wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2021 – 07:47 AM EDT

PDB ID	:	1JXZ
Title	:	Structure of the H90Q mutant of 4-Chlorobenzoyl-Coenzyme A Dehalogenase complexed with 4-hydroxybenzoyl-Coenzyme A (product)
Authors	:	Thoden, J.B.; Zhang, W.; Wei, Y.; Luo, L.; Taylor, K.L.; Yang, G.; Dunaway-Mariano, D.; Benning, M.M.; Holden, H.M.
Deposited on	:	2001-09-10
Resolution	:	1.90 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:

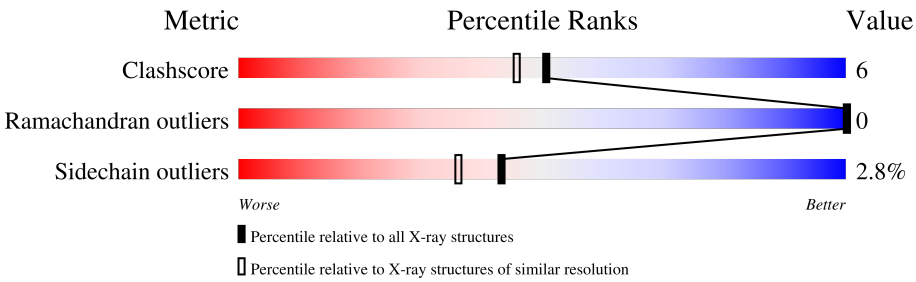
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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%

Mol	Chain	Length	Quality of chain
1	A	269	78% 22%
1	B	269	75% 21% • •
1	C	269	72% 22% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7199 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 4-chlorobenzoyl Coenzyme A dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	268	2088	1319	377	377	15	0	1	0
1	B	269	2097	1324	378	379	16	0	2	0
1	C	264	2051	1299	365	371	16	0	1	0

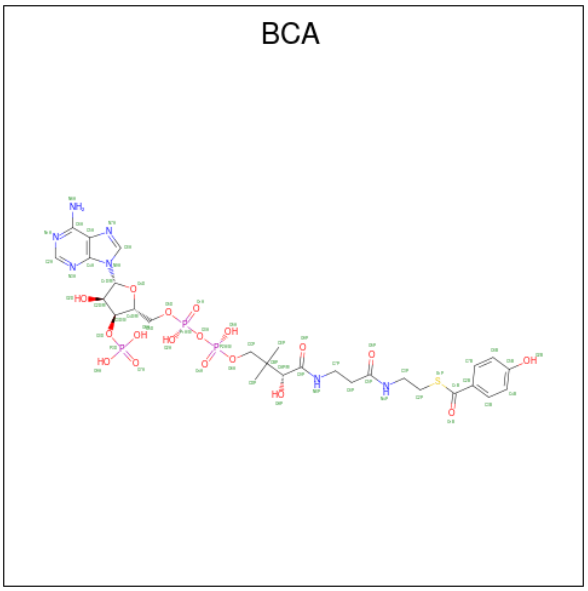
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	ALA	GLY	conflict	PIR 419529
A	90	GLN	HIS	engineered mutation	PIR 419529
B	85	ALA	GLY	conflict	PIR 419529
B	90	GLN	HIS	engineered mutation	PIR 419529
C	85	ALA	GLY	conflict	PIR 419529
C	90	GLN	HIS	engineered mutation	PIR 419529

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

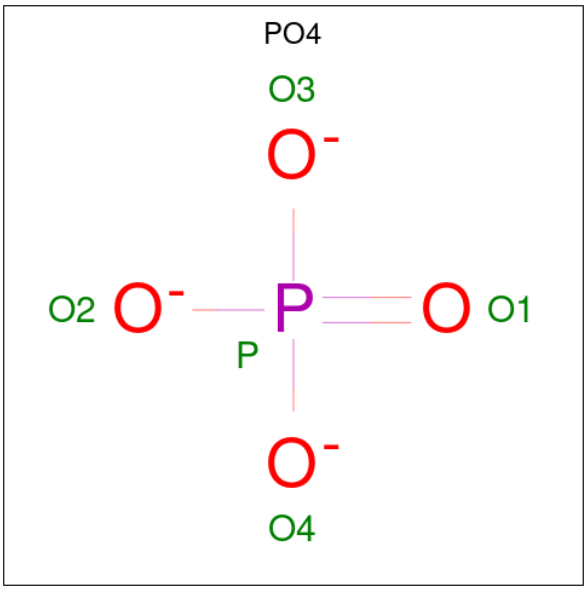
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0

- Molecule 3 is 4-HYDROXYBENZOYL COENZYME A (three-letter code: BCA) (formula: $C_{28}H_{40}N_7O_{18}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	A	1	53	28	7	15	2	1	0	0
3	B	1	53	28	7	15	2	1	0	0
3	C	1	53	28	7	15	2	1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is water.

