



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 10:33 PM BST

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1  
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) : 2.13.1

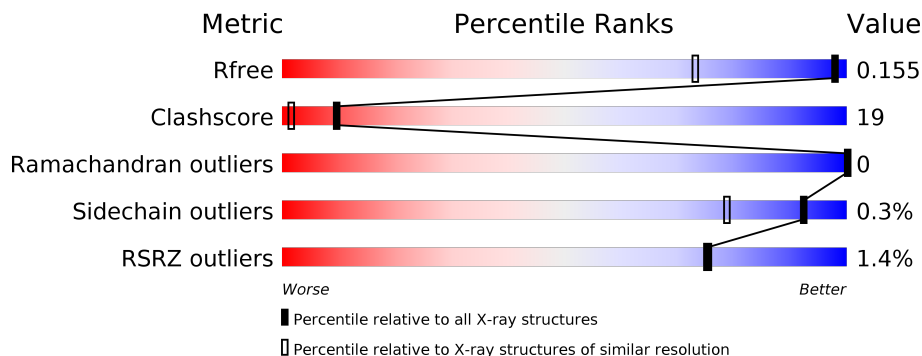
# 1 Overall quality at a glance i

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div>
1	B	139	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>
1	C	139	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>
1	D	139	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>
1	E	139	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>
1	F	139	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
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

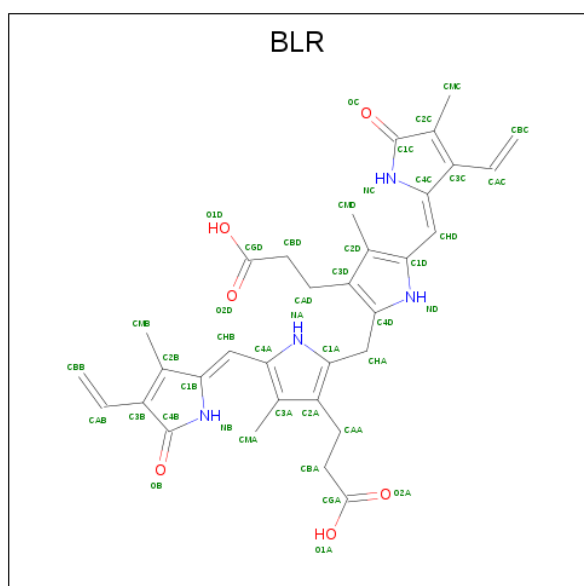
There are 4 unique types of molecules in this entry. The entry contains 17639 atoms, of which 8031 are hydrogens and 0 are deuteriums.

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.

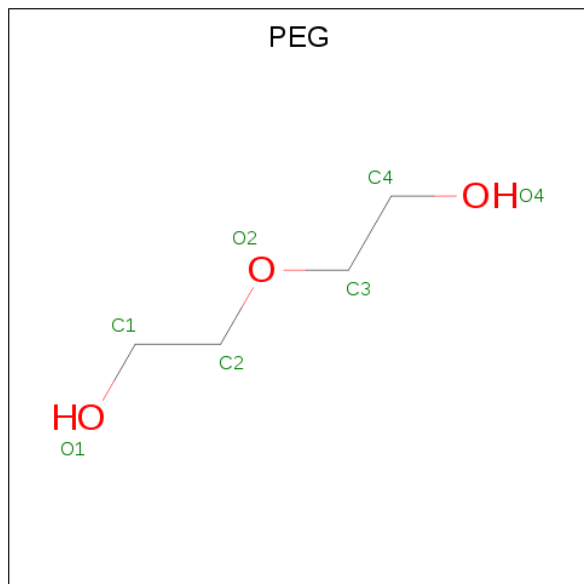
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	139	Total 2668	C 828	H 1377	N 210	O 249	S 4	0	43	0
1	B	138	Total 2526	C 789	H 1302	N 199	O 232	S 4	0	29	0
1	C	138	Total 2453	C 767	H 1243	N 203	O 237	S 3	0	27	0
1	D	138	Total 2472	C 771	H 1272	N 198	O 227	S 4	0	23	0
1	E	139	Total 2490	C 775	H 1278	N 204	O 229	S 4	0	24	0
1	F	137	Total 2504	C 782	H 1277	N 204	O 238	S 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<sub>33</sub>H<sub>36</sub>N<sub>4</sub>O<sub>6</sub>).



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<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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
3	F	1	Total	C	H	O	0	0
			17	4	10	3		
3	F	1	Total	C	H	O	0	0
			17	4	10	3		
3	F	1	Total	C	H	O	0	0
			17	4	10	3		

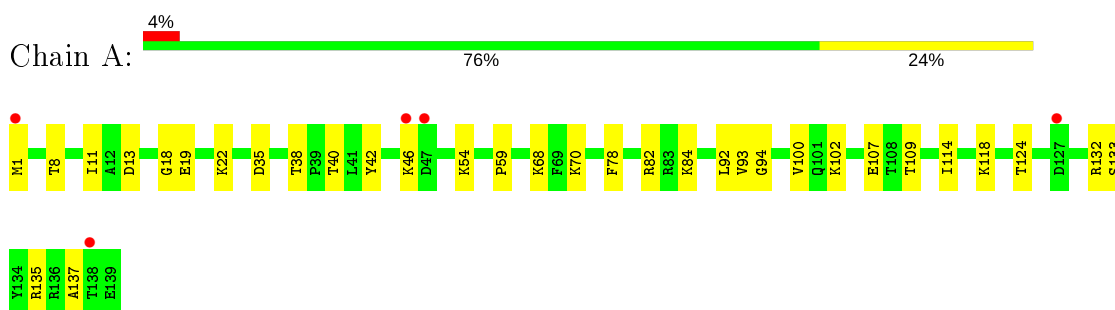
- Molecule 4 is water.

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

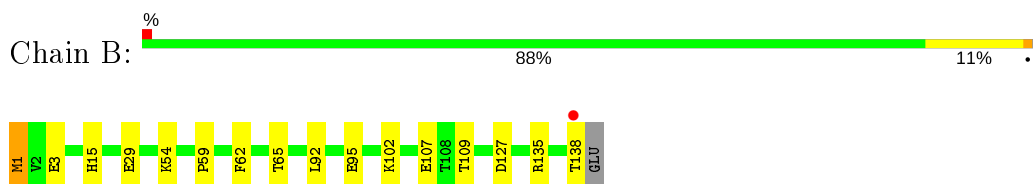
### 3 Residue-property plots [i](#)

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.

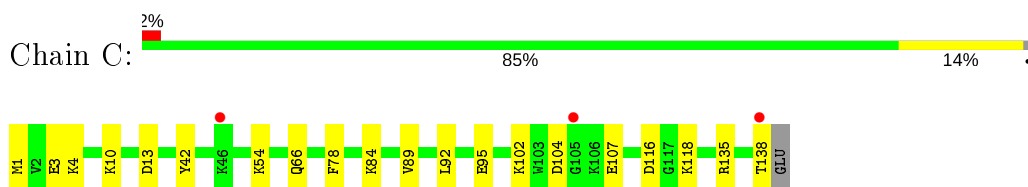
- Molecule 1: Bilirubin-inducible fluorescent protein UnaG



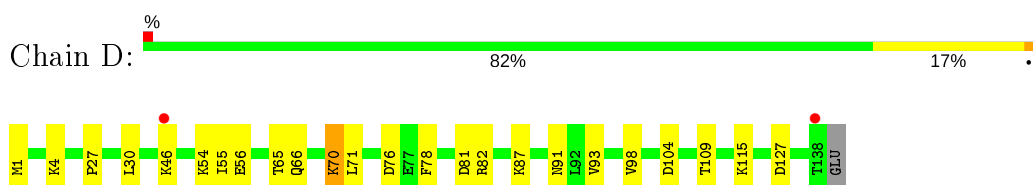
- Molecule 1: Bilirubin-inducible fluorescent protein UnaG



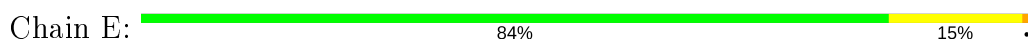
- Molecule 1: Bilirubin-inducible fluorescent protein UnaG



- Molecule 1: Bilirubin-inducible fluorescent protein UnaG

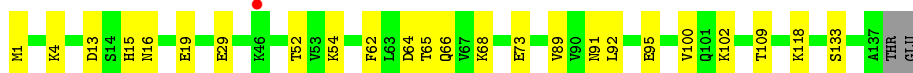
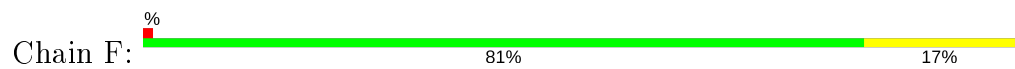


- Molecule 1: Bilirubin-inducible fluorescent protein UnaG





- Molecule 1: Bilirubin-inducible fluorescent protein UnaG





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 1.20Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.129 , 0.159 0.128 , 0.155	Depositor DCC
$R_{free}$ test set	11461 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.5	Xtrriage
Anisotropy	0.284	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 76.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	17639	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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(°)	Ideal(°)
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.

