



# Full wwPDB X-ray Structure Validation Report ⓘ

May 6, 2021 – 11:56 am BST

PDB ID : 6YX7  
Title : The high resolution structure of allophycocyanin from cyanobacterium Nostoc sp. WR13, the P21212 crystal form.  
Authors : Patel, H.M.; Roszak, A.W.; Madamwar, D.; Cogdell, R.J.  
Deposited on : 2020-04-30  
Resolution : 1.42 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 : 2.18  
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) : 2.18

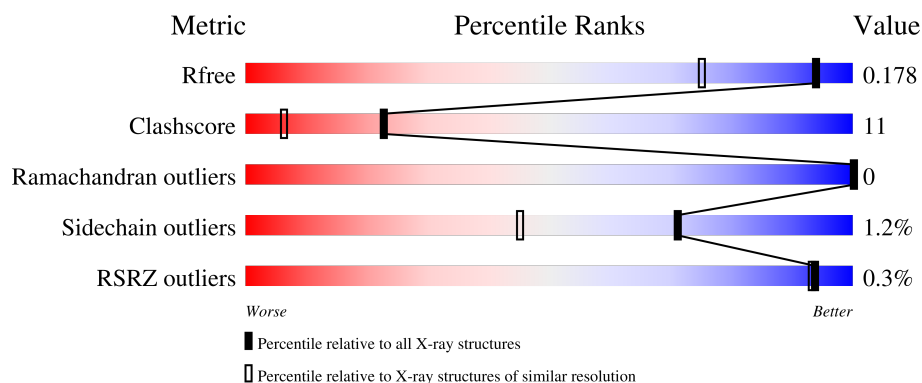
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.42 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.





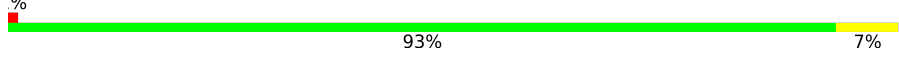

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2579 (1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632 (1.44-1.40)
Sidechain outliers	138945	2631 (1.44-1.40)
RSRZ outliers	127900	2528 (1.44-1.40)

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  $\geq 3$ , 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	AAA	160	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>12%</div> </div> </div>
1	CCC	160	<div> <div></div> <div>88%</div> <div>12%</div> <div>.</div> </div>
1	EEE	160	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>.</div> </div> </div>
1	GGG	160	<div> <div></div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	III	160	<div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain	
1	KKK	160		
2	BBB	161		
2	DDD	161		
2	FFF	161		
2	HHH	161		
2	JJJ	161		
2	LLL	161		

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
10	P6G	CCC	202	-	-	-	X
15	PGE	GGG	203	-	-	X	-
15	PGE	LLL	204	-	-	-	X
4	PG4	AAA	202	-	-	X	-
4	PG4	CCC	203	-	-	X	X
4	PG4	FFF	204	-	-	-	X
7	1PE	BBB	204	-	-	X	-
8	PEG	BBB	205	-	-	X	-
8	PEG	BBB	208	-	-	X	-
8	PEG	CCC	204	-	-	X	-
8	PEG	HHH	204	-	-	X	-
8	PEG	JJJ	205	-	-	X	-
9	EDO	KKK	203	-	-	X	-
9	EDO	KKK	204	-	-	X	-

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 19418 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.

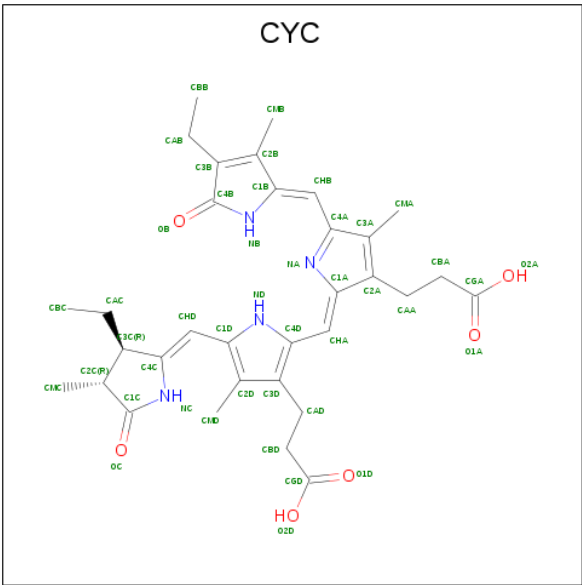
- Molecule 1 is a protein called Allophycocyanin alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	160	Total	C	N	O	S	0	10	0
			1272	800	222	243	7			
1	CCC	160	Total	C	N	O	S	0	15	0
			1292	820	223	243	6			
1	EEE	160	Total	C	N	O	S	0	12	0
			1285	808	226	245	6			
1	GGG	160	Total	C	N	O	S	0	13	0
			1272	803	220	243	6			
1	III	160	Total	C	N	O	S	0	8	0
			1247	785	215	241	6			
1	KKK	160	Total	C	N	O	S	0	16	0
			1319	830	230	252	7			

- Molecule 2 is a protein called Allophycocyanin beta.

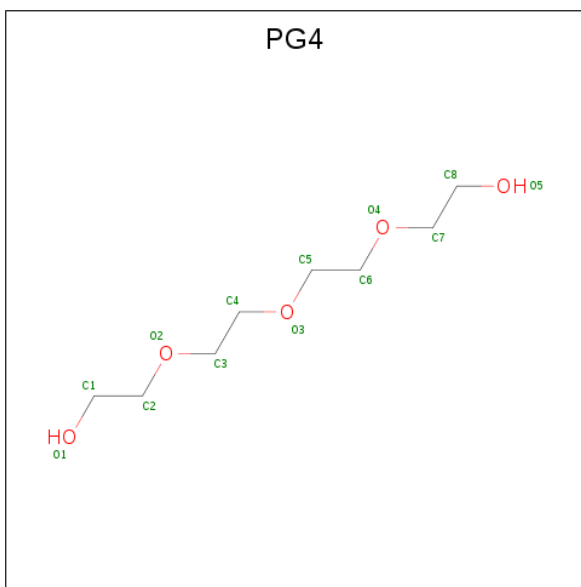
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	161	Total	C	N	O	S	0	15	0
			1303	831	213	253	6			
2	DDD	161	Total	C	N	O	S	0	19	0
			1309	837	210	256	6			
2	FFF	161	Total	C	N	O	S	0	3	0
			1236	779	207	244	6			
2	HHH	161	Total	C	N	O	S	0	13	0
			1290	818	210	256	6			
2	JJJ	161	Total	C	N	O	S	0	9	0
			1258	797	209	246	6			
2	LLL	161	Total	C	N	O	S	0	11	0
			1280	813	213	248	6			

- Molecule 3 is PHYCOCYANOBILIN (three-letter code: CYC) (formula:  $C_{33}H_{40}N_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



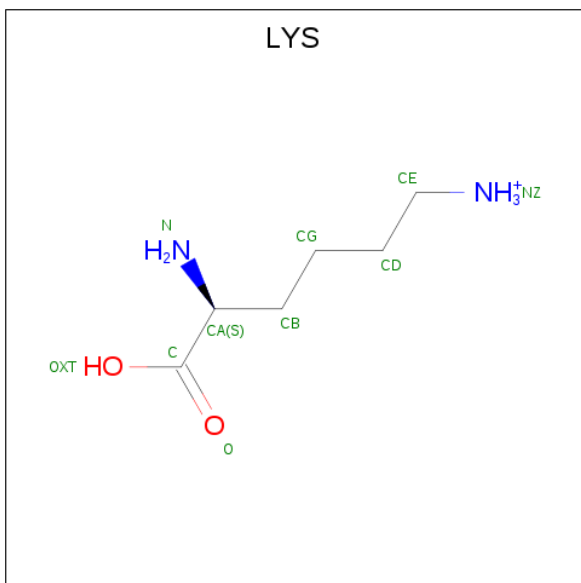
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	0	0
			43	33	4	6		
3	BBB	1	Total	C	N	O	0	0
			43	33	4	6		
3	CCC	1	Total	C	N	O	0	0
			43	33	4	6		
3	DDD	1	Total	C	N	O	0	0
			43	33	4	6		
3	EEE	1	Total	C	N	O	0	0
			43	33	4	6		
3	FFF	1	Total	C	N	O	0	0
			43	33	4	6		
3	GGG	1	Total	C	N	O	0	0
			43	33	4	6		
3	HHH	1	Total	C	N	O	0	0
			43	33	4	6		
3	III	1	Total	C	N	O	0	0
			43	33	4	6		
3	JJJ	1	Total	C	N	O	0	0
			43	33	4	6		
3	KKK	1	Total	C	N	O	0	0
			43	33	4	6		
3	LLL	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



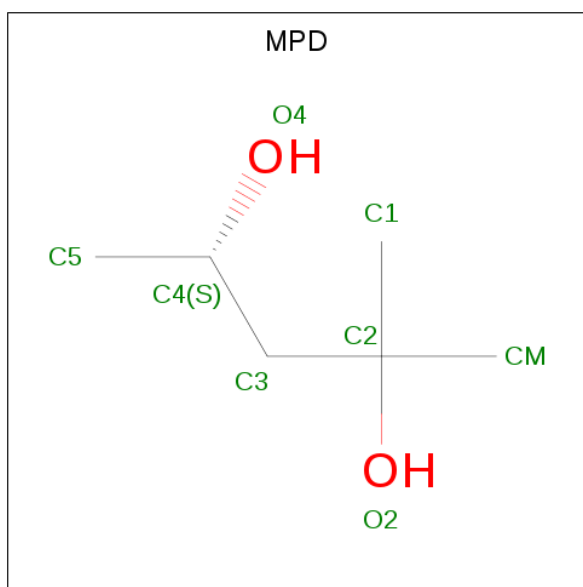
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			13	8	5		
4	CCC	1	Total	C	O	0	0
			13	8	5		
4	FFF	1	Total	C	O	0	0
			13	8	5		
4	JJJ	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is LYSINE (three-letter code: LYS) (formula:  $C_6H_{15}N_2O_2$ ).



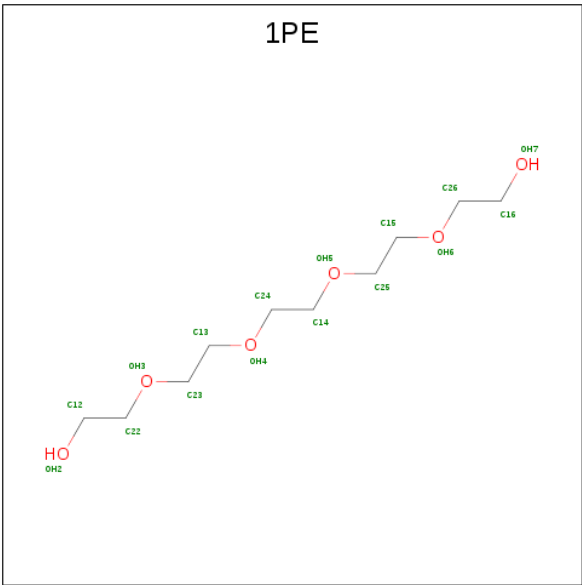
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	BBB	1	Total	C	N	O	0	1
			16	11	3	2		
5	III	1	Total	C	N	O	0	0
			10	6	2	2		
5	KKK	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



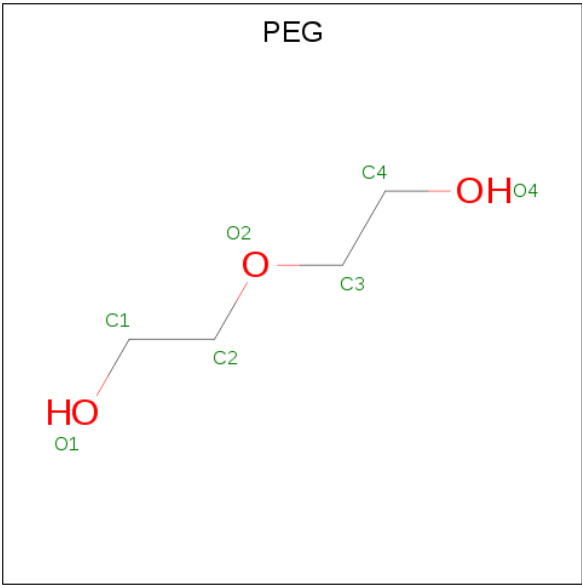
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	BBB	1	Total	C	O	0	0
			8	6	2		
6	DDD	1	Total	C	O	0	0
			8	6	2		
6	EEE	1	Total	C	O	0	0
			8	6	2		
6	FFF	1	Total	C	O	0	0
			8	6	2		
6	HHH	1	Total	C	O	0	0
			8	6	2		
6	JJJ	1	Total	C	O	0	0
			8	6	2		
6	LLL	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	BBB	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 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
8	BBB	1	Total	C	O	0	0
			7	4	3		
8	BBB	1	Total	C	O	0	0
			7	4	3		
8	BBB	1	Total	C	O	0	0
			7	4	3		

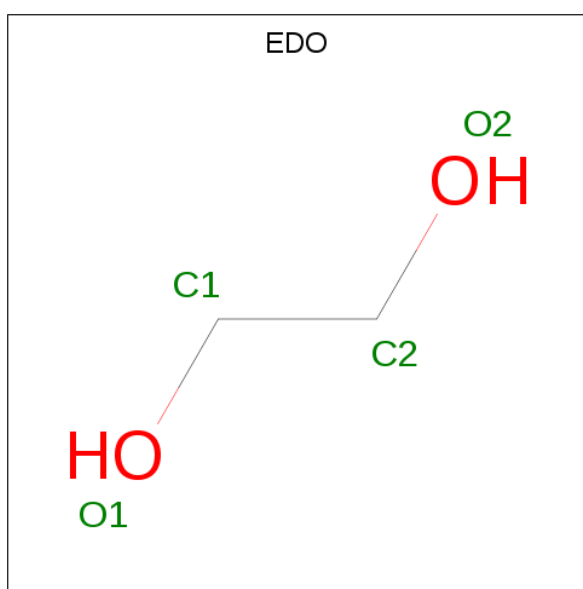
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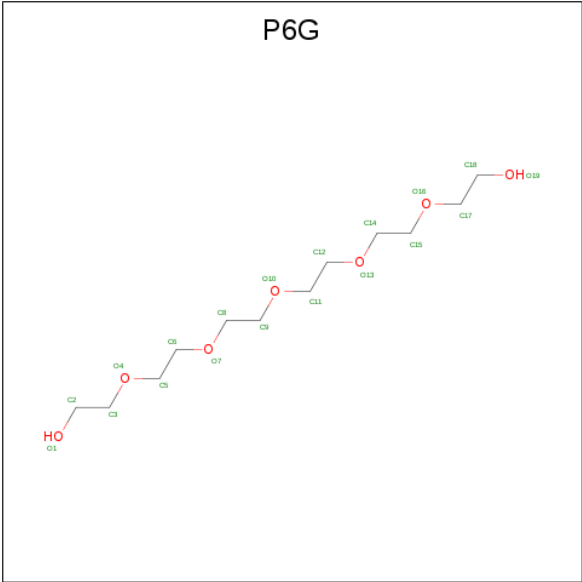
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	CCC	1	Total	C	O	0	0
			7	4	3		
8	GGG	1	Total	C	O	0	0
			7	4	3		
8	HHH	1	Total	C	O	0	0
			7	4	3		
8	JJJ	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



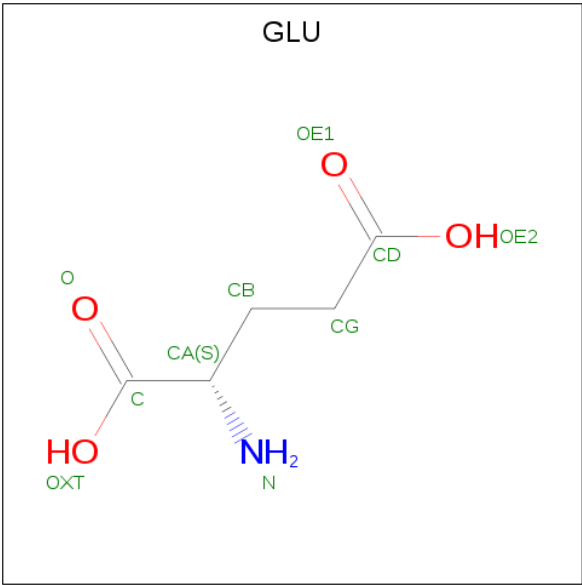
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	BBB	1	Total	C	O	0	0
			4	2	2		
9	CCC	1	Total	C	O	0	0
			4	2	2		
9	CCC	1	Total	C	O	0	0
			4	2	2		
9	KKK	1	Total	C	O	0	0
			4	2	2		
9	KKK	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



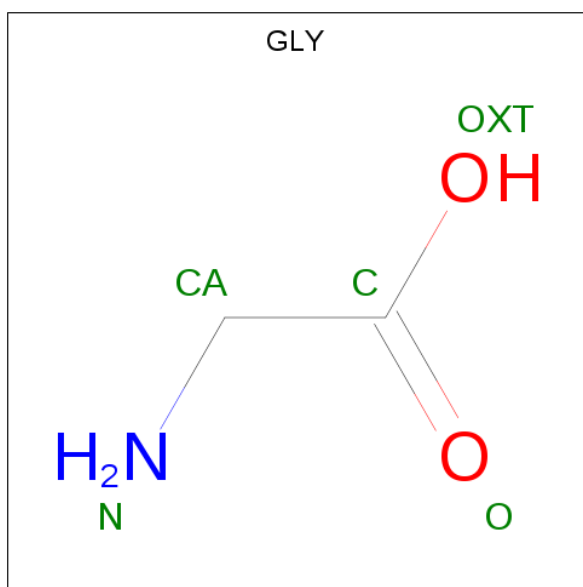
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	CCC	1	Total	C	O	0	0
			19	12	7		

- Molecule 11 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



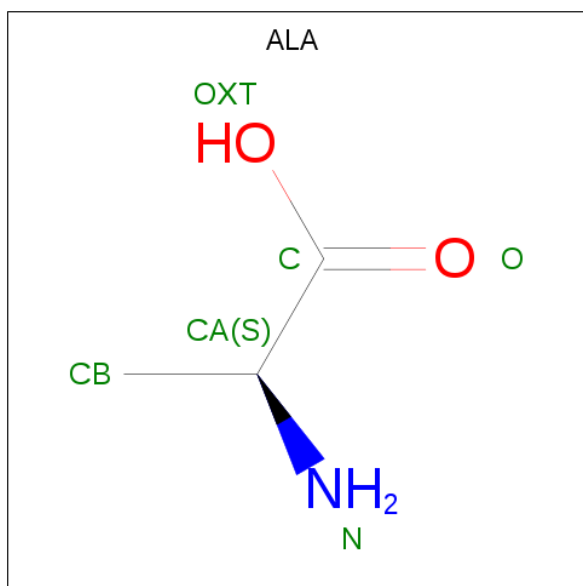
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	DDD	1	Total	C	N	O	0	0
			10	5	1	4		
11	HHH	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 12 is GLYCINE (three-letter code: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	EEE	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 13 is ALANINE (three-letter code: ALA) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	FFF	1	Total	C	N	O	0	0
			6	3	1	2		

- Molecule 14 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



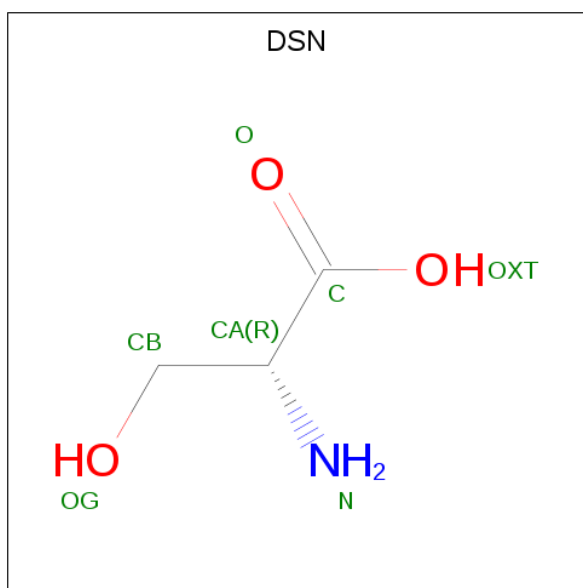
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	GGG	1	Total	C	O	0	0
			8	6	2		

- Molecule 15 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	GGG	1	Total	C	O	0	0
			10	6	4		
15	GGG	1	Total	C	O	0	0
			10	6	4		
15	LLL	1	Total	C	O	0	0
			10	6	4		

