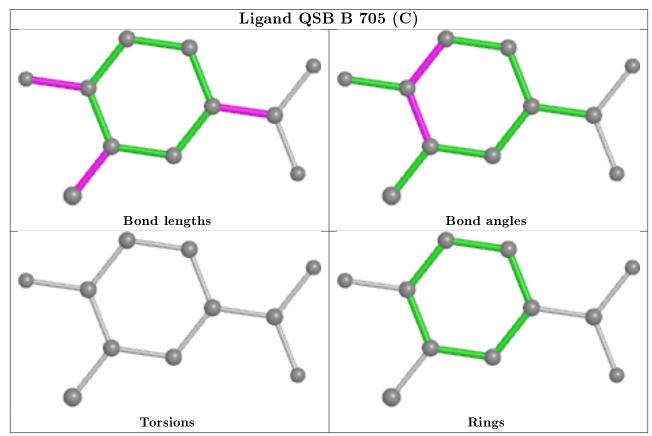
11 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	B12	19	0
3	С	703	B12	25	0
2	С	701	SF4	1	0
5	В	705[A]	QSB	2	0
5	A	705[A]	QSB	1	0
5	С	705[A]	QSB	1	0
5	A	705[B]	QSB	1	0
5	A	705[C]	QSB	1	0
3	В	703	B12	20	0
5	В	705[B]	QSB	1	0
5	С	705[B]	QSB	1	0

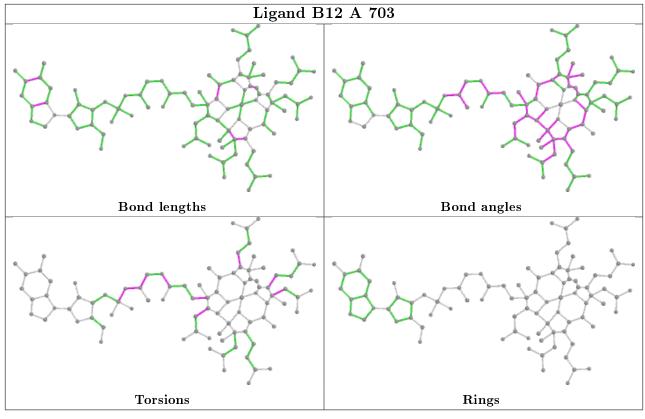
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

