wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 04:49 PM JST

PDB ID	:	6LLH / pdb_00006llh
Title	:	Biphenyl-2,3-diol-soaked resting complex of Oxy and Fd in carbazole 1,9a-dioxygenase
Authors	:	Wang, Y.X.; Suzuki-Minakuchi, C.; Nojiri, H.
Deposited on	:	2019-12-23
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:

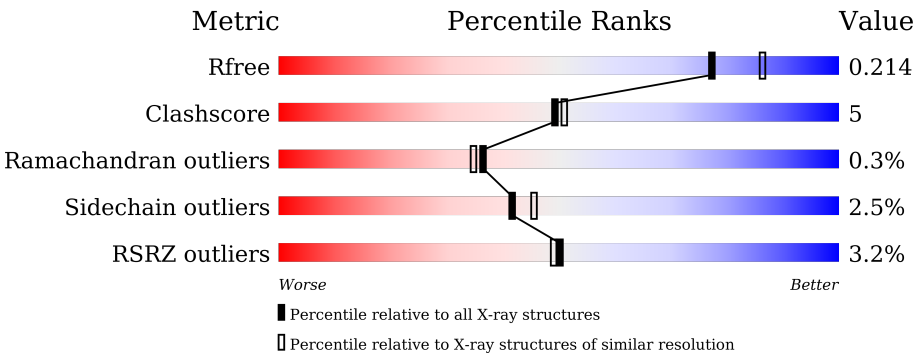
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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	392	2%, 86%, 12%, ••
1	B	392	2%, 86%, 12%, ••
1	C	392	%, 87%, 11%, ••
2	D	115	13%, 82%, 10%, 9%
2	E	115	2%, 87%, 5%, 8%
2	F	115	11%, 82%, 9%, •, 9%

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
5	BPY	A	503	-	-	X	-
6	EDO	B	504	-	-	X	-
6	EDO	C	506	-	-	X	-
6	EDO	C	507	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 13006 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 Terminal oxygenase component of carbazole.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3147	2013	537	584	13	0	3	0
1	B	388	3143	2008	538	584	13	0	2	0
1	C	388	3162	2022	541	586	13	0	5	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	385	LEU	-	expression tag	UNP Q84II6
A	386	GLU	-	expression tag	UNP Q84II6
A	387	HIS	-	expression tag	UNP Q84II6
A	388	HIS	-	expression tag	UNP Q84II6
A	389	HIS	-	expression tag	UNP Q84II6
A	390	HIS	-	expression tag	UNP Q84II6
A	391	HIS	-	expression tag	UNP Q84II6
A	392	HIS	-	expression tag	UNP Q84II6
B	385	LEU	-	expression tag	UNP Q84II6
B	386	GLU	-	expression tag	UNP Q84II6
B	387	HIS	-	expression tag	UNP Q84II6
B	388	HIS	-	expression tag	UNP Q84II6
B	389	HIS	-	expression tag	UNP Q84II6
B	390	HIS	-	expression tag	UNP Q84II6
B	391	HIS	-	expression tag	UNP Q84II6
B	392	HIS	-	expression tag	UNP Q84II6
C	385	LEU	-	expression tag	UNP Q84II6
C	386	GLU	-	expression tag	UNP Q84II6
C	387	HIS	-	expression tag	UNP Q84II6
C	388	HIS	-	expression tag	UNP Q84II6
C	389	HIS	-	expression tag	UNP Q84II6
C	390	HIS	-	expression tag	UNP Q84II6
C	391	HIS	-	expression tag	UNP Q84II6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	392	HIS	-	expression tag	UNP Q84II6

- Molecule 2 is a protein called Ferredoxin CarAc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	105	776	489	130	150	7	0	0	0
			Total	C	N	O	S			
2	E	106	785	494	132	152	7	0	0	0
			Total	C	N	O	S			
2	F	105	793	500	133	153	7	0	3	0

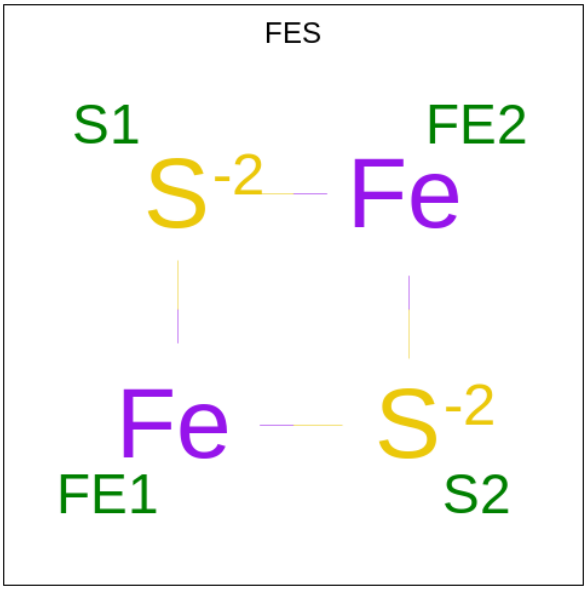
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	108	LEU	-	expression tag	UNP Q8GI16
D	109	GLU	-	expression tag	UNP Q8GI16
D	110	HIS	-	expression tag	UNP Q8GI16
D	111	HIS	-	expression tag	UNP Q8GI16
D	112	HIS	-	expression tag	UNP Q8GI16
D	113	HIS	-	expression tag	UNP Q8GI16
D	114	HIS	-	expression tag	UNP Q8GI16
D	115	HIS	-	expression tag	UNP Q8GI16
E	108	LEU	-	expression tag	UNP Q8GI16
E	109	GLU	-	expression tag	UNP Q8GI16
E	110	HIS	-	expression tag	UNP Q8GI16
E	111	HIS	-	expression tag	UNP Q8GI16
E	112	HIS	-	expression tag	UNP Q8GI16
E	113	HIS	-	expression tag	UNP Q8GI16
E	114	HIS	-	expression tag	UNP Q8GI16
E	115	HIS	-	expression tag	UNP Q8GI16
F	108	LEU	-	expression tag	UNP Q8GI16
F	109	GLU	-	expression tag	UNP Q8GI16
F	110	HIS	-	expression tag	UNP Q8GI16
F	111	HIS	-	expression tag	UNP Q8GI16
F	112	HIS	-	expression tag	UNP Q8GI16
F	113	HIS	-	expression tag	UNP Q8GI16
F	114	HIS	-	expression tag	UNP Q8GI16
F	115	HIS	-	expression tag	UNP Q8GI16

- Molecule 3 is FE (II) ION (CCD ID: FE2) (formula: Fe).