- Molecule 16 is D-SERINE (three-letter code: DSN) (formula:  $C_3H_7NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	JJJ	1	Total	C	N	O	0	0
			7	3	1	3		
16	LLL	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	AAA	230	Total	O	0	0
			230	230		
17	BBB	281	Total	O	0	0
			281	281		
17	CCC	299	Total	O	0	0
			299	299		
17	DDD	303	Total	O	0	0
			303	303		
17	EEE	246	Total	O	0	0
			246	246		
17	FFF	286	Total	O	0	0
			286	286		
17	GGG	241	Total	O	0	0
			241	241		
17	HHH	284	Total	O	0	0
			284	284		
17	III	252	Total	O	0	0
			252	252		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	JJJ	284	Total 284	O 284	0	0
17	KKK	238	Total 238	O 238	0	0
17	LLL	264	Total 264	O 264	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: Allophycocyanin alpha



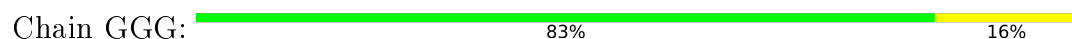
- Molecule 1: Allophycocyanin alpha



- Molecule 1: Allophycocyanin alpha



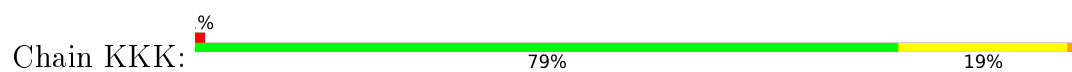
- Molecule 1: Allophycocyanin alpha



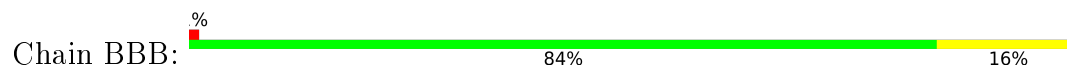
- Molecule 1: Allophycocyanin alpha



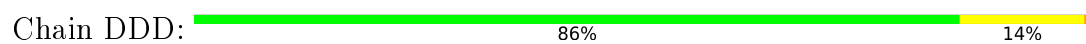
- Molecule 1: Allophycocyanin alpha



- Molecule 2: Allophycocyanin beta



- Molecule 2: Allophycocyanin beta



- Molecule 2: Allophycocyanin beta



- Molecule 2: Allophycocyanin beta



- Molecule 2: Allophycocyanin beta



- Molecule 2: Allophycocyanin beta





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.69 Å   177.73 Å   106.37 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	106.37 – 1.42 106.37 – 1.42	Depositor EDS
% Data completeness (in resolution range)	87.3 (106.37-1.42) 87.3 (106.37-1.42)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 1.42 Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.126   ,   0.175 0.130   ,   0.178	Depositor DCC
$R_{free}$ test set	19133 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	19418	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	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 48.78 % 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 8.1971e-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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CYC, MPD, PG4, PGE, 1PE, MEN, DSN, MRD, P6G, PEG, EDO

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	AAA	0.67	0/1320	0.79	1/1780 (0.1%)
1	CCC	0.70	0/1358	0.81	0/1831
1	EEE	0.69	0/1342	0.80	3/1808 (0.2%)
1	GGG	0.70	0/1326	0.84	2/1790 (0.1%)
1	III	0.71	0/1286	0.79	1/1735 (0.1%)
1	KKK	0.71	0/1358	0.84	2/1834 (0.1%)
2	BBB	0.67	0/1358	0.75	0/1836
2	DDD	0.73	0/1373	0.78	0/1857
2	FFF	0.67	0/1249	0.78	1/1689 (0.1%)
2	HHH	0.72	0/1333	0.76	0/1804
2	JJJ	0.65	0/1292	0.77	1/1746 (0.1%)
2	LLL	0.66	0/1317	0.76	1/1781 (0.1%)
All	All	0.69	0/15912	0.79	12/21491 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	FFF	116	TYR	CB-CG-CD1	5.72	124.44	121.00
2	JJJ	116	TYR	CB-CG-CD1	5.52	124.31	121.00
1	III	35	ARG	CG-CD-NE	-5.36	100.56	111.80
2	LLL	94	TYR	CB-CG-CD1	5.34	124.21	121.00
1	EEE	35[A]	ARG	CG-CD-NE	-5.32	100.64	111.80
1	EEE	35[B]	ARG	CG-CD-NE	-5.32	100.64	111.80
1	GGG	86	TYR	CB-CG-CD1	5.31	124.19	121.00
1	AAA	86	TYR	CB-CG-CD1	5.30	124.18	121.00
1	KKK	58[A]	PHE	CB-CA-C	5.27	120.94	110.40
1	KKK	58[B]	PHE	CB-CA-C	5.27	120.94	110.40
1	EEE	86	TYR	CB-CG-CD1	5.17	124.10	121.00
1	GGG	82	ARG	CG-CD-NE	5.16	122.64	111.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	AAA	1272	0	1312	26	0
1	CCC	1292	0	1370	35	0
1	EEE	1285	0	1333	28	0
1	GGG	1272	0	1324	43	0
1	III	1247	0	1282	12	0
1	KKK	1319	0	1349	52	0
2	BBB	1303	0	1359	49	0
2	DDD	1309	0	1372	22	0
2	FFF	1236	0	1247	6	0
2	HHH	1290	0	1322	26	0
2	JJJ	1258	0	1292	13	0
2	LLL	1280	0	1322	17	0
3	AAA	43	0	37	4	0
3	BBB	43	0	37	3	0
3	CCC	43	0	37	3	0
3	DDD	43	0	37	2	0
3	EEE	43	0	37	3	0
3	FFF	43	0	37	2	0
3	GGG	43	0	37	3	0
3	HHH	43	0	37	3	0
3	III	43	0	37	3	0
3	JJJ	43	0	37	2	0
3	KKK	43	0	37	3	0
3	LLL	43	0	37	3	0
4	AAA	13	0	18	11	0
4	CCC	13	0	18	15	0
4	FFF	13	0	18	0	0
4	JJJ	13	0	18	2	0
5	BBB	16	0	24	0	0
5	III	10	0	12	0	0
5	KKK	10	0	12	1	0
6	BBB	8	0	14	0	0
6	DDD	8	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	EEE	8	0	14	5	0
6	FFF	8	0	14	0	0
6	HHH	8	0	14	1	0
6	JJJ	8	0	14	0	0
6	LLL	8	0	14	0	0
7	BBB	16	0	22	8	0
8	BBB	21	0	30	28	0
8	CCC	7	0	10	4	0
8	GGG	7	0	10	0	0
8	HHH	7	0	10	4	0
8	JJJ	7	0	10	4	0
9	BBB	4	0	6	1	0
9	CCC	8	0	12	0	0
9	KKK	8	0	12	10	0
10	CCC	19	0	26	5	0
11	DDD	10	0	5	2	0
11	HHH	10	0	5	0	0
12	EEE	5	0	2	3	0
13	FFF	6	0	4	2	0
14	GGG	8	0	14	0	0
15	GGG	20	0	28	18	0
15	LLL	10	0	14	2	0
16	JJJ	7	0	6	1	0
16	LLL	7	0	6	0	0
17	AAA	230	0	0	5	0
17	BBB	281	0	0	17	0
17	CCC	299	0	0	7	0
17	DDD	303	0	0	11	0
17	EEE	246	0	0	7	0
17	FFF	286	0	0	2	0
17	GGG	241	0	0	18	0
17	HHH	284	0	0	13	0
17	III	252	0	0	5	1
17	JJJ	284	0	0	6	0
17	KKK	238	0	0	16	0
17	LLL	264	0	0	8	1
All	All	19418	0	16778	379	1

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 11.