All (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
1:C:104[B]:ASP:OD1	4:C:638:HOH:O	1.62	1.15
1:A:137:ALA:N	4:A:550:HOH:O	1.83	1.09
1:D:82[A]:ARG:NE	4:D:545:HOH:O	1.85	1.08
1:F:13[A]:ASP:OD2	4:F:532:HOH:O	1.73	1.07
1:C:13[A]:ASP:OD2	4:C:634:HOH:O	1.71	1.06
1:D:46[A]:LYS:HB3	4:D:609:HOH:O	1.56	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54[A]:LYS:NZ	4:C:503:HOH:O	1.88	1.05
3:F:203:PEG:O4	4:F:583:HOH:O	1.74	1.05
1:D:82[A]:ARG:NH2	4:D:523:HOH:O	1.91	1.03
1:A:46:LYS:HB3	4:A:556:HOH:O	1.59	1.02
1:C:89:VAL:CB	4:C:555:HOH:O	1.69	1.02
1:D:66:GLN:NE2	4:D:581:HOH:O	1.70	1.01
1:B:3[B]:GLU:OE2	4:B:600:HOH:O	1.79	1.00
1:A:107[A]:GLU:CD	4:A:569:HOH:O	1.99	0.99
1:F:19[B]:GLU:OE2	4:F:581:HOH:O	1.81	0.98
1:E:3[A]:GLU:OE1	4:E:573:HOH:O	1.80	0.97
1:C:116[A]:ASP:OD2	4:C:439:HOH:O	1.81	0.97
4:B:591:HOH:O	1:D:54[A]:LYS:CE	2.12	0.95
1:A:82[B]:ARG:NE	4:A:560:HOH:O	1.98	0.95
1:A:1[A]:MET:HG3	4:A:523:HOH:O	1.66	0.94
1:C:89:VAL:CG1	4:C:555:HOH:O	2.02	0.94
1:E:115[B]:LYS:CE	4:E:598:HOH:O	2.15	0.92
1:F:54[B]:LYS:NZ	4:F:525:HOH:O	2.01	0.92
1:C:13[B]:ASP:OD2	4:C:578:HOH:O	1.86	0.91
1:F:13[B]:ASP:OD1	4:F:502:HOH:O	1.89	0.90
1:E:66[B]:GLN:OE1	4:E:596:HOH:O	1.88	0.90
1:D:82[A]:ARG:CZ	4:D:545:HOH:O	2.13	0.90
1:A:93:VAL:N	4:A:503:HOH:O	2.04	0.89
1:A:46:LYS:CB	4:A:556:HOH:O	2.17	0.88
4:B:591:HOH:O	1:D:54[A]:LYS:HD3	1.73	0.87
1:D:46[B]:LYS:NZ	4:D:591:HOH:O	2.07	0.87
4:B:591:HOH:O	1:D:54[A]:LYS:CD	2.24	0.84
1:E:107:GLU:OE2	4:E:549:HOH:O	1.92	0.84
1:B:109[B]:THR:HG23	4:B:580:HOH:O	1.77	0.84
1:F:1:MET:HE1	4:F:600:HOH:O	1.76	0.84
1:C:10:LYS:NZ	4:C:511:HOH:O	1.98	0.83
1:D:54[C]:LYS:CG	4:D:581:HOH:O	2.26	0.83
1:D:46[A]:LYS:CD	4:D:588:HOH:O	2.25	0.83
1:E:115[B]:LYS:HE3	4:E:598:HOH:O	1.74	0.83
1:B:127[A]:ASP:HB3	3:B:204:PEG:H21	1.61	0.82
1:A:107[A]:GLU:OE2	4:A:569:HOH:O	1.94	0.82
1:F:91:ASN:OD1	4:F:544:HOH:O	1.98	0.81
1:D:82[A]:ARG:NH2	4:D:545:HOH:O	2.09	0.81
1:A:84[A]:LYS:NZ	4:A:494:HOH:O	2.12	0.81
1:E:109[B]:THR:HG23	4:E:439:HOH:O	1.81	0.80
1:C:138:THR:HG22	4:F:566:HOH:O	1.81	0.79
1:A:13:ASP:OD1	4:A:351:HOH:O	2.01	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LYS:CG	4:A:553:HOH:O	2.31	0.79
1:C:95[A]:GLU:OE2	4:C:630:HOH:O	2.00	0.78
3:E:202:PEG:O4	4:E:596:HOH:O	2.01	0.78
1:D:87:LYS:NZ	4:D:600:HOH:O	2.09	0.78
1:D:82[B]:ARG:NH1	4:D:473:HOH:O	2.17	0.78
1:C:116[A]:ASP:OD1	4:C:417:HOH:O	2.01	0.77
1:B:127[A]:ASP:CB	3:B:204:PEG:H21	2.13	0.77
1:F:64:ASP:O	3:F:203:PEG:H11	1.85	0.77
1:D:54[C]:LYS:HG2	4:D:581:HOH:O	1.83	0.75
1:A:19:GLU:HG3	4:A:557:HOH:O	1.86	0.75
1:A:124[B]:THR:HG21	4:A:568:HOH:O	1.84	0.75
1:A:22[A]:LYS:HG2	4:A:360:HOH:O	1.87	0.75
1:A:92:LEU:HB3	4:A:503:HOH:O	1.87	0.75
1:B:109[A]:THR:HG21	4:B:530:HOH:O	1.86	0.74
1:F:95[A]:GLU:OE2	4:F:423:HOH:O	2.05	0.74
1:F:13[A]:ASP:OD1	4:F:440:HOH:O	2.05	0.74
1:E:68[B]:LYS:HE2	4:E:555:HOH:O	1.89	0.73
1:A:13:ASP:OD2	4:A:485:HOH:O	2.06	0.73
1:A:18:GLY:HA3	3:A:202:PEG:H21	1.70	0.72
1:A:13:ASP:OD1	1:A:133[A]:SER:OG	2.06	0.72
1:D:109[B]:THR:HG21	4:D:445:HOH:O	1.88	0.72
3:E:202:PEG:O1	4:E:528:HOH:O	2.06	0.72
1:A:109[B]:THR:HG23	4:A:587:HOH:O	1.89	0.72
1:A:1[A]:MET:CG	4:A:523:HOH:O	2.31	0.71
1:A:118[A]:LYS:HE2	4:A:518:HOH:O	1.90	0.71
1:C:4:LYS:HE2	4:C:589:HOH:O	1.89	0.71
1:A:93:VAL:CG2	1:D:93:VAL:HG11	2.20	0.71
1:D:46[B]:LYS:HE3	4:D:591:HOH:O	1.90	0.71
1:B:54[B]:LYS:HD2	4:B:605:HOH:O	1.90	0.71
1:A:82[A]:ARG:NH2	4:A:495:HOH:O	2.09	0.71
1:D:46[B]:LYS:CE	4:D:591:HOH:O	2.38	0.70
1:A:93:VAL:HG23	1:D:93:VAL:HG11	1.74	0.70
1:D:46[A]:LYS:HD2	4:D:588:HOH:O	1.91	0.70
1:A:92:LEU:C	4:A:503:HOH:O	2.27	0.70
1:F:102[A]:LYS:NZ	4:F:523:HOH:O	2.25	0.70
1:C:102[B]:LYS:NZ	1:C:107[B]:GLU:OE2	2.22	0.70
1:A:82[A]:ARG:HB2	4:A:560:HOH:O	1.92	0.69
1:F:29[B]:GLU:OE2	4:F:575:HOH:O	2.11	0.69
1:F:73[B]:GLU:HG2	4:F:309:HOH:O	1.92	0.69
1:B:15[B]:HIS:ND1	4:B:603:HOH:O	2.19	0.68
1:C:4:LYS:NZ	4:C:587:HOH:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LYS:HG3	4:A:553:HOH:O	1.91	0.68
1:A:82[B]:ARG:CZ	4:F:405:HOH:O	2.42	0.68
1:A:82[B]:ARG:HB2	4:A:560:HOH:O	1.93	0.67
1:C:3:GLU:HB2	4:C:617:HOH:O	1.94	0.67
1:D:30:LEU:CD2	4:D:554:HOH:O	2.42	0.67
3:F:202:PEG:H42	4:F:544:HOH:O	1.94	0.67
1:A:92:LEU:HD13	4:A:523:HOH:O	1.93	0.66
1:B:138:THR:HG21	1:E:4:LYS:HB3	1.76	0.66
1:E:54:LYS:HE3	4:E:608:HOH:O	1.94	0.66
1:B:54[B]:LYS:HE2	1:D:76:ASP:OD2	1.96	0.66
1:C:1:MET:HB2	1:C:92:LEU:HD21	1.77	0.66
1:A:8[B]:THR:HG22	1:A:42:TYR:CD1	2.31	0.64
4:B:591:HOH:O	1:D:54[A]:LYS:HE3	1.86	0.64
1:F:1:MET:CE	1:F:4[A]:LYS:CE	2.76	0.64
1:E:29:GLU:HG3	4:E:607:HOH:O	1.97	0.64
1:F:54[B]:LYS:NZ	4:F:520:HOH:O	2.20	0.64
1:D:27:PRO:HG3	4:D:555:HOH:O	1.98	0.64
1:B:127[B]:ASP:CB	3:B:204:PEG:H21	2.27	0.63
1:E:138:THR:HG22	4:E:583:HOH:O	1.97	0.63
1:F:19[B]:GLU:OE1	4:F:582:HOH:O	2.13	0.63
1:F:133[A]:SER:OG	4:F:502:HOH:O	2.15	0.63
1:B:127[B]:ASP:HB2	3:B:204:PEG:H21	1.77	0.63
1:D:87:LYS:CE	4:D:600:HOH:O	2.45	0.63
1:B:62:PHE:HZ	3:B:203:PEG:H11	1.63	0.63
1:A:18:GLY:HA3	3:A:202:PEG:C2	2.29	0.63
1:F:109[A]:THR:HG21	4:F:548:HOH:O	1.99	0.63
1:B:65:THR:OG1	3:B:202:PEG:H32	1.99	0.62
1:E:73[B]:GLU:HG2	4:E:588:HOH:O	1.98	0.62
1:D:98:VAL:HB	3:D:202:PEG:H12	1.83	0.61
1:F:1:MET:HA	1:F:1:MET:HE3	1.82	0.61
3:F:203:PEG:H32	4:F:583:HOH:O	2.01	0.61
1:D:109[B]:THR:HG23	4:D:442:HOH:O	2.00	0.61
1:A:82[A]:ARG:HB3	4:A:494:HOH:O	2.01	0.60
1:D:54[C]:LYS:CD	4:D:581:HOH:O	2.48	0.59
1:F:29[A]:GLU:OE1	4:F:575:HOH:O	2.17	0.59
1:D:46[A]:LYS:HE3	4:D:591:HOH:O	2.02	0.59
1:A:135[B]:ARG:NH1	4:A:341:HOH:O	2.30	0.59
1:A:84[B]:LYS:HE3	4:A:494:HOH:O	2.03	0.59
1:D:46[B]:LYS:CD	4:D:588:HOH:O	2.51	0.59
1:A:1[B]:MET:N	4:A:508:HOH:O	2.34	0.58
1:F:65:THR:OG1	3:F:203:PEG:H32	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54[B]:LYS:HE3	1:D:78:PHE:HZ	1.68	0.58
1:A:93:VAL:CG2	1:D:93:VAL:CG1	2.81	0.58
4:A:520:HOH:O	3:F:203:PEG:H21	2.02	0.58
1:F:29[B]:GLU:CD	4:F:575:HOH:O	2.41	0.58
1:E:115[A]:LYS:HD2	4:E:598:HOH:O	2.03	0.58
1:F:19[B]:GLU:CD	4:F:582:HOH:O	2.42	0.57
1:E:22[B]:LYS:NZ	4:E:606:HOH:O	2.36	0.57
1:D:1[A]:MET:HB2	4:D:369:HOH:O	2.04	0.57
3:E:202:PEG:H11	4:E:520:HOH:O	2.04	0.57
1:C:78:PHE:HB2	3:E:202:PEG:H12	1.87	0.57
1:B:62:PHE:CZ	3:B:203:PEG:H11	2.40	0.56
1:A:82[B]:ARG:HB3	4:A:494:HOH:O	2.05	0.56
1:E:46[B]:LYS:NZ	4:E:560:HOH:O	2.21	0.56
1:B:127[A]:ASP:HB3	3:B:204:PEG:C2	2.35	0.56
1:E:115[A]:LYS:CE	4:E:598:HOH:O	2.53	0.56
1:D:82[B]:ARG:HD3	4:D:473:HOH:O	2.06	0.56
1:D:46[A]:LYS:CG	4:D:588:HOH:O	2.54	0.55