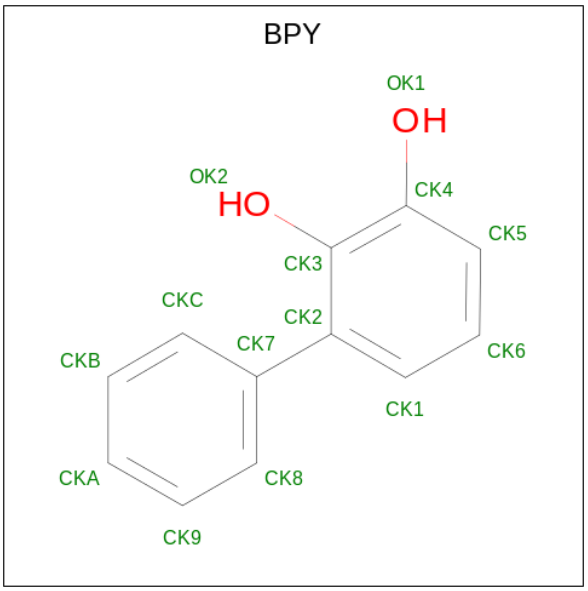
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
3	A	1	1	1	0	0
			Total	Fe		
3	B	1	1	1	0	0
			Total	Fe		
3	C	1	1	1	0	0

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



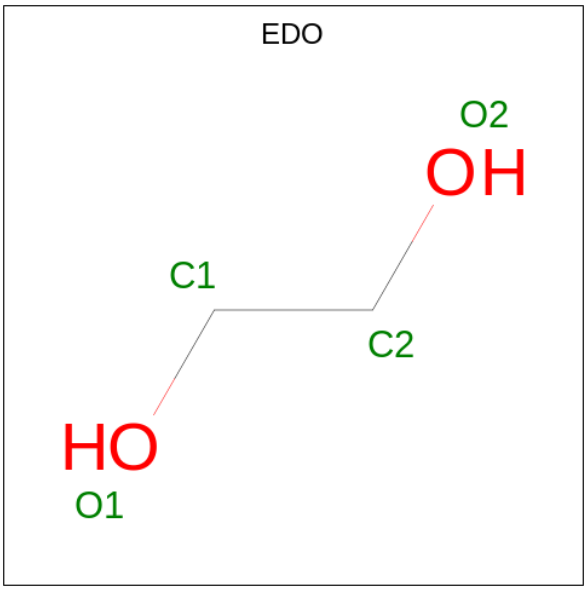
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	A	1	4	2	2	0	0
			Total	Fe	S		
4	B	1	4	2	2	0	0
			Total	Fe	S		
4	C	1	4	2	2	0	0
			Total	Fe	S		
4	D	1	4	2	2	0	0
			Total	Fe	S		
4	E	1	4	2	2	0	0
			Total	Fe	S		
4	F	1	4	2	2	0	0

- Molecule 5 is BIPHENYL-2,3-DIOL (CCD ID: BPY) (formula: $C_{12}H_{10}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	14	12	2	0	0
			Total	C	O		
5	B	1	14	12	2	0	0
			Total	C	O		
5	C	1	14	12	2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	4	2	2	0	0

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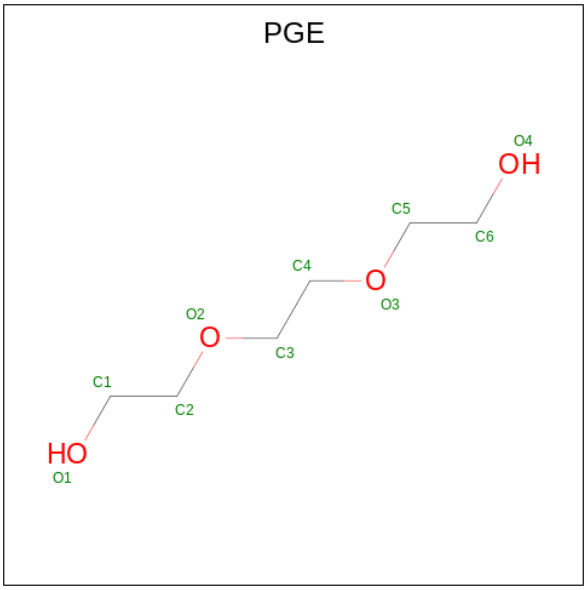
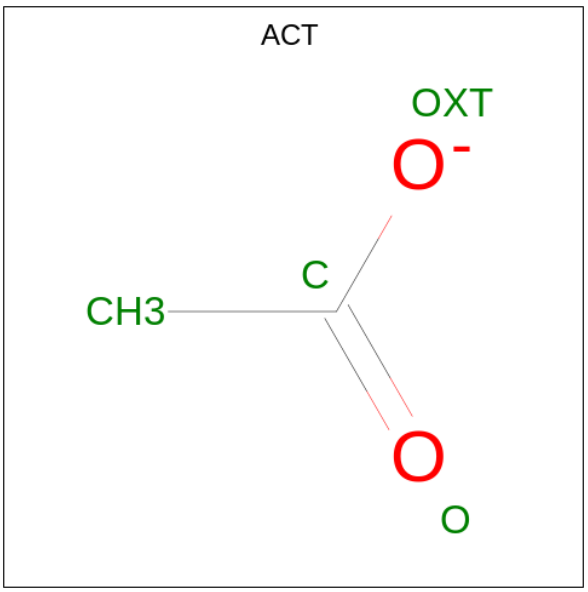
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	4	2	2	0	0
6	B	1	4	2	2	0	0
6	B	1	4	2	2	0	0
6	B	1	4	2	2	0	0
6	B	1	4	2	2	0	0
6	B	1	4	2	2	0	0
6	C	1	4	2	2	0	0
6	C	1	4	2	2	0	0
6	C	1	4	2	2	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