All (379) 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:CCC:48[A]:ARG:NH2	4:CCC:203:PG4:H41	1.29	1.46
2:HHH:35[C]:GLU:HG3	17:HHH:301:HOH:O	1.37	1.24
2:LLL:131[B]:GLN:NE2	17:LLL:301:HOH:O	1.73	1.19
2:DDD:86[B]:ASP:OD1	17:DDD:302:HOH:O	1.60	1.18
2:DDD:15[B]:GLN:OE1	17:DDD:303:HOH:O	1.65	1.13
1:GGG:76[A]:MET:HE2	17:GGG:428:HOH:O	0.97	1.13
1:EEE:37[C]:ARG:CZ	17:EEE:303:HOH:O	1.97	1.12
2:DDD:15[B]:GLN:NE2	17:DDD:304:HOH:O	1.80	1.11
10:CCC:202:P6G:H122	4:CCC:203:PG4:H71	1.30	1.10
1:CCC:48[A]:ARG:HH22	4:CCC:203:PG4:C4	1.65	1.10
1:AAA:46[B]:ARG:HG3	1:AAA:46[B]:ARG:HH11	1.18	1.08
2:HHH:35[C]:GLU:CG	17:HHH:301:HOH:O	1.91	1.08
1:CCC:48[B]:ARG:NH2	4:CCC:203:PG4:H41	1.69	1.07
1:GGG:56[B]:GLN:NE2	17:GGG:303:HOH:O	1.90	1.04
1:CCC:4[B]:THR:HG21	17:CCC:368:HOH:O	1.57	1.04
1:CCC:48[A]:ARG:NH2	4:CCC:203:PG4:C4	2.21	1.03
10:CCC:202:P6G:H122	4:CCC:203:PG4:C7	1.88	1.03
1:EEE:147[B]:GLU:OE1	12:EEE:202:GLY:N	1.91	1.02
2:HHH:21[B]:ASN:OD1	17:HHH:303:HOH:O	1.79	1.01
2:BBB:39[B]:ARG:CD	8:BBB:208:PEG:O4	2.09	1.00
1:CCC:35[A]:ARG:NH1	17:CCC:302:HOH:O	1.84	1.00
9:KKK:203:EDO:H12	17:KKK:305:HOH:O	1.60	1.00
2:LLL:6[B]:THR:HG22	17:LLL:348:HOH:O	1.59	0.99
17:CCC:308:HOH:O	2:DDD:6[A]:THR:HG22	1.63	0.98
2:BBB:117[B]:ASN:OD1	17:BBB:302:HOH:O	1.81	0.97
2:DDD:54[B]:GLU:OE2	17:DDD:305:HOH:O	1.83	0.97
8:BBB:208:PEG:O4	17:BBB:303:HOH:O	1.85	0.95
2:BBB:39[B]:ARG:HD2	8:BBB:208:PEG:O4	1.67	0.94
2:BBB:39[B]:ARG:CZ	8:BBB:208:PEG:H31	1.97	0.94
1:GGG:133:LYS:HE2	15:GGG:203:PGE:H3	1.49	0.93
1:GGG:76[A]:MET:HE1	17:GGG:505:HOH:O	1.66	0.93
11:DDD:202:GLU:HG2	11:DDD:202:GLU:OXT	1.66	0.93
8:BBB:208:PEG:C2	15:GGG:203:PGE:H32	2.00	0.92
2:LLL:6[B]:THR:CG2	17:LLL:348:HOH:O	2.14	0.91
2:BBB:39[B]:ARG:CZ	8:BBB:208:PEG:C3	2.48	0.91
8:BBB:208:PEG:H21	15:GGG:203:PGE:H32	1.53	0.90
10:CCC:202:P6G:C12	4:CCC:203:PG4:H71	2.03	0.89
2:DDD:45[B]:SER:OG	17:DDD:306:HOH:O	1.89	0.88
3:KKK:201:CYC:HMA1	3:KKK:201:CYC:HB	1.38	0.88
2:JJJ:15[B]:GLN:CD	17:JJJ:302:HOH:O	2.12	0.87
1:AAA:48[A]:ARG:HH21	1:AAA:139:LEU:HD21	1.38	0.87
2:JJJ:15[B]:GLN:OE1	17:JJJ:302:HOH:O	1.92	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:EEE:201:CYC:HB	3:EEE:201:CYC:HMA1	1.39	0.86
2:HHH:35[C]:GLU:CD	17:HHH:301:HOH:O	2.08	0.86
1:EEE:37[B]:ARG:HG2	1:EEE:37[B]:ARG:HH11	1.39	0.86
2:HHH:35[A]:GLU:OE1	17:HHH:304:HOH:O	1.92	0.86
3:III:201:CYC:HB	3:III:201:CYC:HMA1	1.40	0.85
1:GGG:134[A]:SER:HA	15:GGG:203:PGE:H6	1.56	0.85
2:HHH:86[B]:ASP:OD2	17:HHH:305:HOH:O	1.93	0.85
1:KKK:61[A]:ARG:NH1	1:KKK:63[A]:ASP:OD1	2.10	0.85
3:GGG:201:CYC:HMA1	3:GGG:201:CYC:HB	1.40	0.85
1:AAA:27:SER:OG	1:GGG:24[B]:ARG:CZ	2.25	0.84
1:GGG:134[B]:SER:HA	15:GGG:203:PGE:H6	1.56	0.84
3:AAA:201:CYC:HB	3:AAA:201:CYC:HMA1	1.40	0.84
2:BBB:39[B]:ARG:NH1	8:BBB:208:PEG:H31	1.91	0.84
2:BBB:39[B]:ARG:NH1	17:BBB:304:HOH:O	2.10	0.83
1:KKK:156:VAL:O	1:KKK:160:GLN:HG3	1.78	0.83
1:EEE:60:LYS:O	9:KKK:204:EDO:H22	1.80	0.82
2:DDD:14[B]:VAL:HG23	17:DDD:368:HOH:O	1.78	0.82
3:CCC:201:CYC:HMA1	3:CCC:201:CYC:HB	1.43	0.82
1:CCC:48[B]:ARG:HH22	4:CCC:203:PG4:H41	1.42	0.81
2:DDD:86[B]:ASP:OD2	17:DDD:308:HOH:O	1.99	0.80
2:DDD:86[B]:ASP:OD2	17:DDD:307:HOH:O	1.98	0.80
6:EEE:203:MPD:O2	17:EEE:302:HOH:O	1.99	0.80
8:BBB:208:PEG:H21	15:GGG:203:PGE:C3	2.12	0.79
1:AAA:11:ASP:OD2	4:AAA:202:PG4:H11	1.83	0.79
2:JJJ:15[B]:GLN:NE2	17:JJJ:302:HOH:O	2.15	0.78
4:AAA:202:PG4:H72	2:BBB:87:TYR:CE1	2.19	0.77
1:GGG:133:LYS:HE2	15:GGG:203:PGE:H5	1.67	0.77
1:CCC:34[B]:GLN:HG3	1:CCC:37[B]:ARG:HH12	1.49	0.77
1:EEE:37[B]:ARG:HH11	1:EEE:37[B]:ARG:CG	1.98	0.75
1:KKK:61[A]:ARG:HH11	1:KKK:61[A]:ARG:HB3	1.48	0.75
2:HHH:21[B]:ASN:ND2	17:HHH:308:HOH:O	2.19	0.75
2:BBB:131[A]:GLN:OE1	2:BBB:134:LYS:HE2	1.88	0.74
1:GGG:28:PHE:CE1	1:GGG:35[A]:ARG:NH2	2.55	0.74
1:GGG:76[A]:MET:CE	17:GGG:428:HOH:O	1.76	0.74
1:EEE:147[B]:GLU:OE1	12:EEE:202:GLY:CA	2.35	0.74
1:CCC:48[A]:ARG:HH22	4:CCC:203:PG4:H41	0.93	0.73
1:GGG:2:ILE:HD11	1:GGG:24[B]:ARG:HB3	1.70	0.73
8:HHH:204:PEG:H41	17:HHH:318:HOH:O	1.88	0.73
1:EEE:37[C]:ARG:NH2	17:EEE:303:HOH:O	2.11	0.73
11:DDD:202:GLU:OXT	11:DDD:202:GLU:CG	2.35	0.73
8:BBB:208:PEG:H41	17:BBB:307:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:KKK:204:EDO:H21	17:KKK:327:HOH:O	1.89	0.72
2:BBB:39[B]:ARG:HD2	8:BBB:208:PEG:HO4	1.55	0.72
1:CCC:48[A]:ARG:HH21	4:CCC:203:PG4:H41	1.45	0.72
1:GGG:137:ALA:HB2	15:GGG:203:PGE:H22	1.72	0.71
1:CCC:28:PHE:CE1	1:CCC:35[A]:ARG:NH2	2.58	0.71
1:KKK:37[A]:ARG:NH1	17:KKK:304:HOH:O	2.23	0.71
1:GGG:24[B]:ARG:NE	1:GGG:24[B]:ARG:HA	2.06	0.70
1:KKK:48[C]:ARG:HH11	1:KKK:48[C]:ARG:HB3	1.54	0.70
1:AAA:96[B]:VAL:HG11	2:BBB:27:LEU:HD13	1.73	0.70
1:GGG:56[B]:GLN:NE2	17:GGG:302:HOH:O	1.79	0.70
1:EEE:56:GLN:O	1:EEE:60:LYS:HD3	1.92	0.69
1:GGG:51[A]:LYS:NZ	17:GGG:306:HOH:O	2.26	0.69
1:GGG:2:ILE:HD11	1:GGG:24[A]:ARG:HB3	1.74	0.69
1:KKK:48[C]:ARG:HH11	1:KKK:48[C]:ARG:CB	2.07	0.68
1:EEE:37[C]:ARG:NE	17:EEE:303:HOH:O	2.17	0.68
1:EEE:40:GLN:HE22	2:FFF:24:LEU:HD11	1.59	0.67
1:III:37:ARG:HH21	1:III:40[A]:GLN:NE2	1.92	0.67
6:EEE:203:MPD:C1	6:EEE:203:MPD:H53	2.23	0.67
6:EEE:203:MPD:H53	6:EEE:203:MPD:H13	1.76	0.67
8:BBB:208:PEG:C4	17:BBB:303:HOH:O	2.40	0.67
2:BBB:35:GLU:OE1	2:BBB:39[B]:ARG:CG	2.43	0.66
2:BBB:65[B]:ILE:HG13	17:BBB:488:HOH:O	1.95	0.66
1:EEE:24:ARG:HG2	17:III:496:HOH:O	1.95	0.66
3:GGG:201:CYC:HMD2	3:GGG:201:CYC:HC	1.60	0.66
3:III:201:CYC:HMD2	3:III:201:CYC:HC	1.60	0.66
3:AAA:201:CYC:HMD2	3:AAA:201:CYC:HC	1.60	0.66
1:CCC:2[B]:ILE:HD11	1:CCC:24:ARG:NH1	2.10	0.66
2:BBB:39[B]:ARG:CZ	8:BBB:208:PEG:H32	2.26	0.66
3:KKK:201:CYC:HC	3:KKK:201:CYC:HMD2	1.61	0.66
3:EEE:201:CYC:HC	3:EEE:201:CYC:HMD2	1.61	0.65
1:GGG:35[A]:ARG:NH1	17:GGG:305:HOH:O	2.23	0.65
2:BBB:143:PRO:HA	7:BBB:204:1PE:C12	2.27	0.65
2:BBB:143:PRO:HA	7:BBB:204:1PE:H121	1.79	0.65
1:EEE:37[B]:ARG:HG2	1:EEE:37[B]:ARG:NH1	2.11	0.65
2:BBB:5[A]:ILE:HD12	2:BBB:27:LEU:HD22	1.79	0.64
2:HHH:116:TYR:OH	17:HHH:306:HOH:O	2.14	0.64
2:DDD:2[A]:GLN:NE2	17:DDD:301:HOH:O	2.29	0.64
1:KKK:57:LEU:O	1:KKK:61[B]:ARG:HB2	1.97	0.64
2:BBB:39[A]:ARG:HH22	8:BBB:205:PEG:H11	1.62	0.64
1:KKK:23[B]:ASP:OD2	17:KKK:301:HOH:O	2.15	0.64
1:EEE:40:GLN:NE2	2:FFF:24:LEU:CD1	2.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:EEE:203:MPD:H4	17:EEE:384:HOH:O	1.98	0.64
9:BBB:207:EDO:H12	17:BBB:443:HOH:O	1.97	0.63
2:LLL:39[B]:ARG:NH2	15:LLL:204:PGE:O4	2.31	0.63
2:DDD:21[B]:ASN:ND2	17:DDD:312:HOH:O	2.27	0.63
1:III:48[A]:ARG:NH2	1:III:139:LEU:HD21	2.13	0.63
1:EEE:40:GLN:NE2	2:FFF:24:LEU:HD11	2.14	0.63
1:AAA:46[B]:ARG:HG3	1:AAA:46[B]:ARG:NH1	1.97	0.63
1:GGG:24[A]:ARG:NH2	17:GGG:307:HOH:O	2.31	0.62
2:DDD:43:THR:CG2	2:DDD:140[B]:LEU:HG	2.29	0.62
1:GGG:52:GLN:NE2	17:GGG:308:HOH:O	2.32	0.62
3:DDD:201:CYC:HMD2	3:DDD:201:CYC:HC	1.65	0.62
1:KKK:56:GLN:O	1:KKK:60[B]:LYS:HB3	1.98	0.62
1:KKK:66[A]:SER:HB2	9:KKK:204:EDO:O1	1.99	0.61
15:GGG:203:PGE:H62	17:GGG:438:HOH:O	2.00	0.61
1:AAA:2:ILE:HG12	1:AAA:24[A]:ARG:HG3	1.82	0.61
1:KKK:64[A]:VAL:HG12	1:KKK:121:PRO:HG3	1.81	0.61
1:KKK:63[A]:ASP:HB2	9:KKK:204:EDO:H21	1.82	0.61
3:LLL:201:CYC:HMD2	3:LLL:201:CYC:HC	1.65	0.61
1:AAA:27:SER:OG	1:GGG:24[B]:ARG:NE	2.33	0.60
1:GGG:112[B]:ARG:HH22	1:GGG:160:GLN:C	2.05	0.60
1:KKK:59[B]:GLN:NE2	17:KKK:306:HOH:O	2.34	0.60
1:CCC:112[B]:ARG:NH2	1:CCC:160:GLN:O	2.34	0.60
3:CCC:201:CYC:HMD2	3:CCC:201:CYC:HC	1.67	0.60
1:GGG:137:ALA:HB2	15:GGG:203:PGE:C2	2.31	0.59
2:LLL:65[B]:ILE:HG13	17:LLL:481:HOH:O	2.02	0.59
1:GGG:51[A]:LYS:HE2	1:GGG:51[A]:LYS:HA	1.85	0.59
1:KKK:40:GLN:HE22	2:LLL:24:LEU:HD11	1.67	0.59
1:III:56[A]:GLN:NE2	17:III:305:HOH:O	2.31	0.59
3:BBB:201:CYC:HC	3:BBB:201:CYC:HMD2	1.67	0.59
1:AAA:48[B]:ARG:CB	1:AAA:48[B]:ARG:CZ	2.82	0.58
1:KKK:123:ASP:CG	17:KKK:303:HOH:O	2.42	0.58
1:III:37:ARG:HH21	1:III:40[A]:GLN:HE21	1.49	0.58
2:BBB:131[A]:GLN:OE1	2:BBB:134:LYS:CE	2.52	0.58
1:CCC:24:ARG:NH2	1:KKK:23[B]:ASP:OD2	2.35	0.58
2:HHH:6[A]:THR:HG23	17:HHH:390:HOH:O	2.03	0.58
2:BBB:143:PRO:HD3	7:BBB:204:1PE:H132	1.85	0.58
2:BBB:35:GLU:OE1	2:BBB:39[B]:ARG:HG3	2.04	0.58
1:III:112:ARG:NH2	1:III:158:ALA:O	2.36	0.58
2:JJJ:78:TYR:CG	1:KKK:114[B]:MET:HE2	2.38	0.57
2:HHH:86[B]:ASP:OD1	17:HHH:307:HOH:O	2.17	0.57
3:AAA:201:CYC:HMA1	3:AAA:201:CYC:NB	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:HHH:201:CYC:HC	3:HHH:201:CYC:HMD2	1.68	0.57
1:KKK:65[B]:VAL:HB	9:KKK:203:EDO:O1	2.05	0.57
8:BBB:208:PEG:H22	15:GGG:203:PGE:H32	1.85	0.56
2:BBB:39[A]:ARG:NH2	8:BBB:205:PEG:H11	2.20	0.56
2:BBB:106[B]:GLU:HG3	17:BBB:344:HOH:O	2.04	0.56
2:DDD:21[B]:ASN:OD1	17:DDD:309:HOH:O	2.18	0.56
2:BBB:5[A]:ILE:HD12	2:BBB:27:LEU:CD2	2.35	0.56
2:JJJ:21[B]:ASN:ND2	17:JJJ:303:HOH:O	2.39	0.56
1:III:48[A]:ARG:HH22	1:III:139:LEU:HD21	1.71	0.56
1:AAA:2:ILE:HG12	1:AAA:24[B]:ARG:HG3	1.87	0.56
2:HHH:7[A]:SER:OG	8:HHH:204:PEG:H11	2.06	0.56
1:GGG:17:LEU:O	17:GGG:304:HOH:O	2.17	0.55
2:BBB:35:GLU:OE1	2:BBB:39[B]:ARG:HG2	2.05	0.55
3:GGG:201:CYC:HMA1	3:GGG:201:CYC:NB	2.17	0.55
1:GGG:96[B]:VAL:HG11	2:HHH:27:LEU:HD13	1.87	0.55
2:HHH:14[A]:VAL:HG13	17:HHH:458:HOH:O	2.06	0.55
3:III:201:CYC:HMA1	3:III:201:CYC:NB	2.17	0.55
1:AAA:14:ALA:HB2	4:AAA:202:PG4:H52	1.88	0.55
1:CCC:96[B]:VAL:HG11	2:DDD:27:LEU:HD13	1.89	0.55
1:CCC:48[A]:ARG:NH1	17:CCC:305:HOH:O	2.40	0.54
1:CCC:48[B]:ARG:HH22	4:CCC:203:PG4:C4	2.19	0.54
1:CCC:2[B]:ILE:HG21	1:CCC:28:PHE:CG	2.43	0.53
1:EEE:60:LYS:O	9:KKK:204:EDO:C2	2.54	0.53
1:AAA:36:LEU:HD23	1:AAA:96[B]:VAL:HG22	1.91	0.53
4:AAA:202:PG4:H22	4:AAA:202:PG4:O3	2.09	0.53
1:EEE:31:GLY:C	1:EEE:35[B]:ARG:HH12	2.11	0.53
3:KKK:201:CYC:HMA1	3:KKK:201:CYC:NB	2.16	0.53
2:BBB:39[B]:ARG:NH2	8:BBB:208:PEG:H31	2.23	0.53
13:FFF:202:ALA:N	17:FFF:303:HOH:O	2.40	0.53
8:BBB:208:PEG:C3	17:BBB:307:HOH:O	2.57	0.53
17:CCC:308:HOH:O	2:DDD:6[A]:THR:CG2	2.39	0.53
2:LLL:143:PRO:HD3	15:LLL:204:PGE:H12	1.90	0.53
3:JJJ:201:CYC:HMD2	3:JJJ:201:CYC:HC	1.74	0.52
2:BBB:39[B]:ARG:NH2	8:BBB:208:PEG:C3	2.72	0.52
2:HHH:43:THR:CG2	2:HHH:140[B]:LEU:HG	2.40	0.52
1:KKK:50:VAL:HG22	1:KKK:132[B]:MET:HE1	1.92	0.52
2:BBB:39[B]:ARG:NE	8:BBB:208:PEG:O4	2.42	0.52
1:KKK:57:LEU:O	1:KKK:61[B]:ARG:N	2.43	0.52
1:AAA:11:ASP:OD2	4:AAA:202:PG4:C1	2.56	0.52
2:HHH:33:THR:HB	6:HHH:203:MPD:HM3	1.92	0.52
1:CCC:34[B]:GLN:CG	1:CCC:37[B]:ARG:HH12	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GGG:143:GLU:CD	1:GGG:143:GLU:H	2.12	0.51
1:AAA:76[C]:MET:HG2	17:AAA:402:HOH:O	2.10	0.51
15:GGG:203:PGE:H22	15:GGG:203:PGE:H52	1.93	0.51
1:GGG:24[B]:ARG:NH1	17:GGG:307:HOH:O	2.42	0.51
1:EEE:160:GLN:HE21	1:EEE:160:GLN:HA	1.76	0.51
3:CCC:201:CYC:HMA1	3:CCC:201:CYC:NB	2.20	0.51
1:EEE:40:GLN:HE22	2:FFF:24:LEU:CD1	2.21	0.51
2:BBB:143:PRO:CA	7:BBB:204:1PE:H121	2.39	0.51
3:EEE:201:CYC:HMA1	3:EEE:201:CYC:NB	2.16	0.51
8:BBB:208:PEG:C4	17:BBB:307:HOH:O	2.55	0.51
2:HHH:7[A]:SER:OG	8:HHH:204:PEG:C1	2.58	0.51
2:BBB:131[A]:GLN:CD	17:BBB:314:HOH:O	2.49	0.50
8:CCC:204:PEG:H42	17:KKK:301:HOH:O	2.10	0.50
3:FFF:201:CYC:HMD2	3:FFF:201:CYC:HC	1.76	0.50
1:GGG:2:ILE:HD12	1:GGG:24[A]:ARG:NH1	2.26	0.50
2:DDD:43:THR:HG22	2:DDD:140[B]:LEU:HG	1.93	0.50
10:CCC:202:P6G:C12	4:CCC:203:PG4:C7	2.74	0.50
1:KKK:88:LEU:HB2	1:KKK:132[B]:MET:HE1	1.93	0.50
1:CCC:51[B]:LYS:HE2	17:CCC:420:HOH:O	2.11	0.50
2:LLL:117[B]:ASN:OD1	17:LLL:302:HOH:O	2.18	0.50
1:GGG:24[B]:ARG:HD3	17:GGG:307:HOH:O	2.12	0.49
2:JJJ:78:TYR:CB	1:KKK:114[B]:MET:HE2	2.41	0.49
2:JJJ:128:GLN:OE1	8:JJJ:205:PEG:H11	2.13	0.49
1:EEE:160:GLN:HG3	1:KKK:116:LYS:HE3	1.94	0.49
2:DDD:131:GLN:HE22	2:DDD:134[A]:LYS:NZ	2.10	0.49
3:JJJ:201:CYC:HMA1	16:JJJ:202:DSN:HB2	1.93	0.49
1:CCC:2[C]:ILE:HG12	1:CCC:98:GLY:O	2.13	0.49
2:DDD:56:VAL:HG21	2:DDD:82[B]:ILE:HD12	1.95	0.49
1:EEE:31:GLY:C	1:EEE:35[B]:ARG:NH1	2.66	0.49
2:LLL:77[B]:ARG:NH1	17:LLL:305:HOH:O	2.44	0.49
1:AAA:104:GLU:HA	1:AAA:108:ILE:HB	1.95	0.49
2:BBB:15[B]:GLN:NE2	17:BBB:310:HOH:O	2.45	0.49
2:HHH:26:LYS:HE2	8:HHH:204:PEG:H21	1.94	0.48
2:HHH:131:GLN:HE22	2:HHH:134:LYS:NZ	2.11	0.48
1:KKK:50:VAL:HG22	1:KKK:132[B]:MET:CE	2.43	0.48
1:KKK:102:PRO:HD3	17:KKK:308:HOH:O	2.11	0.48
1:GGG:24[A]:ARG:CZ	17:GGG:307:HOH:O	2.61	0.48
2:DDD:85[A]:LEU:HD13	3:DDD:201:CYC:HBC1	1.96	0.48
2:BBB:39[A]:ARG:HH12	8:BBB:205:PEG:C1	2.26	0.48
1:EEE:5:LYS:HE2	17:EEE:325:HOH:O	2.13	0.48
1:KKK:55:ASP:O	1:KKK:59[B]:GLN:N	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:71:ALA:HA	1:CCC:76[B]:MET:HB3	1.96	0.47
1:KKK:61[A]:ARG:HH12	1:KKK:63[A]:ASP:CG	2.18	0.47
17:BBB:366:HOH:O	1:CCC:76[B]:MET:CE	2.62	0.47
1:KKK:66[A]:SER:HB2	9:KKK:204:EDO:HO1	1.79	0.47
1:KKK:49:ILE:HG22	1:KKK:132[B]:MET:CE	2.44	0.47
1:AAA:48[B]:ARG:CZ	1:AAA:48[B]:ARG:HB2	2.45	0.47
1:AAA:123:ASP:OD2	17:AAA:302:HOH:O	2.20	0.47
1:KKK:104:GLU:HA	1:KKK:108:ILE:HB	1.95	0.47
1:CCC:51[A]:LYS:HE3	17:CCC:506:HOH:O	2.15	0.47
1:GGG:71:ALA:HA	1:GGG:76[A]:MET:HB3	1.96	0.47
2:JJJ:131:GLN:HE22	2:JJJ:134:LYS:NZ	2.13	0.47
1:KKK:65[B]:VAL:CG1	9:KKK:203:EDO:O1	2.63	0.47
2:BBB:39[B]:ARG:HD3	8:BBB:208:PEG:O4	2.08	0.47
2:JJJ:63:SER:HB2	8:JJJ:205:PEG:H31	1.96	0.47
1:KKK:61[A]:ARG:NH1	1:KKK:63[A]:ASP:CG	2.68	0.47
1:KKK:88:LEU:HB2	1:KKK:132[B]:MET:CE	2.45	0.46
1:AAA:48[A]:ARG:NH2	1:AAA:139:LEU:HD21	2.19	0.46
1:GGG:48:ARG:HH11	1:GGG:139:LEU:HD11	1.80	0.46
2:BBB:143:PRO:HA	7:BBB:204:1PE:H122	1.94	0.46
6:EEE:203:MPD:C1	6:EEE:203:MPD:C5	2.91	0.46
1:III:71:ALA:HA	1:III:76[B]:MET:HB3	1.97	0.46
4:JJJ:204:PG4:H41	17:JJJ:461:HOH:O	2.15	0.45
1:KKK:40:GLN:NE2	2:LLL:24:LEU:HD11	2.31	0.45
1:GGG:145:ALA:HB1	15:GGG:203:PGE:H2	1.98	0.45
15:GGG:203:PGE:H3	15:GGG:203:PGE:H5	1.52	0.45
1:CCC:2[A]:ILE:HG21	1:CCC:28:PHE:CG	2.51	0.45
1:EEE:147[B]:GLU:OE1	12:EEE:202:GLY:C	2.55	0.45
1:KKK:76:MET:HG2	17:KKK:424:HOH:O	2.17	0.45
4:AAA:202:PG4:C6	2:BBB:90:ARG:HH22	2.30	0.45
4:AAA:202:PG4:H61	2:BBB:90:ARG:HH22	1.80	0.45
1:EEE:2:ILE:HG21	1:EEE:28:PHE:CG	2.52	0.45
1:KKK:64[A]:VAL:HA	17:KKK:349:HOH:O	2.16	0.45
4:CCC:203:PG4:H41	4:CCC:203:PG4:H22	1.69	0.45
1:GGG:133:LYS:HG3	15:GGG:203:PGE:H1	1.98	0.45
8:JJJ:205:PEG:H31	17:JJJ:480:HOH:O	2.17	0.45
1:KKK:66[A]:SER:CB	17:KKK:403:HOH:O	2.64	0.45
2:DDD:130:ILE:HG21	2:DDD:157:CYS:SG	2.57	0.45
1:KKK:55:ASP:O	1:KKK:59[A]:GLN:OE1	2.35	0.45
1:KKK:63[A]:ASP:C	17:KKK:327:HOH:O	2.54	0.45
1:GGG:60:LYS:NZ	17:GGG:320:HOH:O	2.49	0.45
2:HHH:58:LYS:HD2	17:HHH:309:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:59:GLN:HG2	17:AAA:440:HOH:O	2.16	0.45
8:JJJ:205:PEG:H42	8:JJJ:205:PEG:H21	1.62	0.45
1:KKK:65[B]:VAL:CG1	9:KKK:203:EDO:HO1	2.30	0.45
1:GGG:96[B]:VAL:CG1	2:HHH:27:LEU:HD13	2.46	0.44
1:KKK:24:ARG:NE	17:KKK:317:HOH:O	2.50	0.44
1:KKK:49:ILE:HG22	1:KKK:132[B]:MET:HE2	1.99	0.44
1:EEE:60:LYS:N	1:EEE:60:LYS:CD	2.80	0.44
2:HHH:130:ILE:HG21	2:HHH:157:CYS:SG	2.57	0.44
1:CCC:2[C]:ILE:HD11	1:CCC:98:GLY:O	2.18	0.44
1:CCC:24:ARG:HA	8:CCC:204:PEG:H41	2.00	0.44
2:BBB:63:SER:OG	2:BBB:65[A]:ILE:HG22	2.17	0.44
1:CCC:27:SER:CB	8:CCC:204:PEG:H22	2.48	0.44
1:EEE:71:ALA:HA	1:EEE:76[B]:MET:HB3	1.97	0.44
1:GGG:56[B]:GLN:HG2	17:GGG:303:HOH:O	2.18	0.44
1:AAA:11:ASP:CG	4:AAA:202:PG4:H11	2.38	0.44
2:DDD:63:SER:OG	2:DDD:65[B]:ILE:HG22	2.17	0.43
2:FFF:131:GLN:HE22	2:FFF:134:LYS:NZ	2.16	0.43
1:GGG:112[A]:ARG:CZ	17:GGG:393:HOH:O	2.66	0.43
1:AAA:71:ALA:HA	1:AAA:76[A]:MET:HB3	1.98	0.43
2:BBB:39[B]:ARG:NH1	8:BBB:208:PEG:C3	2.67	0.43
1:GGG:104:GLU:HA	1:GGG:108:ILE:HB	1.99	0.43
2:JJJ:62:TYR:CE2	5:KKK:202:LYS:HA	2.53	0.43
1:KKK:47[B]:GLU:HG2	17:KKK:486:HOH:O	2.18	0.43
2:HHH:115:THR:HG21	3:HHH:201:CYC:HMA2	1.99	0.43
2:JJJ:39:ARG:HH12	4:JJJ:204:PG4:H12	1.82	0.43
2:BBB:39[A]:ARG:HH22	8:BBB:205:PEG:C1	2.30	0.43
2:BBB:83:ARG:NH1	3:BBB:201:CYC:O1A	2.52	0.43
1:AAA:11:ASP:O	4:AAA:202:PG4:C5	2.66	0.43
7:BBB:204:1PE:OH7	8:BBB:206:PEG:O4	2.13	0.42
1:CCC:23:ASP:OD2	8:CCC:204:PEG:C1	2.66	0.42
1:CCC:104:GLU:HA	1:CCC:108:ILE:HB	2.00	0.42
1:EEE:51[A]:LYS:HE2	1:EEE:51[A]:LYS:HB3	1.76	0.42
2:BBB:39[B]:ARG:NH2	8:BBB:208:PEG:H32	2.33	0.42
2:HHH:83:ARG:NH1	3:HHH:201:CYC:O1A	2.51	0.42
1:KKK:60[B]:LYS:O	1:KKK:60[B]:LYS:HG3	2.19	0.42
10:CCC:202:P6G:H112	10:CCC:202:P6G:H141	1.65	0.42
3:FFF:201:CYC:HAB2	13:FFF:202:ALA:HB3	2.02	0.42
1:KKK:61[A]:ARG:HH11	1:KKK:61[A]:ARG:CB	2.24	0.42
2:BBB:77[A]:ARG:NH1	17:BBB:316:HOH:O	2.52	0.42
1:GGG:134[A]:SER:CA	15:GGG:203:PGE:H6	2.39	0.42
4:AAA:202:PG4:O3	4:AAA:202:PG4:C2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KKK:64[A]:VAL:HG12	1:KKK:121:PRO:CG	2.48	0.42
2:LLL:63:SER:OG	2:LLL:65[A]:ILE:HG22	2.20	0.42
1:AAA:40:GLN:HE22	2:BBB:24:LEU:HD11	1.84	0.42
1:CCC:2[C]:ILE:CG1	1:CCC:98:GLY:O	2.68	0.42
2:LLL:115:THR:HG21	3:LLL:201:CYC:HMA2	2.01	0.42
1:EEE:37[B]:ARG:HH11	1:EEE:37[B]:ARG:CB	2.33	0.42
4:CCC:203:PG4:H62	4:CCC:203:PG4:H81	1.16	0.42
17:BBB:366:HOH:O	1:CCC:76[B]:MET:HE3	2.20	0.42
1:AAA:46[B]:ARG:NH2	17:AAA:315:HOH:O	2.52	0.41
2:BBB:39[B]:ARG:HD2	2:BBB:39[B]:ARG:HA	1.86	0.41
2:BBB:53:LYS:NZ	17:BBB:317:HOH:O	2.53	0.41
1:GGG:48:ARG:NH2	1:GGG:52:GLN:HE22	2.18	0.41
1:KKK:2:ILE:HB	17:KKK:460:HOH:O	2.20	0.41
1:AAA:27:SER:OG	1:GGG:24[B]:ARG:NH1	2.52	0.41
1:CCC:48[A]:ARG:NH2	4:CCC:203:PG4:H22	2.35	0.41
2:LLL:43:THR:CG2	2:LLL:140[B]:LEU:HG	2.50	0.41
1:KKK:58[B]:PHE:CZ	1:KKK:77:THR:HG23	2.54	0.41
2:LLL:117[B]:ASN:CG	17:LLL:302:HOH:O	2.58	0.41
4:AAA:202:PG4:H62	4:AAA:202:PG4:H82	1.67	0.41
2:BBB:130:ILE:HG21	2:BBB:157:CYS:SG	2.61	0.41
7:BBB:204:1PE:H152	7:BBB:204:1PE:H162	1.77	0.41
1:III:59[A]:GLN:HG3	17:III:382:HOH:O	2.20	0.41
2:LLL:15[B]:GLN:NE2	17:LLL:312:HOH:O	2.53	0.41
2:JJJ:78:TYR:CD1	1:KKK:114[A]:MET:HG3	2.55	0.41
2:LLL:130:ILE:HG21	2:LLL:157:CYS:SG	2.61	0.41
3:AAA:201:CYC:HMD2	3:AAA:201:CYC:NC	2.31	0.41
2:JJJ:130:ILE:HG21	2:JJJ:157:CYS:SG	2.61	0.41
2:LLL:83:ARG:NH1	3:LLL:201:CYC:O1A	2.53	0.41
1:AAA:46[B]:ARG:NH2	17:AAA:316:HOH:O	2.53	0.41
2:HHH:43:THR:HG22	2:HHH:140[B]:LEU:HG	2.01	0.41
1:III:76[A]:MET:CE	17:III:327:HOH:O	2.69	0.41
1:CCC:2[B]:ILE:CD1	1:CCC:24:ARG:NH1	2.83	0.41
2:BBB:26:LYS:NZ	17:BBB:308:HOH:O	2.44	0.41
1:CCC:34[B]:GLN:HG3	1:CCC:37[B]:ARG:NH1	2.27	0.41
2:FFF:53:LYS:NZ	17:FFF:306:HOH:O	2.50	0.41
2:HHH:58:LYS:HB3	2:HHH:58:LYS:HE3	1.89	0.41
1:III:40[B]:GLN:NE2	17:III:310:HOH:O	2.44	0.41
1:KKK:65[B]:VAL:HG12	1:KKK:77:THR:OG1	2.21	0.41
2:BBB:115:THR:HG21	3:BBB:201:CYC:HMA2	2.01	0.41
1:KKK:50:VAL:CG2	1:KKK:132[B]:MET:HE1	2.51	0.41
15:GGG:203:PGE:C6	17:GGG:438:HOH:O	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BBB:204:1PE:H262	8:BBB:205:PEG:H41	2.03	0.40
1:GGG:133:LYS:CE	15:GGG:203:PGE:H3	2.35	0.40
1:KKK:5:LYS:HG3	17:KKK:309:HOH:O	2.21	0.40
2:BBB:25:GLU:OE2	2:BBB:28:LYS:NZ	2.50	0.40
2:DDD:43:THR:HG22	2:DDD:140[B]:LEU:CD2	2.51	0.40
2:HHH:63:SER:OG	2:HHH:65[B]:ILE:HG22	2.21	0.40
1:EEE:59:GLN:NE2	17:EEE:304:HOH:O	2.12	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:III:428:HOH:O	17:LLL:475:HOH:O[4_454]	2.19	0.01