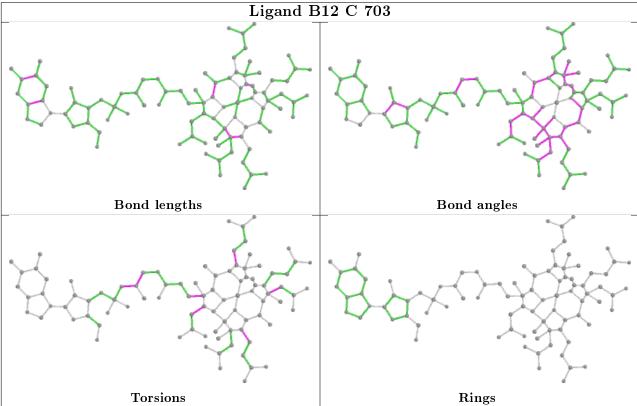


Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

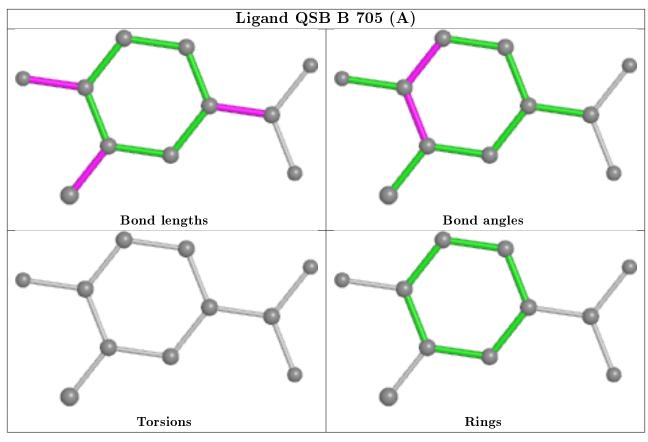


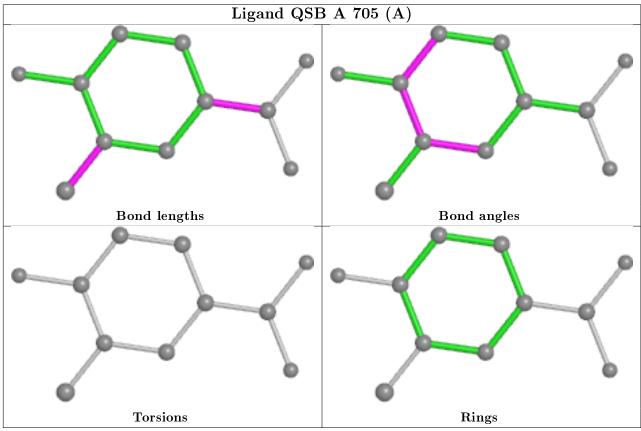




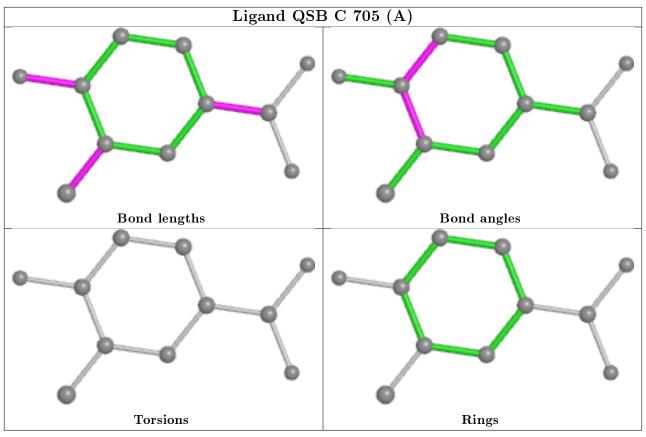


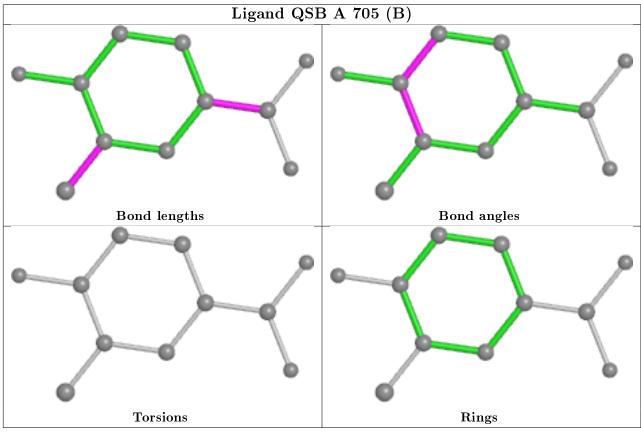




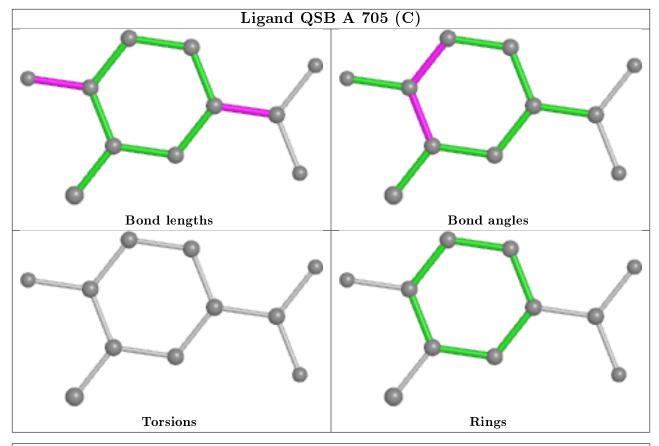


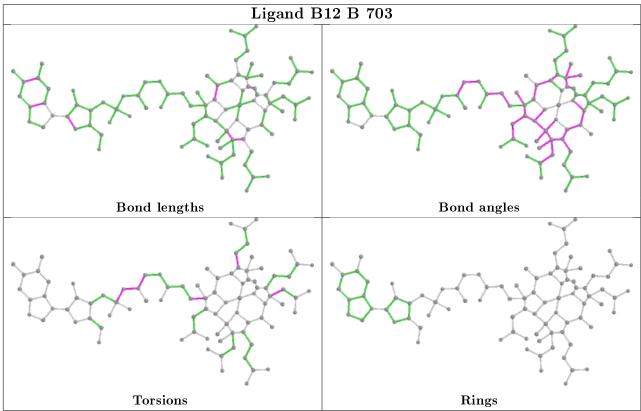




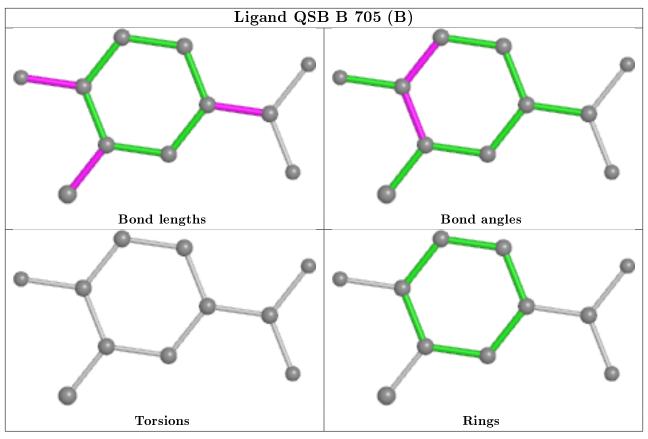


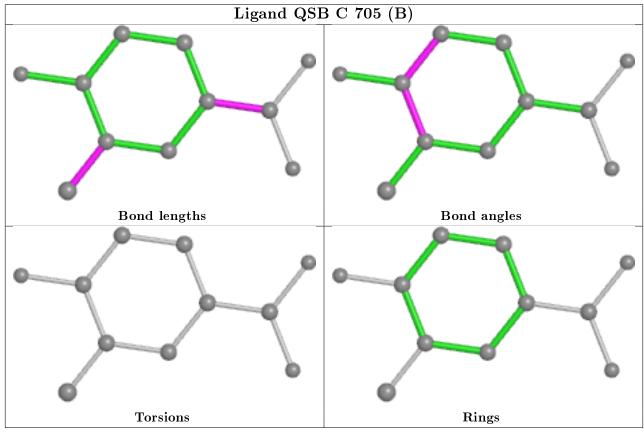




