wwPDB X-ray Structure Validation Summary Report (i)

Jun 13, 2024 – 09:26 AM EDT

PDB ID	:	4I3B
Title	:	Crystal structure of fluorescent protein UnaG wild type
Authors	:	Kumagai, A.; Ando, R.; Miyatake, H.; Miyawaki, A.
Deposited on	:	2012-11-26
Resolution	:	1.20 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:

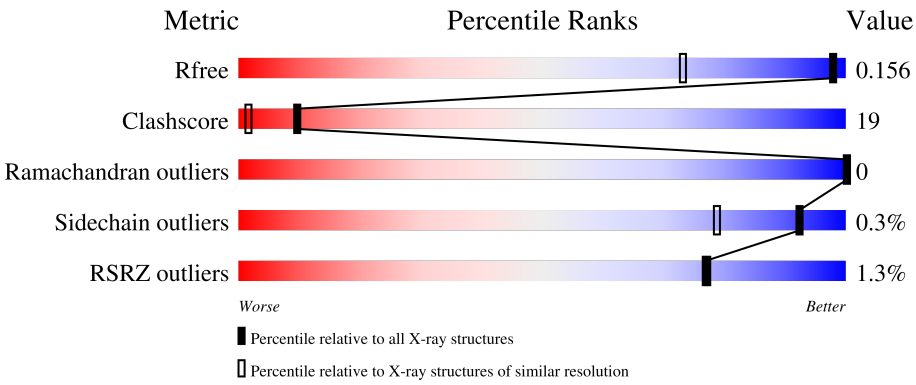
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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	139	4% 76% 24%
1	B	139	% 88% 11% ••
1	C	139	2% 85% 14% •
1	D	139	% 82% 17% ••
1	E	139	84% 15% •

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Mol	Chain	Length	Quality of chain
1	F	139	% 81% 17%

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	PEG	A	202	-	-	X	-
3	PEG	B	202	-	-	X	-
3	PEG	B	204	-	-	X	-
3	PEG	D	202	-	-	X	-
3	PEG	E	202	-	-	X	-
3	PEG	F	203	-	-	X	-

2 Entry composition (i)

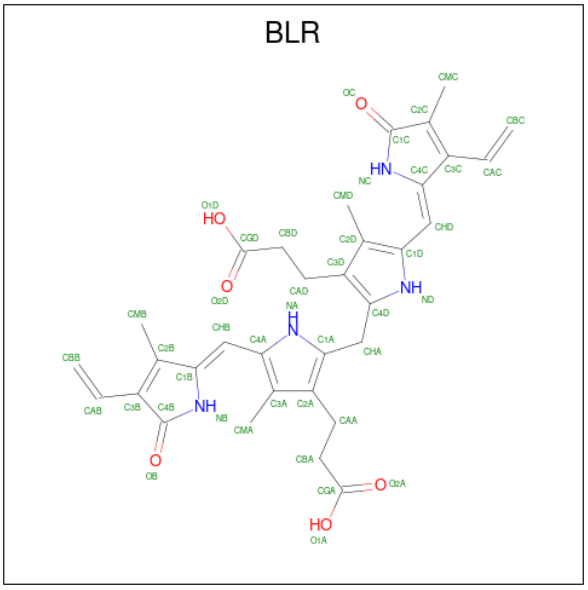
There are 4 unique types of molecules in this entry. The entry contains 17639 atoms, of which 8031 are hydrogens and 0 are deuteriums.

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 Bilirubin-inducible fluorescent protein UnaG.

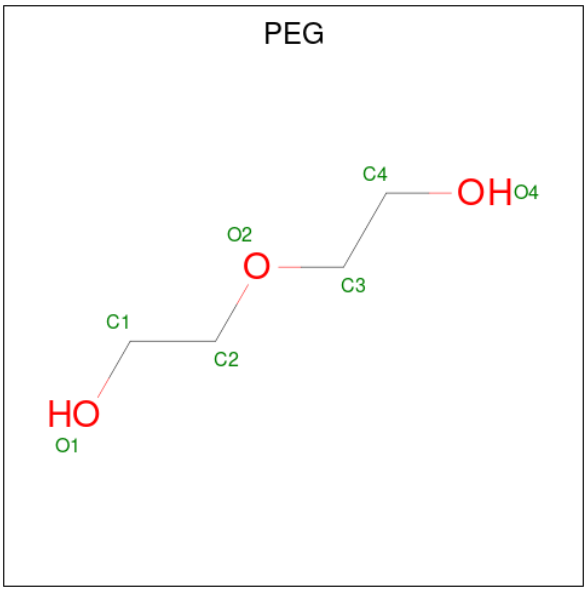
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	139	2668	828	1377	210	249	4	0	43	0
1	B	138	2526	789	1302	199	232	4	0	29	0
1	C	138	2453	767	1243	203	237	3	0	27	0
1	D	138	2472	771	1272	198	227	4	0	23	0
1	E	139	2490	775	1278	204	229	4	0	24	0
1	F	137	2504	782	1277	204	238	3	0	34	0

- Molecule 2 is 3-[5-[(Z)-(4-ethenyl-3-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-2-[[5-[(Z)-(3-ethenyl-4-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-3-(3-hydroxy-3-oxopropyl)-4-methyl-1H-pyrrol-2-yl]methyl]-4-methyl-1H-pyrrol-3-yl]propanoic acid (three-letter code: BLR) (formula: $C_{33}H_{36}N_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			75	33	32	4	6		
2	B	1	Total	C	H	N	O	0	0
			75	33	32	4	6		
2	C	1	Total	C	H	N	O	0	0
			75	33	32	4	6		
2	D	1	Total	C	H	N	O	0	0
			75	33	32	4	6		
2	E	1	Total	C	H	N	O	0	0
			75	33	32	4	6		
2	F	1	Total	C	H	N	O	0	0
			75	33	32	4	6		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	D	1	Total	C	H	O	0	0
			17	4	10	3		
3	E	1	Total	C	H	O	0	0
			17	4	10	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	F	1	17	4	10	3	0	0
			Total	C	H	O		
3	F	1	17	4	10	3	0	0
			Total	C	H	O		
3	F	1	17	4	10	3	0	0

- Molecule 4 is water.