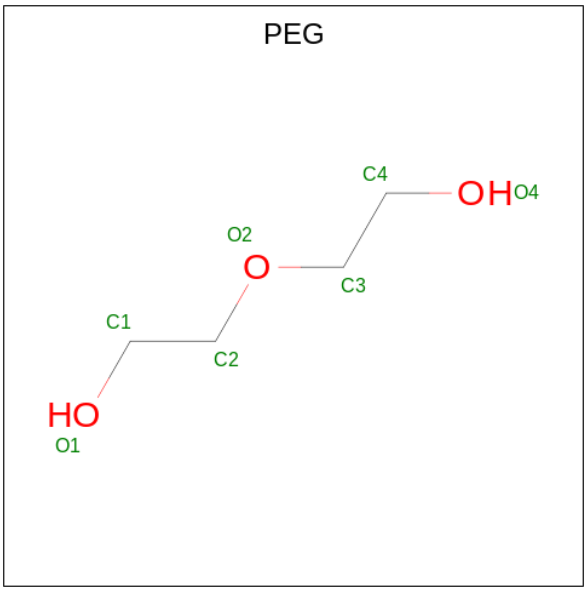
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	10	6	4	0	0
7	E	1	10	6	4	0	0

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	4	2	2	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	7	4	3	0	0
			Total	C	O		
9	B	1	7	4	3	0	0

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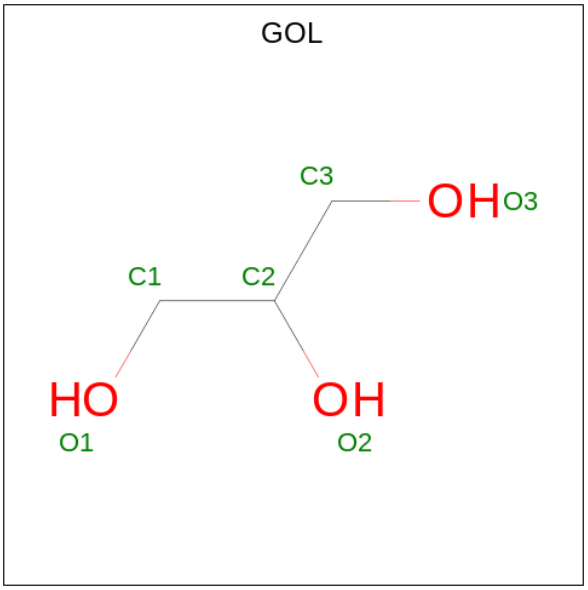
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	E	1	7	4	3	0	0

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 11 is water.

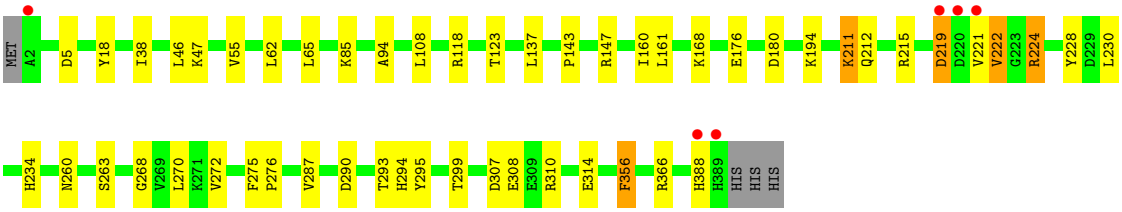
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	312	312	312	0	0
11	B	291	291	291	0	0
11	C	293	293	293	0	0
11	D	28	28	28	0	0
11	E	59	59	59	0	0
11	F	57	57	57	0	0

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.

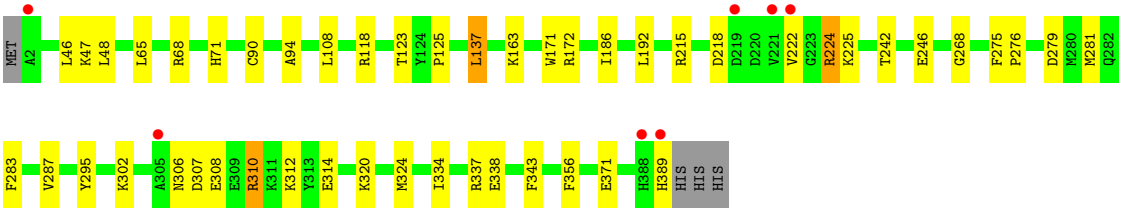
• Molecule 1: Terminal oxygenase component of carbazole

Chain A:



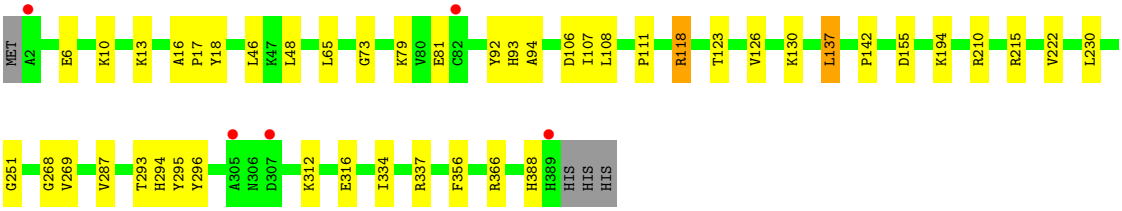
• Molecule 1: Terminal oxygenase component of carbazole

Chain B:



• Molecule 1: Terminal oxygenase component of carbazole

Chain C:

