



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:03 AM UTC

PDB ID : 9EF6 / pdb\_00009ef6  
Title : Crystal structure of Cryptosporidium parvum N-myristoyltransferase with bound myristoyl-CoA and inhibitor 20045  
Authors : Fenwick, M.K.; Staker, B.L.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2024-11-19  
Resolution : 1.95 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

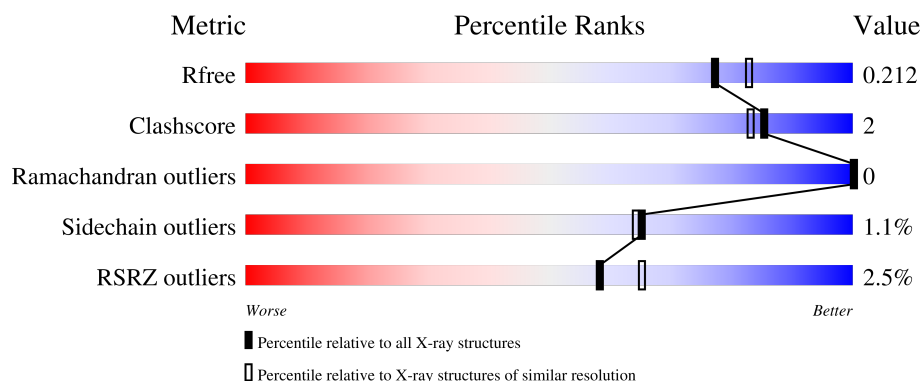
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

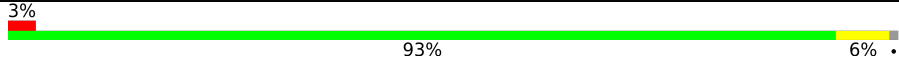
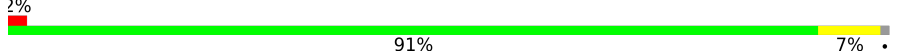
The reported resolution of this entry is 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	A	431	
1	B	431	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15969 atoms, of which 7615 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.

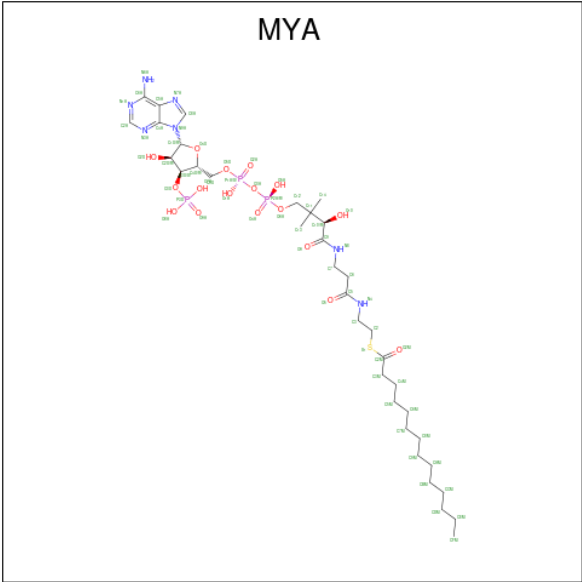
- Molecule 1 is a protein called Glycylpeptide N-tetradecanoyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	426	Total	C	H	N	O	S	0	28	0
			7338	2365	3658	625	669	21			
1	B	426	Total	C	H	N	O	S	0	43	0
			7459	2403	3720	632	682	22			

There are 8 discrepancies between the modelled and reference sequences:

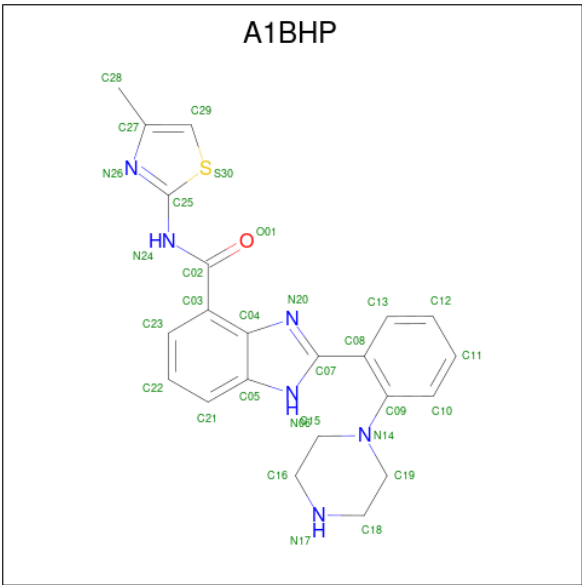
Chain	Residue	Modelled	Actual	Comment	Reference
A	36	GLY	-	expression tag	UNP Q5CV46
A	37	PRO	-	expression tag	UNP Q5CV46
A	38	GLY	-	expression tag	UNP Q5CV46
A	39	SER	-	expression tag	UNP Q5CV46
B	36	GLY	-	expression tag	UNP Q5CV46
B	37	PRO	-	expression tag	UNP Q5CV46
B	38	GLY	-	expression tag	UNP Q5CV46
B	39	SER	-	expression tag	UNP Q5CV46

- Molecule 2 is TETRADECANOYL-COA (CCD ID: MYA) (formula:  $C_{35}H_{62}N_7O_{17}P_3S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	0	0
			121	35	58	7	17	3	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			121	35	58	7	17	3	1		

- Molecule 3 is (2M)-N-(4-methyl-1,3-thiazol-2-yl)-2-[2-(piperazin-1-yl)phenyl]-1H-1,3-benzimidazole-4-carboxamide (CCD ID: A1BHP) (formula: C<sub>22</sub>H<sub>22</sub>N<sub>6</sub>OS) (labeled as "Ligand of Interest" by depositor).