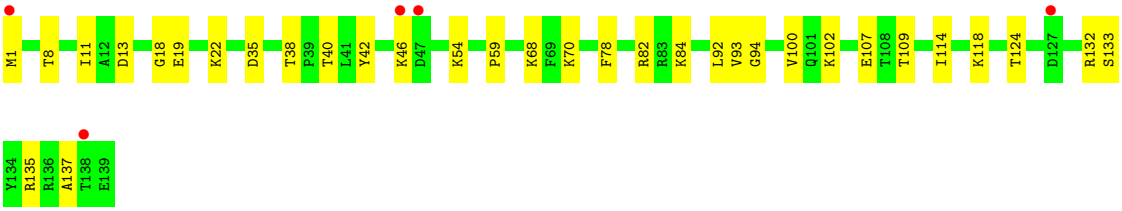
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	288	288	288	0	0
			Total	O		
4	B	347	347	347	0	0
			Total	O		
4	C	348	348	348	0	0
			Total	O		
4	D	311	311	311	0	0
			Total	O		
4	E	325	325	325	0	0
			Total	O		
4	F	304	304	304	0	0

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.

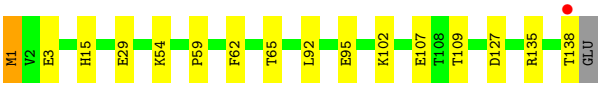
• Molecule 1: Bilirubin-inducible fluorescent protein UnaG

Chain A:



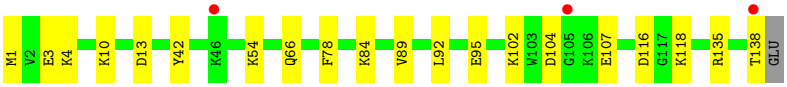
• Molecule 1: Bilirubin-inducible fluorescent protein UnaG

Chain B:



• Molecule 1: Bilirubin-inducible fluorescent protein UnaG

Chain C:

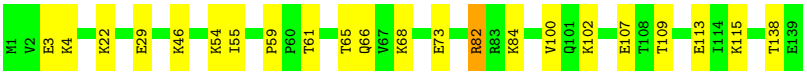


• Molecule 1: Bilirubin-inducible fluorescent protein UnaG

Chain D:

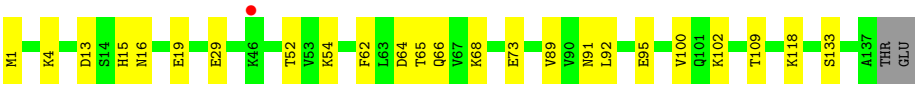
• Molecule 1: Bilirubin-inducible fluorescent protein UnaG

Chain E:



• Molecule 1: Bilirubin-inducible fluorescent protein UnaG

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	44.39Å 73.95Å 124.36Å 90.00° 92.45° 90.00°	Depositor
Resolution (Å)	31.92 – 1.20 31.92 – 1.20	Depositor EDS
% Data completeness (in resolution range)	92.3 (31.92-1.20) 92.3 (31.92-1.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 1.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.129 , 0.159 0.128 , 0.156	Depositor DCC
R_{free} test set	11461 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	11.5	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 76.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	17639	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.0308e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: PEG, BLR

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	0.55	0/1464	0.73	1/1966 (0.1%)
1	B	0.54	0/1346	0.72	0/1806
1	C	0.56	0/1340	0.73	0/1799
1	D	0.55	0/1306	0.74	0/1752
1	E	0.58	0/1331	0.88	4/1785 (0.2%)
1	F	0.49	0/1410	0.69	0/1897
All	All	0.54	0/8197	0.75	5/11005 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	82[A]	ARG	NE-CZ-NH2	-11.49	114.55	120.30
1	E	82[B]	ARG	NE-CZ-NH2	-11.49	114.55	120.30
1	E	82[A]	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	E	82[B]	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	132	ARG	NE-CZ-NH1	5.55	123.08	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	1291	1377	1241	63	0
1	B	1224	1302	1225	35	0
1	C	1210	1243	1137	25	0
1	D	1200	1272	1225	59	0
1	E	1212	1278	1196	38	0
1	F	1227	1277	1126	53	0
2	A	43	32	34	2	0
2	B	43	32	34	2	0
2	C	43	32	34	2	0
2	D	43	32	34	3	0
2	E	43	32	34	4	0
2	F	43	32	34	2	0
3	A	7	10	10	4	0
3	B	21	30	30	19	0
3	D	7	10	10	5	0
3	E	7	10	10	10	0
3	F	21	30	30	16	0
4	A	288	0	0	52	0
4	B	347	0	0	22	0
4	C	348	0	0	21	0
4	D	311	0	0	38	0
4	E	325	0	0	30	0
4	F	304	0	0	43	0
All	All	9608	8031	7444	303	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 19.

The worst 5 of 303 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:66[B]:GLN:NE2	4:C:635:HOH:O	1.62	1.30
1:F:66[B]:GLN:NE2	4:F:601:HOH:O	1.63	1.25
1:B:15[B]:HIS:CD2	4:B:602:HOH:O	1.83	1.22
1:D:46[B]:LYS:HB3	4:D:609:HOH:O	1.40	1.19
1:C:89:VAL:HB	4:C:555:HOH:O	1.02	1.18

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	179/139 (129%)	177 (99%)	2 (1%)	0	100	100
1	B	164/139 (118%)	164 (100%)	0	0	100	100
1	C	163/139 (117%)	163 (100%)	0	0	100	100
1	D	158/139 (114%)	156 (99%)	2 (1%)	0	100	100
1	E	160/139 (115%)	158 (99%)	2 (1%)	0	100	100
1	F	169/139 (122%)	168 (99%)	1 (1%)	0	100	100
All	All	993/834 (119%)	986 (99%)	7 (1%)	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	160/120 (133%)	160 (100%)	0	100	100
1	B	146/120 (122%)	144 (99%)	2 (1%)	67	32
1	C	144/120 (120%)	144 (100%)	0	100	100
1	D	141/120 (118%)	140 (99%)	1 (1%)	84	59
1	E	143/120 (119%)	143 (100%)	0	100	100
1	F	151/120 (126%)	151 (100%)	0	100	100
All	All	885/720 (123%)	882 (100%)	3 (0%)	92	79

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1[A]	MET
1	B	1[B]	MET
1	D	70	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	15	HIS

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)

15 ligands are modelled in this entry.