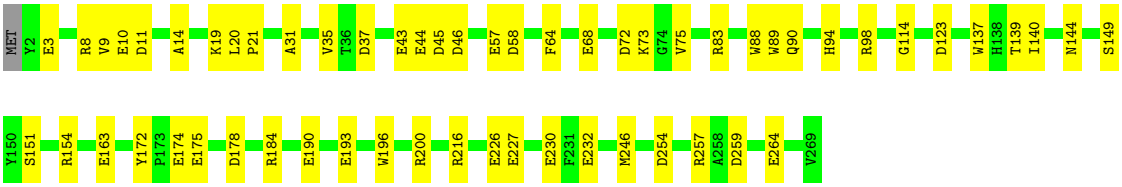
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	324	324	324	0	0
			Total	O		
5	B	248	248	248	0	0
			Total	O		
5	C	224	224	224	0	0

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. 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. 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.

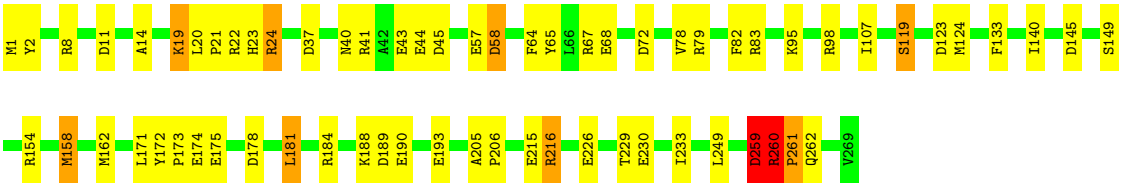
• Molecule 1: 4-chlorobenzoyl Coenzyme A dehalogenase

Chain A:



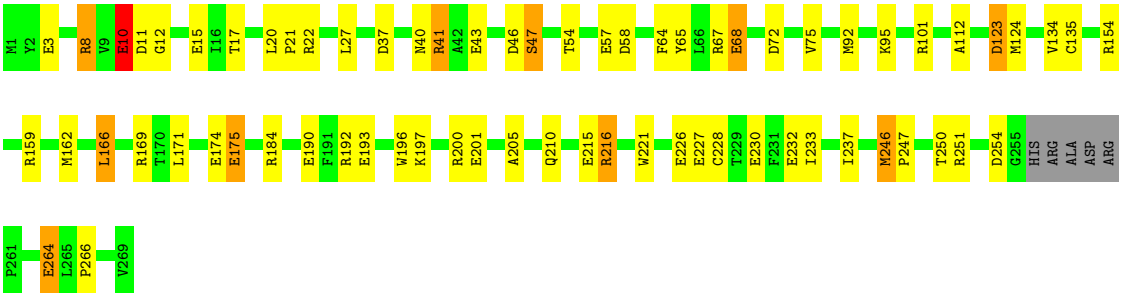
• Molecule 1: 4-chlorobenzoyl Coenzyme A dehalogenase

Chain B:



• Molecule 1: 4-chlorobenzoyl Coenzyme A dehalogenase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	108.10Å 102.70Å 90.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 46.38 – 1.68	Depositor EDS
% Data completeness (in resolution range)	88.0 (30.00-1.90) 79.9 (46.38-1.68)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 1.68Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.195 , (Not available) 0.303 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	11.0	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 90.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	7199	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: CA, BCA, PO4

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	1.24	17/2139 (0.8%)	1.34	27/2898 (0.9%)
1	B	1.20	11/2153 (0.5%)	1.43	34/2916 (1.2%)
1	C	1.17	15/2100 (0.7%)	1.38	28/2843 (1.0%)
All	All	1.21	43/6392 (0.7%)	1.38	89/8657 (1.0%)