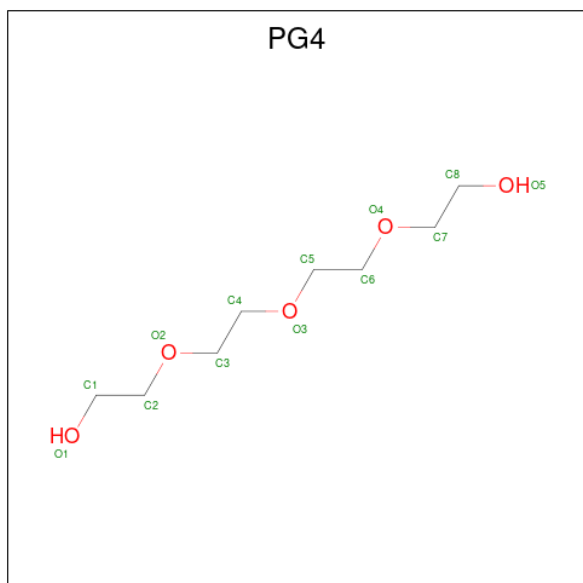


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			53	22	23	6	1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

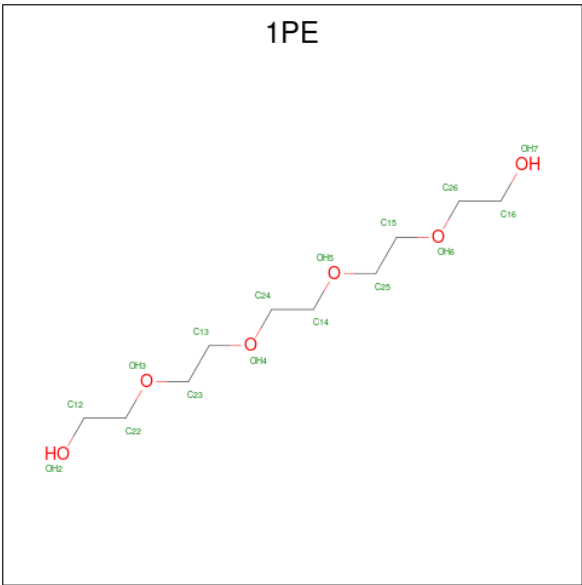
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	4	Total	Cl	0	1
			4	4		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



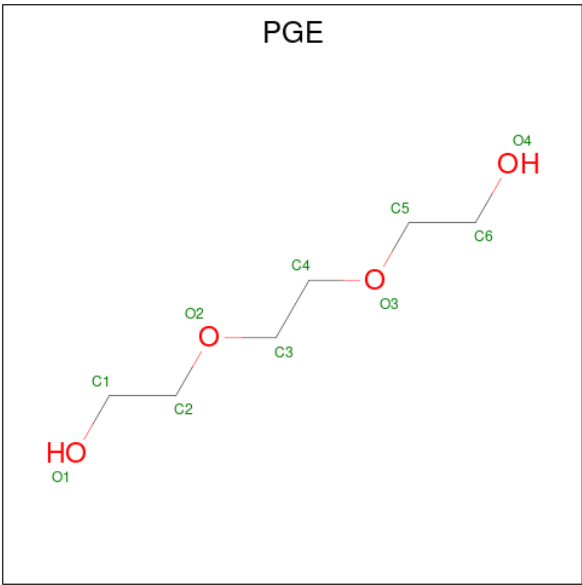
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			38	10	22	6		
6	A	1	Total	C	H	O	0	0
			38	10	22	6		
6	B	1	Total	C	H	O	0	1
			38	10	22	6		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			24	6	14	4		

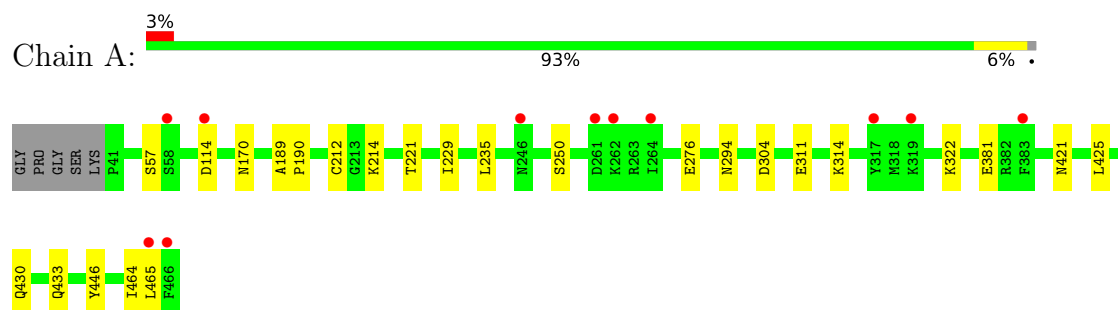
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	370	Total 372	O 372	0	14
8	B	325	Total 330	O 330	0	25