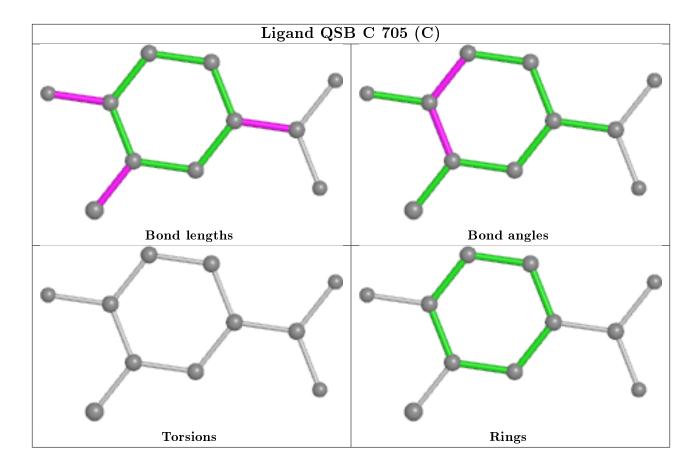












5.7 Other polymers (i)

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, 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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(m \AA^2)$	Q < 0.9
1	A	700/725~(96%)	-0.07	0 100 100	11, 19, 32, 48	0
1	В	$696/725 \; (96\%)$	-0.26	3 (0%) 92 92	13, 20, 35, 57	0
1	С	$695/725 \ (95\%)$	0.01	14 (2%) 65 63	17, 28, 42, 62	0