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	226	GLU	CD-OE2	11.35	1.38	1.25
1	A	68	GLU	CD-OE1	-10.57	1.14	1.25
1	A	57	GLU	CD-OE2	9.82	1.36	1.25
1	B	193	GLU	CD-OE2	9.35	1.35	1.25
1	A	190	GLU	CD-OE2	8.75	1.35	1.25

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	216	ARG	NE-CZ-NH1	13.91	127.25	120.30
1	B	216	ARG	NE-CZ-NH2	-12.98	113.81	120.30
1	A	72	ASP	CB-CG-OD1	8.97	126.37	118.30
1	B	145	ASP	CB-CG-OD2	-8.88	110.31	118.30
1	C	169	ARG	NE-CZ-NH1	8.80	124.70	120.30

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	2088	0	2075	19	0
1	B	2097	0	2088	27	0
1	C	2051	0	2045	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	53	0	36	1	0
3	B	53	0	36	1	0
3	C	53	0	36	1	0
4	B	5	0	0	0	0
5	A	324	0	0	6	2
5	B	248	0	0	2	1
5	C	224	0	0	5	0
All	All	7199	0	6316	72	2

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 6.

The worst 5 of 72 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:C:65:TYR:CD1	1:C:68:GLU:HG3	2.14	0.83
1:B:65:TYR:CD1	1:B:68:GLU:HG3	2.14	0.82
1:B:140:ILE:HG13	1:B:140:ILE:O	1.94	0.68
1:C:41:ARG:NH1	5:C:457:HOH:O	2.25	0.68
1:A:21:PRO:HD2	5:A:591:HOH:O	1.97	0.64

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:438:HOH:O	5:B:403:HOH:O[2_575]	2.11	0.09
5:A:356:HOH:O	5:A:423:HOH:O[3_546]	2.14	0.06

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	267/269 (99%)	258 (97%)	9 (3%)	0	100	100
1	B	269/269 (100%)	257 (96%)	12 (4%)	0	100	100
1	C	261/269 (97%)	250 (96%)	11 (4%)	0	100	100
All	All	797/807 (99%)	765 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	214/214 (100%)	213 (100%)	1 (0%)	88	89
1	B	216/214 (101%)	204 (94%)	12 (6%)	21	11
1	C	211/214 (99%)	205 (97%)	6 (3%)	43	36
All	All	641/642 (100%)	622 (97%)	19 (3%)	43	33

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	10	GLU
1	C	166	LEU
1	C	246	MET
1	C	47	SER
1	B	158	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	235	ASN
1	C	90	GLN
1	B	235	ASN
1	B	33	GLN
1	C	33	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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	BCA	B	272	-	48,56,60	2.04	6 (12%)	60,82,89	2.37	14 (23%)
3	BCA	C	271	-	48,56,60	1.71	8 (16%)	60,82,89	1.77	12 (20%)
4	PO4	B	271	-	4,4,4	2.06	2 (50%)	6,6,6	0.63	0
3	BCA	A	271	-	48,56,60	1.77	5 (10%)	60,82,89	1.54	9 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BCA	B	272	-	-	6/46/66/71	0/4/4/4
3	BCA	C	271	-	-	8/46/66/71	0/4/4/4
3	BCA	A	271	-	-	1/46/66/71	0/4/4/4

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	272	BCA	C9P-N8P	7.95	1.51	1.33
3	A	271	BCA	C9P-N8P	6.86	1.48	1.33
3	A	271	BCA	C5P-N4P	6.61	1.48	1.33
3	B	272	BCA	C5P-N4P	6.13	1.47	1.33
3	C	271	BCA	C5P-N4P	6.09	1.47	1.33

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	272	BCA	CDP-CBP-CAP	7.65	122.08	108.82
3	B	272	BCA	CEP-CBP-CAP	-7.54	95.74	108.82
3	B	272	BCA	C2P-S1P-C1B	6.85	108.40	99.80
3	B	272	BCA	C3P-N4P-C5P	-6.47	110.82	122.84
3	A	271	BCA	C7P-N8P-C9P	-6.29	111.36	122.59

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	272	BCA	CAP-CBP-CCP-O6A
3	C	271	BCA	CCP-O6A-P2A-O5A
3	C	271	BCA	CDP-CBP-CCP-O6A
3	C	271	BCA	CEP-CBP-CCP-O6A
3	C	271	BCA	CAP-CBP-CCP-O6A

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	272	BCA	1	0
3	C	271	BCA	1	0