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	BLR	D	201	-	40,46,46	2.89	13 (32%)	47,67,67	1.72	12 (25%)
2	BLR	E	201	-	40,46,46	2.58	12 (30%)	47,67,67	1.66	8 (17%)
2	BLR	F	201	-	40,46,46	2.91	12 (30%)	47,67,67	1.85	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BLR	C	200	-	40,46,46	2.76	13 (32%)	47,67,67	1.66	8 (17%)
3	PEG	B	203	-	6,6,6	0.71	0	5,5,5	0.50	0
3	PEG	E	202	-	6,6,6	0.72	0	5,5,5	0.74	0
3	PEG	F	203	-	6,6,6	0.65	0	5,5,5	1.32	1 (20%)
3	PEG	F	204	-	6,6,6	0.69	0	5,5,5	0.63	0
2	BLR	B	201	-	40,46,46	2.82	11 (27%)	47,67,67	1.59	7 (14%)
2	BLR	A	201	-	40,46,46	3.14	12 (30%)	47,67,67	1.59	11 (23%)
3	PEG	A	202	-	6,6,6	0.70	0	5,5,5	0.85	0
3	PEG	F	202	-	6,6,6	0.58	0	5,5,5	1.72	1 (20%)
3	PEG	B	202	-	6,6,6	0.53	0	5,5,5	1.39	1 (20%)
3	PEG	B	204	-	6,6,6	0.68	0	5,5,5	0.99	0
3	PEG	D	202	-	6,6,6	0.66	0	5,5,5	0.92	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
2	BLR	D	201	-	-	2/24/58/58	0/4/4/4
2	BLR	E	201	-	-	4/24/58/58	0/4/4/4
2	BLR	F	201	-	-	2/24/58/58	0/4/4/4
2	BLR	C	200	-	-	3/24/58/58	0/4/4/4
3	PEG	B	203	-	-	3/4/4/4	-
3	PEG	E	202	-	-	2/4/4/4	-
3	PEG	F	203	-	-	0/4/4/4	-
3	PEG	F	204	-	-	1/4/4/4	-
2	BLR	B	201	-	-	3/24/58/58	0/4/4/4
2	BLR	A	201	-	-	3/24/58/58	0/4/4/4
3	PEG	A	202	-	-	2/4/4/4	-
3	PEG	F	202	-	-	2/4/4/4	-
3	PEG	B	202	-	-	2/4/4/4	-
3	PEG	B	204	-	-	2/4/4/4	-
3	PEG	D	202	-	-	2/4/4/4	-

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	BLR	CHA-C4D	-13.35	1.41	1.51
2	F	201	BLR	CHA-C4D	-11.98	1.42	1.51
2	B	201	BLR	CHA-C4D	-11.37	1.43	1.51
2	D	201	BLR	CHA-C4D	-11.36	1.43	1.51
2	C	200	BLR	CHA-C4D	-10.89	1.43	1.51

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	201	BLR	C3B-C4B-NB	-6.79	97.60	106.13
2	E	201	BLR	C3B-C4B-NB	-5.90	98.72	106.13
2	C	200	BLR	C3B-C4B-NB	-5.48	99.25	106.13
2	A	201	BLR	C3B-C4B-NB	-5.00	99.85	106.13
2	B	201	BLR	C3B-C4B-NB	-4.82	100.08	106.13

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	202	PEG	C4-C3-O2-C2
3	B	202	PEG	C1-C2-O2-C3
3	B	204	PEG	O1-C1-C2-O2
3	F	204	PEG	O2-C3-C4-O4
3	B	203	PEG	O1-C1-C2-O2

There are no ring outliers.

14 monomers are involved in 69 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	201	BLR	3	0
2	E	201	BLR	4	0
2	F	201	BLR	2	0
2	C	200	BLR	2	0
3	B	203	PEG	3	0
3	E	202	PEG	10	0
3	F	203	PEG	13	0
2	B	201	BLR	2	0
2	A	201	BLR	2	0
3	A	202	PEG	4	0
3	F	202	PEG	3	0
3	B	202	PEG	6	0
3	B	204	PEG	10	0

Continued on next page...

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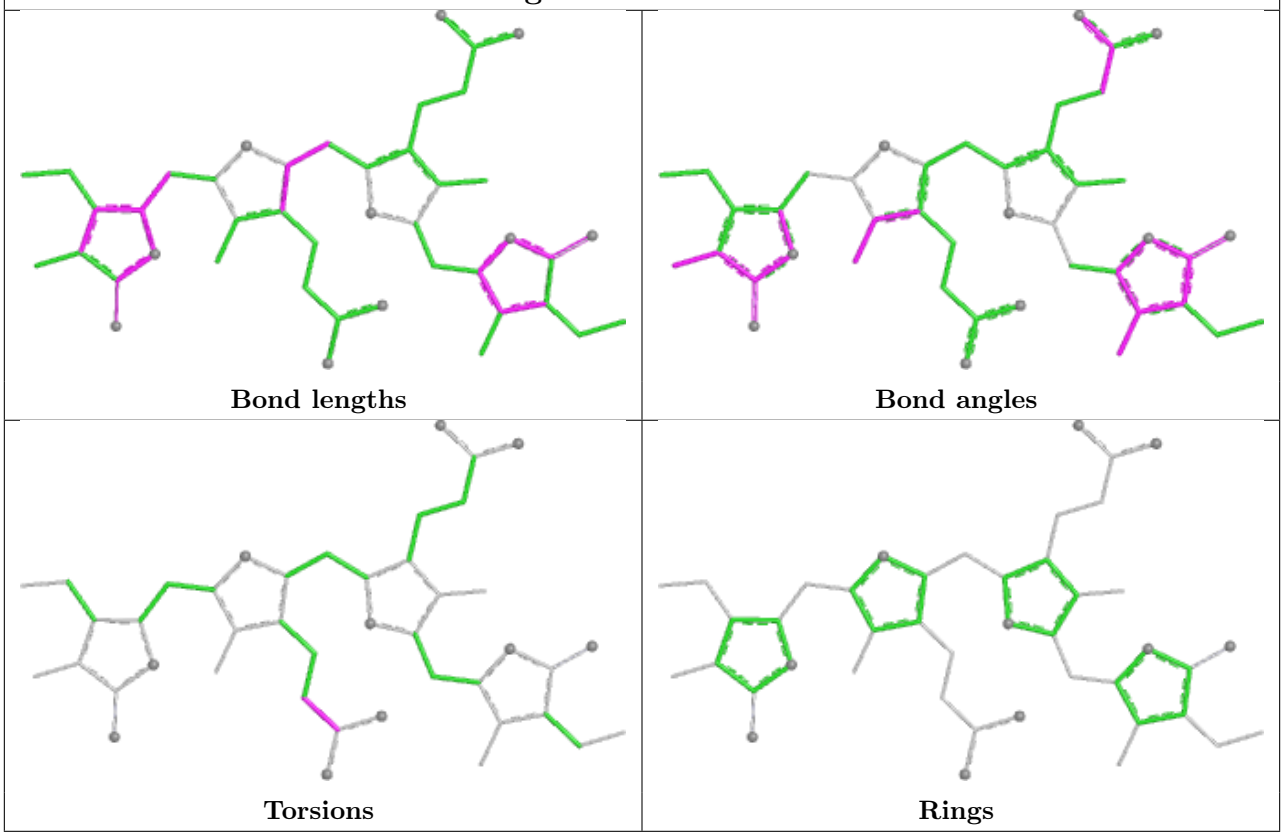
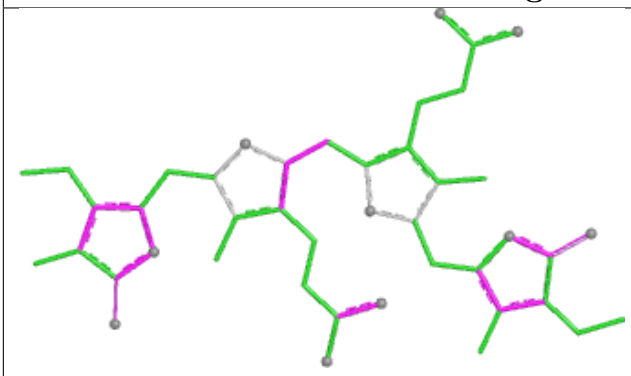
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	202	PEG	5	0