4:A:520:HOH:O	3:F:203:PEG:C2	2.55	0.55
1:A:93:VAL:C	4:A:503:HOH:O	2.44	0.55
1:A:78:PHE:O	3:F:203:PEG:H22	2.07	0.55
1:F:1:MET:CE	1:F:4[A]:LYS:HE2	2.37	0.55
2:C:200:BLR:H25	2:C:200:BLR:H21	1.88	0.54
1:D:54[C]:LYS:HD3	4:D:581:HOH:O	2.07	0.54
1:F:29[B]:GLU:HG3	4:F:575:HOH:O	2.07	0.54
1:B:1[A]:MET:N	4:B:368:HOH:O	2.36	0.54
1:B:54[B]:LYS:NZ	4:B:555:HOH:O	2.40	0.54
1:F:1:MET:HE3	1:F:4[A]:LYS:HE2	1.89	0.54
1:A:11[A]:ILE:HG21	1:A:38:THR:HA	1.89	0.54
1:B:127[B]:ASP:CG	3:B:204:PEG:H21	2.27	0.54
1:C:1:MET:CB	1:C:92:LEU:HD21	2.38	0.54
1:D:87:LYS:HE3	4:D:600:HOH:O	2.07	0.54
1:B:138:THR:O	1:B:138:THR:HG22	2.08	0.54
1:F:1:MET:CA	1:F:1:MET:HE3	2.36	0.54
1:A:94:GLY:N	4:A:503:HOH:O	2.41	0.54
1:D:46[B]:LYS:HB3	4:D:588:HOH:O	2.08	0.54
1:A:1[B]:MET:HB2	4:A:537:HOH:O	2.08	0.53
1:E:115[A]:LYS:NZ	4:E:367:HOH:O	2.42	0.53
1:F:15:HIS:CE1	1:F:16[B]:ASN:ND2	2.77	0.53
3:B:202:PEG:H12	4:B:519:HOH:O	2.07	0.53
1:B:1[A]:MET:HB3	4:B:468:HOH:O	2.07	0.53
1:D:91:ASN:HB2	3:D:202:PEG:H11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:LYS:HE3	4:C:577:HOH:O	2.09	0.53
1:F:65:THR:OG1	3:F:203:PEG:C3	2.57	0.53
1:E:82[A]:ARG:NH2	4:E:501:HOH:O	1.99	0.52
1:A:109[B]:THR:OG1	1:A:124[B]:THR:OG1	2.27	0.52
1:F:4[A]:LYS:CE	4:F:600:HOH:O	2.57	0.52
1:A:54:LYS:HG2	4:A:553:HOH:O	2.01	0.52
2:E:201:BLR:H25	2:E:201:BLR:H21	1.91	0.52
1:F:19[B]:GLU:CG	4:F:581:HOH:O	2.57	0.52
1:F:4[A]:LYS:HE2	4:F:600:HOH:O	2.10	0.52
1:A:93:VAL:CA	4:A:503:HOH:O	2.53	0.52
1:B:59:PRO:HB3	3:B:203:PEG:H12	1.91	0.52
1:E:115[A]:LYS:CD	4:E:598:HOH:O	2.58	0.52
2:A:201:BLR:CBC	2:A:201:BLR:H21	2.41	0.51
3:B:204:PEG:C3	4:B:567:HOH:O	2.59	0.51
3:F:203:PEG:H42	4:F:328:HOH:O	2.10	0.51
1:F:29[B]:GLU:CG	4:F:575:HOH:O	2.59	0.51
1:C:84[A]:LYS:NZ	4:C:558:HOH:O	2.44	0.51
1:B:54[B]:LYS:HE3	1:D:78:PHE:CZ	2.47	0.50
1:B:1[A]:MET:HG3	1:B:92:LEU:HD21	1.93	0.50
2:B:201:BLR:H25	2:B:201:BLR:H21	1.94	0.50
4:C:468:HOH:O	3:E:202:PEG:H31	2.12	0.49
4:A:494:HOH:O	1:F:62:PHE:O	2.19	0.49
1:A:92:LEU:HD22	4:A:460:HOH:O	2.12	0.49
1:C:135[A]:ARG:NH1	4:C:505:HOH:O	2.40	0.49
1:A:40[B]:THR:HG21	4:A:551:HOH:O	2.12	0.49
1:B:102[B]:LYS:HE2	1:B:107[B]:GLU:CD	2.33	0.49
3:F:203:PEG:C3	4:F:583:HOH:O	2.58	0.49
1:D:46[B]:LYS:CG	4:D:588:HOH:O	2.61	0.49
1:B:102[B]:LYS:HG2	1:B:107[B]:GLU:HG2	1.95	0.49
2:D:201:BLR:H25	2:D:201:BLR:H21	1.95	0.49
2:A:201:BLR:H21	2:A:201:BLR:H25	1.94	0.49
1:E:65:THR:OG1	3:E:202:PEG:H22	2.14	0.48
1:E:66[B]:GLN:CG	4:E:596:HOH:O	2.61	0.48
1:B:135:ARG:NH1	4:B:601:HOH:O	2.28	0.47
1:F:1:MET:HE1	1:F:4[A]:LYS:NZ	2.29	0.47
1:B:65:THR:OG1	3:B:202:PEG:C3	2.61	0.47
1:F:92:LEU:O	3:F:202:PEG:C3	2.62	0.47
3:F:202:PEG:C4	4:F:544:HOH:O	2.58	0.47
1:D:115[B]:LYS:HE3	4:D:463:HOH:O	2.15	0.47
1:F:4[B]:LYS:HE3	4:F:600:HOH:O	2.13	0.47
1:A:46:LYS:CA	4:A:556:HOH:O	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:ASP:O	1:D:82[B]:ARG:HB2	2.15	0.47
3:F:203:PEG:H41	4:F:574:HOH:O	2.15	0.47
1:B:138:THR:HG21	1:E:4:LYS:CB	2.44	0.46
1:A:102:LYS:HG2	1:A:107[B]:GLU:HG2	1.97	0.46
1:E:84[B]:LYS:NZ	4:E:561:HOH:O	2.47	0.46
1:E:102[B]:LYS:NZ	1:E:107:GLU:OE1	2.49	0.46
1:E:65:THR:HG1	3:E:202:PEG:H22	1.79	0.46
1:A:35:ASP:OD2	3:A:202:PEG:H32	2.15	0.46
1:E:115[B]:LYS:NZ	4:E:598:HOH:O	2.23	0.46
1:A:68[A]:LYS:HE3	1:A:68[A]:LYS:HB3	1.79	0.46
1:B:54[B]:LYS:CE	1:D:76:ASP:OD2	2.63	0.46
1:B:95[B]:GLU:OE1	4:B:517:HOH:O	2.20	0.46
1:F:4[A]:LYS:NZ	4:F:600:HOH:O	2.30	0.46
1:D:46[A]:LYS:CB	4:D:609:HOH:O	2.36	0.46
1:A:68[B]:LYS:HE3	4:A:416:HOH:O	2.16	0.45
1:A:114[B]:ILE:HA	1:A:118[B]:LYS:O	2.15	0.45
1:A:1[A]:MET:CB	4:A:523:HOH:O	2.60	0.45
3:A:202:PEG:H32	4:A:339:HOH:O	2.16	0.45
1:F:89[A]:VAL:CG1	4:F:523:HOH:O	2.64	0.45
1:E:100:VAL:HG22	1:E:109[B]:THR:HG22	1.98	0.45
1:F:1:MET:CE	1:F:4[A]:LYS:NZ	2.80	0.45
1:F:64:ASP:O	3:F:203:PEG:C1	2.60	0.45
1:F:1:MET:HE1	1:F:95[A]:GLU:OE1	2.16	0.45
1:A:54:LYS:HE3	4:A:553:HOH:O	2.16	0.45
1:A:84[A]:LYS:HD2	1:F:64:ASP:OD2	2.17	0.45
1:E:65:THR:HG1	3:E:202:PEG:C2	2.30	0.45
1:B:54[B]:LYS:CD	4:B:605:HOH:O	2.58	0.44
1:D:109[A]:THR:HG21	3:D:202:PEG:O4	2.17	0.44
1:A:93:VAL:HG23	1:D:93:VAL:CG1	2.46	0.44
1:C:4:LYS:CE	4:C:589:HOH:O	2.58	0.44
1:A:100:VAL:HG22	1:A:109[B]:THR:HG22	1.99	0.44
2:C:200:BLR:CBC	2:C:200:BLR:H21	2.46	0.44
1:D:104[A]:ASP:OD1	4:D:502:HOH:O	2.21	0.44
1:A:107[A]:GLU:CG	4:A:569:HOH:O	2.54	0.44
1:F:68[B]:LYS:NZ	4:F:603:HOH:O	2.50	0.44
1:E:65:THR:OG1	3:E:202:PEG:C2	2.66	0.44
2:F:201:BLR:H21	2:F:201:BLR:H25	1.99	0.44
1:F:1:MET:HE1	1:F:4[A]:LYS:HZ3	1.82	0.44
1:E:109[B]:THR:HG21	4:E:458:HOH:O	2.17	0.44
1:F:118:LYS:CD	4:F:563:HOH:O	2.65	0.44
1:D:82[B]:ARG:CD	4:D:473:HOH:O	2.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:201:BLR:CBC	2:E:201:BLR:H21	2.47	0.43
1:F:118:LYS:HD3	4:F:563:HOH:O	2.18	0.43
1:B:102[B]:LYS:HE2	1:B:107[B]:GLU:OE2	2.17	0.43
1:F:100:VAL:HG22	1:F:109[A]:THR:HG22	1.99	0.43
1:A:59:PRO:HD2	4:A:435:HOH:O	2.18	0.43
3:B:204:PEG:H22	3:B:204:PEG:O4	2.17	0.43
1:E:59:PRO:HD2	4:E:408:HOH:O	2.18	0.43
1:E:68[B]:LYS:CE	4:E:555:HOH:O	2.56	0.43
1:B:29[A]:GLU:HG2	4:B:418:HOH:O	2.19	0.43
1:C:42:TYR:CD1	1:C:54[A]:LYS:HE3	2.54	0.43
1:D:46[A]:LYS:HB3	4:D:588:HOH:O	2.18	0.43
1:A:46:LYS:CG	4:A:556:HOH:O	2.62	0.42
1:F:52:THR:HG23	1:F:68[A]:LYS:HG2	2.02	0.42
3:E:202:PEG:H42	4:E:507:HOH:O	2.20	0.42
3:F:203:PEG:C4	4:F:583:HOH:O	2.50	0.42
4:B:464:HOH:O	1:E:3[A]:GLU:HG2	2.20	0.42
1:E:113:GLU:CD	1:E:115[B]:LYS:HE3	2.40	0.42
1:E:66[B]:GLN:HG3	1:E:66[B]:GLN:O	2.20	0.42
1:D:55:ILE:HD13	2:D:201:BLR:H6	2.02	0.42
1:E:115[B]:LYS:CD	4:E:598:HOH:O	2.61	0.42
1:F:1:MET:CA	4:F:507:HOH:O	2.68	0.42
3:B:202:PEG:H11	4:B:333:HOH:O	2.20	0.41
1:D:70:LYS:HG3	1:D:71:LEU:N	2.35	0.41
1:F:89[A]:VAL:HG11	4:F:523:HOH:O	2.19	0.41
1:E:61:THR:HG21	2:E:201:BLR:H22	2.02	0.41
2:D:201:BLR:H21	2:D:201:BLR:CBC	2.51	0.41
3:B:202:PEG:H22	1:D:65:THR:HA	2.03	0.41
1:A:70[A]:LYS:HE2	4:A:380:HOH:O	2.20	0.41
1:E:55:ILE:HD13	2:E:201:BLR:H6	2.03	0.41
2:F:201:BLR:CBC	2:F:201:BLR:H21	2.50	0.41
4:A:376:HOH:O	3:D:202:PEG:C2	2.69	0.41
1:F:13[B]:ASP:CG	1:F:133[B]:SER:HG	2.23	0.41
2:B:201:BLR:CBC	2:B:201:BLR:H21	2.50	0.40
1:D:127[B]:ASP:OD1	4:D:377:HOH:O	2.20	0.40
1:F:1:MET:O	1:F:4[A]:LYS:HG2	2.21	0.40
3:B:202:PEG:H31	3:B:202:PEG:H12	1.85	0.40
3:B:204:PEG:H31	4:B:567:HOH:O	2.22	0.40
4:A:345:HOH:O	3:D:202:PEG:H22	2.21	0.40
1:D:54[A]:LYS:HZ2	1:D:56:GLU:HG3	1.87	0.40
1:D:76:ASP:OD1	1:D:87:LYS:NZ	2.51	0.40
1:D:4:LYS:HG2	4:D:598:HOH:O	2.21	0.40