All	All	2091/2175 (96%)	-0.11	17 (0%) 86 85	11, 22, 39, 62	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	${f Res}$	Type	RSRZ	
1	С	696	SER	4.4	
1	В	39	PHE	3.6	
1	С	693	LEU	3.1	
1	С	100	LEU	2.9	
1	В	641	GLY	2.9	

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)

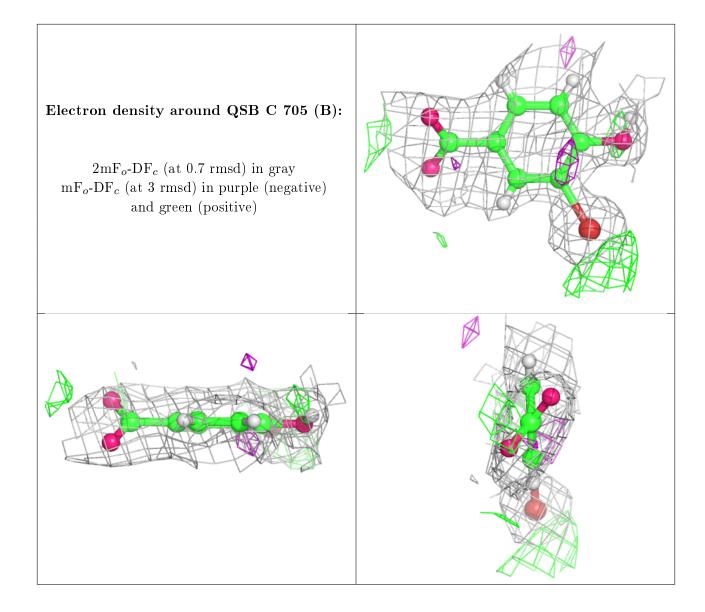
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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