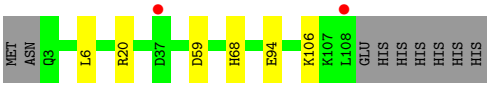


• Molecule 2: Ferredoxin CarAc

Chain D:

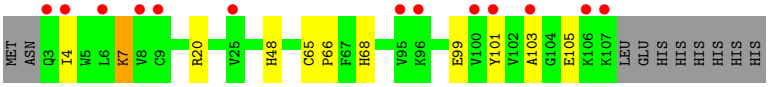
• Molecule 2: Ferredoxin CarAc

Chain E:



• Molecule 2: Ferredoxin CarAc

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.26Å 89.79Å 105.44Å 90.00° 103.99° 90.00°	Depositor
Resolution (Å)	36.59 – 1.99 36.59 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.7 (36.59-1.99) 98.7 (36.59-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.96 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.162 , 0.207 0.172 , 0.214	Depositor DCC
R_{free} test set	6097 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13006	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: PGE, PEG, GOL, FE2, FES, EDO, ACT, BPY

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	1.01	1/3238 (0.0%)	1.05	5/4394 (0.1%)
1	B	0.94	2/3231 (0.1%)	0.99	1/4386 (0.0%)
1	C	1.01	3/3259 (0.1%)	1.02	1/4423 (0.0%)
2	D	0.88	0/792	0.93	0/1077
2	E	0.99	0/801	1.02	1/1089 (0.1%)
2	F	0.99	1/815 (0.1%)	0.99	0/1107
All	All	0.98	7/12136 (0.1%)	1.01	8/16476 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	4
2	E	0	1
2	F	0	1
All	All	0	12

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	92	TYR	C-O	-7.26	1.17	1.23
2	F	48	HIS	CE1-NE2	5.81	1.38	1.32
1	C	251	GLY	C-O	5.73	1.28	1.23
1	A	294	HIS	CE1-NE2	5.47	1.38	1.32
1	C	294	HIS	CE1-NE2	5.43	1.38	1.32

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	356	PHE	CA-CB-CG	7.34	121.14	113.80
1	B	224	ARG	CB-CA-C	-6.34	99.19	109.72
1	A	290	ASP	CA-CB-CG	5.83	118.43	112.60
1	C	142	PRO	O-C-N	-5.64	118.72	121.31
1	A	224	ARG	CB-CA-C	-5.13	100.09	109.54

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ARG	Sidechain
1	A	310	ARG	Sidechain
1	B	215[A]	ARG	Sidechain
1	B	215[B]	ARG	Sidechain
1	B	310	ARG	Sidechain

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	3147	0	3062	32	0
1	B	3143	0	3049	35	0
1	C	3162	0	3079	29	0
2	D	776	0	756	4	0
2	E	785	0	764	4	0
2	F	793	0	779	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	1	0
4	D	4	0	0	0	0
4	E	4	0	0	1	0
4	F	4	0	0	1	0
5	A	14	0	8	10	0
5	B	14	0	9	3	0
5	C	14	0	9	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	8	0	12	1	0
6	B	20	0	30	9	0
6	C	12	0	18	12	0
7	A	10	0	14	5	0
7	E	10	0	14	5	0
8	A	4	0	3	0	0
9	A	7	0	10	0	0
9	B	7	0	10	0	0
9	E	7	0	10	2	0
10	C	6	0	8	0	0
11	A	312	0	0	6	0
11	B	291	0	0	9	0
11	C	293	0	0	13	0
11	D	28	0	0	0	0
11	E	59	0	0	1	0
11	F	57	0	0	1	0
All	All	13006	0	11644	127	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 127 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ARG:HH11	6:B:506:EDO:H11	1.11	1.10
1:B:68:ARG:NH1	6:B:506:EDO:H11	1.80	0.97
1:A:272:VAL:HG21	5:A:503:BPY:HCK1	1.51	0.90
1:B:68:ARG:HH11	6:B:506:EDO:C1	1.85	0.89
1:B:389:HIS:C	11:B:680:HOH:O	2.18	0.85

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	389/392 (99%)	373 (96%)	15 (4%)	1 (0%)	36	35
1	B	388/392 (99%)	370 (95%)	17 (4%)	1 (0%)	36	35
1	C	391/392 (100%)	374 (96%)	16 (4%)	1 (0%)	36	35
2	D	103/115 (90%)	98 (95%)	5 (5%)	0	100	100
2	E	104/115 (90%)	103 (99%)	1 (1%)	0	100	100
2	F	106/115 (92%)	103 (97%)	1 (1%)	2 (2%)	6	3
All	All	1481/1521 (97%)	1421 (96%)	55 (4%)	5 (0%)	36	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	4	ILE
1	A	268	GLY
1	B	268	GLY
1	C	268	GLY
2	F	103	ALA

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	338/339 (100%)	326 (96%)	12 (4%)	31	31
1	B	337/339 (99%)	331 (98%)	6 (2%)	51	58
1	C	340/339 (100%)	333 (98%)	7 (2%)	47	52
2	D	83/93 (89%)	80 (96%)	3 (4%)	31	31
2	E	84/93 (90%)	83 (99%)	1 (1%)	63	70
2	F	86/93 (92%)	84 (98%)	2 (2%)	44	49
All	All	1268/1296 (98%)	1237 (98%)	31 (2%)	42	47

