



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:46 PM UTC

PDB ID : 9EF7 / pdb_00009ef7
Title : Crystal structure of Cryptosporidium parvum N-myristoyltransferase with bound myristoyl-CoA and inhibitor 20057
Authors : Fenwick, M.K.; Staker, B.L.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2024-11-19
Resolution : 1.80 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

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>.

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

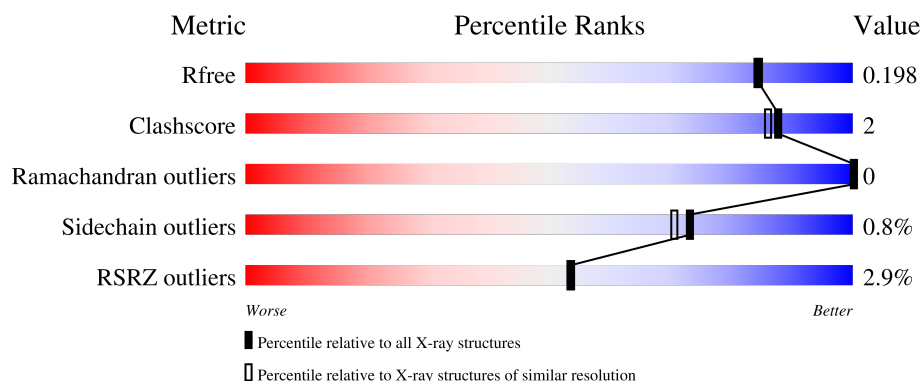
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

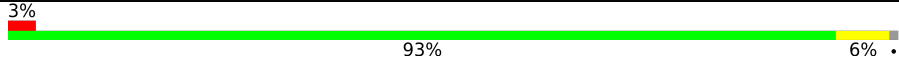
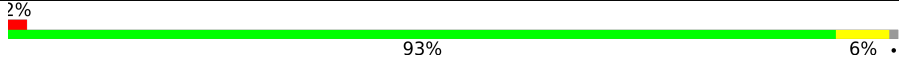
The reported resolution of this entry is 1.80 Å.

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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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 7 unique types of molecules in this entry. The entry contains 16201 atoms, of which 7751 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.

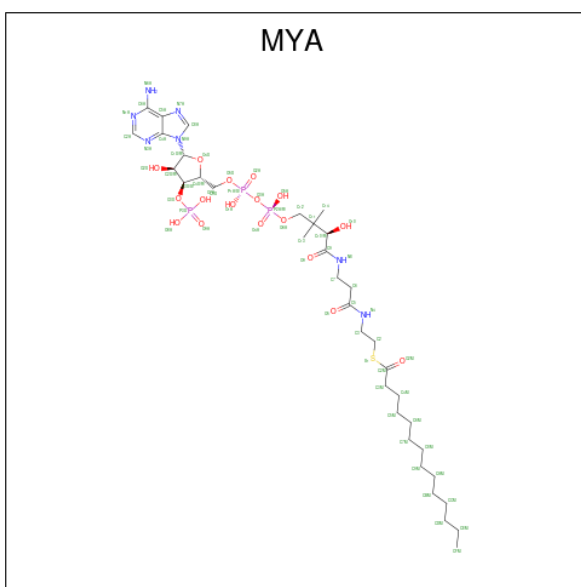
- Molecule 1 is a protein called Glycylpeptide N-tetradecanoyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	426	Total	C	H	N	O	S	0	38	0
			7591	2447	3778	647	697	22			
1	B	426	Total	C	H	N	O	S	0	30	0
			7443	2407	3697	634	682	23			

There are 8 discrepancies between the modelled and reference sequences:

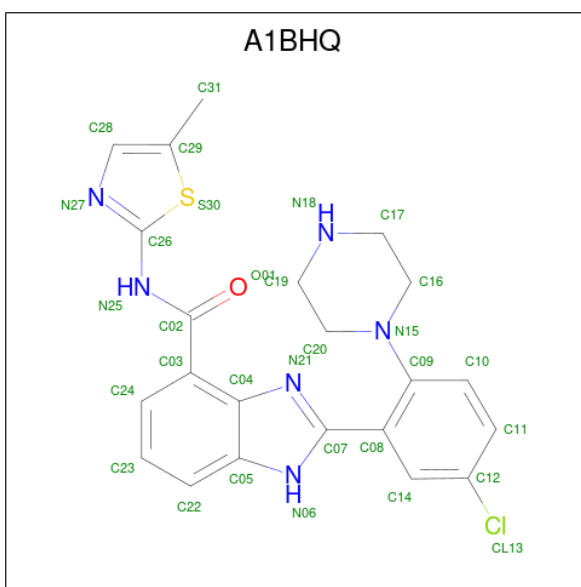
Chain	Residue	Modelled	Actual	Comment	Reference
A	36	GLY	-	expression tag	UNP Q5CV46
A	37	PRO	-	expression tag	UNP Q5CV46
A	38	GLY	-	expression tag	UNP Q5CV46
A	39	SER	-	expression tag	UNP Q5CV46
B	36	GLY	-	expression tag	UNP Q5CV46
B	37	PRO	-	expression tag	UNP Q5CV46
B	38	GLY	-	expression tag	UNP Q5CV46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

- Molecule 2 is TETRADECANOYL-COA (CCD ID: MYA) (formula: C₃₅H₆₂N₇O₁₇P₃S) (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)-2-[5-chloro-2-(piperazin-1-yl)phenyl]-N-(5-methyl-1,3-thiazol-2-yl)-1H-1,3-benzimidazole-4-carboxamide (CCD ID: A1BHQ) (formula: C₂₂H₂₁ClN₆OS) (labeled as "Ligand of Interest" by depositor).

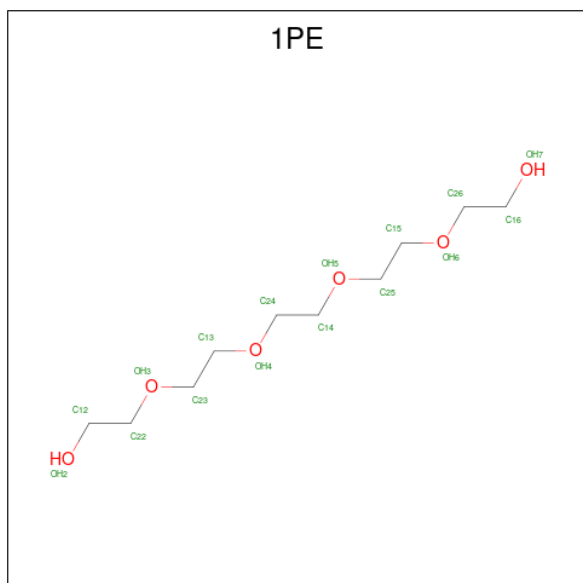


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	H	N	O	S	0	0
			53	22	1	22	6	1	1		

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

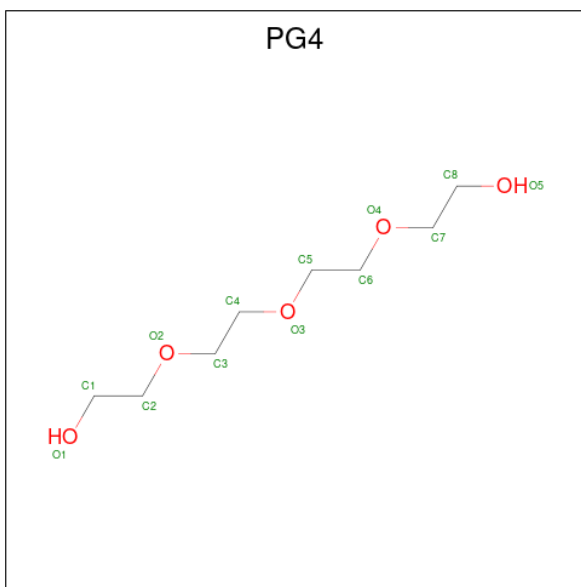
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	3	Total	Cl	0	1
			3	3		