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.

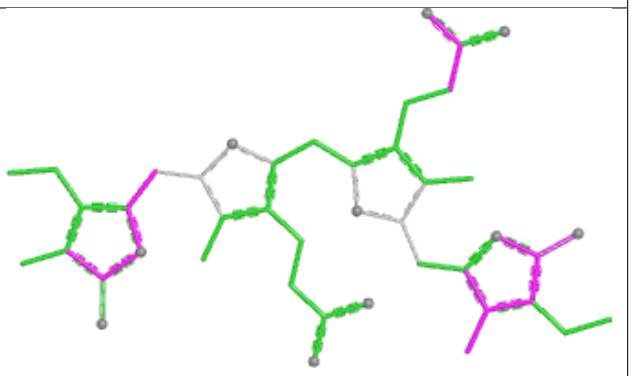
Ligand BLR D 201



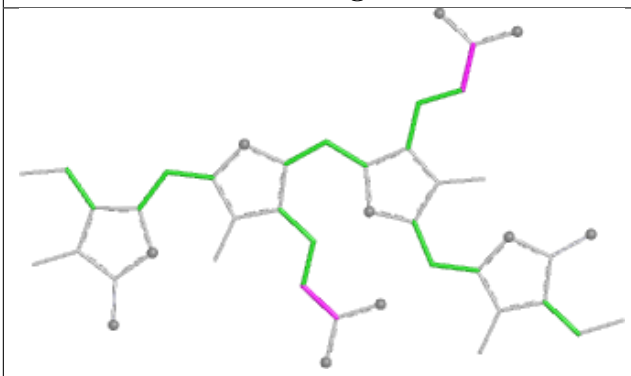
Ligand BLR E 201



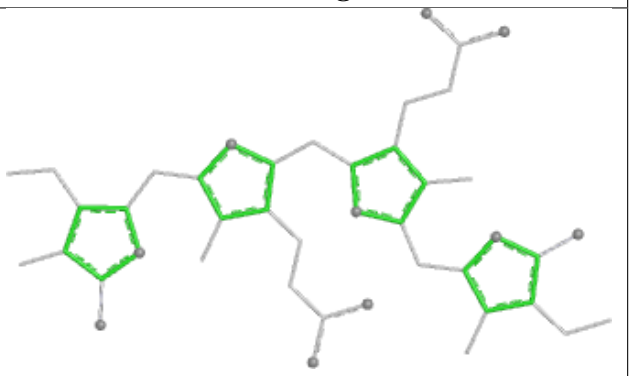
Bond lengths



Bond angles

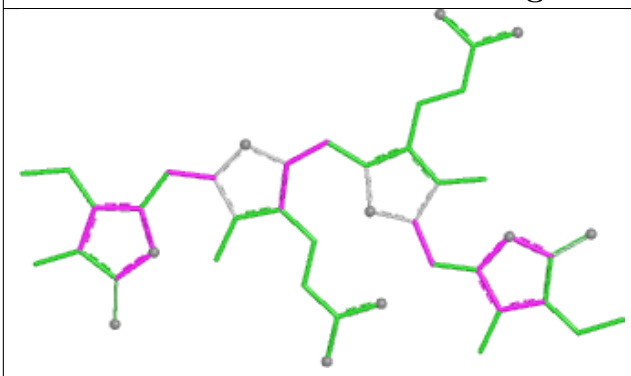


Torsions

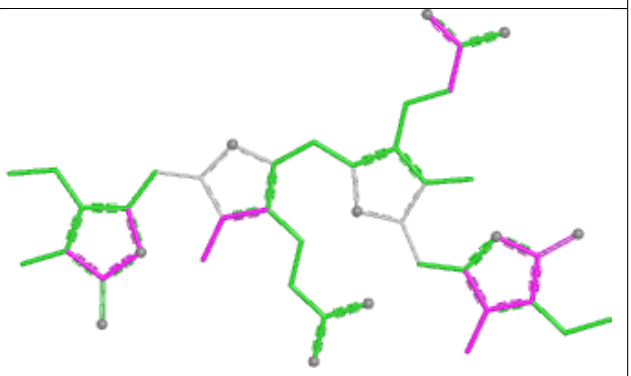


Rings

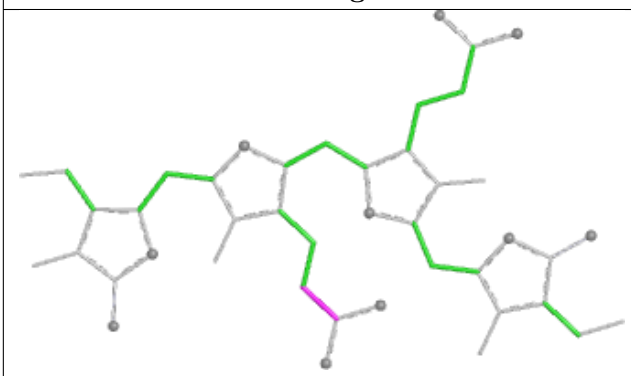
Ligand BLR F 201



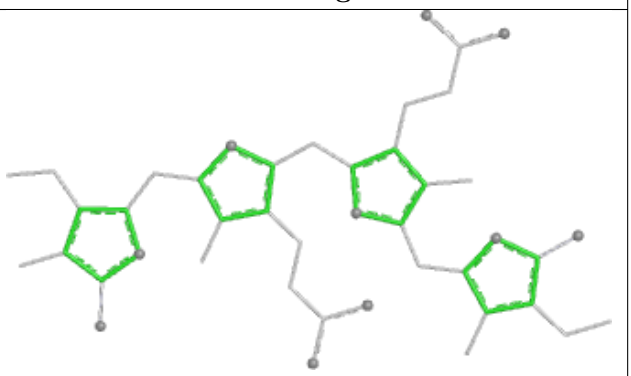
Bond lengths



Bond angles

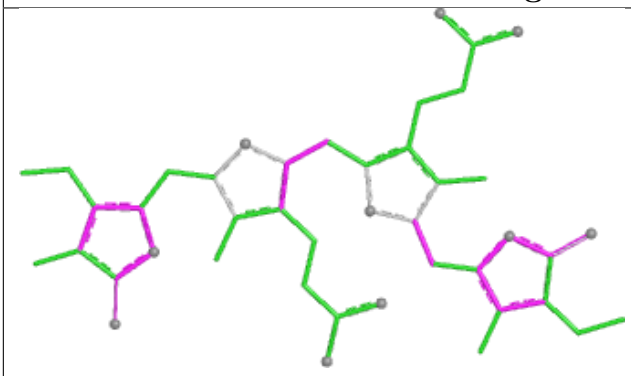


Torsions