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	222	VAL
2	D	92	GLU
1	B	356	PHE
2	F	7	LYS
1	C	388	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	165	GLN
1	C	127	GLN
1	B	234	HIS
1	C	119	GLN
1	B	52	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 29 ligands modelled in this entry, 3 are monoatomic - leaving 26 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	$\#\|Z\| > 2$
4	FES	C	502	1	0,4,4	-	-	-		
5	BPY	B	503	-	15,15,15	2.67	2 (13%)	20,20,20	0.82	0
4	FES	F	201	2	0,4,4	-	-	-		
7	PGE	A	505	-	9,9,9	0.85	0	8,8,8	0.84	0
7	PGE	E	203	-	9,9,9	0.68	0	8,8,8	0.98	0
9	PEG	B	505	-	6,6,6	0.54	0	5,5,5	0.05	0
5	BPY	A	503	3	15,15,15	1.95	4 (26%)	20,20,20	1.94	6 (30%)
6	EDO	A	504	-	3,3,3	0.39	0	2,2,2	0.79	0
6	EDO	B	506	-	3,3,3	0.37	0	2,2,2	0.57	0
5	BPY	C	503	-	15,15,15	2.80	2 (13%)	20,20,20	1.10	1 (5%)
6	EDO	C	506	-	3,3,3	0.14	0	2,2,2	0.58	0
9	PEG	E	202	-	6,6,6	0.41	0	5,5,5	0.45	0
6	EDO	B	508	-	3,3,3	0.59	0	2,2,2	0.14	0
4	FES	E	201	2	0,4,4	-	-	-		
6	EDO	C	507	-	3,3,3	0.36	0	2,2,2	0.19	0
4	FES	A	502	1	0,4,4	-	-	-		
6	EDO	A	508	-	3,3,3	0.69	0	2,2,2	0.23	0
6	EDO	B	504	-	3,3,3	0.32	0	2,2,2	0.12	0
10	GOL	C	505	-	5,5,5	0.43	0	5,5,5	0.74	0
6	EDO	B	507	-	3,3,3	0.42	0	2,2,2	1.01	0
4	FES	B	502	1	0,4,4	-	-	-		
4	FES	D	201	2	0,4,4	-	-	-		
6	EDO	C	504	-	3,3,3	0.38	0	2,2,2	0.58	0
6	EDO	B	509	-	3,3,3	0.42	0	2,2,2	0.47	0
8	ACT	A	506	-	3,3,3	0.88	0	3,3,3	0.86	0
9	PEG	A	507	-	6,6,6	0.61	0	5,5,5	0.65	0

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
4	FES	C	502	1	-	-	0/1/1/1
5	BPY	B	503	-	-	4/4/4/4	0/2/2/2
7	PGE	A	505	-	-	4/7/7/7	-
7	PGE	E	203	-	-	5/7/7/7	-
4	FES	F	201	2	-	-	0/1/1/1
9	PEG	B	505	-	-	1/4/4/4	-
5	BPY	A	503	3	-	2/4/4/4	0/2/2/2
6	EDO	A	504	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	506	-	-	1/1/1/1	-
5	BPY	C	503	-	-	0/4/4/4	0/2/2/2
6	EDO	C	506	-	-	0/1/1/1	-
9	PEG	E	202	-	-	3/4/4/4	-
6	EDO	B	508	-	-	0/1/1/1	-
4	FES	E	201	2	-	-	0/1/1/1
6	EDO	C	507	-	-	0/1/1/1	-
4	FES	A	502	1	-	-	0/1/1/1
6	EDO	A	508	-	-	1/1/1/1	-
6	EDO	B	504	-	-	1/1/1/1	-
10	GOL	C	505	-	-	2/4/4/4	-
6	EDO	B	507	-	-	1/1/1/1	-
4	FES	B	502	1	-	-	0/1/1/1
6	EDO	C	504	-	-	1/1/1/1	-
4	FES	D	201	2	-	-	0/1/1/1
6	EDO	B	509	-	-	0/1/1/1	-
9	PEG	A	507	-	-	4/4/4/4	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	503	BPY	CK4-CK3	8.51	1.50	1.40
5	B	503	BPY	CK4-CK3	8.28	1.49	1.40
5	C	503	BPY	CK2-CK3	6.24	1.51	1.40
5	B	503	BPY	CK2-CK3	5.69	1.50	1.40
5	A	503	BPY	CK4-CK3	4.11	1.44	1.40

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	503	BPY	CK2-CK3-CK4	3.83	122.50	120.03
5	A	503	BPY	CK5-CK6-CK1	3.78	125.61	120.25
5	C	503	BPY	CK2-CK3-CK4	-3.67	117.67	120.03
5	A	503	BPY	CK1-CK2-CK3	-3.46	114.52	117.96
5	A	503	BPY	CK6-CK5-CK4	-2.92	116.35	120.05

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	505	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	A	505	PGE	C1-C2-O2-C3
7	A	505	PGE	O1-C1-C2-O2
7	E	203	PGE	O3-C5-C6-O4
9	A	507	PEG	O1-C1-C2-O2

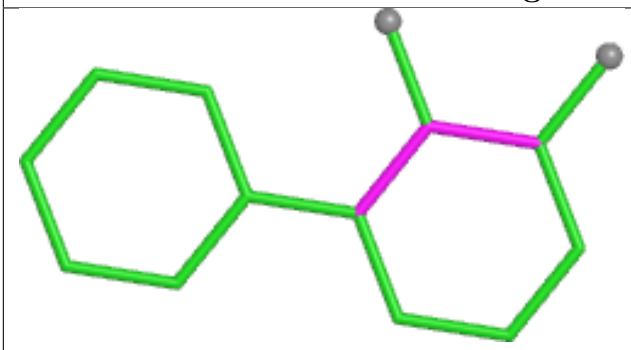
There are no ring outliers.

15 monomers are involved in 52 short contacts:

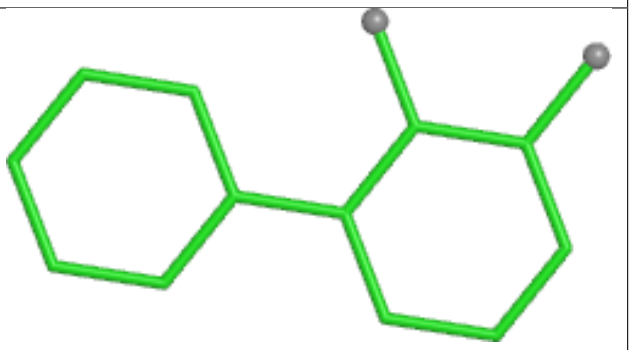
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	FES	1	0
5	B	503	BPY	3	0
4	F	201	FES	1	0
7	A	505	PGE	5	0
7	E	203	PGE	5	0
5	A	503	BPY	10	0
6	B	506	EDO	3	0
5	C	503	BPY	2	0
6	C	506	EDO	7	0
9	E	202	PEG	2	0
4	E	201	FES	1	0
6	C	507	EDO	5	0
6	A	508	EDO	1	0
6	B	504	EDO	4	0
6	B	507	EDO	2	0

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.