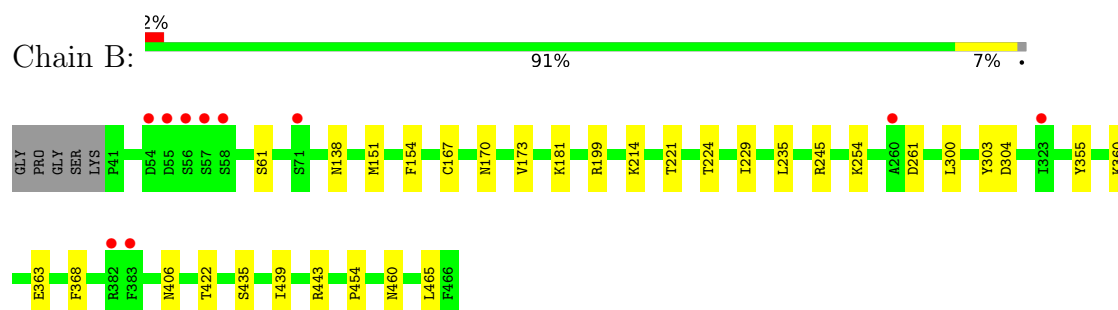
### 3 Residue-property plots [i](#)

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: Glycylpeptide N-tetradecanoyltransferase



#### • Molecule 1: Glycylpeptide N-tetradecanoyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.45Å 88.26Å 98.24Å 90.00° 97.62° 90.00°	Depositor
Resolution (Å)	46.05 – 1.95 46.05 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.05-1.95) 98.7 (46.05-1.95)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.52 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, $R_{free}$	0.167 , 0.192 (Not available) , 0.212	Depositor DCC
$R_{free}$ test set	3236 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 46.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15969	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: CL, 1PE, A1BHP, MYA, PG4, PGE

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	0.43	0/3829	0.44	0/5169
1	B	0.40	0/3935	0.42	0/5321
All	All	0.42	0/7764	0.43	0/10490

There are no bond length outliers.

There are no bond angle outliers.

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	A	3680	3658	3585	11	1
1	B	3739	3720	3588	22	1
2	A	63	58	58	0	0
2	B	63	58	58	0	0
3	A	30	23	0	1	0
4	A	2	0	0	0	0
4	B	4	0	0	2	0
5	A	13	18	18	0	0
6	A	32	44	44	0	0
6	B	16	22	22	0	0
7	B	10	14	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	372	0	0	2	0
8	B	330	0	0	5	0
All	All	8354	7615	7387	33	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 2.

All (33) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224[B]:THR:HG23	8:B:628:HOH:O	1.92	0.68
1:A:229:ILE:HG23	1:A:235:LEU:HD12	1.80	0.63
1:A:433:GLN:NE2	8:A:606:HOH:O	2.30	0.61
1:B:170:ASN:ND2	1:B:304:ASP:OD2	2.31	0.60
1:B:245:ARG:O	8:B:601:HOH:O	2.15	0.59
1:A:170:ASN:ND2	1:A:304:ASP:OD2	2.37	0.58
1:B:224[B]:THR:HG22	1:B:443[B]:ARG:CD	2.39	0.53
1:B:224[B]:THR:HG22	1:B:443[B]:ARG:HD2	1.93	0.50
1:B:181:LYS:NZ	8:B:613:HOH:O	2.42	0.49
1:B:224[A]:THR:CG2	1:B:439[A]:ILE:HD11	2.44	0.47
1:B:460[B]:ASN:ND2	8:B:620[B]:HOH:O	2.48	0.46
1:B:173:VAL:HG11	1:B:465:LEU:HD22	1.99	0.45
1:A:212[A]:CYS:SG	1:A:214:LYS:HG2	2.57	0.45
1:B:254:LYS:NZ	4:B:505:CL:CL	2.85	0.45
1:B:355:TYR:HB2	1:B:368:PHE:CZ	2.53	0.43
1:A:430:GLN:NE2	8:A:633:HOH:O	2.51	0.43
1:B:61:SER:HB3	1:B:454:PRO:HG3	2.00	0.43
1:A:425:LEU:CD1	1:A:464:ILE:HD13	2.48	0.43
1:A:421:ASN:HB3	3:A:502:A1BHP:C12	2.48	0.43
1:B:151:MET:HE2	1:B:154:PHE:HB2	2.02	0.42
1:B:167[B]:CYS:SG	1:B:303:TYR:HB2	2.60	0.42
1:A:465:LEU:N	1:A:465:LEU:HD12	2.35	0.41
1:A:221:THR:HG22	1:A:446:TYR:HB2	2.03	0.41
1:B:138:ASN:O	1:B:199:ARG:HD3	2.20	0.41
1:B:229:ILE:HG23	1:B:235:LEU:HD12	2.03	0.40
1:B:224[A]:THR:HG21	1:B:439[A]:ILE:HD11	2.03	0.40
1:B:435:SER:HB2	4:B:504:CL:CL	2.58	0.40
1:B:406:ASN:HB2	8:B:843[A]:HOH:O	2.20	0.40
1:A:189:ALA:HB3	1:A:190:PRO:HD3	2.02	0.40
1:A:311[A]:GLU:OE1	1:A:314:LYS:NZ	2.54	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)
1:A:381:GLU:OE2	1:B:360:LYS:H[2_556]	1.57	0.03