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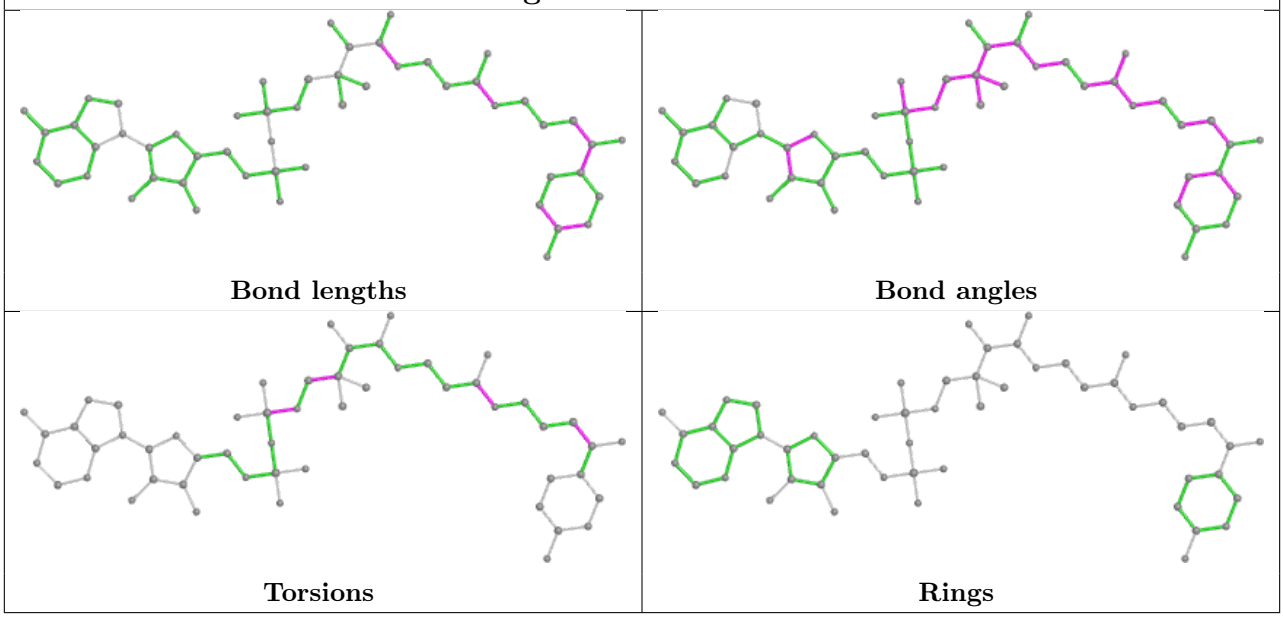
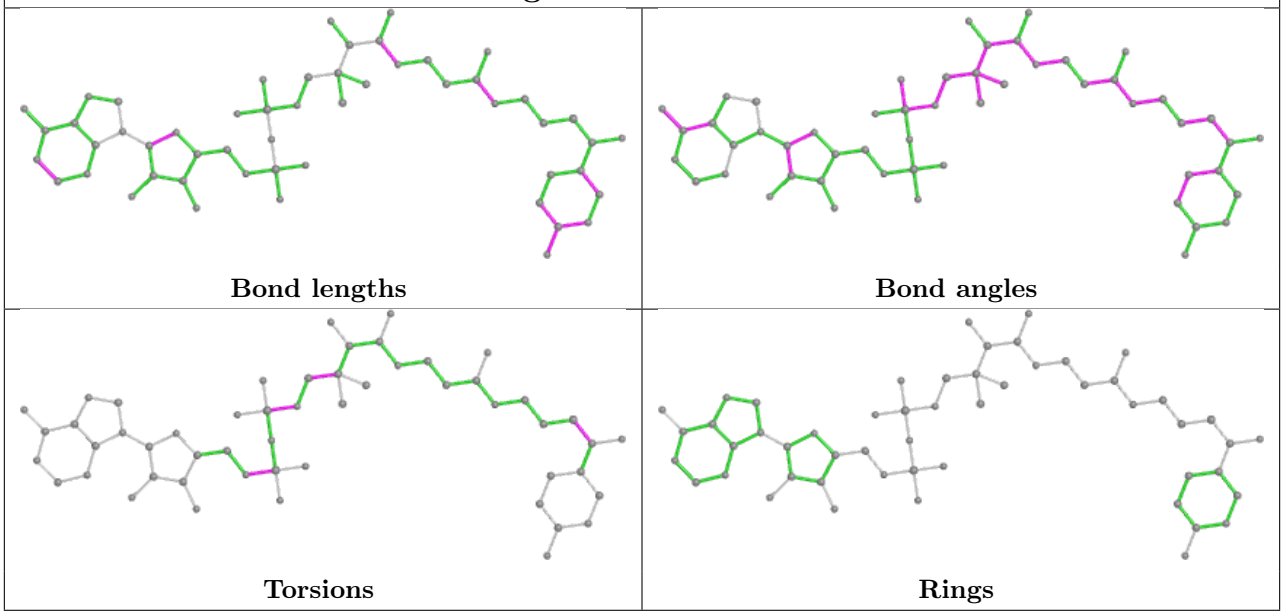
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	271	BCA	1	0