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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

Some 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	A	201	-	34,46,46	3.52	11 (32%)	38,67,67	1.71	9 (23%)
3	PEG	F	204	-	6,6,6	0.68	0	5,5,5	0.64	0
3	PEG	E	202	-	6,6,6	0.71	0	5,5,5	0.74	0
3	PEG	B	204	-	6,6,6	0.67	0	5,5,5	0.99	0
2	BLR	D	201	-	34,46,46	3.24	14 (41%)	38,67,67	1.90	12 (31%)
3	PEG	B	202	-	6,6,6	0.52	0	5,5,5	1.40	1 (20%)
2	BLR	F	201	-	34,46,46	3.27	13 (38%)	38,67,67	2.08	10 (26%)
3	PEG	F	202	-	6,6,6	0.56	0	5,5,5	1.74	1 (20%)
3	PEG	F	203	-	6,6,6	0.65	0	5,5,5	1.32	1 (20%)
2	BLR	B	201	-	34,46,46	3.15	12 (35%)	38,67,67	1.72	5 (13%)
3	PEG	B	203	-	6,6,6	0.70	0	5,5,5	0.50	0
3	PEG	A	202	-	6,6,6	0.69	0	5,5,5	0.86	0
3	PEG	D	202	-	6,6,6	0.65	0	5,5,5	0.93	0
2	BLR	C	200	-	34,46,46	3.08	13 (38%)	38,67,67	1.99	8 (21%)
2	BLR	E	201	-	34,46,46	2.88	11 (32%)	38,67,67	1.80	7 (18%)

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	A	201	-	-	0/20/58/58	0/4/4/4
3	PEG	F	204	-	-	1/4/4/4	-
3	PEG	E	202	-	-	2/4/4/4	-
3	PEG	B	204	-	-	2/4/4/4	-
2	BLR	D	201	-	-	0/20/58/58	0/4/4/4
3	PEG	B	202	-	-	2/4/4/4	-
2	BLR	F	201	-	-	0/20/58/58	0/4/4/4
3	PEG	F	202	-	-	2/4/4/4	-
3	PEG	F	203	-	-	0/4/4/4	-
2	BLR	B	201	-	-	0/20/58/58	0/4/4/4
3	PEG	B	203	-	-	3/4/4/4	-
3	PEG	A	202	-	-	2/4/4/4	-
3	PEG	D	202	-	-	2/4/4/4	-
2	BLR	C	200	-	-	0/20/58/58	0/4/4/4
2	BLR	E	201	-	-	0/20/58/58	0/4/4/4

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	BLR	CHA-C4D	-13.26	1.41	1.51
2	F	201	BLR	CHA-C4D	-11.90	1.42	1.51
2	B	201	BLR	CHA-C4D	-11.29	1.43	1.51
2	D	201	BLR	CHA-C4D	-11.28	1.43	1.51
2	C	200	BLR	CHA-C4D	-10.81	1.43	1.51
2	E	201	BLR	CHA-C4D	-9.56	1.44	1.51
2	A	201	BLR	C1C-NC	7.70	1.54	1.38
2	C	200	BLR	C4B-NB	6.97	1.52	1.38
2	F	201	BLR	C4B-NB	6.94	1.52	1.38
2	A	201	BLR	C4B-NB	6.82	1.52	1.38
2	D	201	BLR	C4B-NB	6.58	1.51	1.38
2	D	201	BLR	C1C-NC	6.55	1.51	1.38
2	F	201	BLR	C1C-NC	6.54	1.51	1.38
2	B	201	BLR	C4B-NB	6.39	1.51	1.38
2	E	201	BLR	C1C-NC	6.09	1.50	1.38
2	E	201	BLR	C4B-NB	5.98	1.50	1.38
2	B	201	BLR	C1C-NC	5.89	1.50	1.38
2	A	201	BLR	C3D-C4D	5.74	1.47	1.39
2	C	200	BLR	C1C-NC	5.66	1.49	1.38
2	D	201	BLR	C3D-C4D	4.86	1.46	1.39
2	B	201	BLR	C3D-C4D	4.86	1.46	1.39
2	D	201	BLR	C3C-C2C	-4.60	1.28	1.37
2	F	201	BLR	C3B-C2B	-4.59	1.28	1.37
2	D	201	BLR	C3B-C2B	-4.56	1.28	1.37
2	B	201	BLR	C1B-NB	4.48	1.45	1.37
2	C	200	BLR	C3B-C2B	-4.41	1.28	1.37
2	A	201	BLR	C3B-C2B	-4.19	1.28	1.37
2	E	201	BLR	C3B-C2B	-4.15	1.28	1.37
2	B	201	BLR	C3C-C2C	-4.09	1.29	1.37
2	A	201	BLR	C3C-C4C	-4.07	1.38	1.45
2	F	201	BLR	C3D-C4D	4.03	1.45	1.39
2	A	201	BLR	C4C-NC	3.97	1.44	1.37
2	E	201	BLR	C3D-C4D	3.97	1.45	1.39
2	C	200	BLR	C3C-C2C	-3.94	1.29	1.37
2	A	201	BLR	C3C-C2C	-3.93	1.29	1.37
2	F	201	BLR	C3C-C2C	-3.87	1.29	1.37
2	C	200	BLR	C3D-C4D	3.86	1.45	1.39
2	B	201	BLR	C3B-C2B	-3.86	1.29	1.37
2	E	201	BLR	C3C-C4C	-3.78	1.39	1.45
2	E	201	BLR	C3C-C2C	-3.61	1.30	1.37
2	F	201	BLR	C1B-C2B	-3.53	1.38	1.45
2	F	201	BLR	C3C-C4C	-3.37	1.39	1.45
2	D	201	BLR	C1B-NB	3.37	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	200	BLR	C1B-C2B	-3.31	1.39	1.45
2	F	201	BLR	C1B-NB	3.29	1.43	1.37
2	E	201	BLR	C1B-C2B	-3.19	1.39	1.45
2	B	201	BLR	C3C-C4C	-3.14	1.40	1.45
2	C	200	BLR	C3C-C4C	-3.06	1.40	1.45
2	D	201	BLR	C1B-C2B	-3.03	1.39	1.45
2	B	201	BLR	C1B-C2B	-2.96	1.39	1.45
2	B	201	BLR	C4C-NC	2.95	1.42	1.37
2	D	201	BLR	C3C-C4C	-2.87	1.40	1.45
2	D	201	BLR	C4C-NC	2.74	1.42	1.37
2	D	201	BLR	OB-C4B	-2.72	1.18	1.23
2	A	201	BLR	OB-C4B	-2.62	1.18	1.23
2	C	200	BLR	C4C-NC	2.61	1.42	1.37
2	C	200	BLR	OB-C4B	-2.52	1.18	1.23
2	C	200	BLR	C4A-CHB	2.50	1.50	1.41
2	F	201	BLR	C4C-NC	2.47	1.41	1.37
2	C	200	BLR	C1B-NB	2.44	1.41	1.37
2	B	201	BLR	OB-C4B	-2.41	1.19	1.23
2	E	201	BLR	OC-C1C	-2.41	1.19	1.23
2	F	201	BLR	C4A-CHB	2.41	1.50	1.41
2	C	200	BLR	OC-C1C	-2.40	1.19	1.23
2	A	201	BLR	C1B-NB	2.32	1.41	1.37
2	E	201	BLR	C4C-NC	2.25	1.41	1.37
2	F	201	BLR	C1D-CHD	2.20	1.49	1.41
2	A	201	BLR	C1B-C2B	-2.16	1.41	1.45
2	D	201	BLR	C1D-CHD	2.15	1.49	1.41
2	F	201	BLR	C3B-C4B	2.14	1.54	1.47
2	D	201	BLR	OC-C1C	-2.11	1.19	1.23
2	D	201	BLR	CHD-C4C	2.11	1.38	1.34
2	E	201	BLR	OB-C4B	-2.09	1.19	1.23
2	B	201	BLR	C4A-CHB	2.04	1.49	1.41