## 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	450/431 (104%)	433 (96%)	17 (4%)	0	100	100
1	B	465/431 (108%)	447 (96%)	18 (4%)	0	100	100
All	All	915/862 (106%)	880 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	420/404 (104%)	413 (98%)	7 (2%)	53	49
1	B	430/404 (106%)	427 (99%)	3 (1%)	76	76
All	All	850/808 (105%)	840 (99%)	10 (1%)	65	61

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	114	ASP
1	A	250	SER
1	A	276	GLU
1	A	294[A]	ASN
1	A	294[B]	ASN
1	A	322	LYS
1	B	214	LYS
1	B	261	ASP
1	B	363	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	120	ASN
1	B	53	ASN
1	B	433	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	MYA	B	501	-	63,65,65	1.56	13 (20%)	85,91,91	1.42	10 (11%)
6	1PE	A	507	-	15,15,15	0.16	0	14,14,14	0.14	0
6	1PE	A	506	-	15,15,15	0.15	0	14,14,14	0.08	0
6	1PE	B	507[B]	-	15,15,15	0.48	0	14,14,14	0.29	0
2	MYA	A	501	-	63,65,65	1.53	15 (23%)	85,91,91	1.45	14 (16%)
7	PGE	B	506	-	9,9,9	0.31	0	8,8,8	0.30	0
3	A1BHP	A	502	-	34,34,34	2.61	12 (35%)	46,48,48	2.41	9 (19%)
5	PG4	A	505	-	12,12,12	0.18	0	11,11,11	0.47	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	MYA	B	501	-	-	8/64/80/80	0/3/3/3
6	1PE	A	507	-	-	3/13/13/13	-
6	1PE	A	506	-	-	3/13/13/13	-
6	1PE	B	507[B]	-	-	7/13/13/13	-
2	MYA	A	501	-	-	3/64/80/80	0/3/3/3
7	PGE	B	506	-	-	2/7/7/7	-
3	A1BHP	A	502	-	-	2/16/24/24	0/5/5/5
5	PG4	A	505	-	-	4/10/10/10	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	A1BHP	C25-S30	-6.91	1.64	1.74
3	A	502	A1BHP	C29-C27	6.10	1.44	1.35
3	A	502	A1BHP	C02-N24	4.59	1.45	1.37
3	A	502	A1BHP	C29-S30	-4.44	1.61	1.71
2	A	501	MYA	C12-C11	4.33	1.59	1.52
2	B	501	MYA	C2M-S1	4.32	1.86	1.76
2	B	501	MYA	C12-C11	3.85	1.58	1.52
3	A	502	A1BHP	C08-C07	3.85	1.54	1.47
3	A	502	A1BHP	C03-C02	3.72	1.57	1.50
2	B	501	MYA	C9-N8	3.60	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	A1BHP	C27-N26	3.59	1.44	1.38
2	A	501	MYA	C5A-C4A	3.53	1.45	1.39
2	B	501	MYA	O3X-C3X	-3.33	1.32	1.44
2	A	501	MYA	O3X-C3X	-3.12	1.33	1.44
2	B	501	MYA	C5A-C4A	3.09	1.44	1.39
2	A	501	MYA	C9-N8	3.05	1.40	1.33
2	A	501	MYA	C2M-S1	3.02	1.83	1.76
2	B	501	MYA	O6A-C12	-2.99	1.34	1.43
2	B	501	MYA	C2A-N1A	2.95	1.39	1.33
2	B	501	MYA	C2X-C3X	2.84	1.59	1.53
2	B	501	MYA	C5-N4	2.82	1.40	1.33
3	A	502	A1BHP	C09-N14	2.77	1.47	1.41
3	A	502	A1BHP	C25-N26	2.74	1.35	1.31
3	A	502	A1BHP	C03-C04	2.73	1.44	1.41
2	A	501	MYA	O6A-C12	-2.71	1.35	1.43
2	A	501	MYA	C3X-C4X	2.70	1.59	1.52
2	A	501	MYA	P1A-O3A	-2.70	1.56	1.59
2	B	501	MYA	C8A-N7A	2.69	1.36	1.31
2	A	501	MYA	C2A-N1A	2.56	1.38	1.33
2	A	501	MYA	C3M-C2M	-2.54	1.48	1.50
2	B	501	MYA	P2A-O3A	-2.53	1.56	1.59
3	A	502	A1BHP	C25-N24	2.44	1.41	1.38
2	A	501	MYA	C8A-N7A	2.26	1.36	1.31
2	A	501	MYA	C5-N4	2.12	1.38	1.33
2	A	501	MYA	C6A-N6A	2.10	1.39	1.34
2	B	501	MYA	C4A-N3A	2.09	1.38	1.34
3	A	502	A1BHP	C05-C04	-2.06	1.38	1.40
2	A	501	MYA	P2A-O3A	-2.06	1.57	1.59
2	A	501	MYA	C8A-N9A	2.04	1.41	1.37
2	B	501	MYA	C8A-N9A	2.02	1.41	1.37