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.

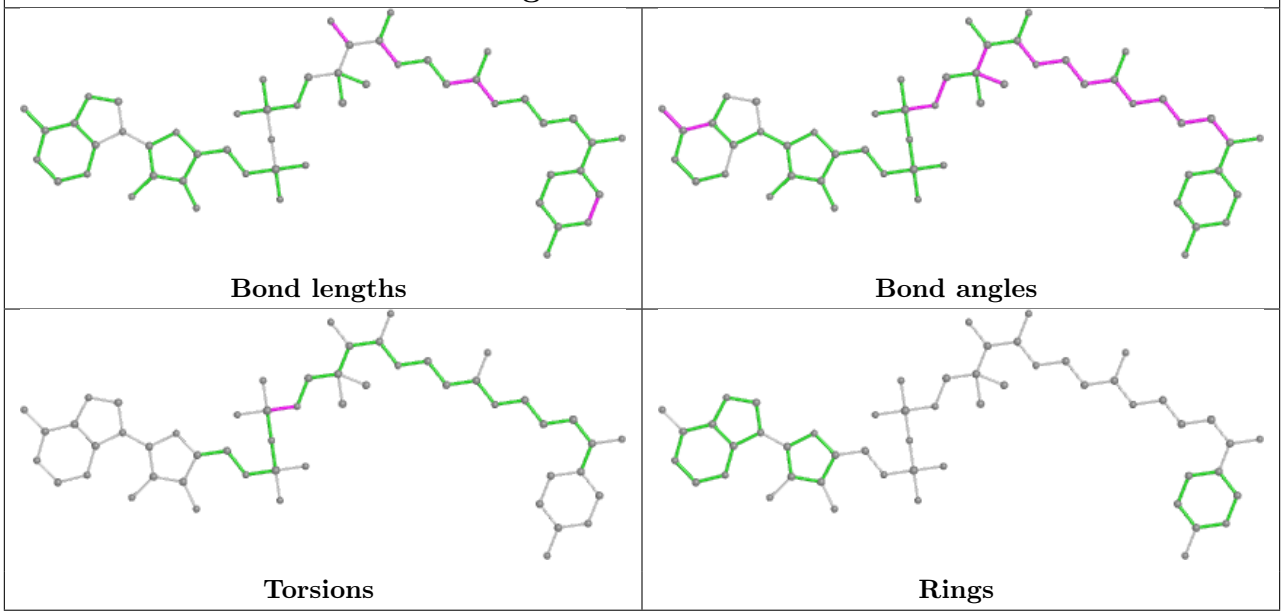
Ligand BCA B 272



Ligand BCA C 271



Ligand BCA A 271



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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

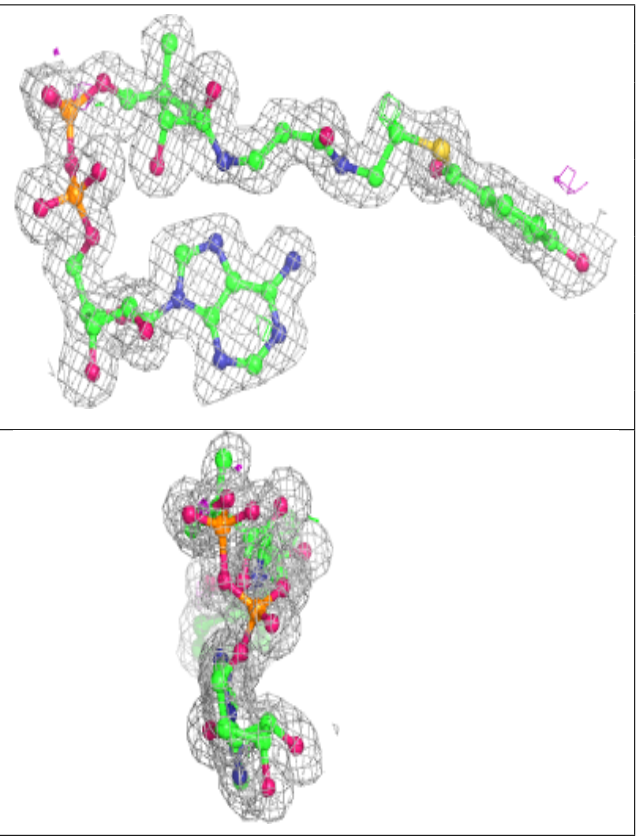
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