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



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

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



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

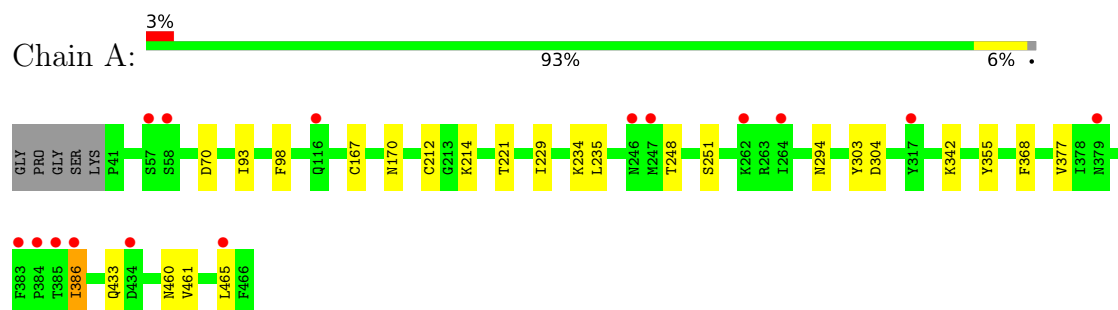
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	314	Total	O	0	28
			323	323		
7	B	300	Total	O	0	21
			306	306		

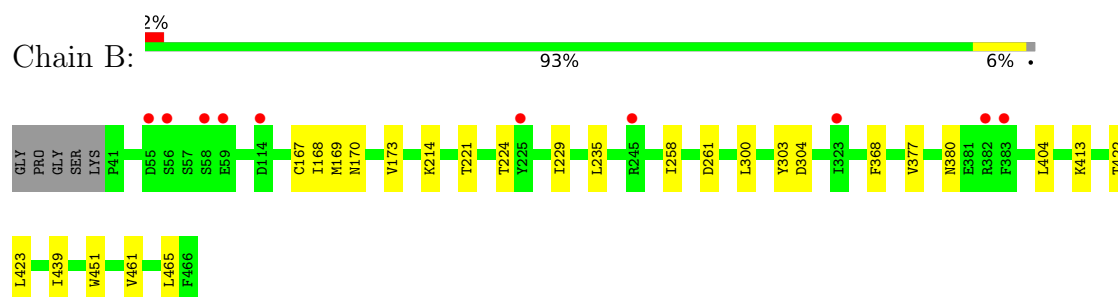
3 Residue-property plots [i](#)

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, α , β , γ	53.81Å 88.16Å 97.98Å 90.00° 97.62° 90.00°	Depositor
Resolution (Å)	38.54 – 1.80 38.54 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.3 (38.54-1.80) 96.4 (38.54-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.81Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.168 , 0.198 0.168 , 0.198	Depositor DCC
R_{free} test set	4090 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16201	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 1PE, PG4, MYA, A1BHQ, CL

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	0.33	0/3906	0.45	0/5272
1	B	0.35	0/3838	0.45	0/5182
All	All	0.34	0/7744	0.45	0/10454