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	AAA	170/160 (106%)	169 (99%)	1 (1%)	0	100	100
1	CCC	176/160 (110%)	176 (100%)	0	0	100	100
1	EEE	172/160 (108%)	172 (100%)	0	0	100	100
1	GGG	172/160 (108%)	172 (100%)	0	0	100	100
1	III	167/160 (104%)	167 (100%)	0	0	100	100
1	KKK	175/160 (109%)	175 (100%)	0	0	100	100
2	BBB	174/161 (108%)	172 (99%)	2 (1%)	0	100	100
2	DDD	177/161 (110%)	175 (99%)	2 (1%)	0	100	100
2	FFF	161/161 (100%)	159 (99%)	2 (1%)	0	100	100
2	HHH	172/161 (107%)	170 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	JJJ	167/161 (104%)	164 (98%)	3 (2%)	0	100	100
2	LLL	169/161 (105%)	167 (99%)	2 (1%)	0	100	100
All	All	2052/1926 (106%)	2038 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	AAA	134/122 (110%)	132 (98%)	2 (2%)	65	36
1	CCC	140/122 (115%)	136 (97%)	4 (3%)	42	10
1	EEE	136/122 (112%)	135 (99%)	1 (1%)	84	65
1	GGG	136/122 (112%)	132 (97%)	4 (3%)	42	10
1	III	131/122 (107%)	126 (96%)	5 (4%)	33	5
1	KKK	139/122 (114%)	135 (97%)	4 (3%)	42	10
2	BBB	141/125 (113%)	140 (99%)	1 (1%)	84	65
2	DDD	144/125 (115%)	139 (96%)	5 (4%)	36	7
2	FFF	128/125 (102%)	128 (100%)	0	100	100
2	HHH	139/125 (111%)	139 (100%)	0	100	100
2	JJJ	133/125 (106%)	133 (100%)	0	100	100
2	LLL	136/125 (109%)	135 (99%)	1 (1%)	84	65
All	All	1637/1482 (110%)	1610 (98%)	27 (2%)	71	32

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	134	SER
1	AAA	140	LEU
2	BBB	36	LEU
1	CCC	2[A]	ILE

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Mol	Chain	Res	Type
1	CCC	2[B]	ILE
1	CCC	2[C]	ILE
1	CCC	60	LYS
2	DDD	11[A]	SER
2	DDD	11[B]	SER
2	DDD	58	LYS
2	DDD	85[A]	LEU
2	DDD	85[B]	LEU
1	EEE	160	GLN
1	GGG	23[A]	ASP
1	GGG	23[B]	ASP
1	GGG	46	ARG
1	GGG	143	GLU
1	III	23	ASP
1	III	51	LYS
1	III	60[A]	LYS
1	III	60[B]	LYS
1	III	60[C]	LYS
1	KKK	59[A]	GLN
1	KKK	59[B]	GLN
1	KKK	61[A]	ARG
1	KKK	61[B]	ARG
2	LLL	128	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues 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	MEN	HHH	71	2	7,8,9	1.32	1 (14%)	6,9,11	0.84	0
2	MEN	JJJ	71	2	7,8,9	0.38	0	6,9,11	0.45	0
2	MEN	FFF	71	2	7,8,9	0.52	0	6,9,11	0.45	0
2	MEN	BBB	71	2	7,8,9	0.81	0	6,9,11	0.92	0
2	MEN	LLL	71	2	7,8,9	1.03	0	6,9,11	1.15	1 (16%)
2	MEN	DDD	71	2	7,8,9	1.29	1 (14%)	6,9,11	0.68	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	MEN	HHH	71	2	-	2/7/8/10	-
2	MEN	JJJ	71	2	-	2/7/8/10	-
2	MEN	FFF	71	2	-	2/7/8/10	-
2	MEN	BBB	71	2	-	2/7/8/10	-
2	MEN	LLL	71	2	-	2/7/8/10	-
2	MEN	DDD	71	2	-	2/7/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	71	MEN	OD1-CG	2.56	1.28	1.23
2	HHH	71	MEN	CE2-ND2	2.48	1.50	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	LLL	71	MEN	OD1-CG-CB	2.57	125.26	121.50

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	71	MEN	CA-CB-CG-OD1
2	DDD	71	MEN	CA-CB-CG-OD1
2	FFF	71	MEN	CA-CB-CG-OD1
2	JJJ	71	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
2	HHH	71	MEN	CA-CB-CG-OD1
2	LLL	71	MEN	CA-CB-CG-OD1
2	BBB	71	MEN	CA-CB-CG-ND2
2	DDD	71	MEN	CA-CB-CG-ND2
2	FFF	71	MEN	CA-CB-CG-ND2
2	HHH	71	MEN	CA-CB-CG-ND2
2	JJJ	71	MEN	CA-CB-CG-ND2
2	LLL	71	MEN	CA-CB-CG-ND2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

51 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	$\# Z  > 2$
3	CYC	KKK	201	1	36,46,46	1.11	1 (2%)	44,67,67	1.35	7 (15%)
4	PG4	FFF	204	-	12,12,12	0.14	0	11,11,11	0.16	0
15	PGE	GGG	204	-	9,9,9	0.18	0	8,8,8	0.19	0
6	MPD	FFF	203	-	7,7,7	0.23	0	9,10,10	0.38	0
3	CYC	CCC	201	1	36,46,46	1.23	1 (2%)	44,67,67	1.39	8 (18%)
4	PG4	JJJ	204	-	12,12,12	0.15	0	11,11,11	0.17	0
4	PG4	CCC	203	-	12,12,12	0.16	0	11,11,11	0.10	0
8	PEG	GGG	205	-	6,6,6	0.18	0	5,5,5	0.09	0
8	PEG	JJJ	205	-	6,6,6	0.50	0	5,5,5	0.36	0
5	LYS	BBB	202[A]	-	5,9,9	0.51	0	4,10,10	0.25	0
6	MPD	DDD	203	-	7,7,7	0.35	0	9,10,10	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MPD	JJJ	203	-	7,7,7	0.20	0	9,10,10	0.50	0
8	PEG	BBB	206	-	6,6,6	0.13	0	5,5,5	0.10	0
3	CYC	III	201	1	36,46,46	1.35	1 (2%)	44,67,67	1.31	8 (18%)
3	CYC	LLL	201	2	36,46,46	1.38	1 (2%)	44,67,67	1.01	2 (4%)
9	EDO	KKK	203	-	3,3,3	0.26	0	2,2,2	0.34	0
8	PEG	BBB	208	-	6,6,6	0.29	0	5,5,5	0.29	0
8	PEG	BBB	205	-	6,6,6	0.19	0	5,5,5	0.24	0
3	CYC	EEE	201	1	36,46,46	1.25	1 (2%)	44,67,67	1.37	7 (15%)
6	MPD	EEE	203	-	7,7,7	0.18	0	9,10,10	0.48	0
5	LYS	BBB	202[B]	-	5,9,9	0.54	0	4,10,10	0.36	0
9	EDO	CCC	206	-	3,3,3	0.30	0	2,2,2	0.69	0
14	MRD	GGG	202	-	7,7,7	0.37	0	9,10,10	0.58	0
9	EDO	CCC	205	-	3,3,3	0.10	0	2,2,2	0.70	0
16	DSN	LLL	202	-	3,6,6	0.73	0	1,7,7	0.23	0
5	LYS	III	202	-	5,9,9	0.46	0	4,10,10	0.34	0
9	EDO	BBB	207	-	3,3,3	0.26	0	2,2,2	0.57	0
3	CYC	FFF	201	2	36,46,46	1.53	1 (2%)	44,67,67	1.08	3 (6%)
3	CYC	GGG	201	1	36,46,46	1.38	1 (2%)	44,67,67	1.42	8 (18%)
3	CYC	HHH	201	2	36,46,46	1.27	1 (2%)	44,67,67	0.98	2 (4%)
8	PEG	HHH	204	-	6,6,6	0.27	0	5,5,5	0.16	0
10	P6G	CCC	202	-	18,18,18	0.85	1 (5%)	17,17,17	0.84	1 (5%)
5	LYS	KKK	202	-	5,9,9	0.46	0	4,10,10	0.25	0
3	CYC	JJJ	201	2	36,46,46	1.47	1 (2%)	44,67,67	1.09	5 (11%)
9	EDO	KKK	204	-	3,3,3	0.16	0	2,2,2	0.61	0
13	ALA	FFF	202	-	2,5,5	0.31	0	2,6,6	0.21	0
3	CYC	DDD	201	2	36,46,46	1.16	1 (2%)	44,67,67	0.90	1 (2%)
3	CYC	AAA	201	1	36,46,46	1.47	1 (2%)	44,67,67	1.41	9 (20%)
11	GLU	DDD	202	-	2,9,9	0.59	0	2,11,11	0.56	0
4	PG4	AAA	202	-	12,12,12	0.15	0	11,11,11	0.33	0
15	PGE	LLL	204	-	9,9,9	0.16	0	8,8,8	0.13	0
6	MPD	BBB	203	-	7,7,7	0.15	0	9,10,10	0.36	0
7	1PE	BBB	204	-	15,15,15	0.76	0	14,14,14	0.77	0
11	GLU	HHH	202	-	2,9,9	0.86	0	2,11,11	0.45	0
15	PGE	GGG	203	-	9,9,9	0.26	0	8,8,8	0.24	0
3	CYC	BBB	201	2	36,46,46	1.41	2 (5%)	44,67,67	1.12	3 (6%)
12	GLY	EEE	202	-	1,4,4	0.07	0	0,4,4	0.00	-
16	DSN	JJJ	202	-	3,6,6	0.73	0	1,7,7	0.45	0
6	MPD	LLL	203	-	7,7,7	0.23	0	9,10,10	0.30	0
6	MPD	HHH	203	-	7,7,7	0.43	0	9,10,10	0.53	0
8	PEG	CCC	204	-	6,6,6	0.17	0	5,5,5	0.18	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
3	CYC	KKK	201	1	-	4/21/74/74	0/4/4/4
4	PG4	FFF	204	-	-	4/10/10/10	-
15	PGE	GGG	204	-	-	5/7/7/7	-
6	MPD	FFF	203	-	-	0/5/5/5	-
3	CYC	CCC	201	1	-	3/21/74/74	0/4/4/4
4	PG4	JJJ	204	-	-	6/10/10/10	-
4	PG4	CCC	203	-	-	10/10/10/10	-
8	PEG	GGG	205	-	-	3/4/4/4	-
8	PEG	JJJ	205	-	-	2/4/4/4	-
5	LYS	BBB	202[A]	-	-	2/5/9/9	-
6	MPD	DDD	203	-	-	0/5/5/5	-
6	MPD	JJJ	203	-	-	0/5/5/5	-
8	PEG	BBB	206	-	-	3/4/4/4	-
3	CYC	III	201	1	-	3/21/74/74	0/4/4/4
3	CYC	LLL	201	2	-	4/21/74/74	0/4/4/4
9	EDO	KKK	203	-	-	1/1/1/1	-
8	PEG	BBB	208	-	-	1/4/4/4	-
8	PEG	BBB	205	-	-	2/4/4/4	-
3	CYC	EEE	201	1	-	4/21/74/74	0/4/4/4
6	MPD	EEE	203	-	-	1/5/5/5	-
5	LYS	BBB	202[B]	-	-	3/5/9/9	-
9	EDO	CCC	206	-	-	1/1/1/1	-
14	MRD	GGG	202	-	-	0/5/5/5	-
9	EDO	CCC	205	-	-	1/1/1/1	-
16	DSN	LLL	202	-	-	2/2/6/6	-
5	LYS	III	202	-	-	1/5/9/9	-
9	EDO	BBB	207	-	-	1/1/1/1	-
3	CYC	FFF	201	2	-	4/21/74/74	0/4/4/4
3	CYC	GGG	201	1	-	3/21/74/74	0/4/4/4
3	CYC	HHH	201	2	-	4/21/74/74	0/4/4/4
8	PEG	HHH	204	-	-	3/4/4/4	-
10	P6G	CCC	202	-	-	11/16/16/16	-
5	LYS	KKK	202	-	-	2/5/9/9	-
3	CYC	JJJ	201	2	-	4/21/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	KKK	204	-	-	0/1/1/1	-
13	ALA	FFF	202	-	-	0/0/4/4	-
3	CYC	DDD	201	2	-	4/21/74/74	0/4/4/4
3	CYC	AAA	201	1	-	4/21/74/74	0/4/4/4
11	GLU	DDD	202	-	-	1/3/9/9	-
4	PG4	AAA	202	-	-	4/10/10/10	-
15	PGE	LLL	204	-	-	4/7/7/7	-
6	MPD	BBB	203	-	-	0/5/5/5	-
7	1PE	BBB	204	-	-	9/13/13/13	-
11	GLU	HHH	202	-	-	1/3/9/9	-
15	PGE	GGG	203	-	-	5/7/7/7	-
3	CYC	BBB	201	2	-	4/21/74/74	0/4/4/4
12	GLY	EEE	202	-	-	0/0/2/2	-
16	DSN	JJJ	202	-	-	2/2/6/6	-
6	MPD	LLL	203	-	-	0/5/5/5	-
6	MPD	HHH	203	-	-	0/5/5/5	-
8	PEG	CCC	204	-	-	3/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	FFF	201	CYC	CHA-C1A	8.49	1.42	1.35
3	JJJ	201	CYC	CHA-C1A	8.08	1.41	1.35
3	AAA	201	CYC	CHA-C1A	8.05	1.41	1.35
3	BBB	201	CYC	CHA-C1A	7.55	1.41	1.35
3	GGG	201	CYC	CHA-C1A	7.52	1.41	1.35
3	LLL	201	CYC	CHA-C1A	7.44	1.41	1.35
3	III	201	CYC	CHA-C1A	6.99	1.41	1.35
3	HHH	201	CYC	CHA-C1A	6.76	1.40	1.35
3	EEE	201	CYC	CHA-C1A	6.74	1.40	1.35
3	CCC	201	CYC	CHA-C1A	6.73	1.40	1.35
3	DDD	201	CYC	CHA-C1A	5.89	1.40	1.35
3	KKK	201	CYC	CHA-C1A	5.62	1.39	1.35
10	CCC	202	P6G	O10-C11	3.03	1.55	1.42
3	BBB	201	CYC	C1B-C2B	-2.20	1.41	1.45

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	201	CYC	C1B-CHB-C4A	4.10	138.10	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	EEE	201	CYC	C1B-CHB-C4A	3.93	137.68	128.08
3	III	201	CYC	C1B-CHB-C4A	3.88	137.57	128.08
3	KKK	201	CYC	C1B-CHB-C4A	3.85	137.48	128.08
3	GGG	201	CYC	CMB-C2B-C1B	3.72	128.81	124.17
3	AAA	201	CYC	C1B-CHB-C4A	3.68	137.06	128.08
3	EEE	201	CYC	CMB-C2B-C1B	3.66	128.74	124.17
3	GGG	201	CYC	C1B-CHB-C4A	3.65	137.01	128.08
3	BBB	201	CYC	CMB-C2B-C1B	3.41	128.42	124.17
3	AAA	201	CYC	CHB-C1B-C2B	-2.98	121.04	126.95
3	KKK	201	CYC	CMA-C3A-C4A	2.89	129.52	125.06
3	CCC	201	CYC	CHB-C4A-NA	-2.86	118.95	124.93
3	AAA	201	CYC	CMA-C3A-C4A	2.84	129.43	125.06
3	GGG	201	CYC	CMA-C3A-C4A	2.83	129.42	125.06
3	CCC	201	CYC	CMB-C2B-C1B	2.79	127.65	124.17
3	CCC	201	CYC	CHB-C4A-C3A	2.77	132.02	124.90
3	CCC	201	CYC	C4D-CHA-C1A	2.75	132.09	128.81
3	KKK	201	CYC	CMB-C2B-C1B	2.66	127.49	124.17
3	KKK	201	CYC	CHB-C4A-NA	-2.60	119.50	124.93
3	III	201	CYC	CHB-C4A-C3A	2.59	131.56	124.90
3	HHH	201	CYC	CHA-C1A-NA	-2.59	125.24	128.83
3	AAA	201	CYC	CMB-C2B-C1B	2.58	127.38	124.17
3	GGG	201	CYC	CHA-C1A-NA	-2.52	125.33	128.83
3	FFF	201	CYC	CMB-C2B-C1B	2.52	127.31	124.17
3	AAA	201	CYC	C2C-C3C-C4C	2.48	105.06	101.34
3	AAA	201	CYC	CHA-C1A-NA	-2.47	125.40	128.83
3	JJJ	201	CYC	CHD-C4C-NC	2.46	128.13	125.20
3	FFF	201	CYC	CHA-C1A-NA	-2.45	125.42	128.83
3	LLL	201	CYC	CMB-C2B-C1B	2.44	127.21	124.17
3	JJJ	201	CYC	C2C-C3C-C4C	2.44	104.99	101.34
3	EEE	201	CYC	CHB-C4A-C3A	2.43	131.16	124.90
3	HHH	201	CYC	C4D-CHA-C1A	2.43	131.71	128.81
3	GGG	201	CYC	CHB-C4A-C3A	2.41	131.10	124.90
3	DDD	201	CYC	C4D-CHA-C1A	2.38	131.65	128.81
10	CCC	202	P6G	O10-C9-C8	-2.38	99.68	110.39
3	EEE	201	CYC	CHB-C4A-NA	-2.37	119.98	124.93
3	EEE	201	CYC	CHA-C1A-NA	-2.36	125.55	128.83
3	BBB	201	CYC	CHA-C1A-NA	-2.35	125.57	128.83
3	FFF	201	CYC	CAC-C3C-C4C	2.34	118.69	112.67
3	KKK	201	CYC	CHB-C4A-C3A	2.31	130.85	124.90
3	CCC	201	CYC	C2C-C3C-C4C	2.31	104.80	101.34
3	GGG	201	CYC	CHB-C1B-C2B	-2.30	122.39	126.95
3	III	201	CYC	CMB-C2B-C1B	2.29	127.03	124.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	III	201	CYC	CMA-C3A-C4A	2.29	128.58	125.06
3	III	201	CYC	CHB-C4A-NA	-2.28	120.15	124.93
3	AAA	201	CYC	CAD-CBD-CGD	2.28	116.50	112.67
3	KKK	201	CYC	CHB-C1B-C2B	-2.28	122.44	126.95
3	KKK	201	CYC	C2C-C3C-C4C	2.27	104.73	101.34
3	CCC	201	CYC	CHA-C1A-NA	-2.25	125.71	128.83
3	JJJ	201	CYC	CHA-C1A-NA	-2.23	125.73	128.83
3	JJJ	201	CYC	CMB-C2B-C1B	2.22	126.94	124.17
3	GGG	201	CYC	C2C-C3C-C4C	2.22	104.66	101.34
3	EEE	201	CYC	CMA-C3A-C4A	2.20	128.45	125.06
3	III	201	CYC	CHA-C1A-NA	-2.20	125.78	128.83
3	JJJ	201	CYC	OC-C1C-C2C	-2.18	124.44	126.17
3	EEE	201	CYC	C2C-C3C-C4C	2.17	104.58	101.34
3	CCC	201	CYC	CMA-C3A-C4A	2.16	128.40	125.06
3	BBB	201	CYC	CHD-C4C-NC	2.15	127.76	125.20
3	LLL	201	CYC	CHA-C1A-NA	-2.13	125.87	128.83
3	GGG	201	CYC	CHB-C4A-NA	-2.12	120.49	124.93
3	AAA	201	CYC	CHB-C1B-NB	2.10	130.57	126.06
3	III	201	CYC	CHB-C1B-C2B	-2.08	122.83	126.95
3	AAA	201	CYC	CHB-C4A-NA	-2.06	120.62	124.93
3	III	201	CYC	C4D-CHA-C1A	2.02	131.22	128.81

There are no chirality outliers.