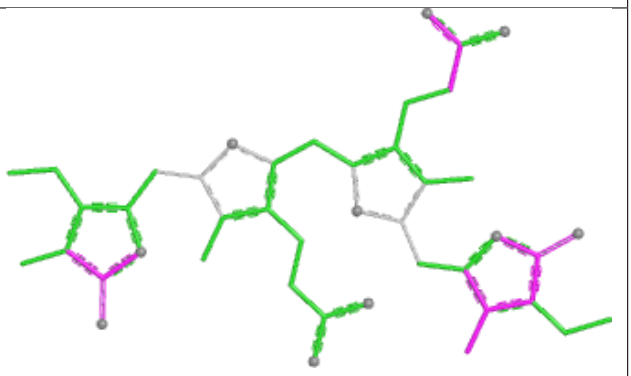


Rings

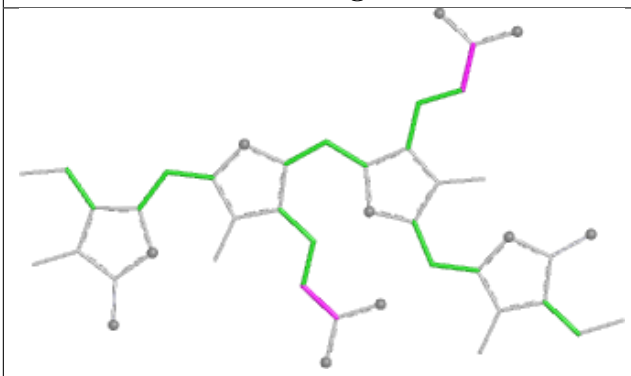
Ligand BLR C 200



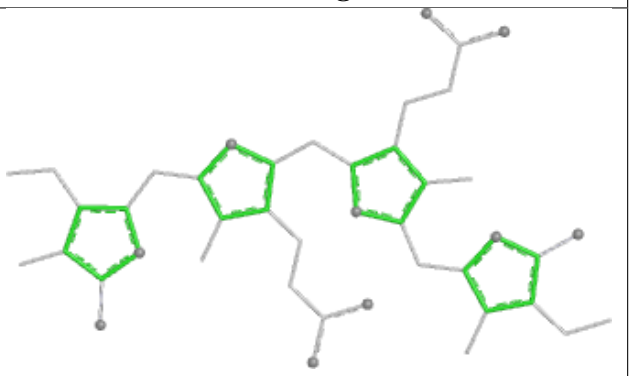
Bond lengths



Bond angles

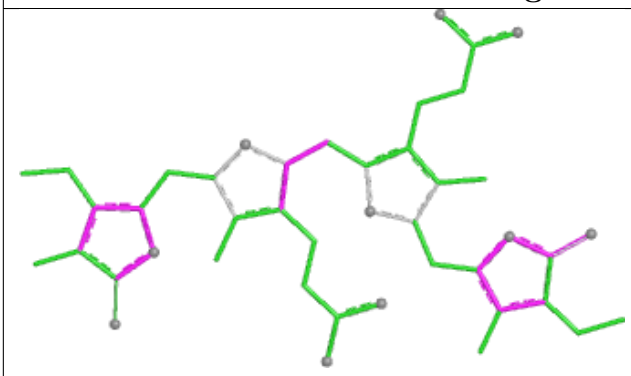


Torsions

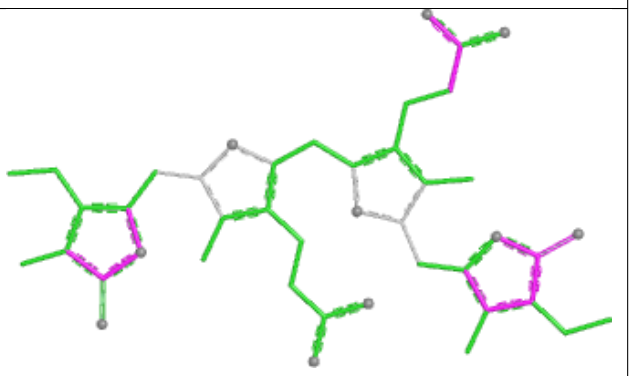


Rings

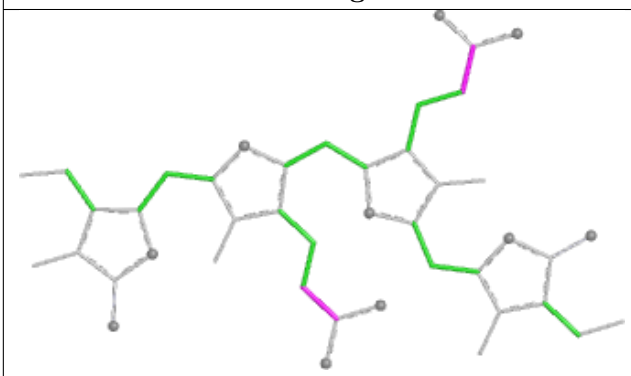
Ligand BLR B 201



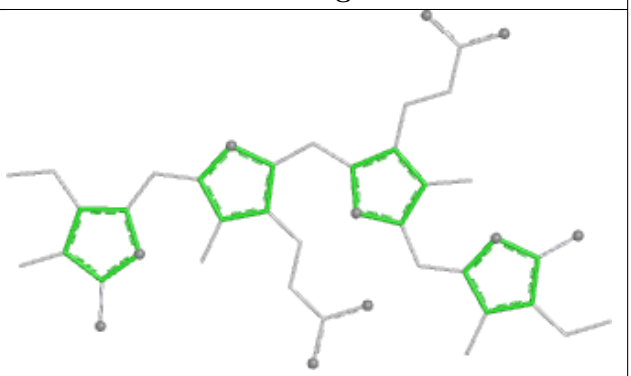
Bond lengths



Bond angles

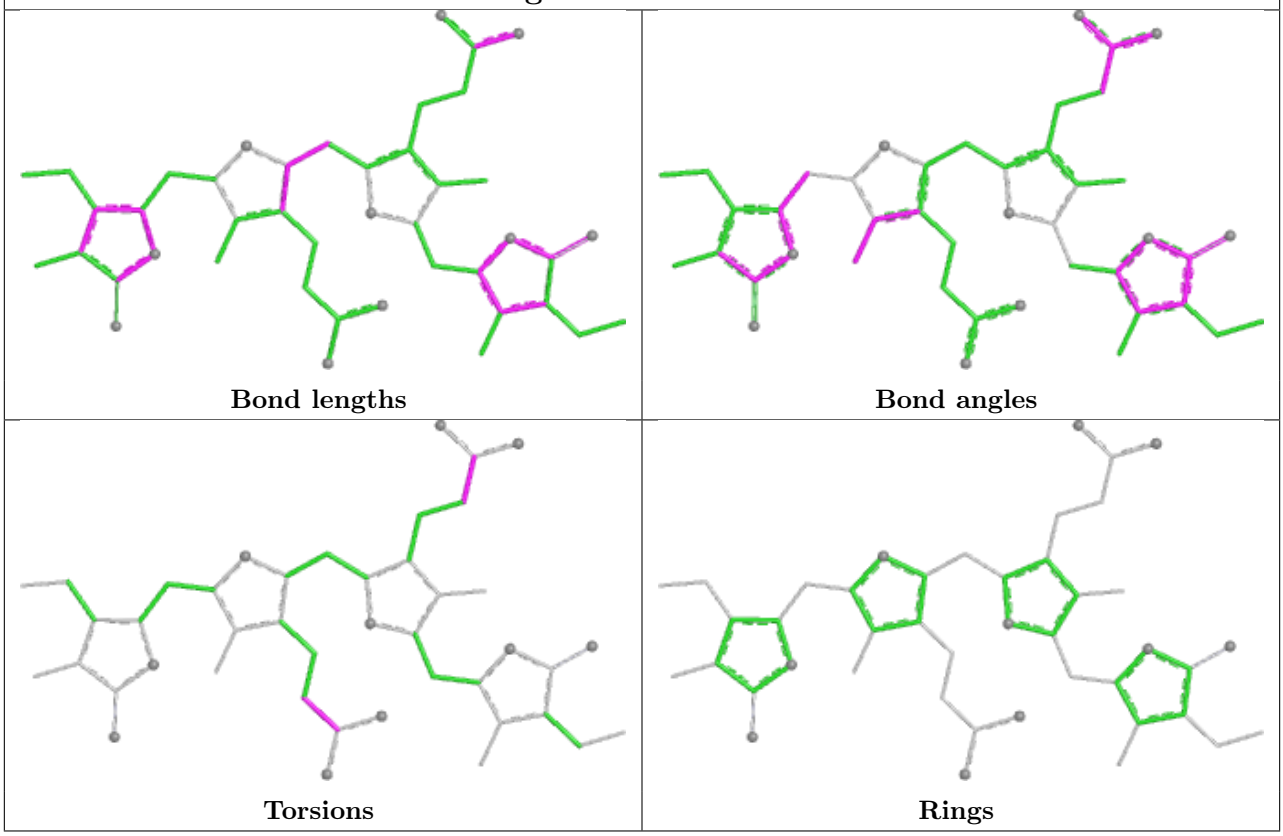


Torsions



Rings

Ligand BLR A 201



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	139/139 (100%)	-0.21	5 (3%)	42	41	8, 13, 25, 35	0
1	B	138/139 (99%)	-0.53	1 (0%)	87	87	7, 11, 19, 22	1 (0%)
1	C	138/139 (99%)	-0.38	3 (2%)	62	61	7, 12, 23, 29	0
1	D	138/139 (99%)	-0.37	1 (0%)	87	87	8, 13, 22, 31	0
1	E	139/139 (100%)	-0.52	0	100	100	6, 10, 18, 24	1 (0%)
1	F	137/139 (98%)	-0.37	1 (0%)	87	87	8, 13, 23, 29	0
All	All	829/834 (99%)	-0.40	11 (1%)	77	77	6, 12, 22, 35	2 (0%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	138	THR	4.5
1	D	138	THR	4.1
1	B	138	THR	3.3
1	A	127[A]	ASP	2.8
1	A	138[A]	THR	2.6

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)