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	201	BLR	C3B-C4B-NB	-7.60	97.60	106.19
2	E	201	BLR	C3B-C4B-NB	-6.61	98.72	106.19
2	C	200	BLR	C3B-C4B-NB	-6.14	99.25	106.19
2	A	201	BLR	C3B-C4B-NB	-5.61	99.85	106.19
2	B	201	BLR	C3B-C4B-NB	-5.41	100.08	106.19
2	D	201	BLR	C3B-C4B-NB	-5.40	100.09	106.19
2	C	200	BLR	CAA-C2A-C1A	-5.14	123.68	127.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	200	BLR	C3B-C2B-C1B	4.09	112.97	108.03
2	F	201	BLR	OB-C4B-C3B	4.02	138.58	129.46
2	F	201	BLR	C3B-C2B-C1B	4.02	112.88	108.03
2	B	201	BLR	C3B-C2B-C1B	3.88	112.72	108.03
2	F	201	BLR	C4B-C3B-C2B	3.84	112.86	107.92
2	E	201	BLR	C3B-C2B-C1B	3.58	112.35	108.03
2	E	201	BLR	OB-C4B-C3B	3.56	137.54	129.46
2	D	201	BLR	C4B-C3B-C2B	3.55	112.48	107.92
2	B	201	BLR	C4B-C3B-C2B	3.49	112.41	107.92
2	D	201	BLR	C3B-C2B-C1B	3.47	112.22	108.03
2	E	201	BLR	C4B-C3B-C2B	3.36	112.24	107.92
2	A	201	BLR	C4B-C3B-C2B	3.36	112.23	107.92
2	D	201	BLR	CAD-C3D-C4D	-3.36	124.94	127.30
2	A	201	BLR	C4C-NC-C1C	-3.14	106.67	110.67
2	C	200	BLR	OB-C4B-C3B	3.12	136.54	129.46
2	D	201	BLR	OB-C4B-C3B	3.09	136.48	129.46
2	C	200	BLR	C4B-C3B-C2B	3.08	111.88	107.92
3	F	202	PEG	C3-O2-C2	3.07	126.58	113.29
2	D	201	BLR	CMB-C2B-C1B	-3.07	120.33	124.17
2	F	201	BLR	CMB-C2B-C1B	-2.99	120.43	124.17
2	D	201	BLR	CMD-C2D-C3D	2.94	130.49	124.94
2	C	200	BLR	CAD-C3D-C4D	-2.89	125.27	127.30
2	C	200	BLR	CMB-C2B-C1B	-2.88	120.56	124.17
2	A	201	BLR	C3B-C2B-C1B	2.75	111.35	108.03
2	D	201	BLR	C4C-NC-C1C	-2.73	107.20	110.67
2	B	201	BLR	OB-C4B-C3B	2.62	135.40	129.46
2	C	200	BLR	C2C-C1C-NC	-2.56	99.60	106.45
3	B	202	PEG	C3-O2-C2	2.55	124.32	113.29
3	F	203	PEG	C3-O2-C2	2.48	124.02	113.29
2	A	201	BLR	OB-C4B-C3B	2.45	135.02	129.46
2	B	201	BLR	C4C-NC-C1C	-2.39	107.62	110.67
2	F	201	BLR	CMD-C2D-C3D	2.31	129.30	124.94
2	F	201	BLR	C4C-NC-C1C	-2.30	107.73	110.67
2	D	201	BLR	C1B-NB-C4B	-2.28	107.76	110.67
2	E	201	BLR	CHD-C4C-NC	-2.24	122.88	130.40
2	F	201	BLR	CAD-C3D-C4D	-2.20	125.75	127.30
2	E	201	BLR	CMB-C2B-C1B	-2.19	121.43	124.17
2	A	201	BLR	C2C-C1C-NC	-2.17	100.67	106.45
2	A	201	BLR	CHD-C4C-NC	-2.15	123.19	130.40
2	E	201	BLR	C2C-C1C-NC	-2.14	100.72	106.45
2	D	201	BLR	C2C-C1C-NC	-2.09	100.86	106.45
2	A	201	BLR	CMD-C2D-C3D	2.08	128.87	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	201	BLR	C2C-C1C-NC	-2.06	100.94	106.45
2	D	201	BLR	CHB-C1B-NB	-2.05	123.52	130.40
2	D	201	BLR	CMC-C2C-C1C	-2.03	116.63	121.39
2	F	201	BLR	CHD-C4C-NC	-2.02	123.63	130.40
2	A	201	BLR	C1B-NB-C4B	-2.00	108.12	110.67

There are no chirality outliers.

All (16) 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	F	204	PEG	O2-C3-C4-O4
3	B	204	PEG	O1-C1-C2-O2
3	B	203	PEG	O1-C1-C2-O2
3	F	202	PEG	O1-C1-C2-O2
3	F	202	PEG	C1-C2-O2-C3
3	D	202	PEG	C1-C2-O2-C3
3	A	202	PEG	C4-C3-O2-C2
3	B	202	PEG	C4-C3-O2-C2
3	B	203	PEG	C4-C3-O2-C2
3	B	203	PEG	C1-C2-O2-C3
3	E	202	PEG	O1-C1-C2-O2
3	D	202	PEG	O2-C3-C4-O4
3	B	204	PEG	C4-C3-O2-C2
3	A	202	PEG	C1-C2-O2-C3

There are no ring outliers.

14 monomers are involved in 69 short contacts:

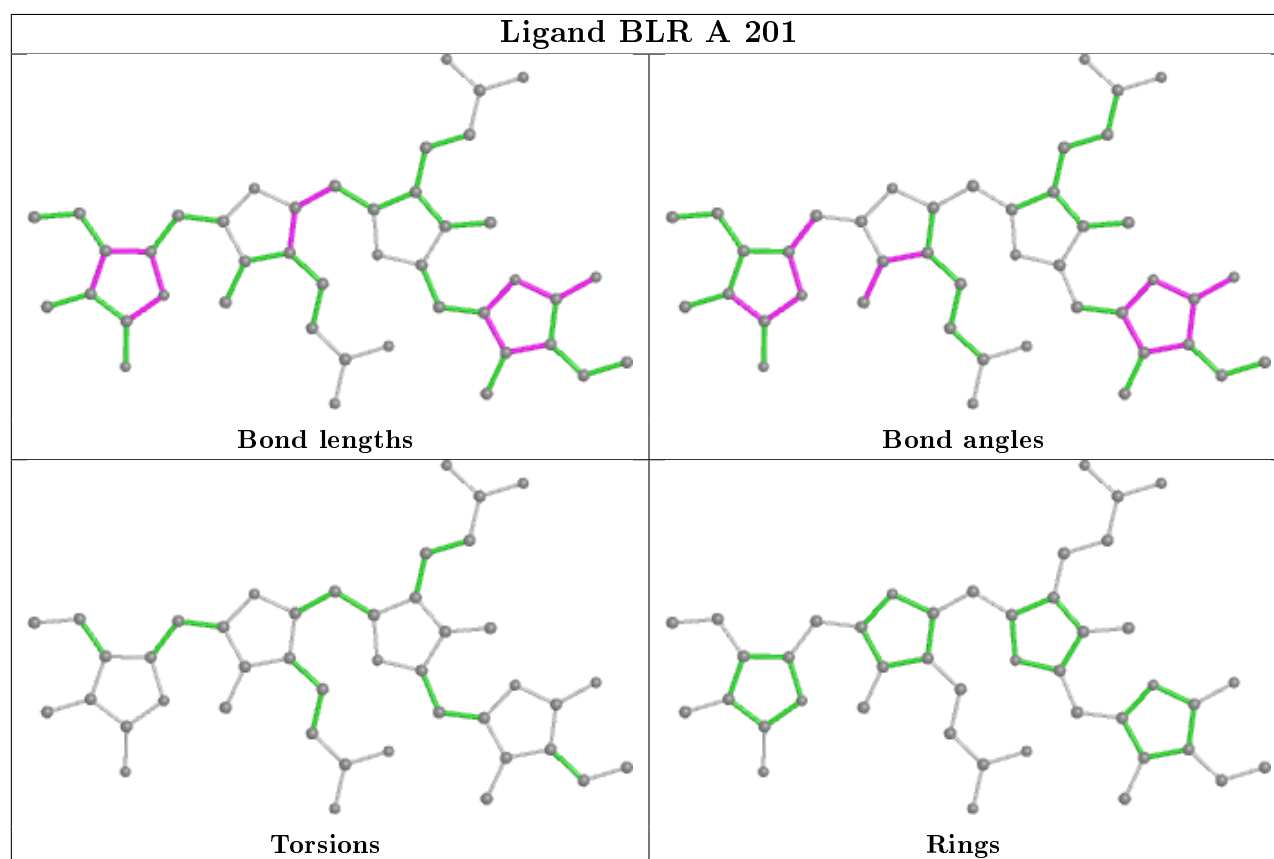
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	BLR	2	0
3	E	202	PEG	10	0
3	B	204	PEG	10	0
2	D	201	BLR	3	0
3	B	202	PEG	6	0
2	F	201	BLR	2	0
3	F	202	PEG	3	0
3	F	203	PEG	13	0
2	B	201	BLR	2	0
3	B	203	PEG	3	0