All (139) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	201	CYC	ND-C1D-CHD-C4C
3	AAA	201	CYC	C2D-C1D-CHD-C4C
3	BBB	201	CYC	NA-C4A-CHB-C1B
3	BBB	201	CYC	C3A-C4A-CHB-C1B
3	BBB	201	CYC	ND-C1D-CHD-C4C
3	BBB	201	CYC	C2D-C1D-CHD-C4C
3	CCC	201	CYC	NA-C4A-CHB-C1B
3	CCC	201	CYC	C3A-C4A-CHB-C1B
3	CCC	201	CYC	ND-C1D-CHD-C4C
3	DDD	201	CYC	NA-C4A-CHB-C1B
3	DDD	201	CYC	C3A-C4A-CHB-C1B
3	DDD	201	CYC	ND-C1D-CHD-C4C
3	DDD	201	CYC	C2D-C1D-CHD-C4C
3	EEE	201	CYC	NA-C4A-CHB-C1B
3	EEE	201	CYC	C3A-C4A-CHB-C1B
3	EEE	201	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
3	EEE	201	CYC	C2D-C1D-CHD-C4C
3	FFF	201	CYC	NA-C4A-CHB-C1B
3	FFF	201	CYC	C3A-C4A-CHB-C1B
3	FFF	201	CYC	ND-C1D-CHD-C4C
3	FFF	201	CYC	C2D-C1D-CHD-C4C
3	GGG	201	CYC	C3A-C4A-CHB-C1B
3	GGG	201	CYC	ND-C1D-CHD-C4C
3	HHH	201	CYC	NA-C4A-CHB-C1B
3	HHH	201	CYC	C3A-C4A-CHB-C1B
3	HHH	201	CYC	ND-C1D-CHD-C4C
3	HHH	201	CYC	C2D-C1D-CHD-C4C
3	III	201	CYC	C3A-C4A-CHB-C1B
3	III	201	CYC	ND-C1D-CHD-C4C
3	JJJ	201	CYC	NA-C4A-CHB-C1B
3	JJJ	201	CYC	C3A-C4A-CHB-C1B
3	JJJ	201	CYC	ND-C1D-CHD-C4C
3	JJJ	201	CYC	C2D-C1D-CHD-C4C
3	KKK	201	CYC	NA-C4A-CHB-C1B
3	KKK	201	CYC	C3A-C4A-CHB-C1B
3	KKK	201	CYC	ND-C1D-CHD-C4C
3	KKK	201	CYC	C2D-C1D-CHD-C4C
3	LLL	201	CYC	NA-C4A-CHB-C1B
3	LLL	201	CYC	C3A-C4A-CHB-C1B
3	LLL	201	CYC	ND-C1D-CHD-C4C
3	LLL	201	CYC	C2D-C1D-CHD-C4C
11	DDD	202	GLU	C-CA-CB-CG
11	HHH	202	GLU	CA-CB-CG-CD
16	JJJ	202	DSN	N-CA-CB-OG
16	LLL	202	DSN	C-CA-CB-OG
4	CCC	203	PG4	C8-C7-O4-C6
8	JJJ	205	PEG	C4-C3-O2-C2
15	LLL	204	PGE	C3-C4-O3-C5
7	BBB	204	1PE	C16-C26-OH6-C15
4	AAA	202	PG4	O1-C1-C2-O2
8	HHH	204	PEG	O1-C1-C2-O2
15	GGG	203	PGE	C3-C4-O3-C5
4	CCC	203	PG4	C4-C3-O2-C2
4	FFF	204	PG4	O2-C3-C4-O3
15	GGG	203	PGE	O2-C3-C4-O3
4	FFF	204	PG4	O3-C5-C6-O4
7	BBB	204	1PE	OH4-C13-C23-OH3
15	LLL	204	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
4	CCC	203	PG4	O3-C5-C6-O4
15	GGG	203	PGE	C4-C3-O2-C2
10	CCC	202	P6G	C11-C12-O13-C14
8	GGG	205	PEG	O2-C3-C4-O4
10	CCC	202	P6G	O16-C17-C18-O19
3	GGG	201	CYC	NA-C4A-CHB-C1B
4	AAA	202	PG4	C8-C7-O4-C6
4	AAA	202	PG4	O4-C7-C8-O5
4	JJJ	204	PG4	O1-C1-C2-O2
8	CCC	204	PEG	O2-C3-C4-O4
8	GGG	205	PEG	O1-C1-C2-O2
8	JJJ	205	PEG	O1-C1-C2-O2
15	GGG	203	PGE	O3-C5-C6-O4
15	LLL	204	PGE	O3-C5-C6-O4
3	AAA	201	CYC	NA-C4A-CHB-C1B
3	III	201	CYC	NA-C4A-CHB-C1B
3	AAA	201	CYC	C3A-C4A-CHB-C1B
5	BBB	202[A]	LYS	CE-CD-CG-CB
16	JJJ	202	DSN	C-CA-CB-OG
8	BBB	205	PEG	O2-C3-C4-O4
8	BBB	206	PEG	O2-C3-C4-O4
9	BBB	207	EDO	O1-C1-C2-O2
9	CCC	205	EDO	O1-C1-C2-O2
15	LLL	204	PGE	O1-C1-C2-O2
5	III	202	LYS	CA-CB-CG-CD
4	CCC	203	PG4	O1-C1-C2-O2
8	BBB	205	PEG	O1-C1-C2-O2
4	CCC	203	PG4	O4-C7-C8-O5
4	FFF	204	PG4	O1-C1-C2-O2
8	HHH	204	PEG	O2-C3-C4-O4
15	GGG	204	PGE	O1-C1-C2-O2
4	AAA	202	PG4	O2-C3-C4-O3
4	FFF	204	PG4	O4-C7-C8-O5
4	JJJ	204	PG4	C1-C2-O2-C3
10	CCC	202	P6G	C6-C5-O4-C3
5	BBB	202[B]	LYS	CE-CD-CG-CB
10	CCC	202	P6G	C8-C9-O10-C11
8	HHH	204	PEG	C4-C3-O2-C2
4	JJJ	204	PG4	O2-C3-C4-O3
8	GGG	205	PEG	C1-C2-O2-C3
8	BBB	206	PEG	C1-C2-O2-C3
4	JJJ	204	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
15	GGG	204	PGE	C3-C4-O3-C5
10	CCC	202	P6G	O1-C2-C3-O4
7	BBB	204	1PE	C14-C24-OH4-C13
10	CCC	202	P6G	C2-C3-O4-C5
7	BBB	204	1PE	C13-C23-OH3-C22
10	CCC	202	P6G	C18-C17-O16-C15
15	GGG	204	PGE	C1-C2-O2-C3
4	CCC	203	PG4	C3-C4-O3-C5
10	CCC	202	P6G	O13-C14-C15-O16
8	CCC	204	PEG	C4-C3-O2-C2
16	LLL	202	DSN	N-CA-CB-OG
7	BBB	204	1PE	OH7-C16-C26-OH6
9	CCC	206	EDO	O1-C1-C2-O2
4	CCC	203	PG4	O2-C3-C4-O3
7	BBB	204	1PE	C25-C15-OH6-C26
5	KKK	202	LYS	CE-CD-CG-CB
4	CCC	203	PG4	C1-C2-O2-C3
4	CCC	203	PG4	C5-C6-O4-C7
7	BBB	204	1PE	C23-C13-OH4-C24
8	BBB	206	PEG	C4-C3-O2-C2
10	CCC	202	P6G	O7-C8-C9-O10
5	BBB	202[A]	LYS	CA-CB-CG-CD
4	JJJ	204	PG4	C5-C6-O4-C7
5	BBB	202[B]	LYS	CA-CB-CG-CD
15	GGG	203	PGE	C1-C2-O2-C3
9	KKK	203	EDO	O1-C1-C2-O2
7	BBB	204	1PE	OH5-C14-C24-OH4
4	JJJ	204	PG4	O4-C7-C8-O5
10	CCC	202	P6G	O10-C11-C12-O13
4	CCC	203	PG4	C6-C5-O3-C4
8	BBB	208	PEG	O2-C3-C4-O4
15	GGG	204	PGE	O3-C5-C6-O4
6	EEE	203	MPD	C2-C3-C4-C5
15	GGG	204	PGE	C6-C5-O3-C4
10	CCC	202	P6G	O4-C5-C6-O7
8	CCC	204	PEG	C1-C2-O2-C3
5	BBB	202[B]	LYS	CG-CD-CE-NZ
5	KKK	202	LYS	CG-CD-CE-NZ
7	BBB	204	1PE	OH6-C15-C25-OH5

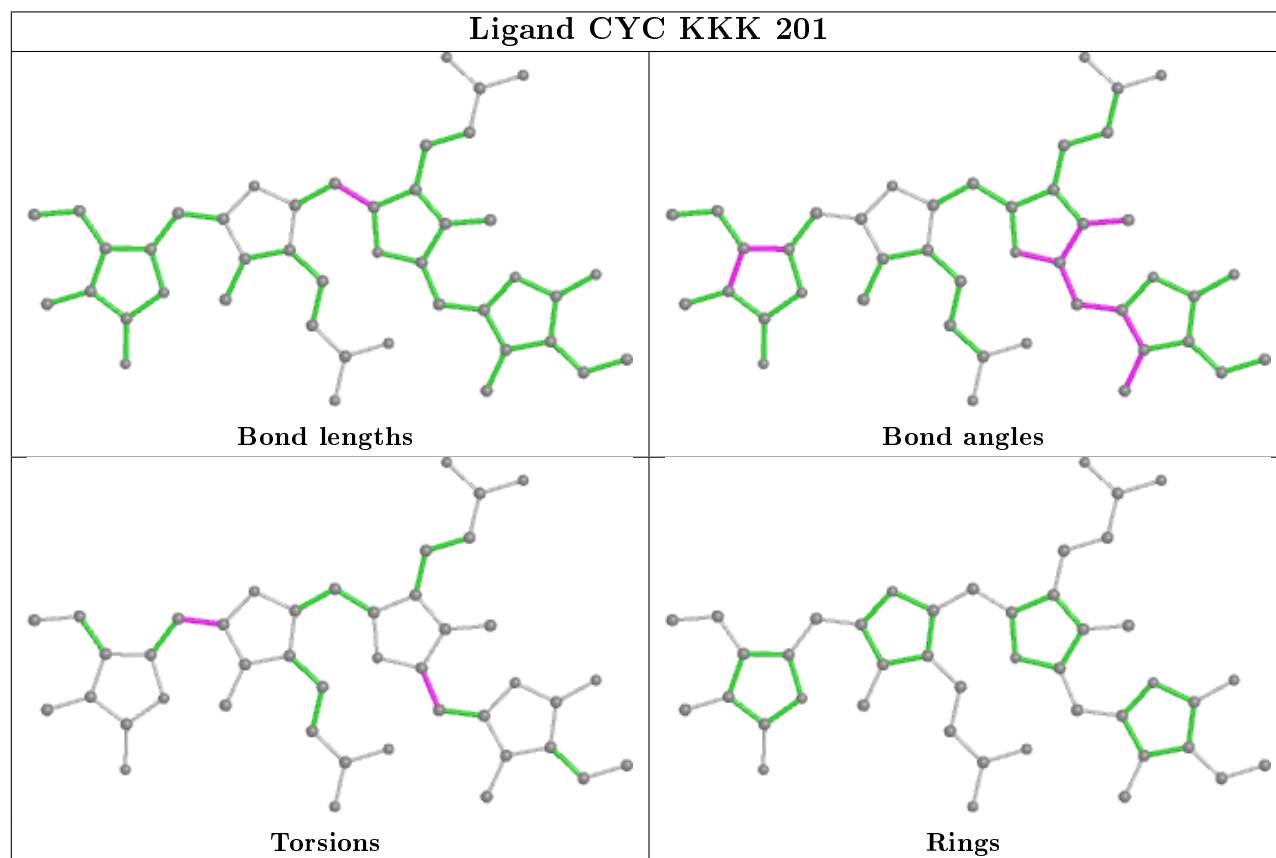
There are no ring outliers.

35 monomers are involved in 149 short contacts:

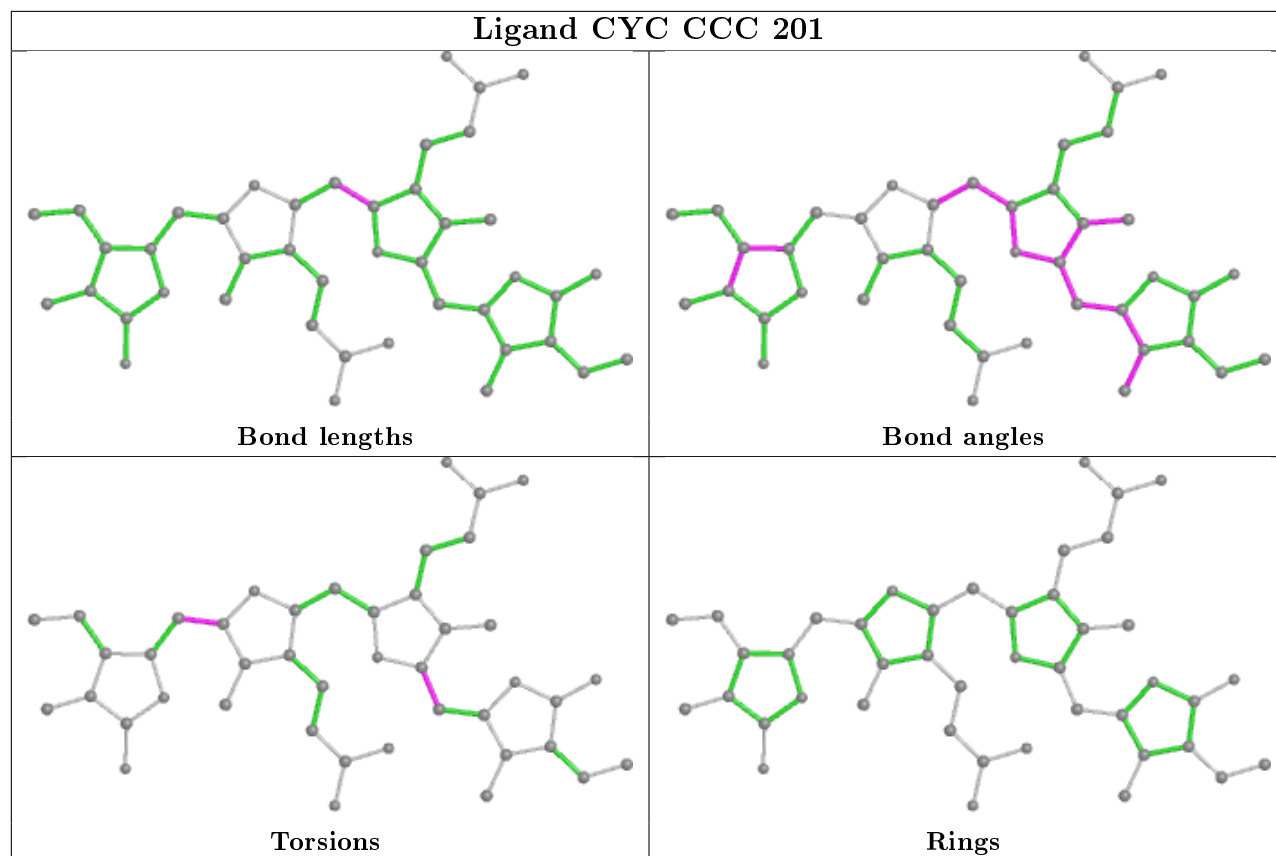
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	KKK	201	CYC	3	0
3	CCC	201	CYC	3	0
4	JJJ	204	PG4	2	0
4	CCC	203	PG4	15	0
8	JJJ	205	PEG	4	0
8	BBB	206	PEG	1	0
3	III	201	CYC	3	0
3	LLL	201	CYC	3	0
9	KKK	203	EDO	4	0
8	BBB	208	PEG	22	0
8	BBB	205	PEG	5	0
3	EEE	201	CYC	3	0
6	EEE	203	MPD	5	0
9	BBB	207	EDO	1	0
3	FFF	201	CYC	2	0
3	GGG	201	CYC	3	0
3	HHH	201	CYC	3	0
8	HHH	204	PEG	4	0
10	CCC	202	P6G	5	0
5	KKK	202	LYS	1	0
3	JJJ	201	CYC	2	0
9	KKK	204	EDO	6	0
13	FFF	202	ALA	2	0
3	DDD	201	CYC	2	0
3	AAA	201	CYC	4	0
11	DDD	202	GLU	2	0
4	AAA	202	PG4	11	0
15	LLL	204	PGE	2	0
7	BBB	204	1PE	8	0
15	GGG	203	PGE	18	0
3	BBB	201	CYC	3	0
12	EEE	202	GLY	3	0
16	JJJ	202	DSN	1	0
6	HHH	203	MPD	1	0
8	CCC	204	PEG	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

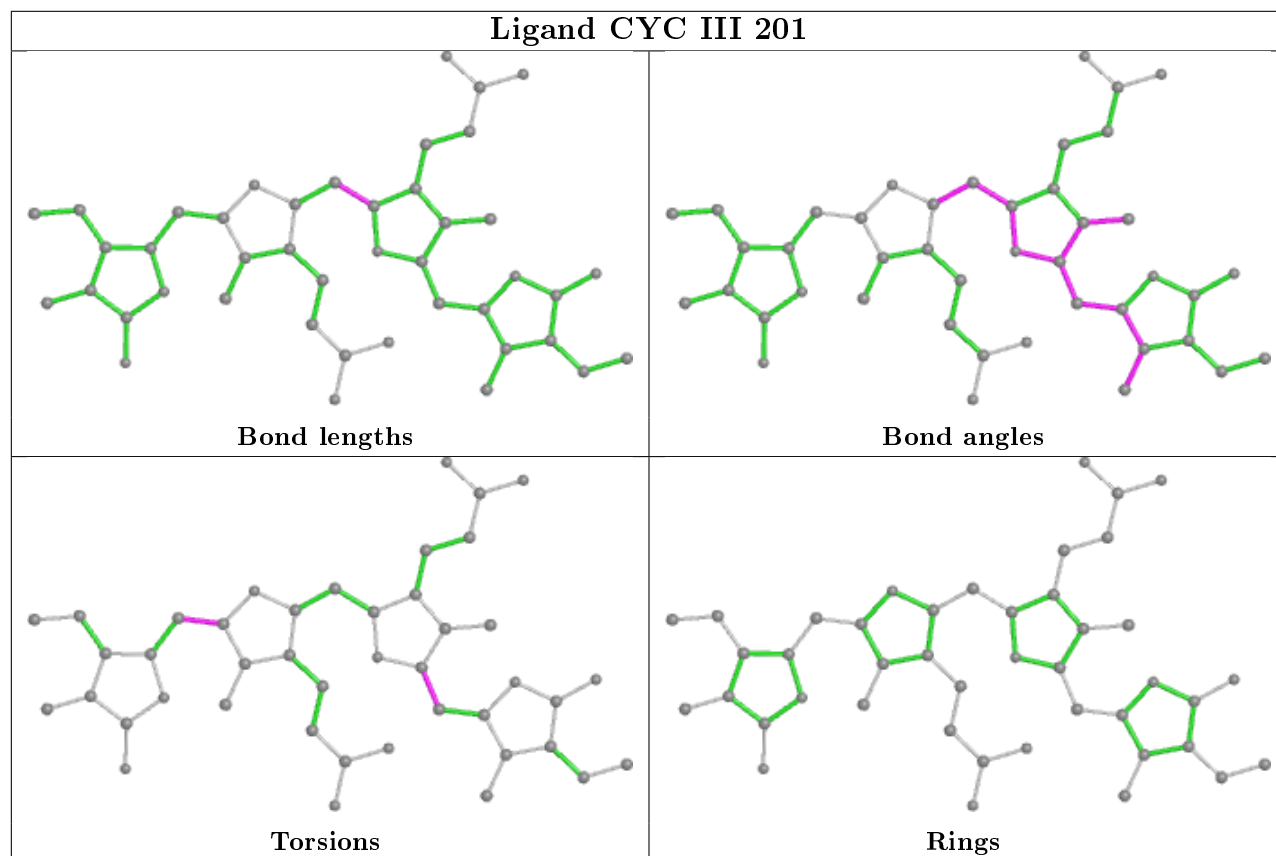
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