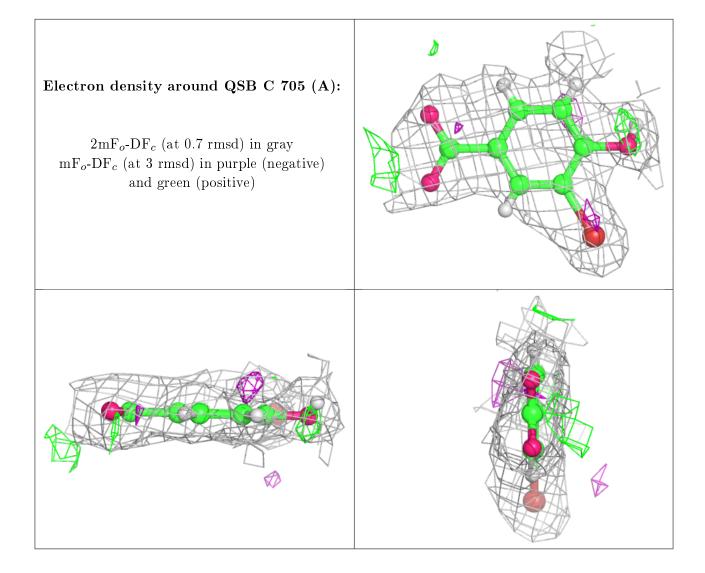
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$oxed{ \mathbf{B\text{-}factors}(\mathbf{\mathring{A}}^2) }$	Q<0.9
5	QSB	С	705[B]	11/11	0.93	0.17	23,28,34,34	15
5	QSB	С	705[A]	11/11	0.93	0.17	23,28,34,34	15
5	QSB	С	705[C]	11/11	0.93	0.17	27,28,35,35	15
4	NA	В	704	1/1	0.94	0.09	34,34,34,34	0
5	QSB	A	705[C]	11/11	0.95	0.17	17,20,25,25	15
5	QSB	В	705[B]	11/11	0.95	0.16	18,22,27,27	15
5	QSB	В	705[C]	11/11	0.95	0.16	21,23,28,28	15
5	QSB	В	705[A]	11/11	0.95	0.16	19,22,27,27	15
5	QSB	A	705[A]	11/11	0.95	0.17	$20,\!21,\!26,\!27$	15
5	QSB	A	705[B]	11/11	0.95	0.17	16,20,25,25	15
4	NA	С	704	1/1	0.96	0.09	32,32,32,32	0
3	B12	С	703	91/91	0.97	0.11	14,22,26,29	0
3	B12	В	703	91/91	0.97	0.11	7,15,19,22	0
4	NA	A	704	1/1	0.97	0.14	25,25,25,25	0
3	B12	A	703	91/91	0.97	0.13	7,14,19,27	0
2	SF4	С	702	8/8	0.99	0.08	17,18,21,21	0
2	SF4	В	701	8/8	0.99	0.07	12,15,17,18	0
2	SF4	С	701	8/8	0.99	0.07	17,19,20,21	0
2	SF4	A	702	8/8	0.99	0.10	10,12,17,18	0
2	SF4	В	702	8/8	0.99	0.06	16,18,20,21	0
2	SF4	A	701	8/8	1.00	0.10	11,14,14,15	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.