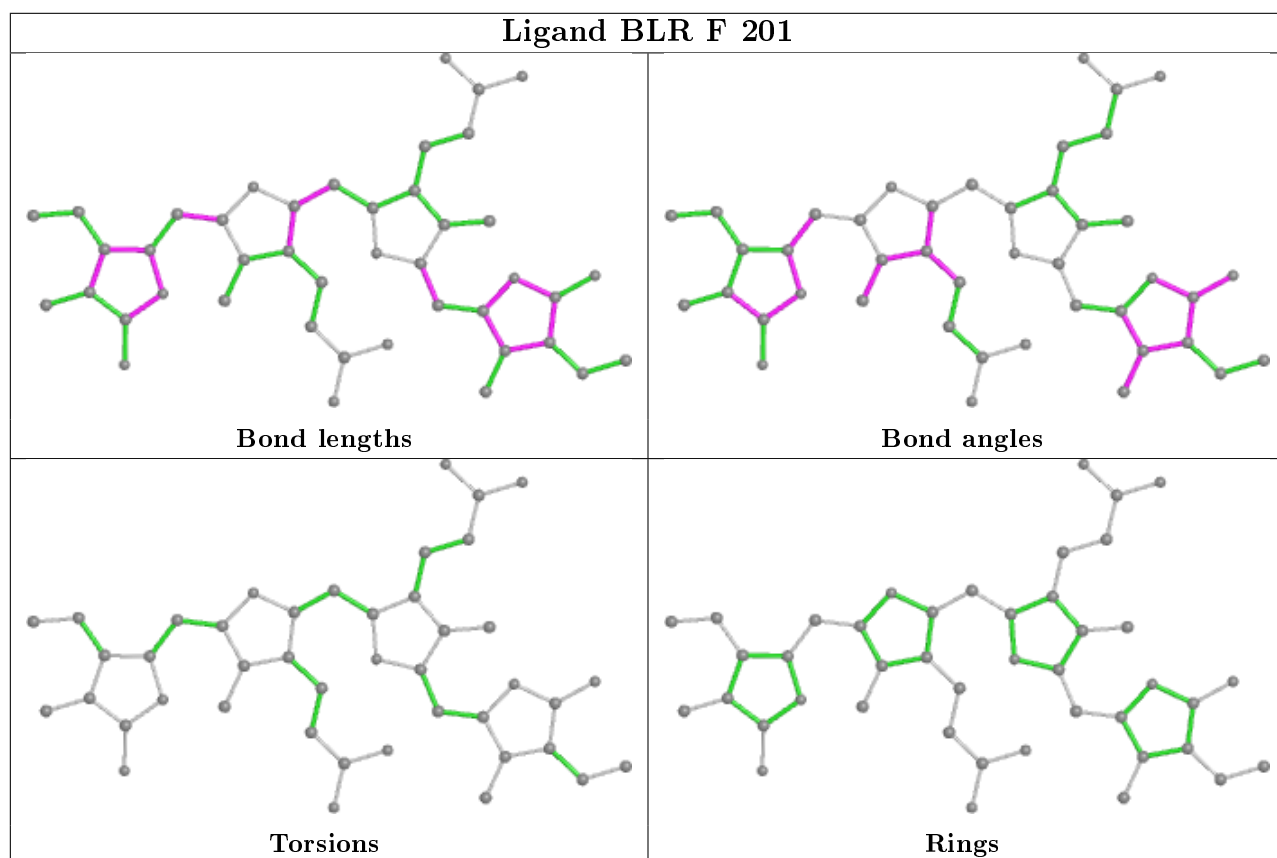
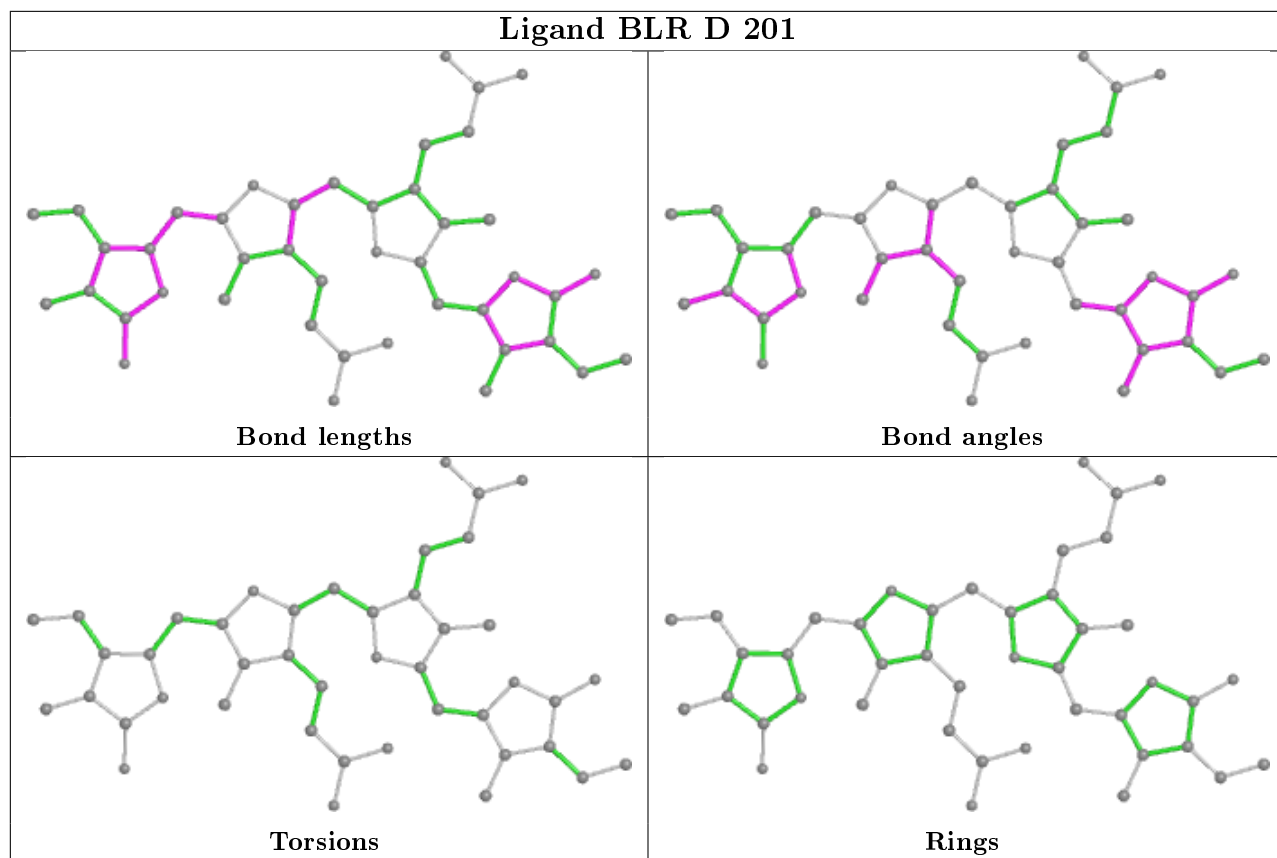
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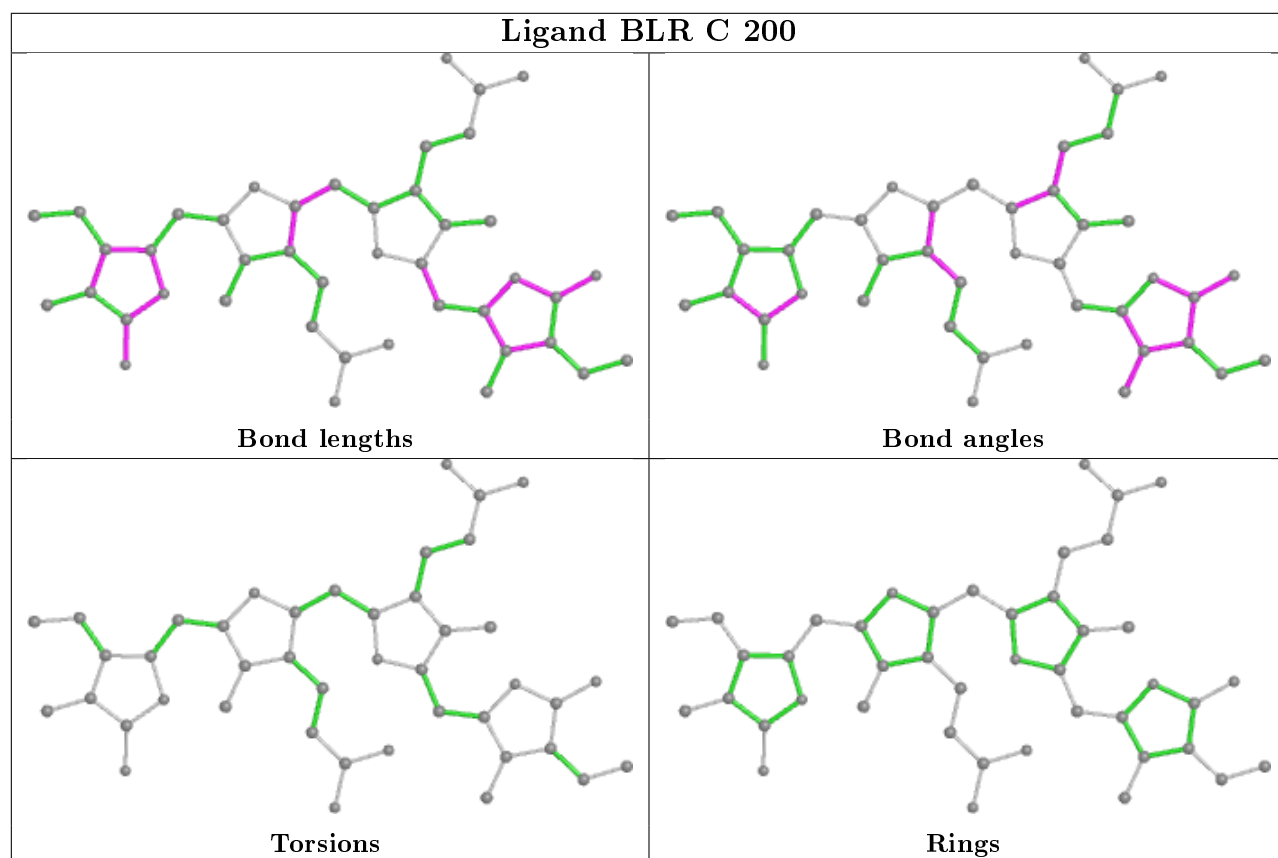
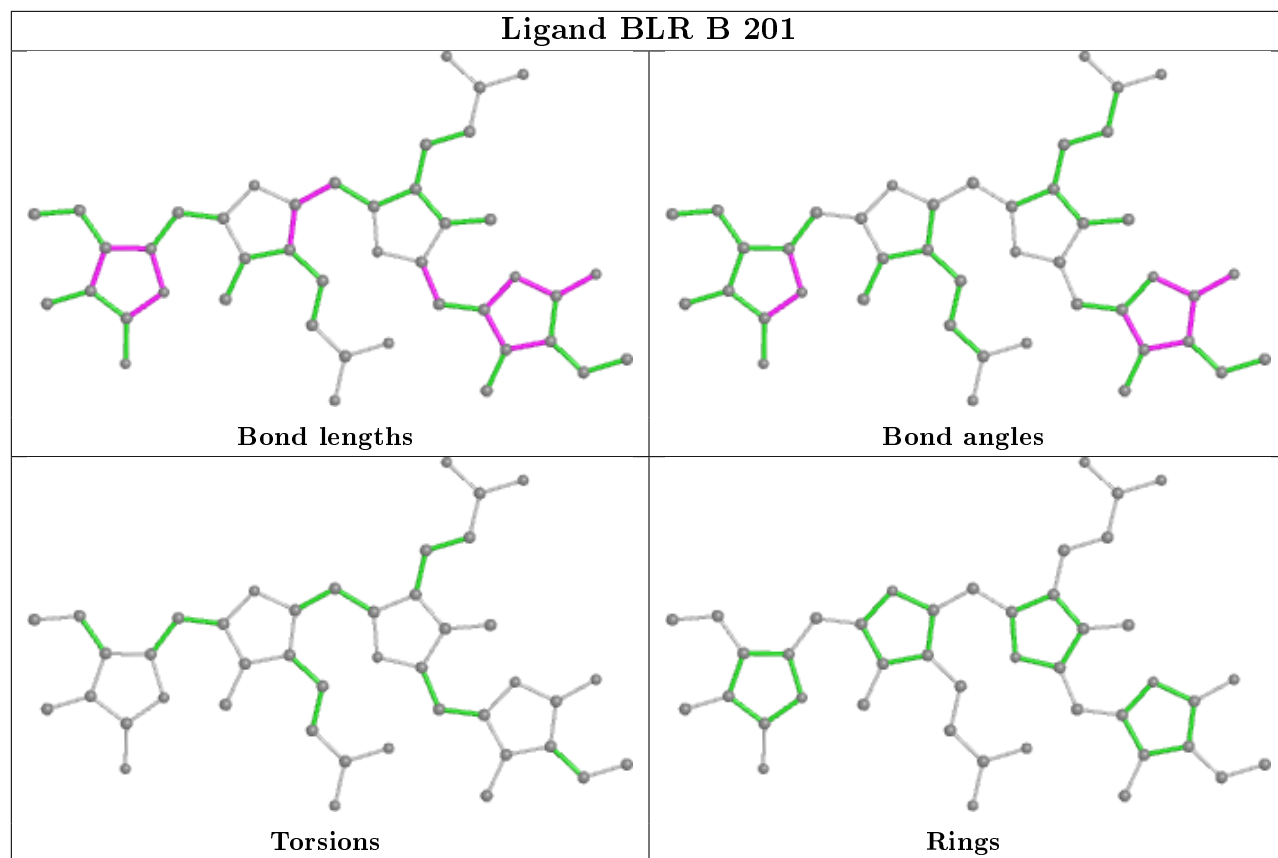