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	A1BHP	C29-S30-C25	10.56	96.61	88.40
3	A	502	A1BHP	C29-C27-N26	-7.05	109.73	114.51
2	B	501	MYA	C6-C5-N4	4.71	124.93	116.34
2	B	501	MYA	C3M-C2M-S1	4.45	118.71	113.40
3	A	502	A1BHP	C05-C04-N20	-3.95	106.89	110.31
2	A	501	MYA	C3M-C2M-S1	3.92	118.07	113.40
3	A	502	A1BHP	C04-C05-N06	3.87	107.33	105.13
3	A	502	A1BHP	S30-C25-N26	-3.81	111.69	115.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	MYA	O5A-P2A-O3A	3.80	117.54	107.27
2	A	501	MYA	C6-C5-N4	3.45	122.63	116.34
2	B	501	MYA	O5-C5-N4	-3.26	116.62	123.03
2	A	501	MYA	C2-S1-C2M	3.25	111.45	101.84
2	A	501	MYA	O5-C5-N4	-3.16	116.83	123.03
2	A	501	MYA	C2X-C3X-C4X	-3.12	97.78	103.24
2	A	501	MYA	O5A-P2A-O3A	3.11	115.68	107.27
2	B	501	MYA	C2-S1-C2M	3.11	111.02	101.84
2	A	501	MYA	O2M-C2M-C3M	-3.00	120.52	123.98
2	A	501	MYA	C5A-C4A-N3A	-2.95	122.66	126.72
3	A	502	A1BHP	C28-C27-N26	2.90	123.53	119.58
2	A	501	MYA	C7-C6-C5	2.84	117.13	112.39
2	A	501	MYA	C10-C9-N8	2.72	121.65	116.48
2	B	501	MYA	O2M-C2M-C3M	-2.64	120.93	123.98
3	A	502	A1BHP	N06-C07-N20	-2.44	108.28	112.44
2	A	501	MYA	O3X-P3X-O9A	-2.40	100.76	109.33
3	A	502	A1BHP	C04-N20-C07	2.40	109.03	105.09
2	B	501	MYA	O3X-P3X-O9A	-2.39	100.82	109.33
2	A	501	MYA	C13-C11-C10	2.32	112.72	108.77
2	B	501	MYA	C5A-C4A-N3A	-2.29	123.56	126.72
2	B	501	MYA	C2X-C3X-C4X	-2.18	99.42	103.24
3	A	502	A1BHP	C21-C05-C04	-2.12	120.57	122.57
2	A	501	MYA	N3A-C4A-N9A	2.08	130.70	127.17
2	B	501	MYA	O2M-C2M-S1	-2.05	120.08	122.68
2	A	501	MYA	C4A-C5A-N7A	-2.00	108.29	110.58

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	MYA	C5X-O5X-P1A-O3A
6	B	507[B]	1PE	OH7-C16-C26-OH6
6	A	507	1PE	OH4-C13-C23-OH3
5	A	505	PG4	O4-C7-C8-O5
5	A	505	PG4	O3-C5-C6-O4
6	B	507[B]	1PE	OH5-C14-C24-OH4
2	B	501	MYA	C3M-C2M-S1-C2
6	B	507[B]	1PE	OH2-C12-C22-OH3
5	A	505	PG4	C3-C4-O3-C5
6	B	507[B]	1PE	C14-C24-OH4-C13
6	B	507[B]	1PE	C15-C25-OH5-C14
7	B	506	PGE	O3-C5-C6-O4