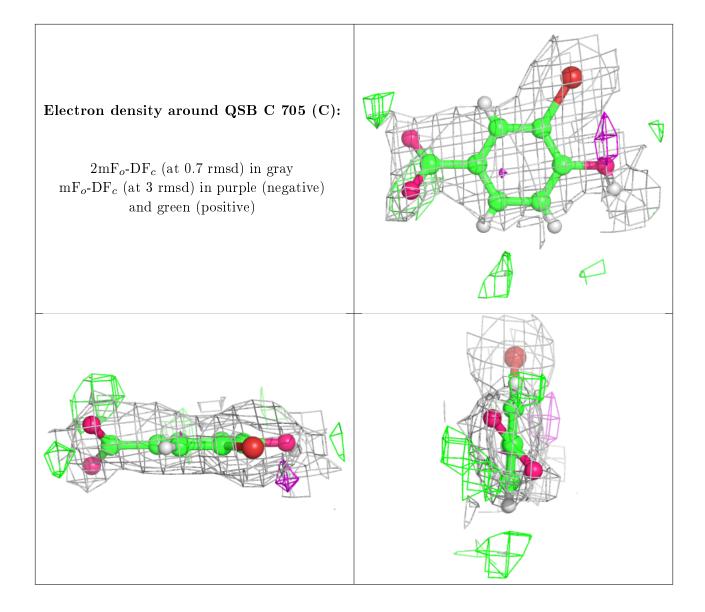




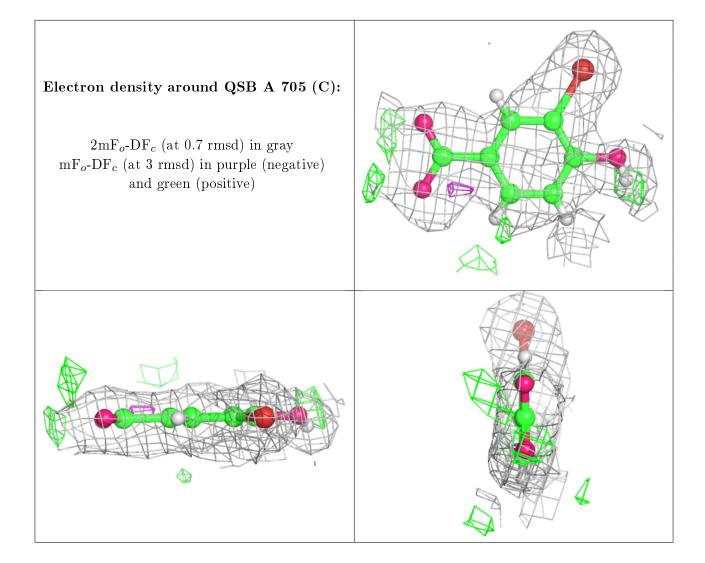




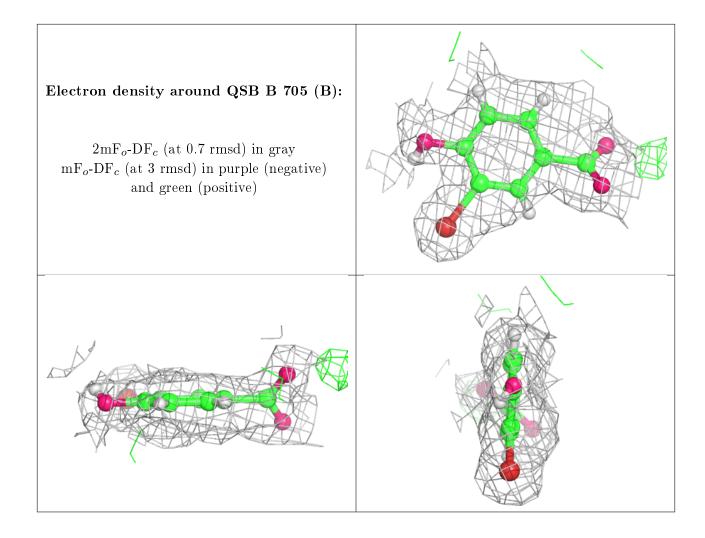




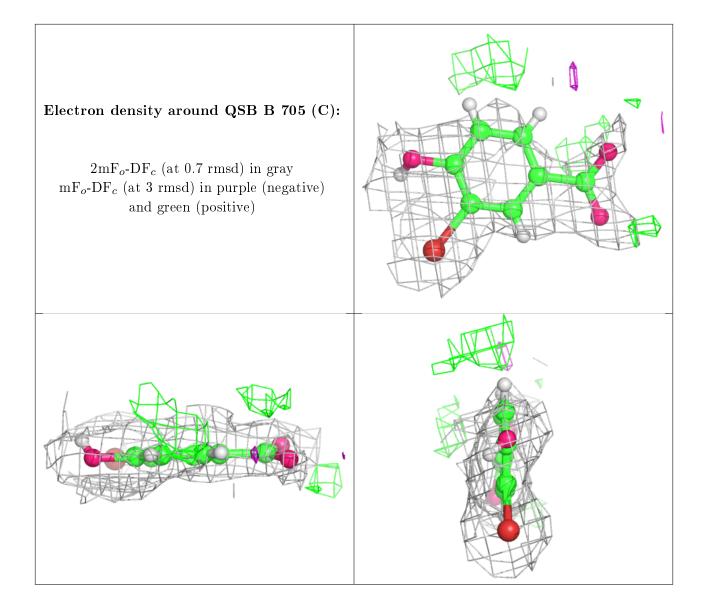