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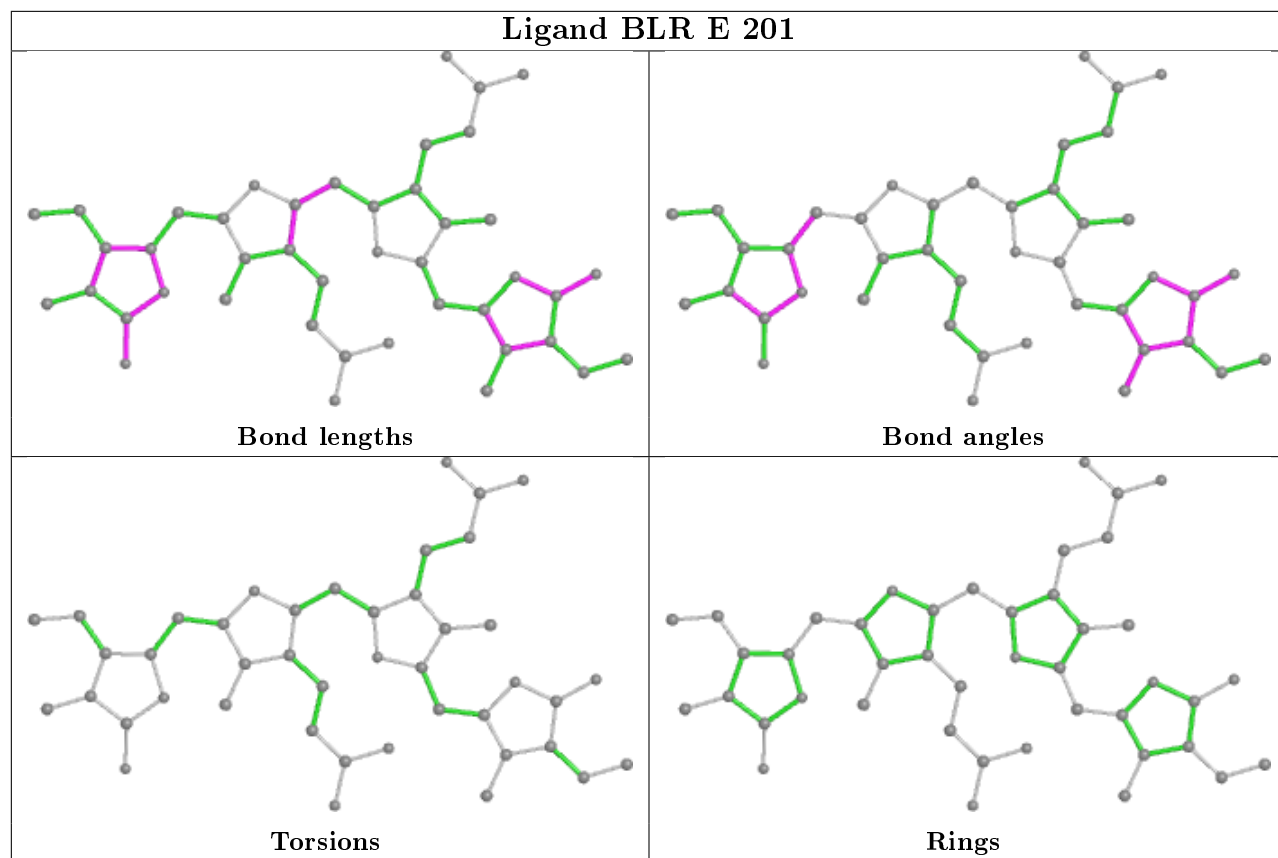
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202	PEG	4	0
3	D	202	PEG	5	0
2	C	200	BLR	2	0
2	E	201	BLR	4	0