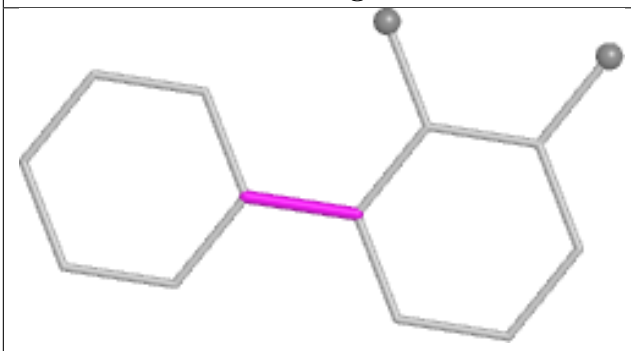
Ligand BPY B 503



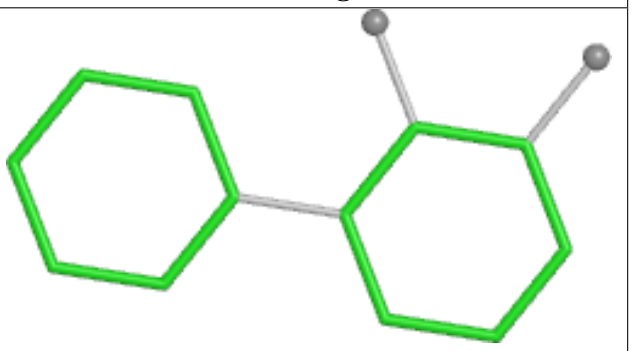
Bond lengths



Bond angles

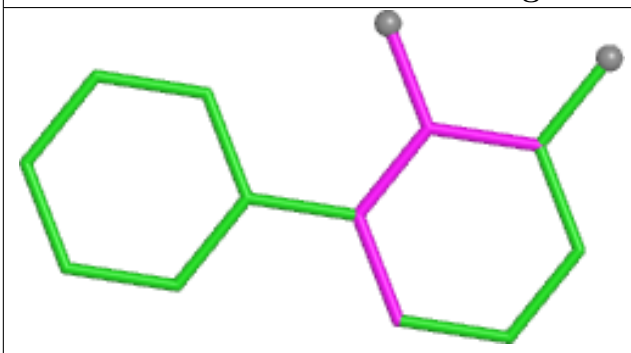


Torsions

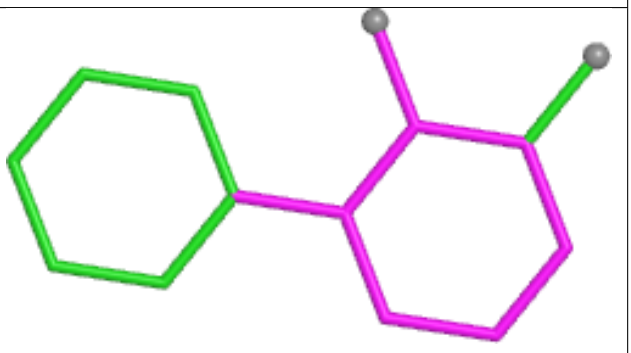


Rings

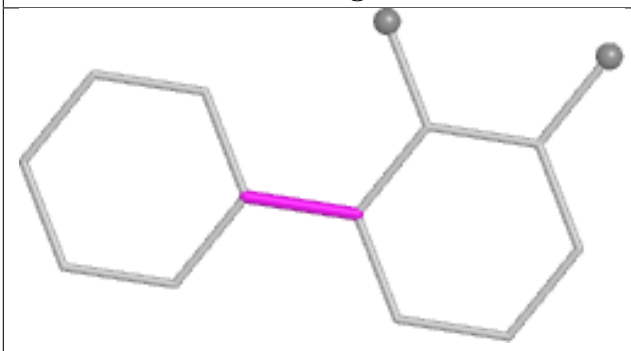
Ligand BPY A 503



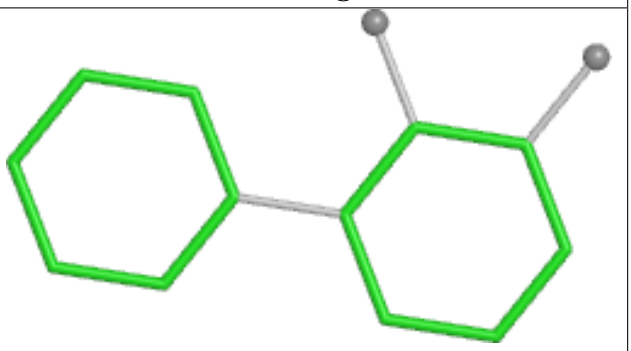
Bond lengths



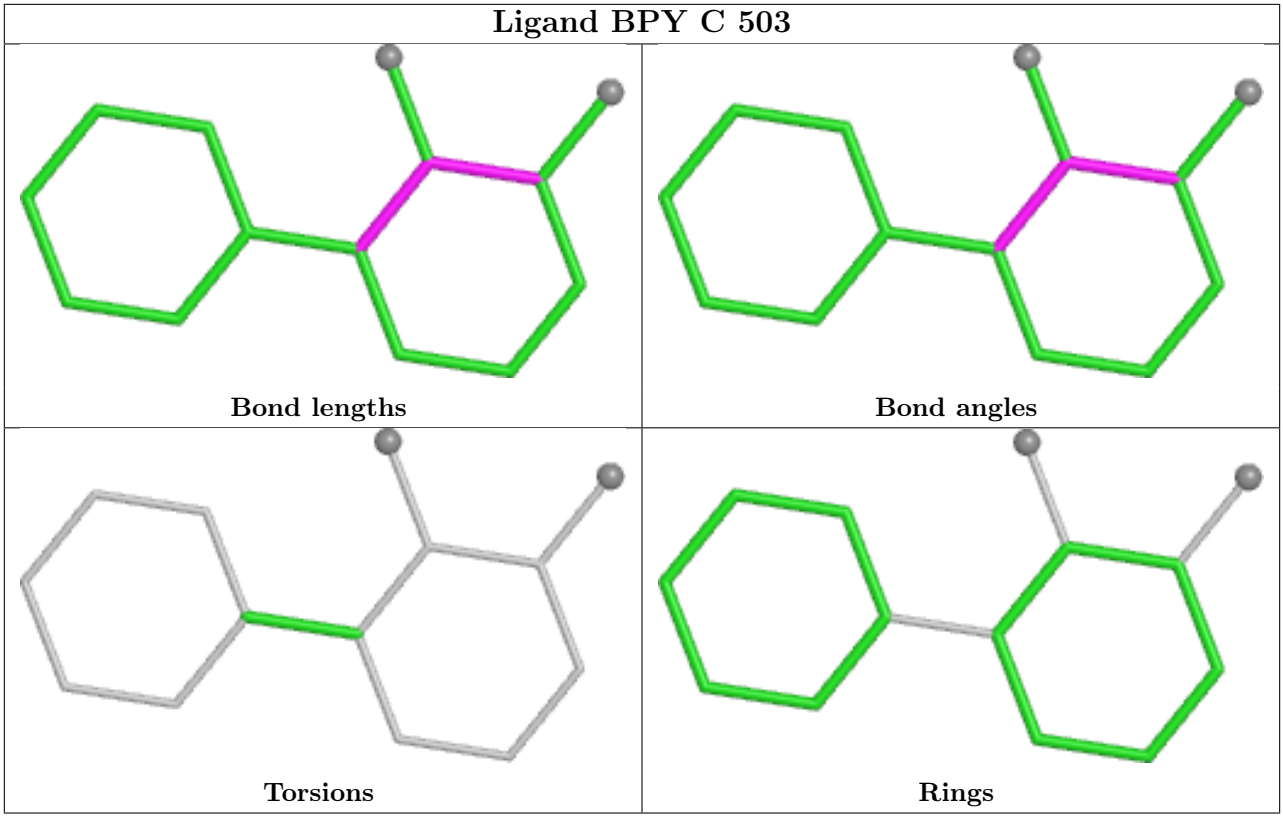
Bond angles



Torsions



Rings



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	388/392 (98%)	-0.22	6 (1%)	72	71	11, 22, 47, 78	3 (0%)
1	B	388/392 (98%)	0.00	7 (1%)	67	67	9, 27, 55, 77	2 (0%)
1	C	388/392 (98%)	-0.08	5 (1%)	75	74	10, 26, 49, 65	5 (1%)
2	D	105/115 (91%)	0.86	15 (14%)	6	5	21, 43, 80, 86	0
2	E	106/115 (92%)	0.28	2 (1%)	66	66	18, 32, 54, 70	0
2	F	105/115 (91%)	0.67	13 (12%)	8	7	18, 36, 61, 79	3 (2%)
All	All	1480/1521 (97%)	0.05	48 (3%)	50	49	9, 26, 57, 86	13 (0%)

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	4	ILE	6.8
2	D	108	LEU	5.7
1	A	220	ASP	5.0
2	E	108	LEU	4.9
2	F	4	ILE	4.2

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)

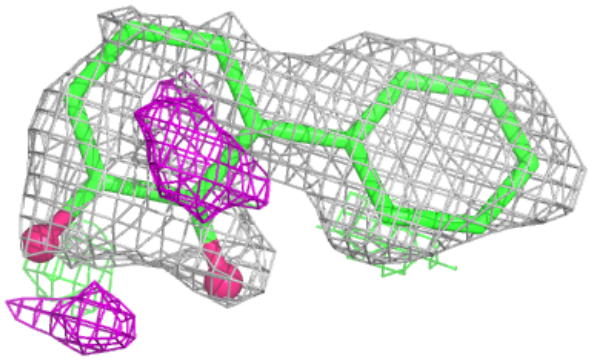
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

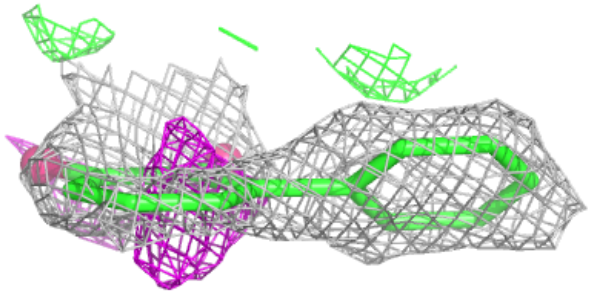