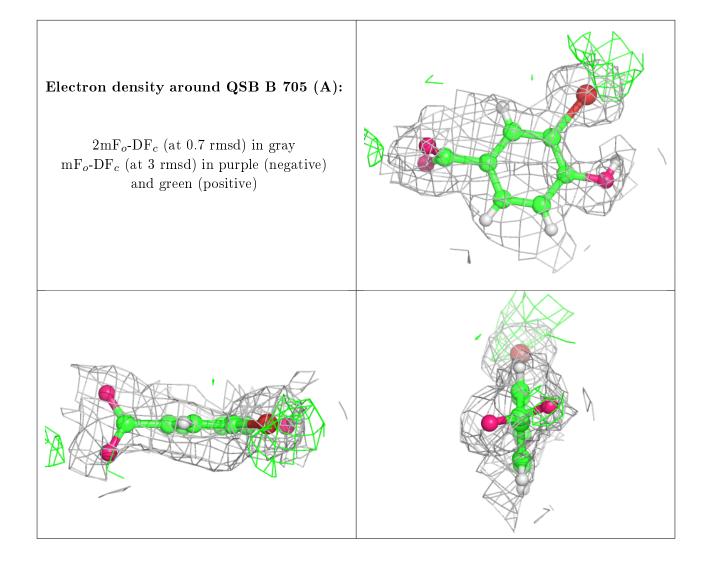




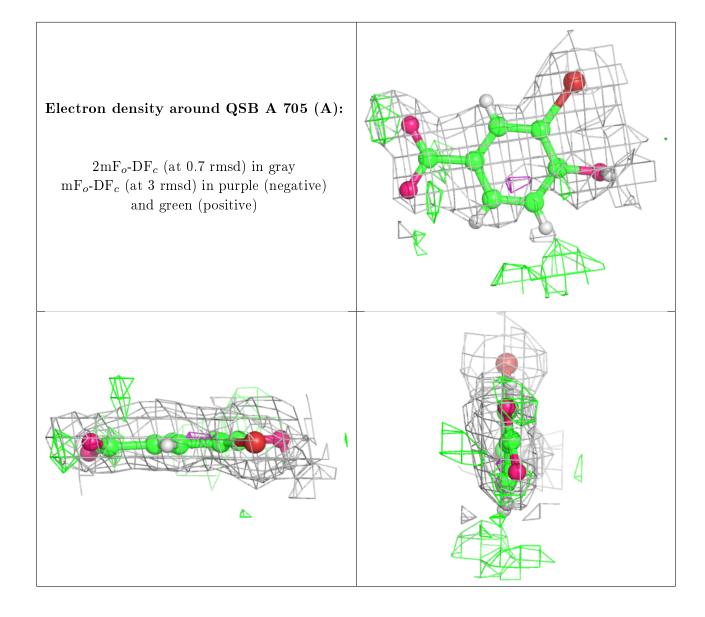




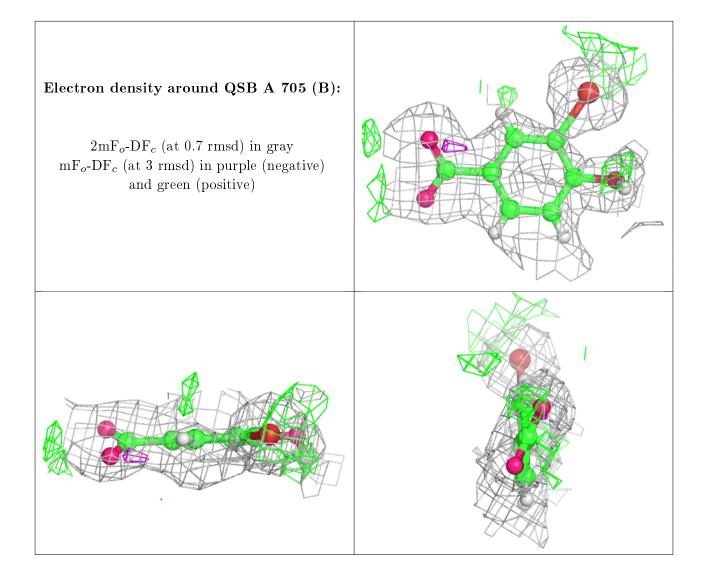




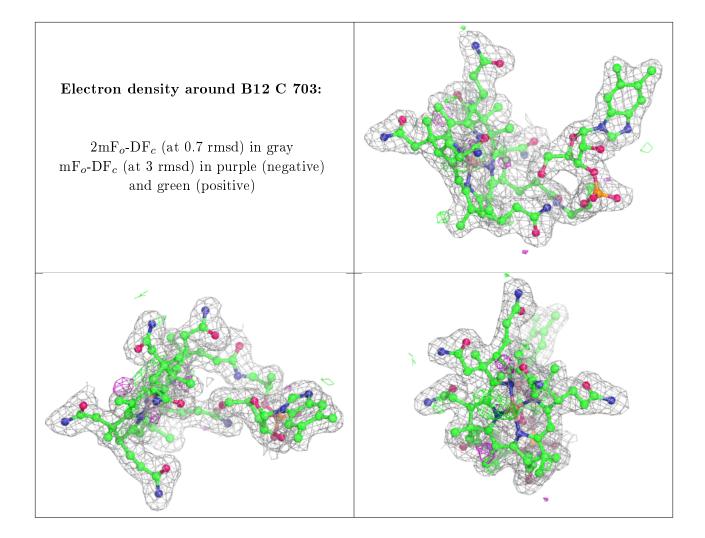