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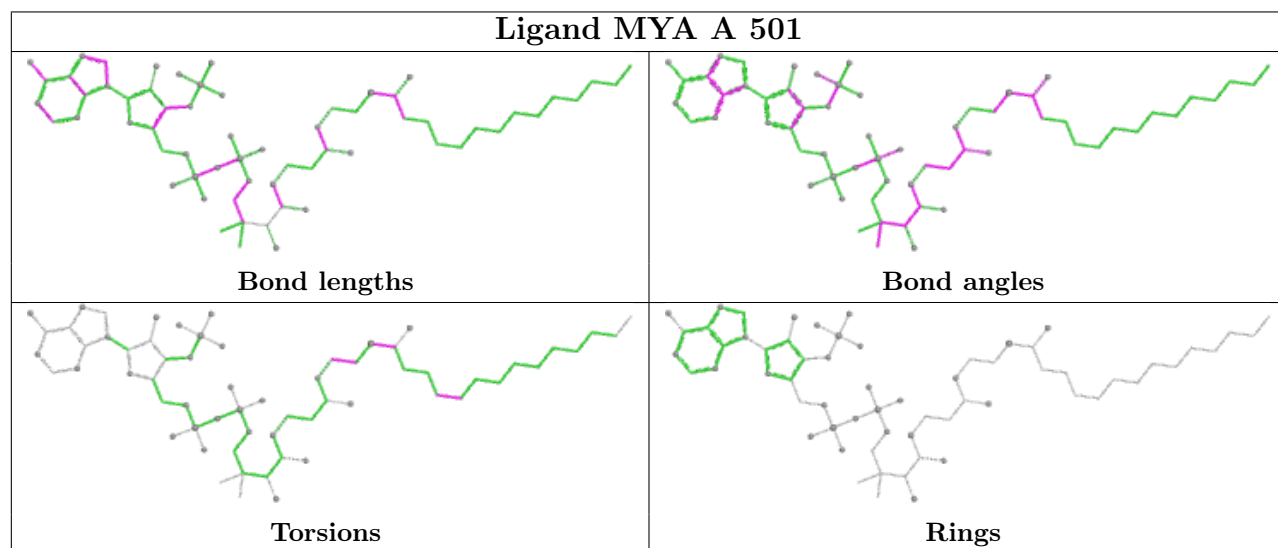
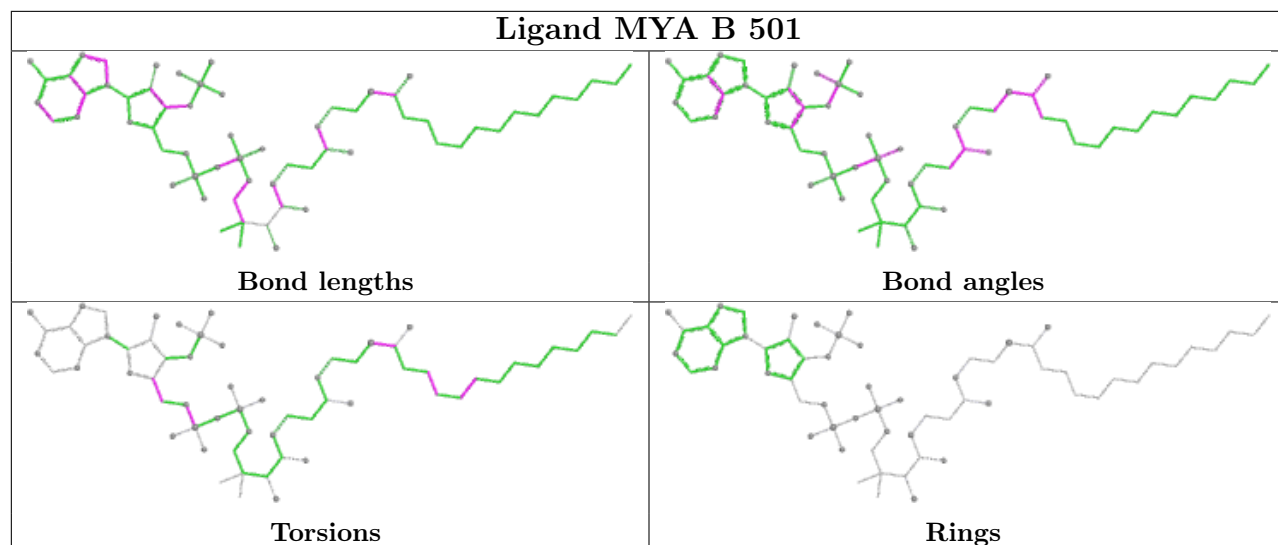
Mol	Chain	Res	Type	Atoms
6	A	506	1PE	C24-C14-OH5-C25
2	B	501	MYA	C3X-C4X-C5X-O5X
7	B	506	PGE	O1-C1-C2-O2
5	A	505	PG4	C1-C2-O2-C3
2	B	501	MYA	C5X-O5X-P1A-O1A
2	B	501	MYA	C5X-O5X-P1A-O2A
3	A	502	A1BHP	O01-C02-C03-C04
2	B	501	MYA	C5M-C6M-C7M-C8M
6	A	506	1PE	OH4-C13-C23-OH3
6	B	507[B]	1PE	C12-C22-OH3-C23
3	A	502	A1BHP	N24-C02-C03-C04
6	A	507	1PE	C13-C23-OH3-C22
2	A	501	MYA	C3M-C2M-S1-C2
6	A	506	1PE	C23-C13-OH4-C24
2	B	501	MYA	C3M-C4M-C5M-C6M
2	A	501	MYA	S1-C2-C3-N4
6	A	507	1PE	C23-C13-OH4-C24
2	B	501	MYA	O4X-C4X-C5X-O5X
6	B	507[B]	1PE	OH6-C15-C25-OH5
2	A	501	MYA	C4M-C5M-C6M-C7M

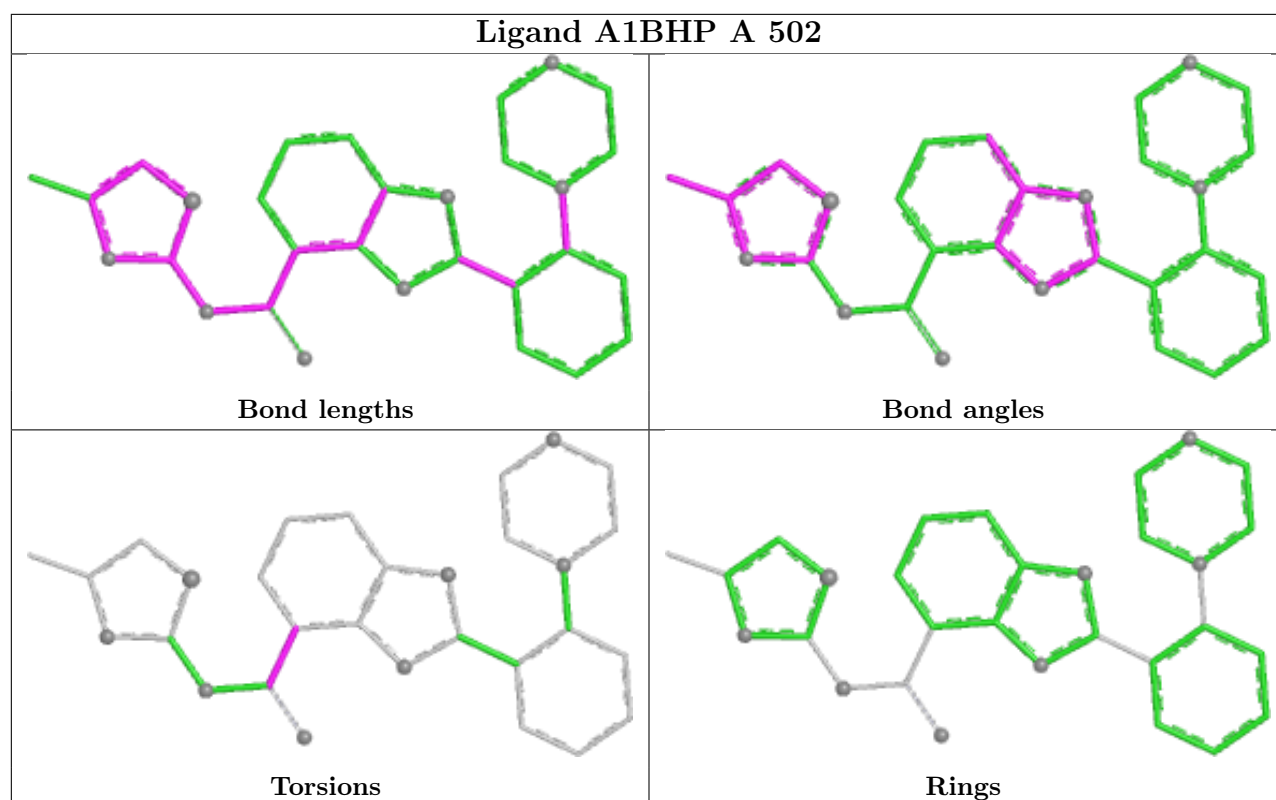
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	A1BHP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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