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PGE	E	203	10/10	0.73	0.21	58,73,78,87	0
6	EDO	A	504	4/4	0.74	0.24	48,52,53,54	0
8	ACT	A	506	4/4	0.74	0.20	52,55,55,58	0
9	PEG	A	507	7/7	0.78	0.17	54,61,65,66	0
9	PEG	B	505	7/7	0.79	0.18	59,61,68,71	0
6	EDO	B	508	4/4	0.82	0.18	45,60,62,62	0
7	PGE	A	505	10/10	0.83	0.15	42,48,54,58	0
10	GOL	C	505	6/6	0.83	0.15	32,53,58,59	0
5	BPY	C	503	14/14	0.85	0.13	46,50,54,54	0
6	EDO	A	508	4/4	0.86	0.15	37,42,42,46	0
9	PEG	E	202	7/7	0.86	0.15	54,59,72,73	0
5	BPY	A	503	14/14	0.86	0.20	46,58,73,75	0
5	BPY	B	503	14/14	0.87	0.15	49,59,62,65	0
6	EDO	B	509	4/4	0.87	0.13	54,55,55,57	0
6	EDO	B	506	4/4	0.87	0.15	37,41,44,56	0
6	EDO	C	504	4/4	0.90	0.11	37,45,47,47	0
6	EDO	B	504	4/4	0.90	0.28	46,46,46,57	0
6	EDO	B	507	4/4	0.91	0.23	32,38,39,39	0
6	EDO	C	507	4/4	0.92	0.16	31,32,35,36	0
6	EDO	C	506	4/4	0.95	0.20	32,34,35,37	0
3	FE2	A	501	1/1	0.99	0.04	25,25,25,25	0
3	FE2	B	501	1/1	0.99	0.04	33,33,33,33	0
4	FES	B	502	4/4	0.99	0.02	13,14,14,14	0
4	FES	C	502	4/4	0.99	0.03	19,20,21,21	0
4	FES	E	201	4/4	0.99	0.03	19,19,20,21	0
4	FES	A	502	4/4	1.00	0.02	15,16,16,16	0
4	FES	D	201	4/4	1.00	0.03	21,22,22,23	0
3	FE2	C	501	1/1	1.00	0.05	27,27,27,27	0
4	FES	F	201	4/4	1.00	0.04	18,18,19,21	0