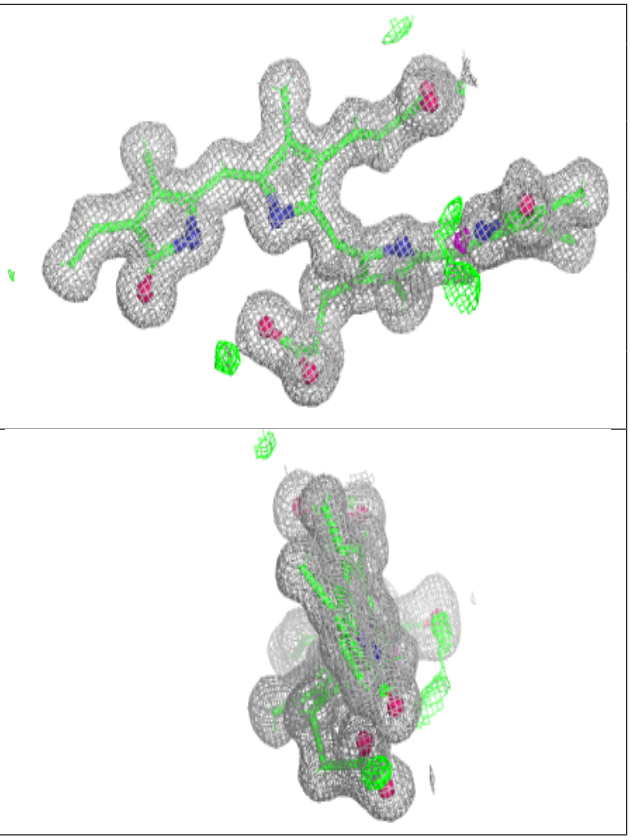
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEG	B	203	7/7	0.71	0.28	18,22,29,29	17
3	PEG	F	204	7/7	0.76	0.35	20,24,29,29	17
3	PEG	B	202	7/7	0.77	0.37	17,21,25,27	17
3	PEG	B	204	7/7	0.78	0.22	18,22,25,29	17
3	PEG	F	202	7/7	0.81	0.28	14,19,23,25	17
3	PEG	F	203	7/7	0.81	0.39	13,21,25,25	17
3	PEG	E	202	7/7	0.81	0.34	15,21,29,33	17
3	PEG	A	202	7/7	0.83	0.23	17,23,29,30	17
3	PEG	D	202	7/7	0.90	0.22	17,20,24,29	17
2	BLR	A	201	43/43	0.98	0.06	7,10,14,15	0
2	BLR	F	201	43/43	0.99	0.06	6,9,12,12	0
2	BLR	B	201	43/43	0.99	0.06	5,7,10,11	0
2	BLR	C	200	43/43	0.99	0.06	5,8,11,11	0
2	BLR	D	201	43/43	0.99	0.06	7,9,12,12	0
2	BLR	E	201	43/43	0.99	0.06	4,7,9,10	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.

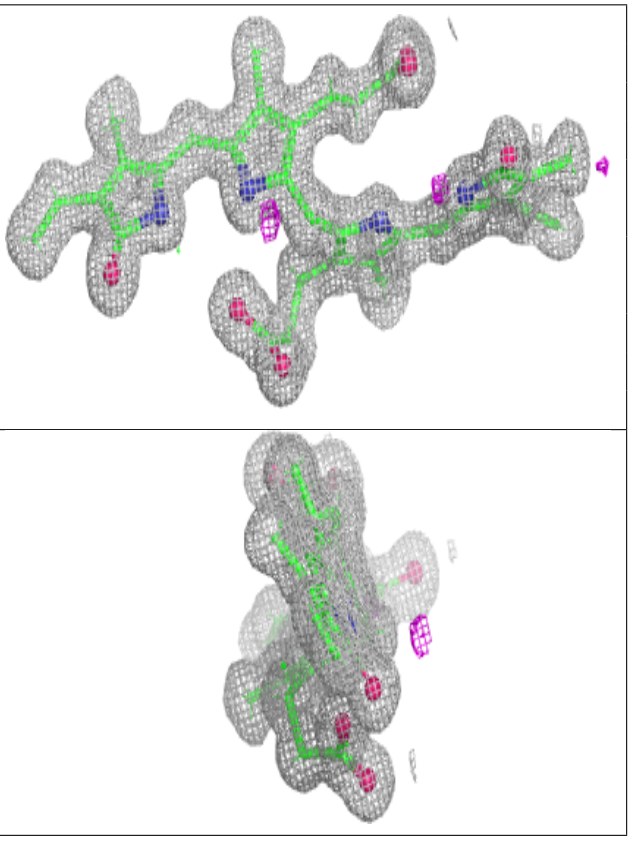
Electron density around BLR A 201:

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



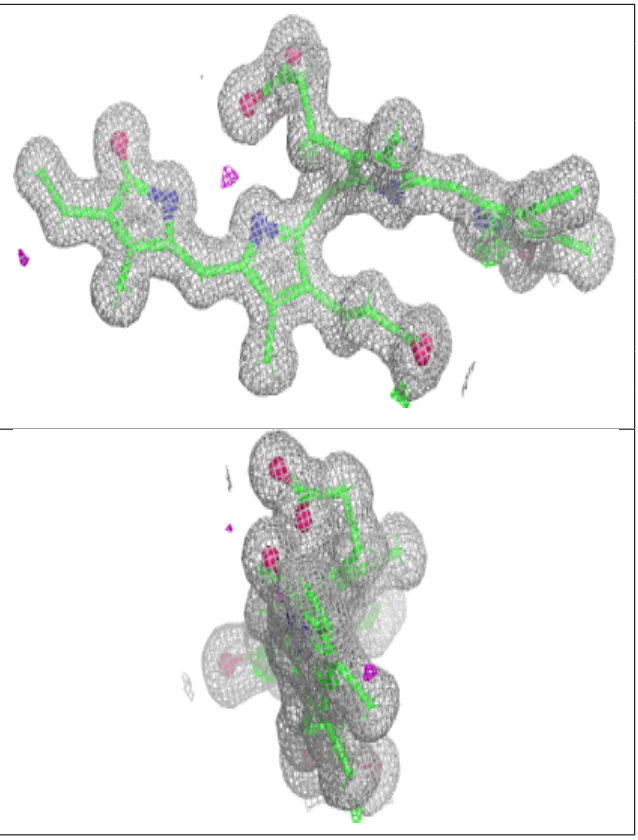
Electron density around BLR F 201:

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



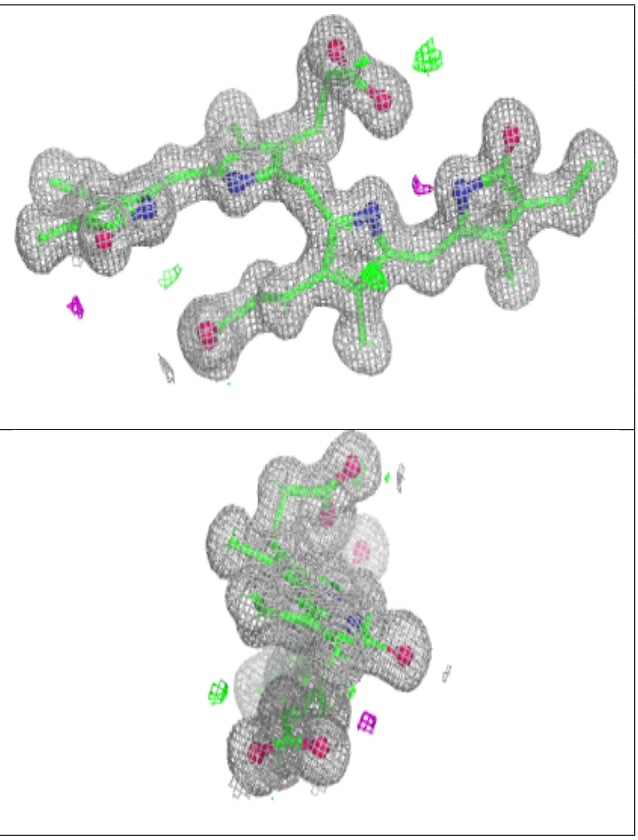
Electron density around BLR B 201:

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



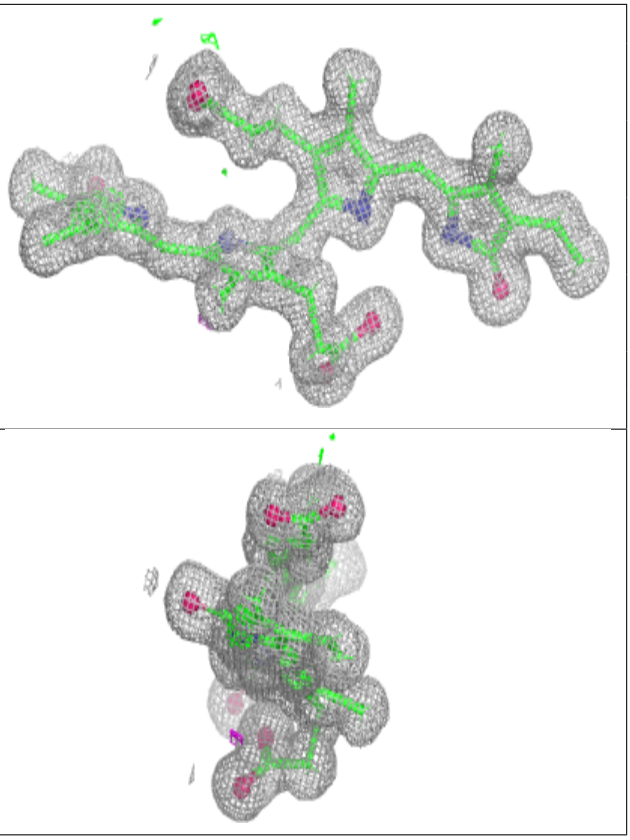
Electron density around BLR C 200:

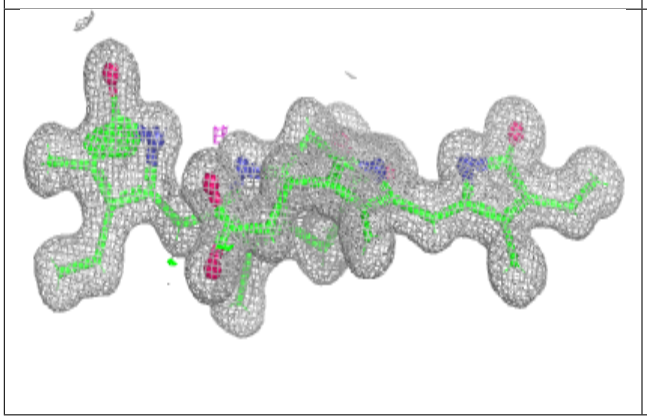
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BLR D 201:

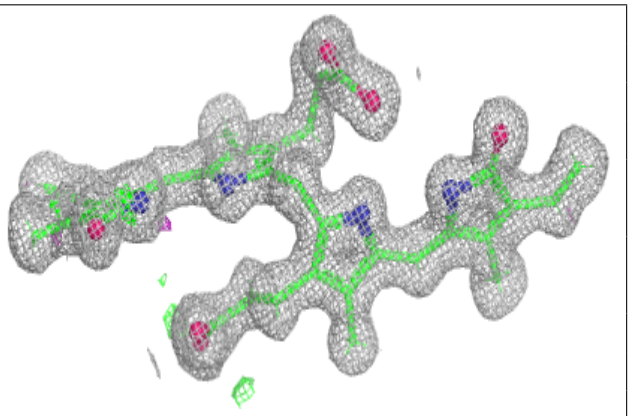
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

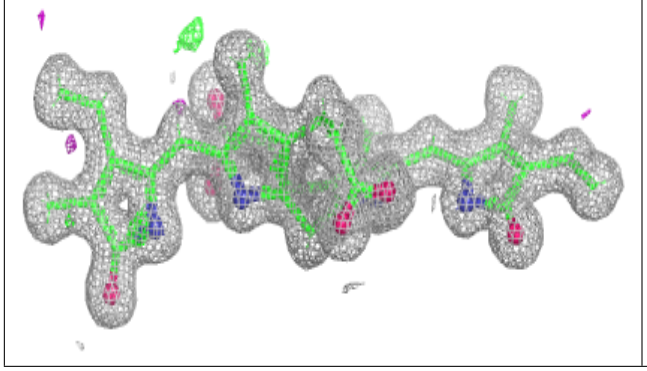


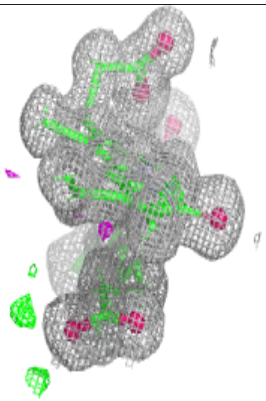


Electron density around BLR E 201:

$2mF_o$-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.