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 than 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	139/139 (100%)	-0.21	5 (3%) 42 41	9, 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	2 (1%) 75 75	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	12 (1%) 75 75	6, 12, 22, 35	2 (0%)

All (12) 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	2.7
1	A	1[A]	MET	2.6
1	A	47	ASP	2.5
1	C	46[A]	LYS	2.4
1	A	46	LYS	2.3
1	F	46	LYS	2.0
1	C	105[A]	GLY	2.0
1	D	46[A]	LYS	2.0

### 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](#)

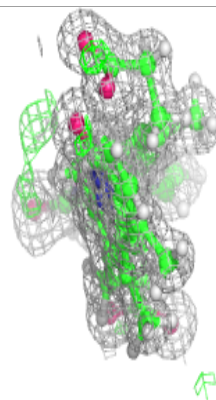
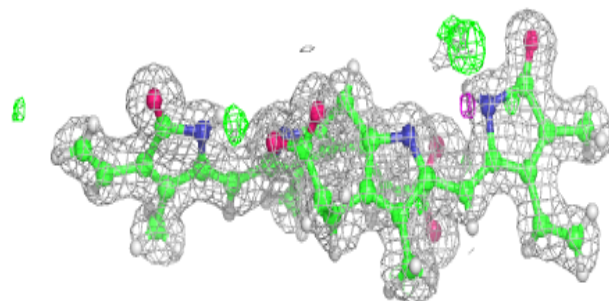
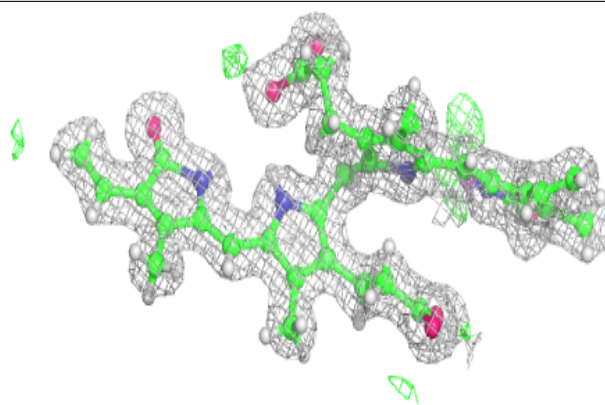
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	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	D	201	43/43	0.99	0.06	7,9,12,12	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	E	201	43/43	0.99	0.06	4,7,9,10	0

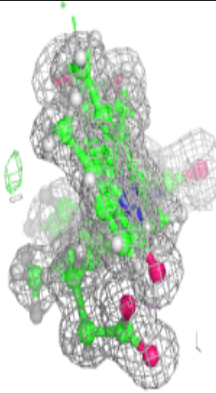
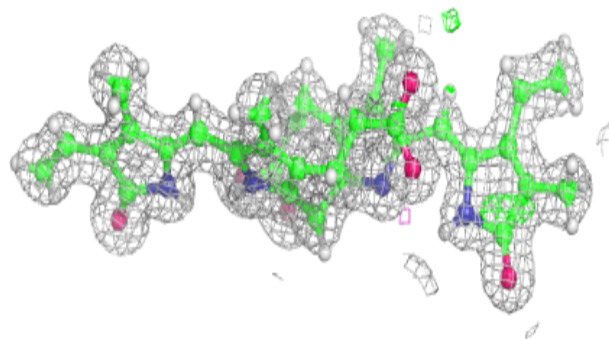
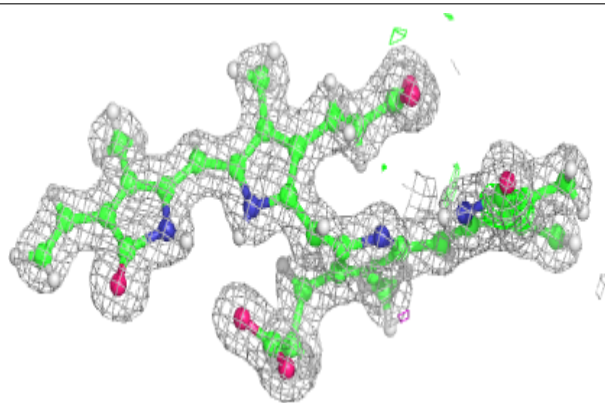
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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 D 201:**

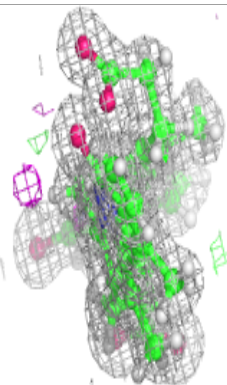
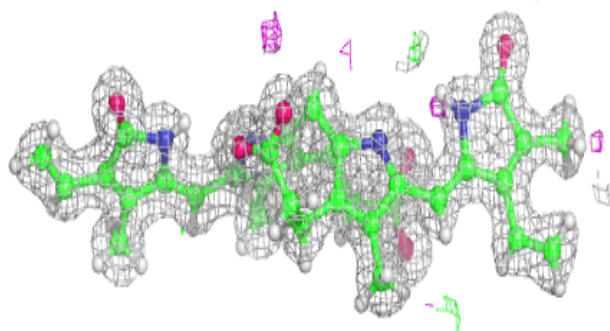
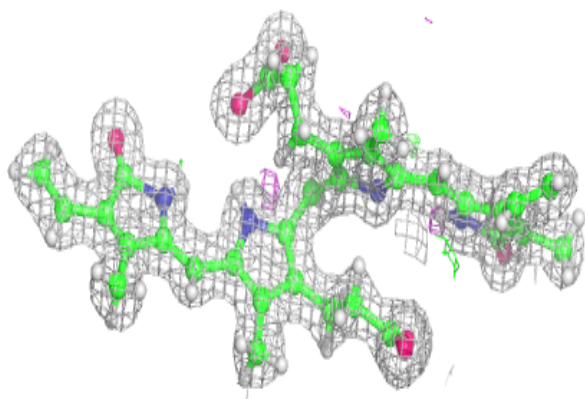
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



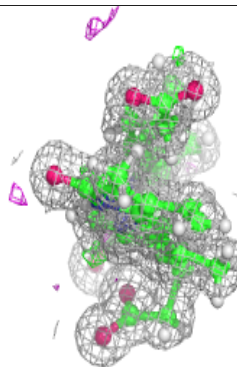
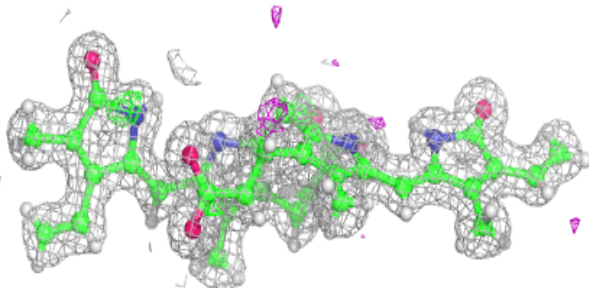
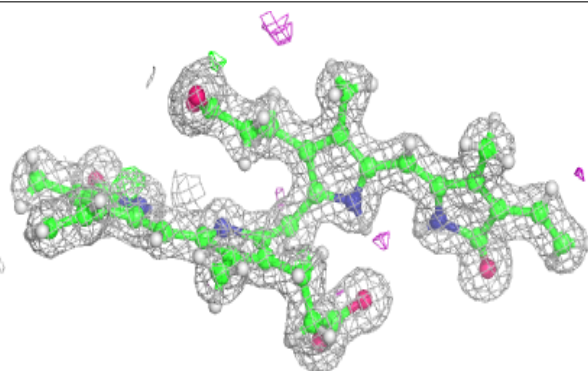


**Electron density around BLR F 201:**

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

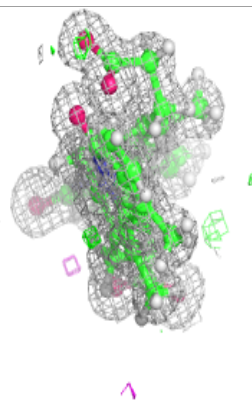
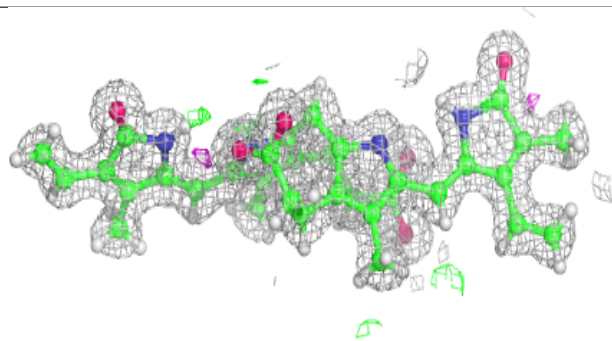
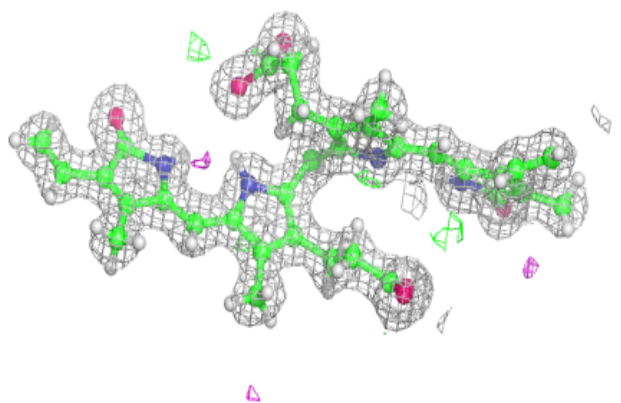
**Electron density around BLR B 201:**

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

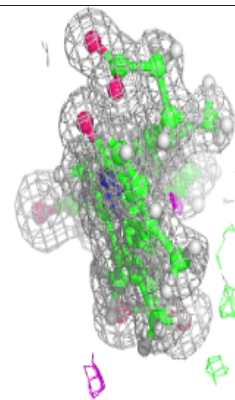
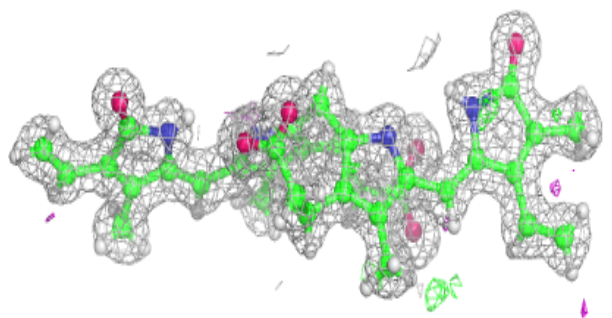
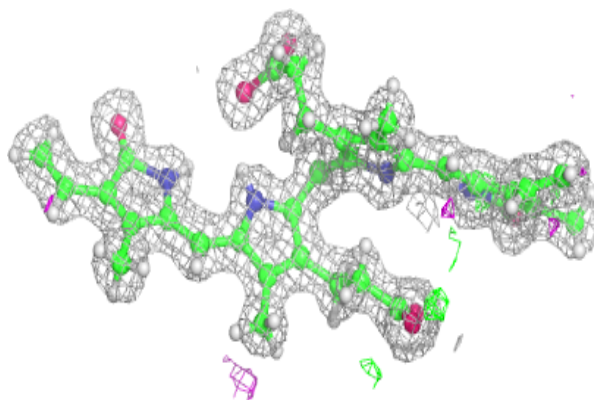


**Electron density around BLR C 200:**

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

**Electron density around BLR 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

There are no such residues in this entry.