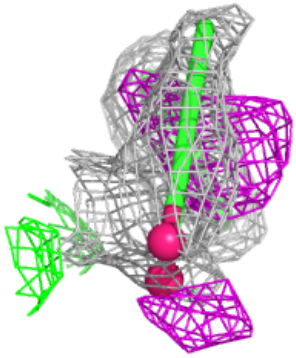
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BPY C 503:

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

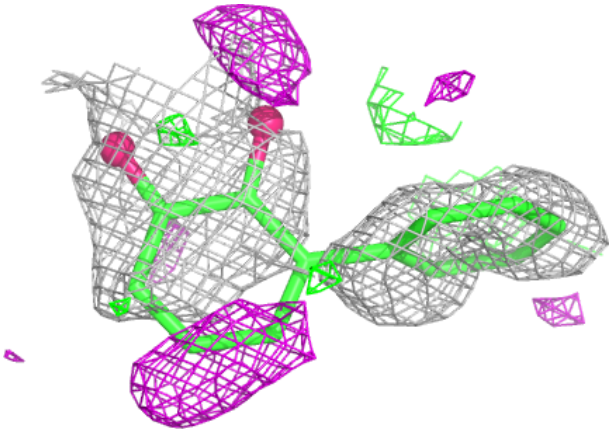


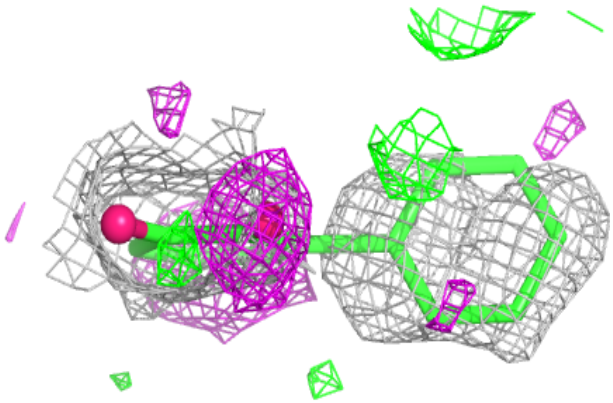


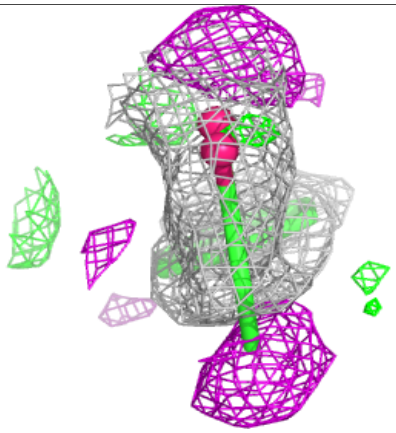


Electron density around BPY A 503:

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

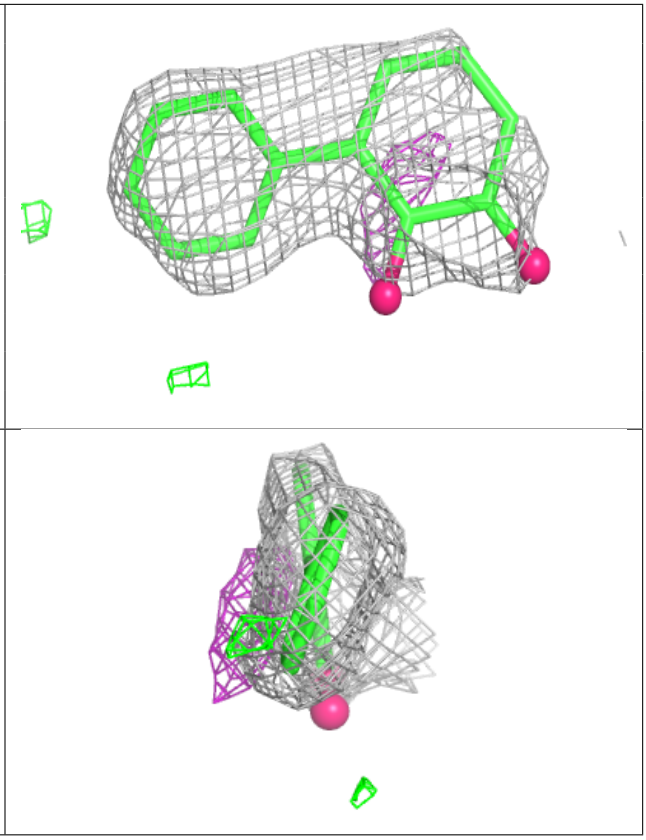






Electron density around BPY B 503:

$2mF_o$-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.