### 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	A	426/431 (98%)	0.08	11 (2%) 57 64	11, 29, 56, 90	21 (4%)
1	B	426/431 (98%)	0.11	10 (2%) 61 68	11, 30, 57, 98	31 (7%)
All	All	852/862 (98%)	0.09	21 (2%) 58 65	11, 29, 57, 98	52 (6%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	SER	3.3
1	B	71	SER	3.3
1	B	323	ILE	3.0
1	A	317[A]	TYR	3.0
1	B	58	SER	2.5
1	B	56	SER	2.5
1	B	382	ARG	2.4
1	A	465	LEU	2.4
1	B	57	SER	2.4
1	A	264	ILE	2.3
1	A	262	LYS	2.3
1	A	319[A]	LYS	2.3
1	B	55	ASP	2.3
1	A	261	ASP	2.2
1	B	54	ASP	2.2
1	A	383	PHE	2.2
1	A	246	ASN	2.2
1	A	114	ASP	2.1
1	B	383	PHE	2.1
1	B	260	ALA	2.1
1	A	466	PHE	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

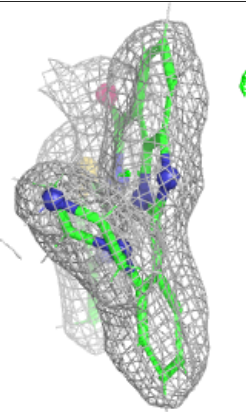
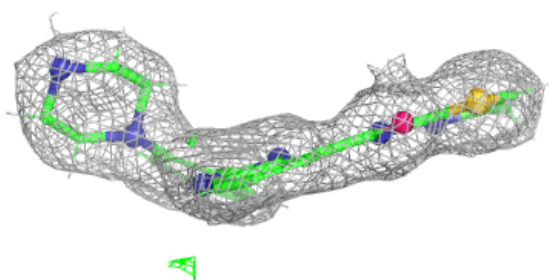
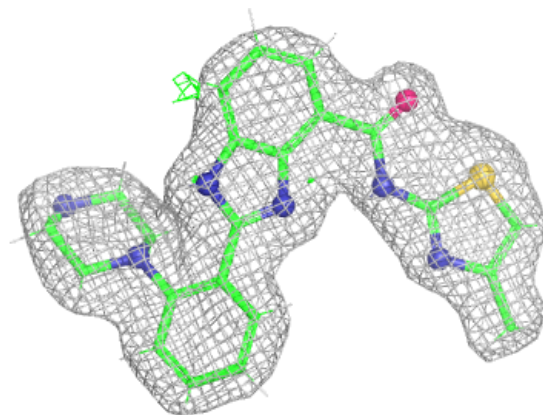
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PG4	A	505	13/13	0.78	0.14	51,62,80,81	0
6	1PE	B	507[B]	16/16	0.79	0.17	42,53,68,70	38
7	PGE	B	506	10/10	0.84	0.12	41,53,62,63	0
6	1PE	A	506	16/16	0.86	0.12	37,52,64,64	0
6	1PE	A	507	16/16	0.89	0.10	33,46,65,81	0
4	CL	B	504	1/1	0.90	0.18	49,49,49,49	0
3	A1BHP	A	502	30/30	0.95	0.07	16,24,30,32	0
4	CL	A	503	1/1	0.95	0.11	41,41,41,41	0
2	MYA	A	501	63/63	0.95	0.07	15,24,31,36	0
2	MYA	B	501	63/63	0.95	0.07	15,27,37,42	0
4	CL	B	505	1/1	0.97	0.13	47,47,47,47	0
4	CL	B	503	1/1	0.97	0.12	45,45,45,45	0
4	CL	B	502[A]	1/1	0.97	0.07	37,37,37,37	1
4	CL	A	504	1/1	0.98	0.11	35,35,35,35	0