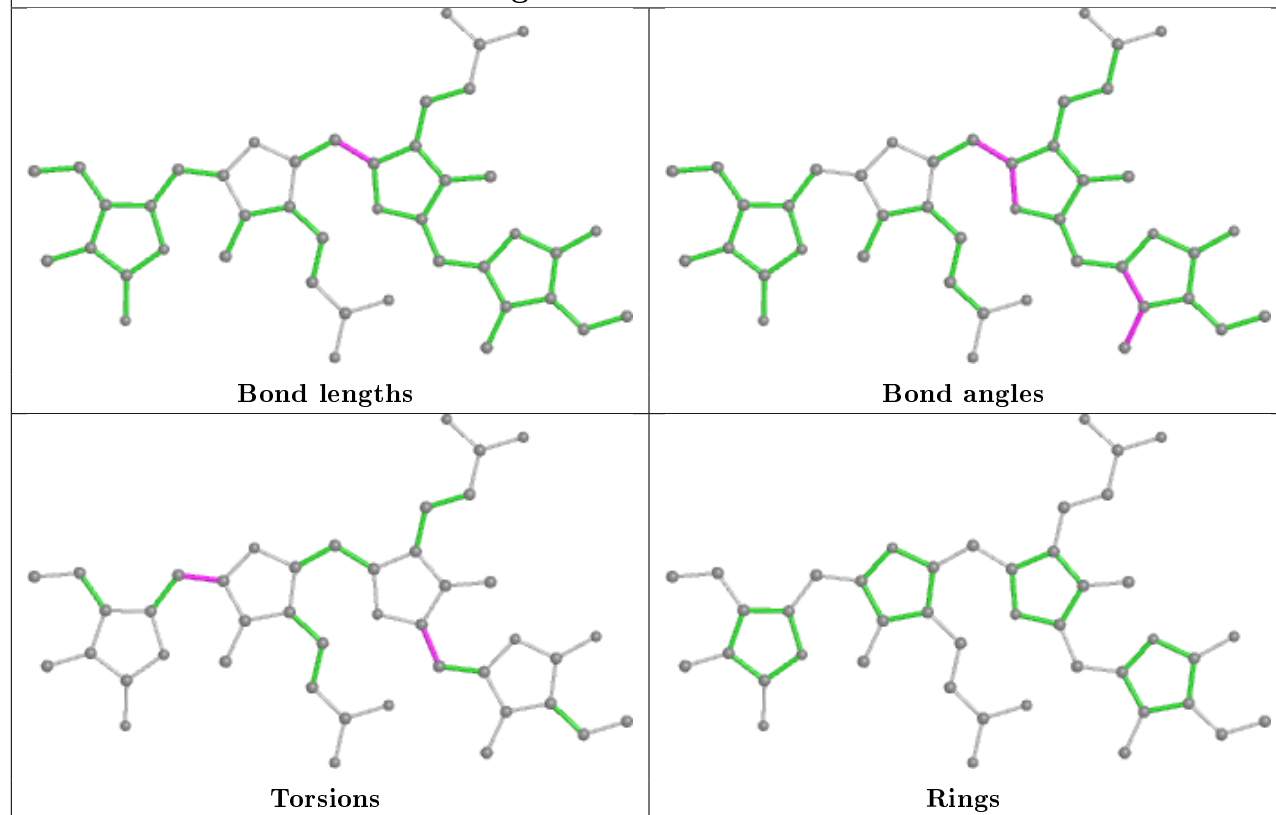
## Ligand CYC CCC 201



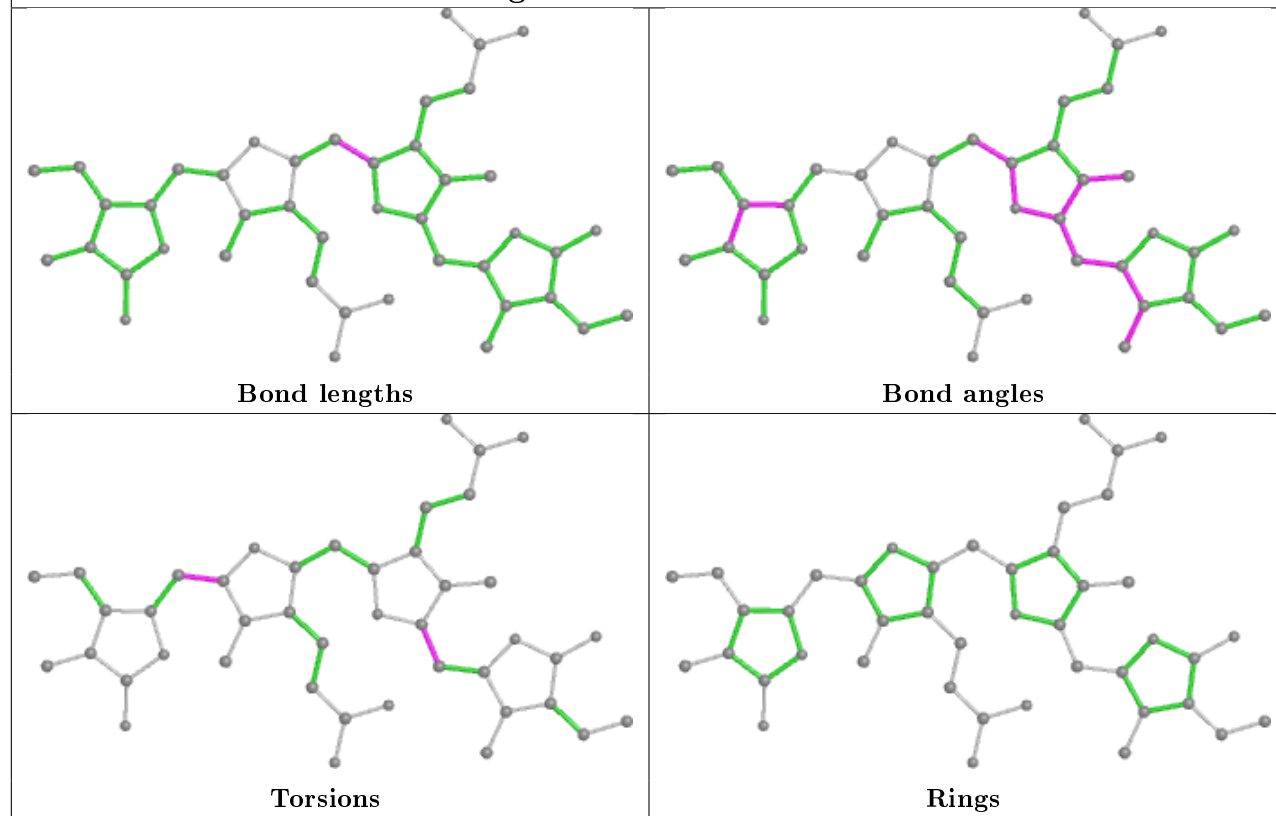
## Ligand CYC III 201



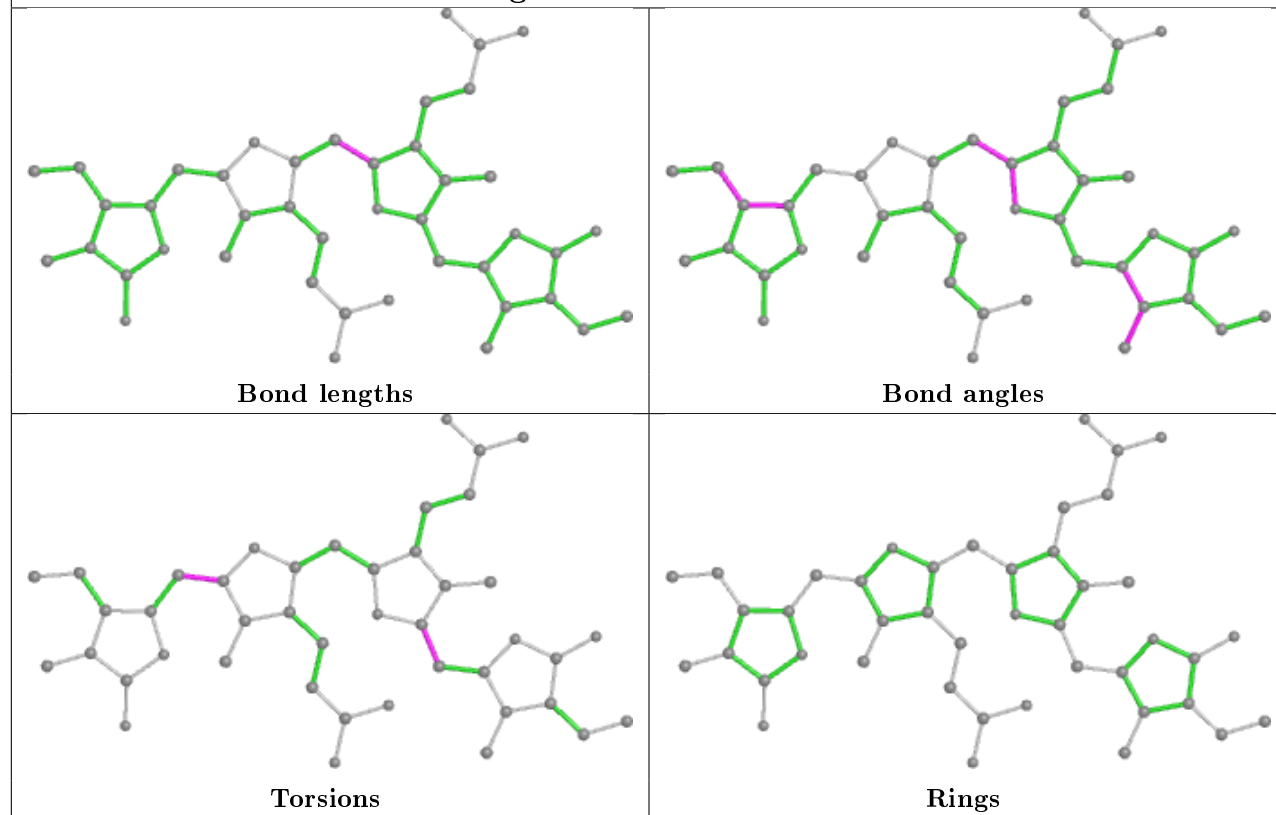
## Ligand CYC LLL 201



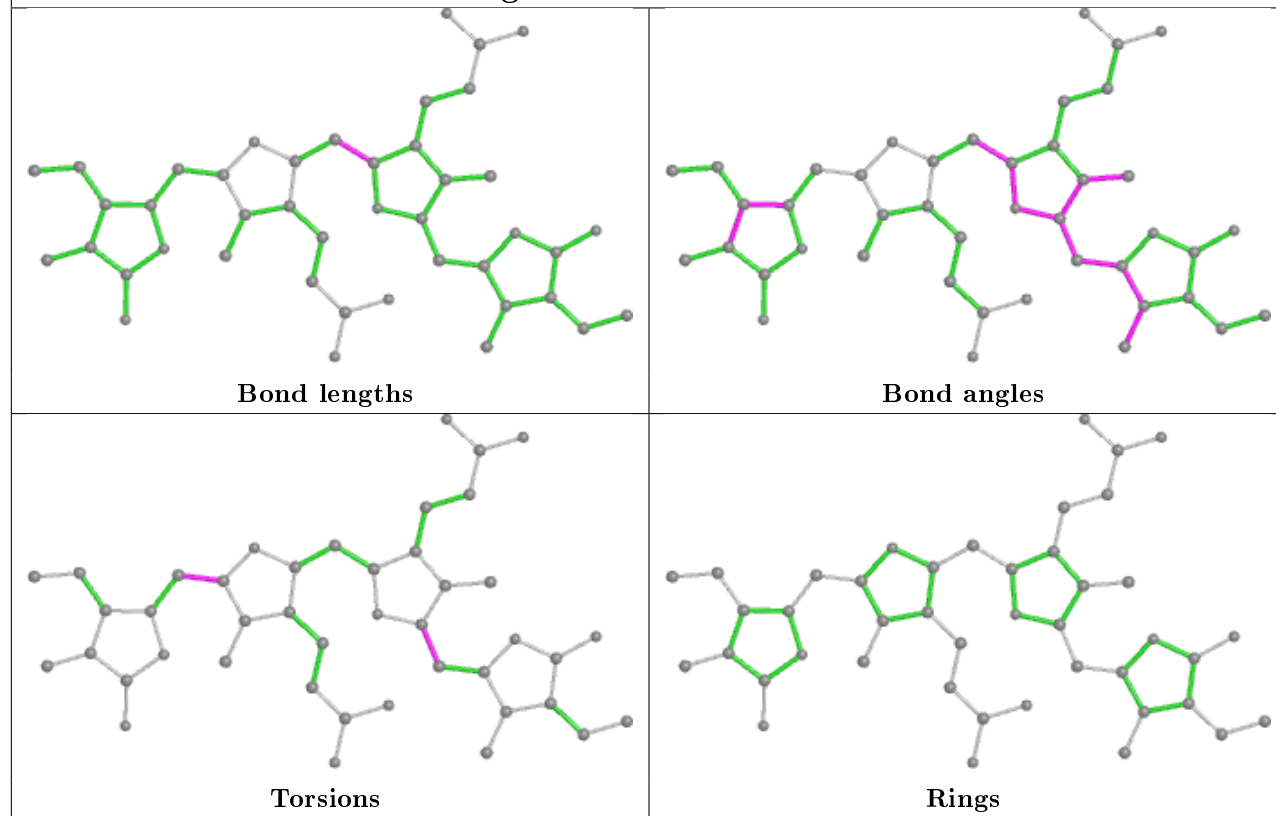
## Ligand CYC EEE 201



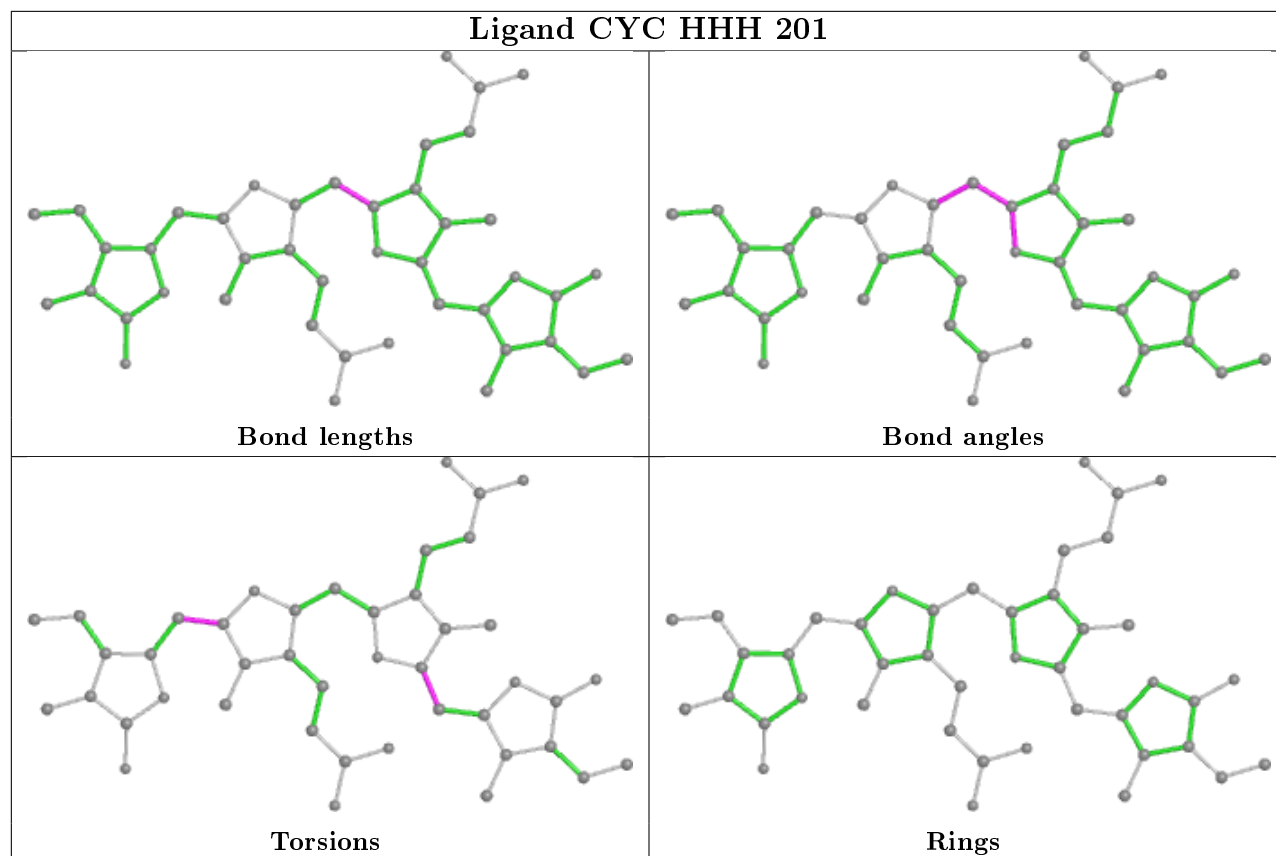
## Ligand CYC FFF 201



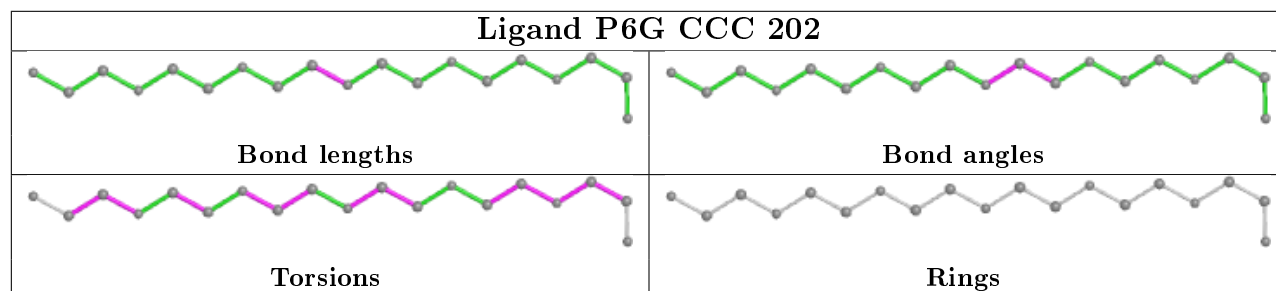
## Ligand CYC GGG 201



## Ligand CYC HHH 201

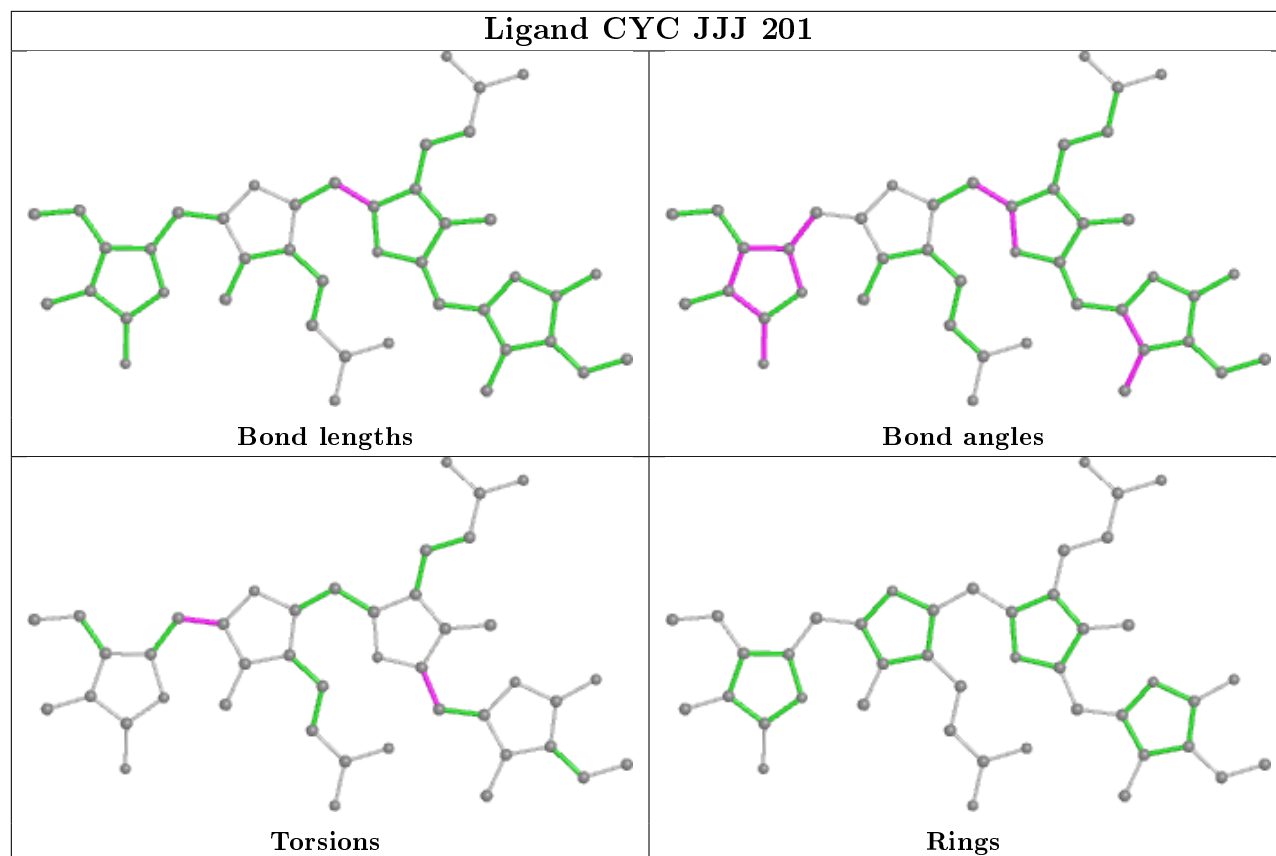


## Ligand P6G CCC 202

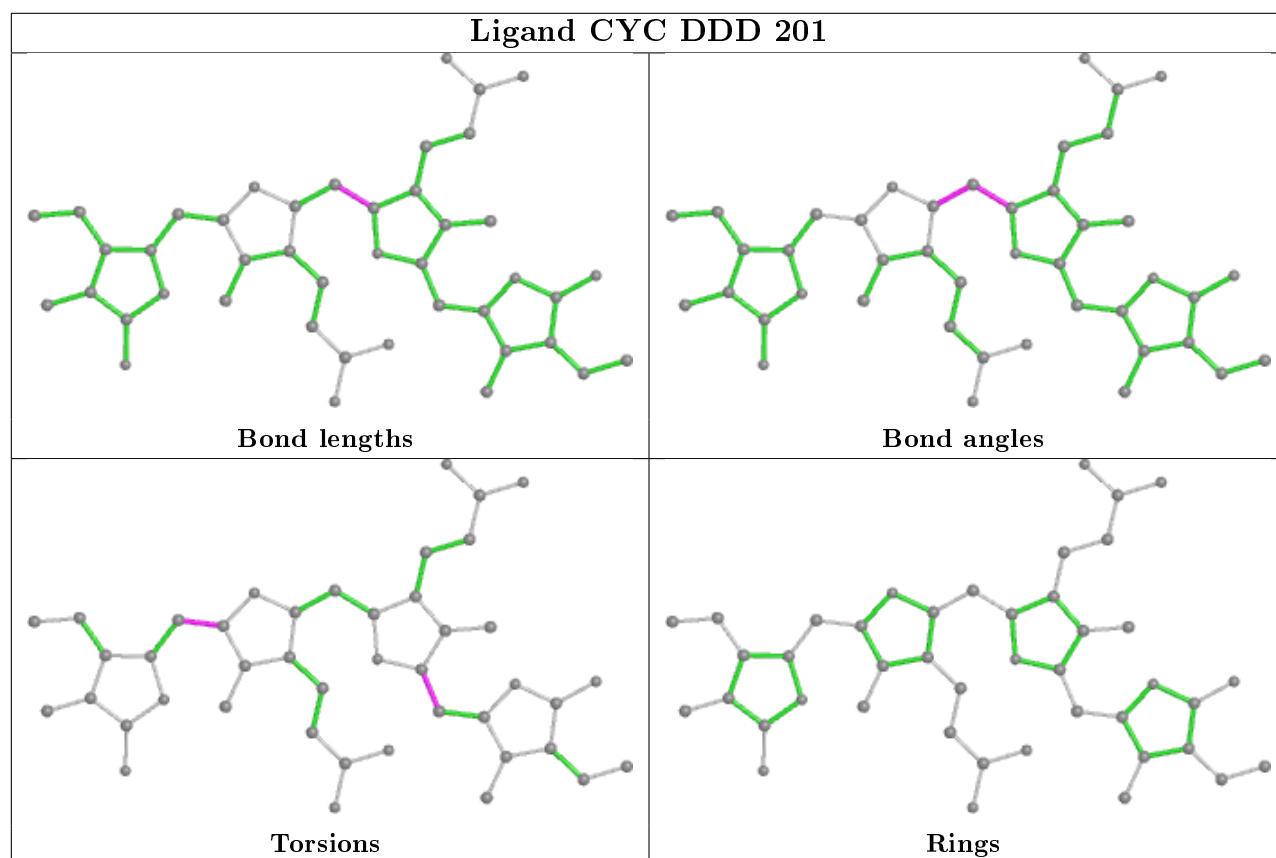




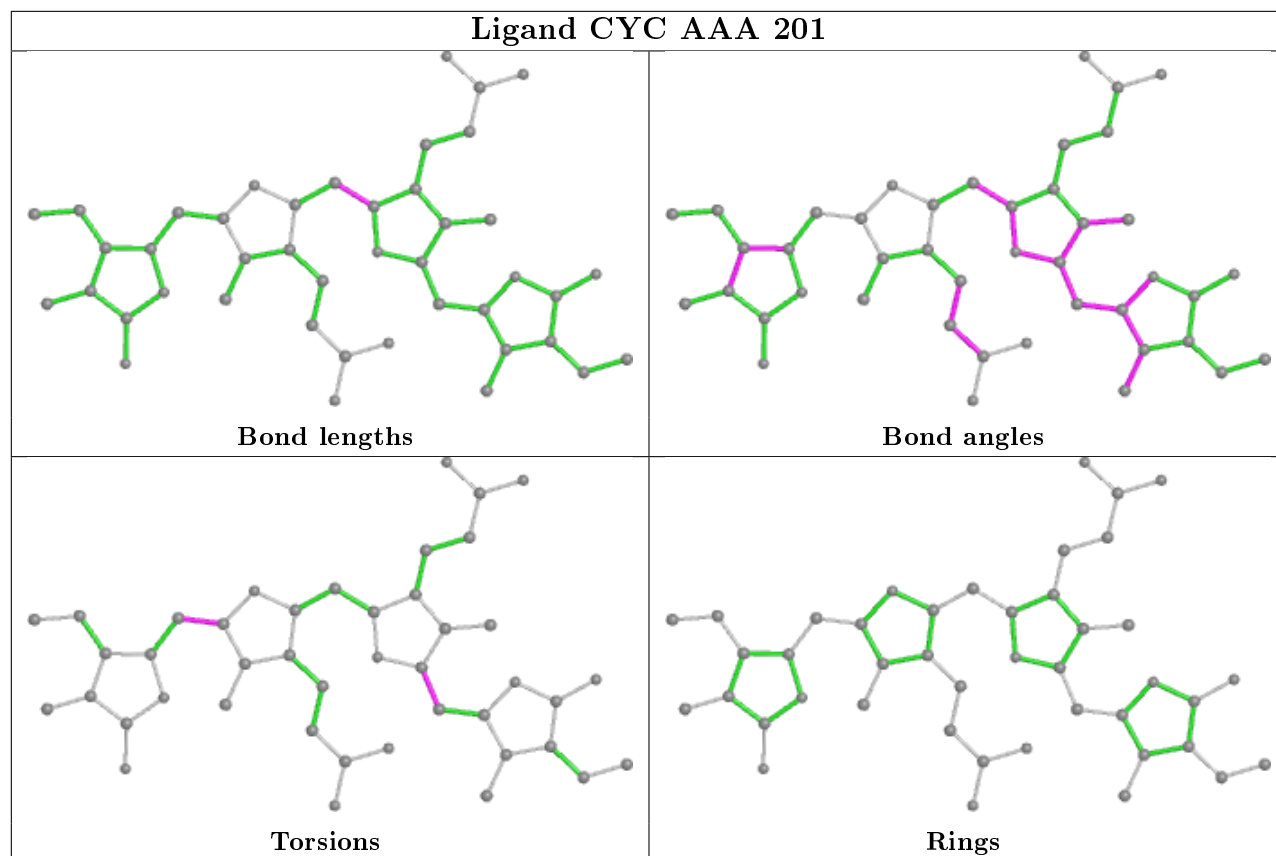
## Ligand CYC JJJ 201



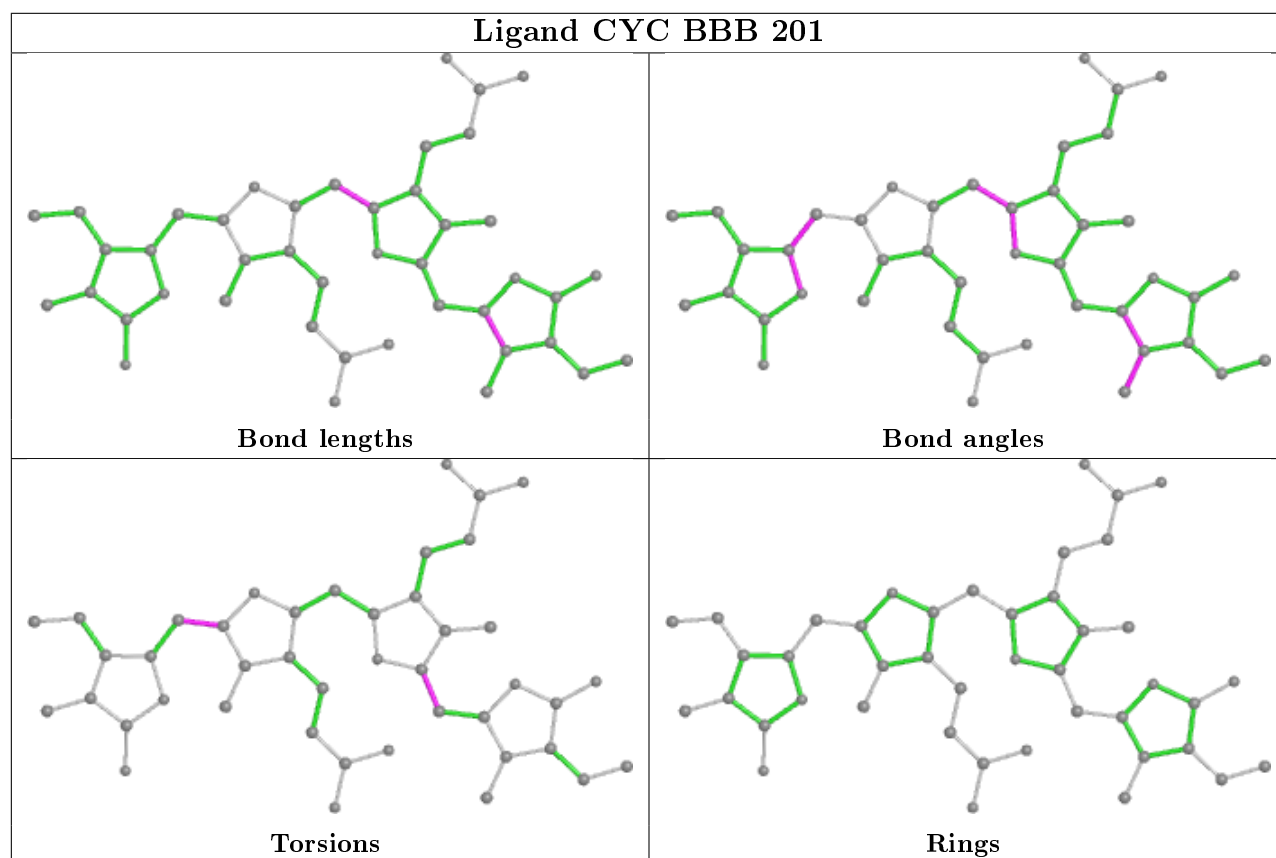
## Ligand CYC DDD 201



## Ligand CYC AAA 201



## Ligand CYC BBB 201



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	AAA	160/160 (100%)	-0.55	1 (0%) 89   88	19, 31, 55, 71	0
1	CCC	160/160 (100%)	-0.60	0 100   100	14, 23, 36, 50	0
1	EEE	160/160 (100%)	-0.60	1 (0%) 89   88	14, 23, 36, 57	0
1	GGG	160/160 (100%)	-0.53	0 100   100	15, 22, 39, 48	0
1	III	160/160 (100%)	-0.55	0 100   100	15, 25, 38, 60	0
1	KKK	160/160 (100%)	-0.45	1 (0%) 89   88	16, 29, 44, 65	0
2	BBB	160/161 (99%)	-0.64	1 (0%) 89   88	14, 23, 39, 69	0
2	DDD	160/161 (99%)	-0.68	0 100   100	15, 21, 35, 62	0
2	FFF	160/161 (99%)	-0.66	0 100   100	17, 22, 35, 58	0
2	HHH	160/161 (99%)	-0.66	0 100   100	16, 21, 37, 60	0
2	JJJ	160/161 (99%)	-0.62	1 (0%) 89   88	14, 21, 35, 56	0
2	LLL	160/161 (99%)	-0.63	0 100   100	15, 22, 35, 65	0
All	All	1920/1926 (99%)	-0.60	5 (0%) 94   93	14, 23, 40, 71	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	160	GLN	2.5
1	KKK	160	GLN	2.4
1	EEE	160	GLN	2.2
2	BBB	161	SER	2.1
2	JJJ	161	SER	2.1

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

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
2	MEN	LLL	71	9/10	0.96	0.06	16,18,21,22	0
2	MEN	DDD	71	9/10	0.97	0.05	20,21,26,28	0
2	MEN	HHH	71	9/10	0.97	0.06	21,24,30,30	0
2	MEN	BBB	71	9/10	0.97	0.06	15,17,20,22	0
2	MEN	JJJ	71	9/10	0.98	0.05	13,14,17,20	0
2	MEN	FFF	71	9/10	0.99	0.05	14,15,18,18	0

### 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
12	GLY	EEE	202	5/5	0.20	0.24	30,31,33,34	5
8	PEG	BBB	206	7/7	0.55	0.23	35,36,37,38	7
11	GLU	HHH	202	10/10	0.61	0.23	37,43,47,47	10
8	PEG	BBB	205	7/7	0.62	0.26	28,34,38,39	7
15	PGE	LLL	204	10/10	0.62	0.49	32,38,40,42	10