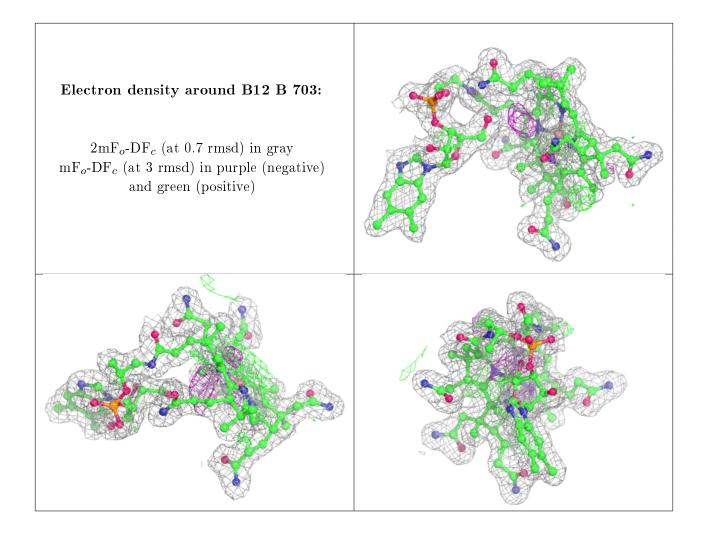




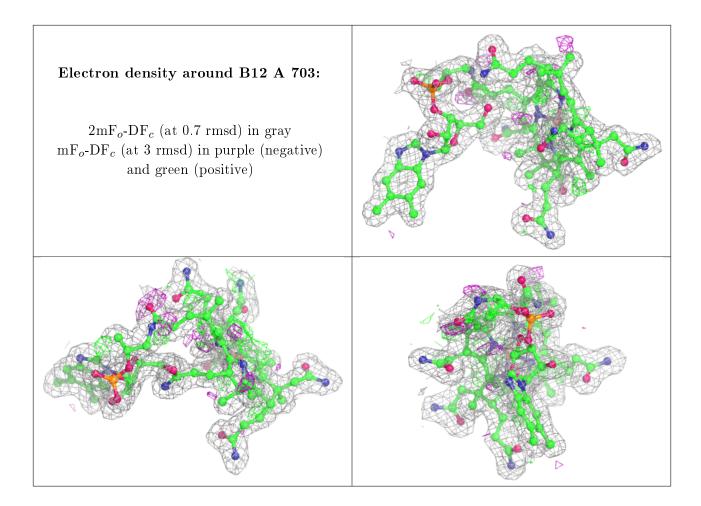












6.5 Other polymers (i)

There are no such residues in this entry.