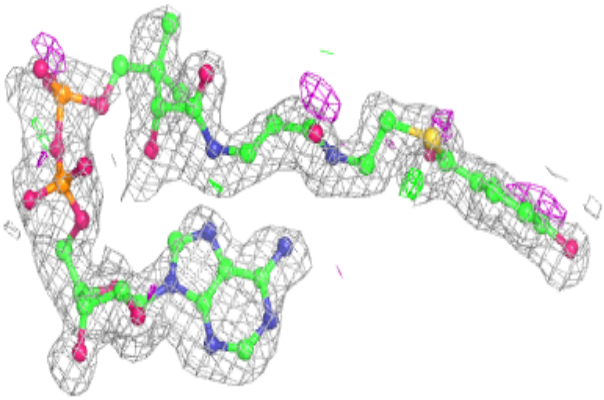
Electron density around BCA A 271:

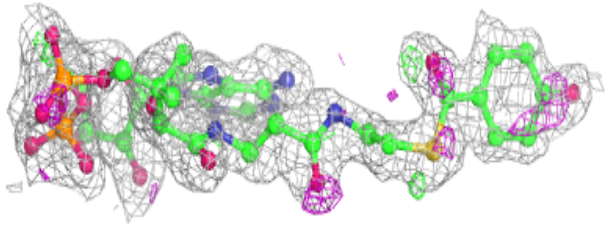
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

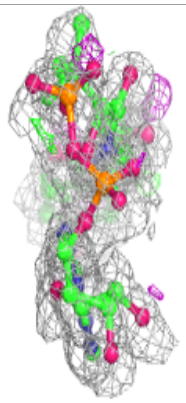


Electron density around BCA B 272:

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

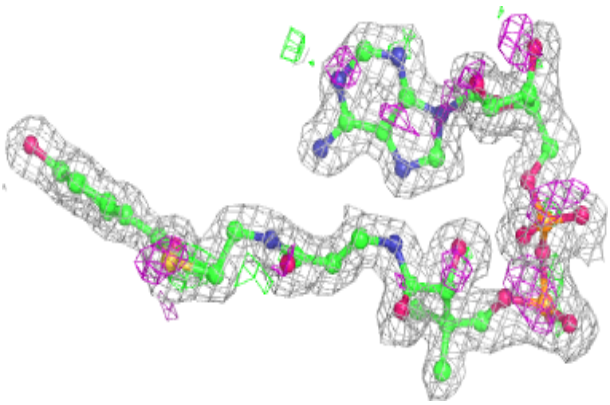


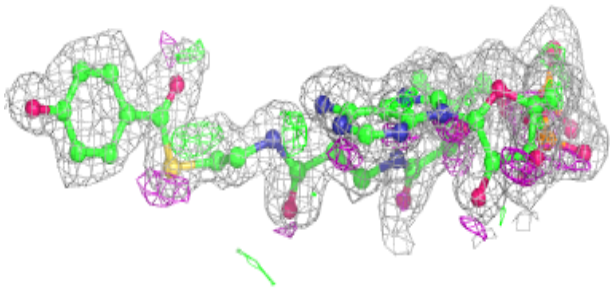


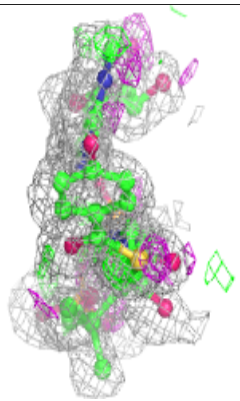


Electron density around BCA C 271:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.