15	PGE	GGG	204	10/10	0.63	0.27	35,38,43,43	10
6	MPD	EEE	203	8/8	0.63	0.26	28,30,31,32	8
11	GLU	DDD	202	10/10	0.66	0.25	35,38,40,41	10
10	P6G	CCC	202	19/19	0.67	0.43	33,37,39,41	19
5	LYS	III	202	10/10	0.69	0.19	35,37,40,43	10
4	PG4	CCC	203	13/13	0.72	0.88	30,32,34,34	13
14	MRD	GGG	202	8/8	0.73	0.17	28,29,32,36	8
4	PG4	FFF	204	13/13	0.74	0.86	20,27,33,37	13
8	PEG	BBB	208	7/7	0.76	0.36	32,33,35,37	7
8	PEG	JJJ	205	7/7	0.77	0.19	24,25,30,32	7
8	PEG	GGG	205	7/7	0.77	0.17	30,32,37,38	7
4	PG4	JJJ	204	13/13	0.80	0.19	28,34,41,43	13
7	1PE	BBB	204	16/16	0.80	0.17	25,38,43,44	16
15	PGE	GGG	203	10/10	0.81	0.20	24,31,34,36	10
16	DSN	JJJ	202	7/7	0.82	0.20	34,37,39,40	7

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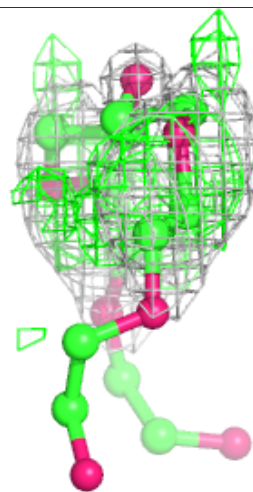
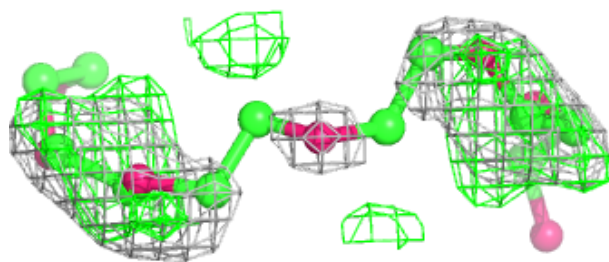
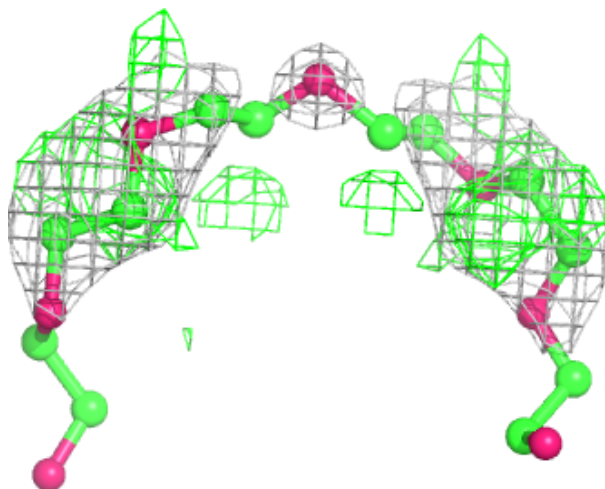
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PG4	AAA	202	13/13	0.84	0.22	25,29,34,36	13
8	PEG	HHH	204	7/7	0.85	0.19	25,29,32,34	7
9	EDO	CCC	205	4/4	0.86	0.18	29,29,30,31	4
5	LYS	KKK	202	10/10	0.87	0.20	21,33,40,43	10
6	MPD	BBB	203	8/8	0.88	0.28	24,27,32,33	8
5	LYS	BBB	202[A]	10/10	0.88	0.27	26,36,39,39	10
13	ALA	FFF	202	6/6	0.88	0.24	37,37,40,43	6
5	LYS	BBB	202[B]	10/10	0.88	0.27	25,36,39,39	10
8	PEG	CCC	204	7/7	0.89	0.32	28,34,37,38	7
16	DSN	LLL	202	7/7	0.89	0.22	33,36,37,38	7
6	MPD	DDD	203	8/8	0.90	0.12	26,29,34,37	8
9	EDO	KKK	204	4/4	0.91	0.14	27,27,27,28	4
9	EDO	BBB	207	4/4	0.92	0.10	28,32,33,33	4
6	MPD	HHH	203	8/8	0.93	0.14	26,29,35,36	8
6	MPD	LLL	203	8/8	0.93	0.31	23,26,32,33	8
9	EDO	CCC	206	4/4	0.93	0.22	24,26,27,27	4
9	EDO	KKK	203	4/4	0.93	0.12	28,29,31,33	4
6	MPD	JJJ	203	8/8	0.94	0.08	23,26,29,34	0
6	MPD	FFF	203	8/8	0.96	0.07	26,29,31,36	8
3	CYC	LLL	201	43/43	0.96	0.06	14,18,31,40	0
3	CYC	EEE	201	43/43	0.96	0.06	14,16,22,28	0
3	CYC	FFF	201	43/43	0.96	0.06	14,21,35,39	0
3	CYC	HHH	201	43/43	0.96	0.06	20,25,36,43	0
3	CYC	III	201	43/43	0.96	0.06	14,17,23,28	0
3	CYC	JJJ	201	43/43	0.96	0.06	14,22,36,40	0
3	CYC	AAA	201	43/43	0.97	0.06	17,19,26,31	0
3	CYC	KKK	201	43/43	0.97	0.06	14,18,26,29	0
3	CYC	BBB	201	43/43	0.97	0.06	14,19,34,43	0
3	CYC	GGG	201	43/43	0.97	0.06	13,15,21,25	0
3	CYC	CCC	201	43/43	0.97	0.06	13,15,22,25	0
3	CYC	DDD	201	43/43	0.97	0.06	17,22,33,37	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.