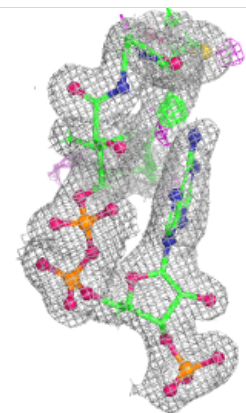
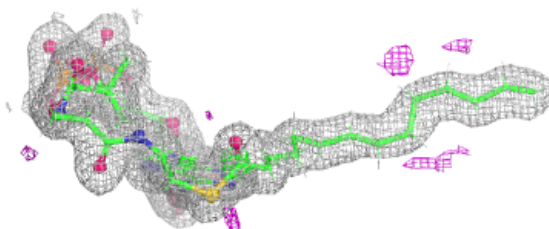
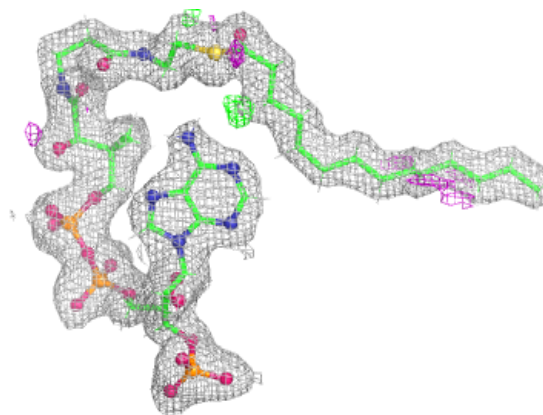
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

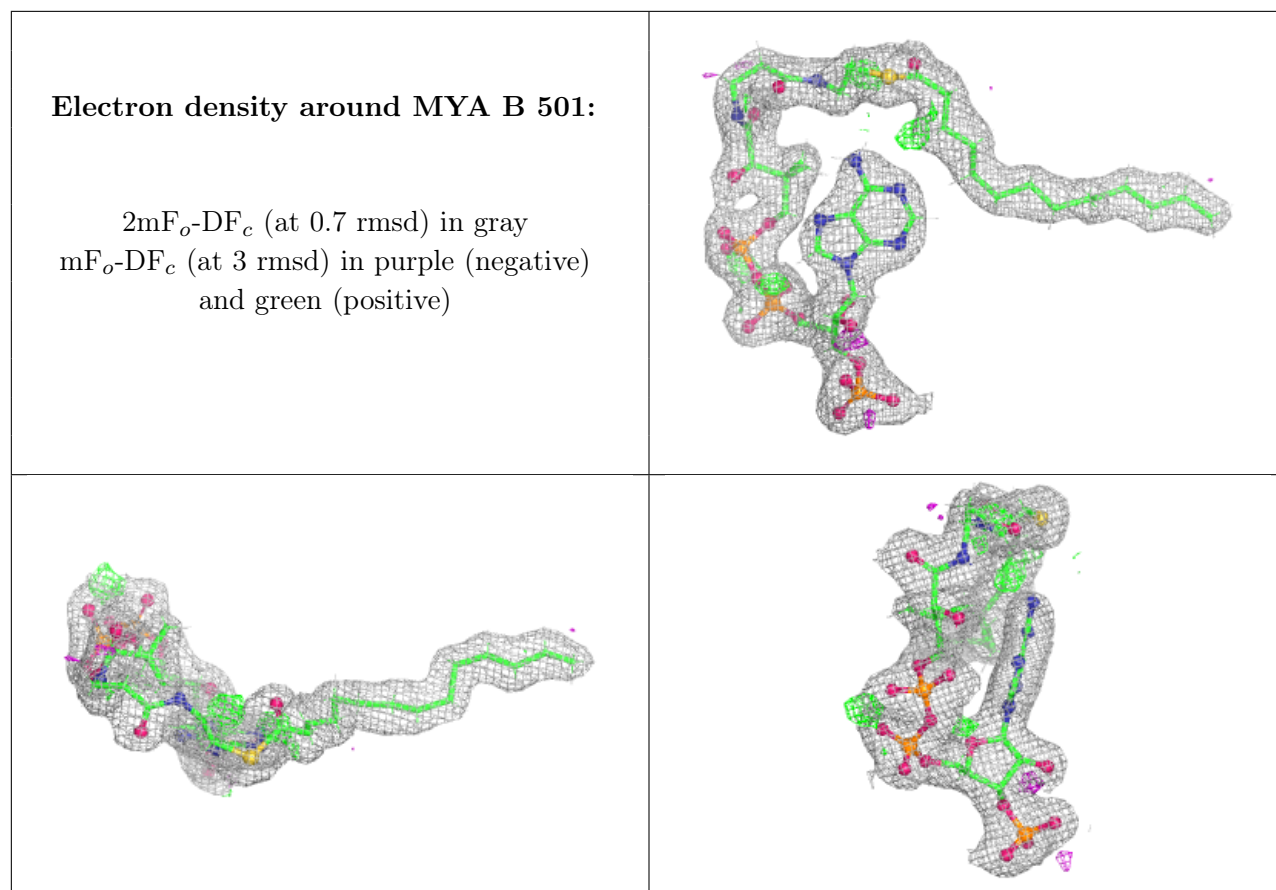
**Electron density around A1BHP A 502:**

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

**Electron density around MYA A 501:**

$2mF_o-DF_c$  (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.