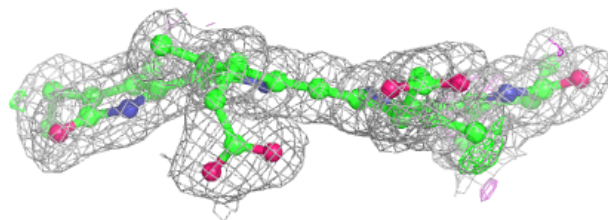
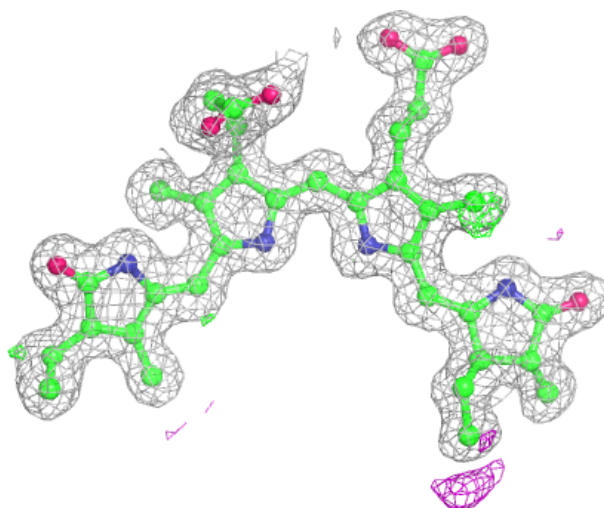
**Electron density around P6G CCC 202:**

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



**Electron density around CYC LLL 201:**

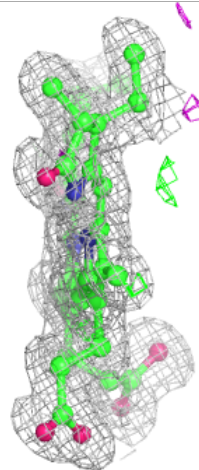
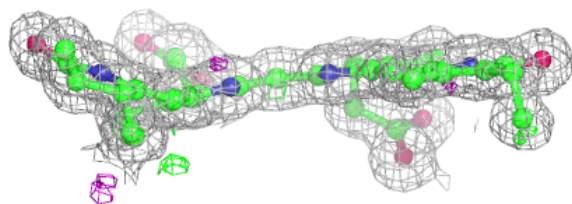
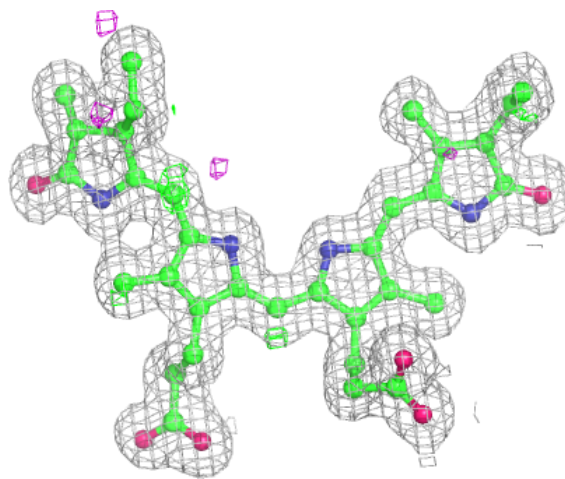
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





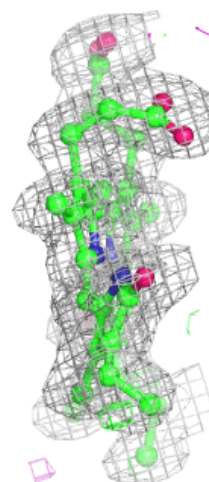
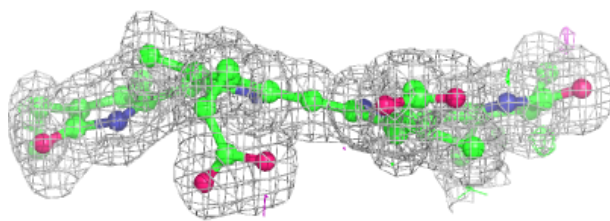
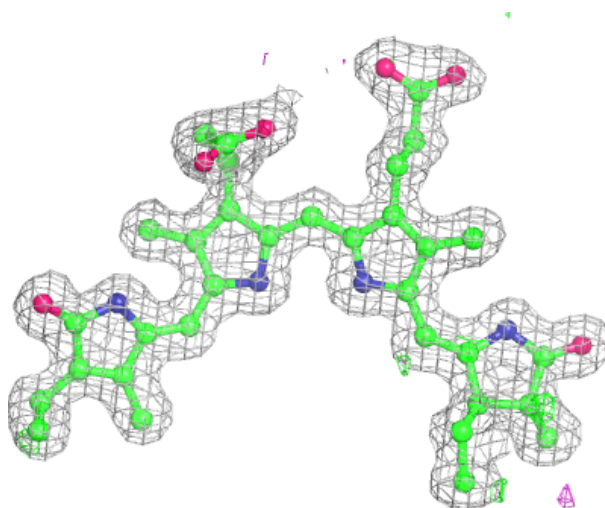
**Electron density around CYC EEE 201:**

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



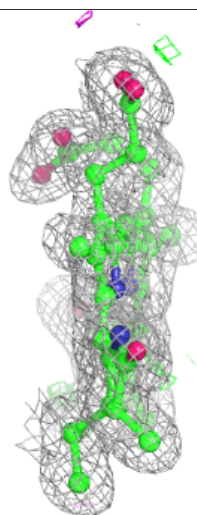
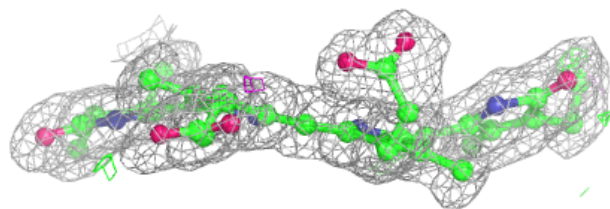
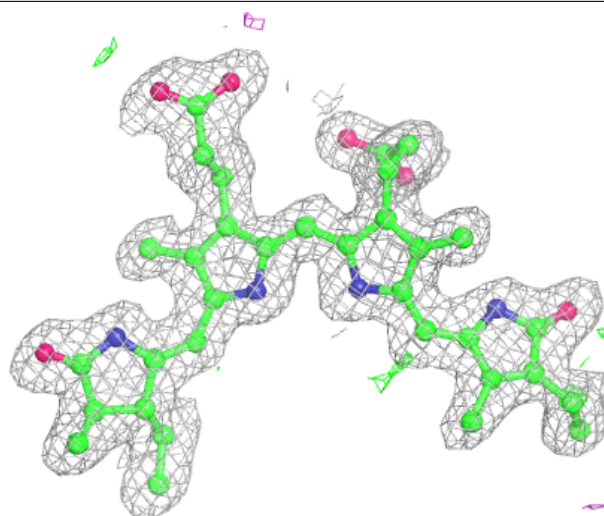
**Electron density around CYC FFF 201:**

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



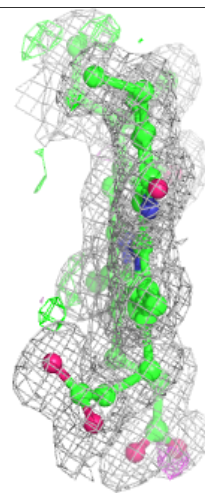
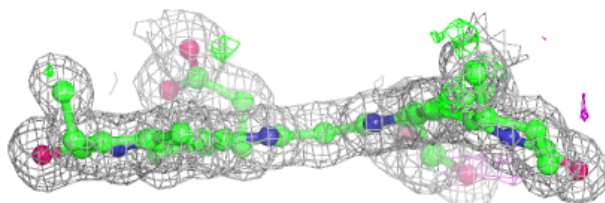
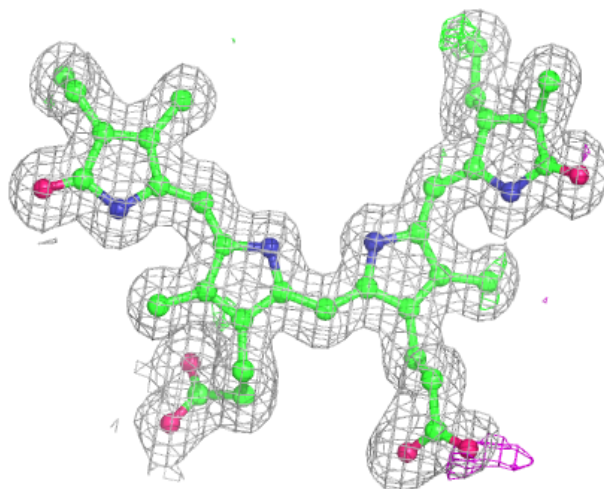
**Electron density around CYC HHH 201:**

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



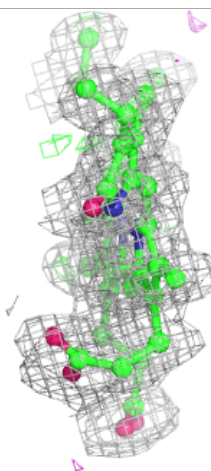
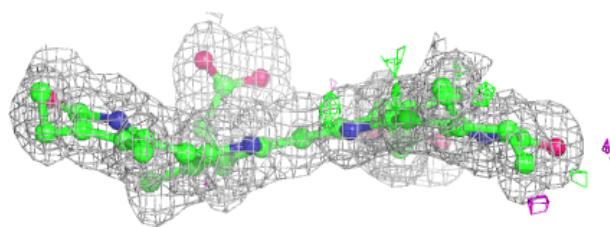
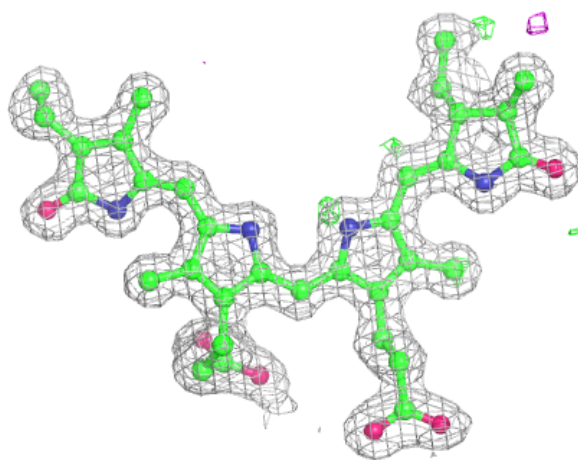
**Electron density around CYC III 201:**

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



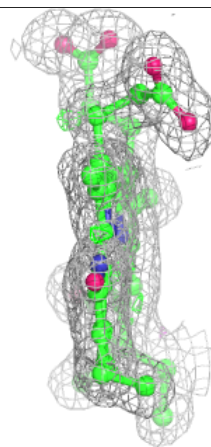
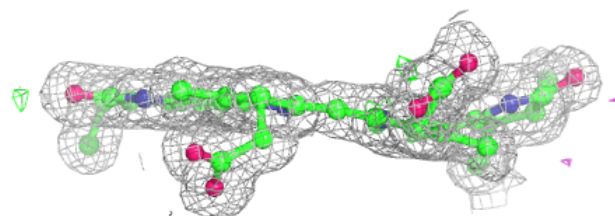
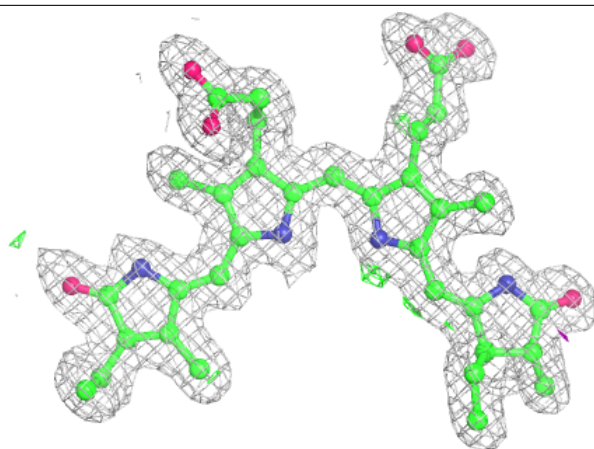
**Electron density around CYC JJJ 201:**

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



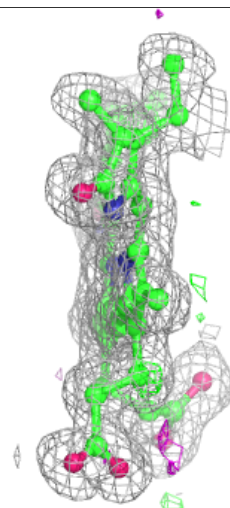
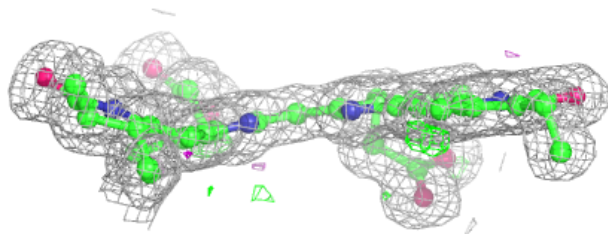
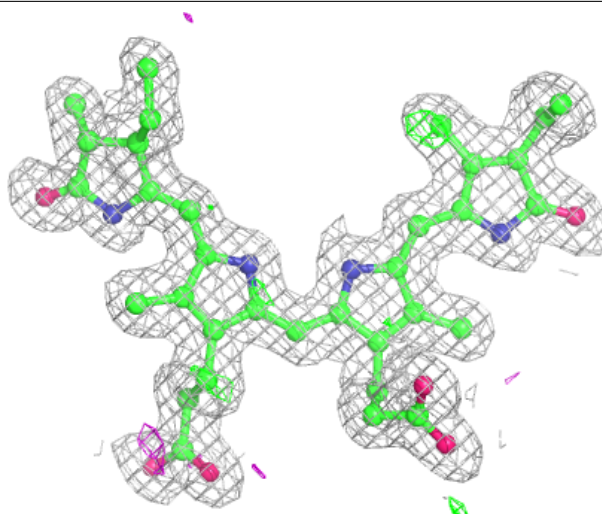
**Electron density around CYC AAA 201:**

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



**Electron density around CYC KKK 201:**

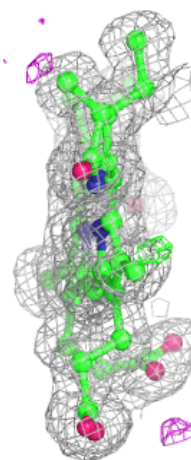
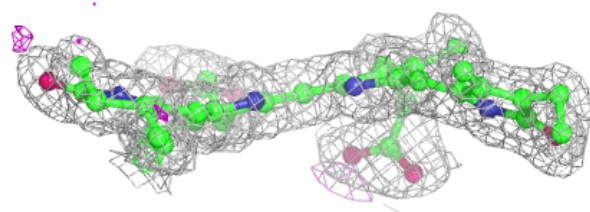
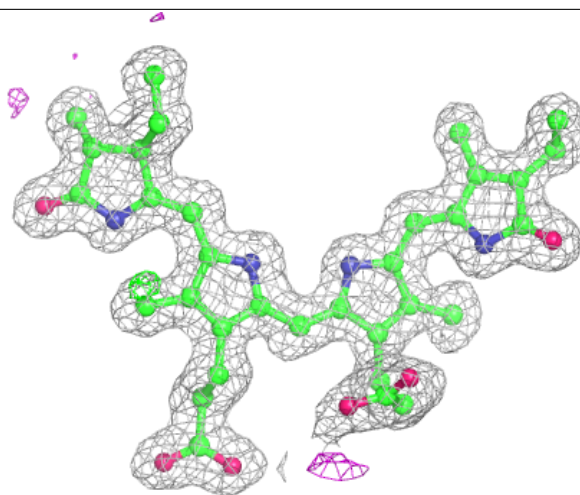
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CYC BBB 201:**

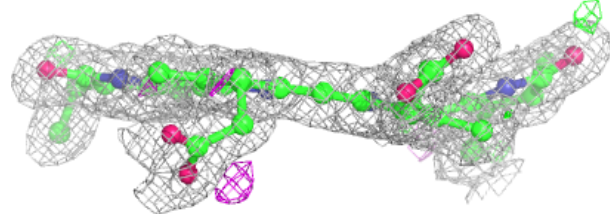
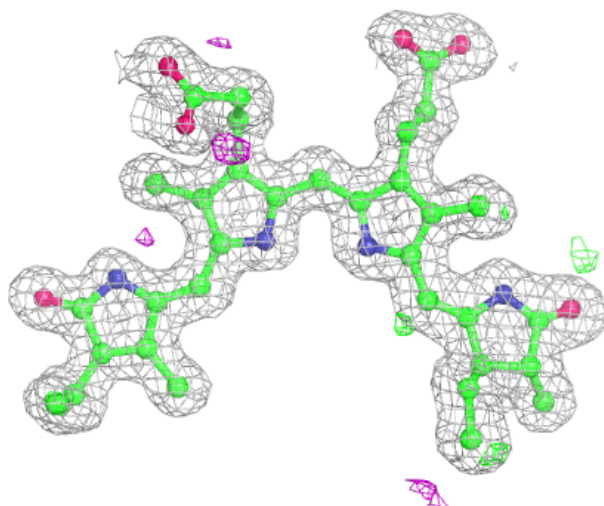
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





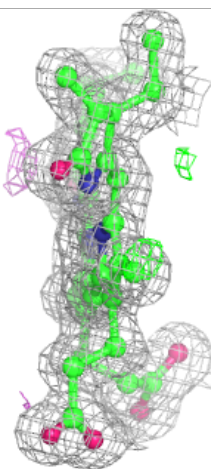
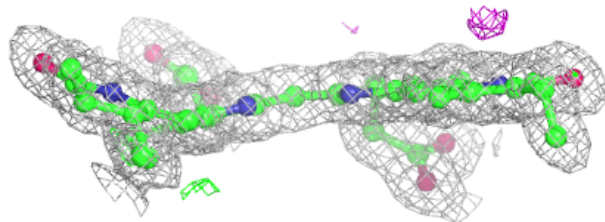
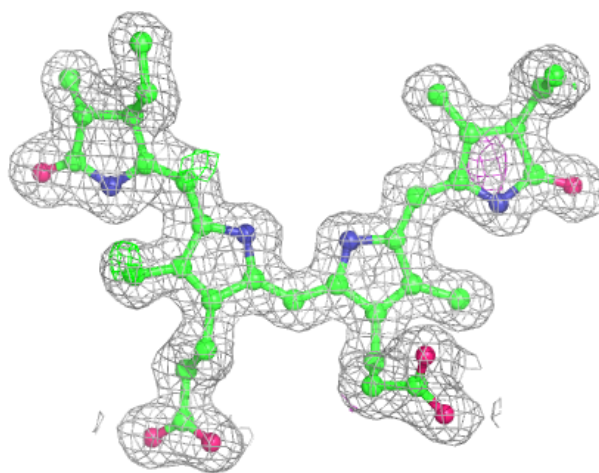
**Electron density around CYC GGG 201:**

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



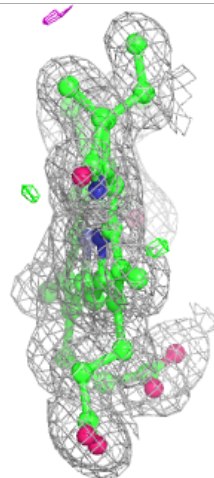
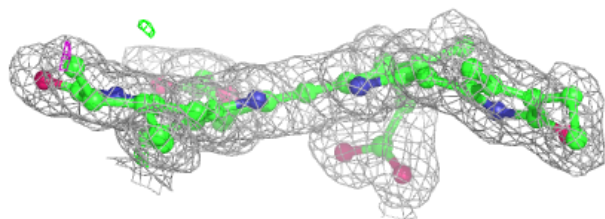
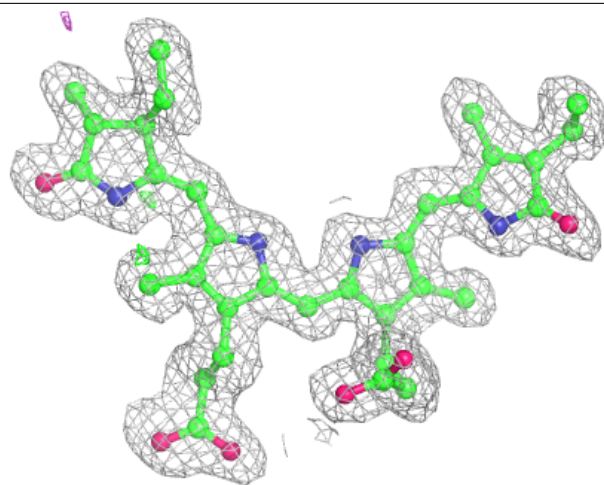
**Electron density around CYC CCC 201:**

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



**Electron density around CYC DDD 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.