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	3813	3778	3752	15	0
1	B	3746	3697	3682	14	0
2	A	63	58	58	0	0
2	B	63	58	58	0	0
3	A	31	22	0	1	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
5	A	32	44	44	0	0
5	B	16	22	22	0	0
6	A	39	54	54	3	0
6	B	13	18	18	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	323	0	0	2	0
7	B	306	0	0	1	0
All	All	8450	7751	7688	31	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (31) 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:258:ILE:HD12	1:B:413:LYS:HD2	1.86	0.56
1:A:212[A]:CYS:SG	1:A:214:LYS:HG2	2.48	0.54
1:A:170:ASN:ND2	1:A:304:ASP:OD2	2.42	0.53
1:A:342:LYS:NZ	6:A:509:PG4:O2	2.43	0.52
1:B:422[B]:THR:HG22	1:B:423:LEU:O	2.09	0.52
1:A:229:ILE:HG23	1:A:235:LEU:HD12	1.94	0.50
1:A:465:LEU:N	1:A:465:LEU:HD12	2.26	0.50
1:A:433:GLN:NE2	7:A:618:HOH:O	2.46	0.48
1:B:221:THR:HG21	1:B:461:VAL:HG21	1.94	0.48
1:A:221:THR:HG21	1:A:461:VAL:HG21	1.95	0.48
1:B:170:ASN:ND2	1:B:304:ASP:OD2	2.46	0.47
1:B:169:MET:HE1	1:B:451:TRP:CZ3	2.50	0.47
1:B:168:ILE:HG23	1:B:300:LEU:HD13	1.96	0.47
1:B:168:ILE:CG2	1:B:300:LEU:HD13	2.45	0.46
1:B:229:ILE:HG23	1:B:235:LEU:HD12	1.97	0.46
1:A:342:LYS:NZ	6:A:509:PG4:O3	2.45	0.46
1:A:460[A]:ASN:ND2	7:A:624:HOH:O	2.49	0.46
1:A:248:THR:H	1:A:251:SER:HG	1.63	0.45
1:B:224:THR:CG2	1:B:439:ILE:HD11	2.47	0.45
1:B:368:PHE:HB3	1:B:404[B]:LEU:HD21	1.99	0.44
1:B:167[B]:CYS:SG	1:B:303:TYR:HB2	2.57	0.44
1:B:173:VAL:HG11	1:B:465:LEU:HD22	1.99	0.44
1:B:404[B]:LEU:C	1:B:404[B]:LEU:HD23	2.44	0.43
1:A:93:ILE:HA	1:A:98:PHE:CD2	2.54	0.42
1:A:355:TYR:HB2	1:A:368:PHE:CZ	2.55	0.42
1:A:167[B]:CYS:SG	1:A:303:TYR:HB2	2.60	0.41
1:B:377:VAL:HG12	1:B:380:ASN:HB2	2.03	0.41
1:A:377:VAL:CG2	1:A:386[B]:ILE:HD11	2.50	0.41
3:A:502:A1BHQ:O01	3:A:502:A1BHQ:S30	2.79	0.40
1:A:342:LYS:NZ	6:A:509:PG4:O4	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	460/431 (107%)	443 (96%)	17 (4%)	0	100	100
1	B	453/431 (105%)	432 (95%)	21 (5%)	0	100	100
All	All	913/862 (106%)	875 (96%)	38 (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	430/404 (106%)	424 (99%)	6 (1%)	59	52
1	B	420/404 (104%)	418 (100%)	2 (0%)	81	80
All	All	850/808 (105%)	842 (99%)	8 (1%)	73	67

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70[A]	ASP
1	A	70[B]	ASP
1	A	234	LYS
1	A	294	ASN
1	A	386[A]	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	386[B]	ILE
1	B	214	LYS
1	B	261	ASP

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	48	GLN
1	B	120	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	$\# Z > 2$
3	A1BHQ	A	502	-	35,35,35	2.94	14 (40%)	49,50,50	2.49	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	1PE	B	505[B]	-	15,15,15	0.13	0	14,14,14	0.12	0
5	1PE	A	505[A]	-	15,15,15	0.14	0	14,14,14	0.10	0
6	PG4	B	506	-	12,12,12	0.16	0	11,11,11	0.48	0
6	PG4	A	509	-	12,12,12	0.17	0	11,11,11	0.47	0
2	MYA	B	501	-	63,65,65	1.61	14 (22%)	85,91,91	1.39	14 (16%)
5	1PE	A	507	-	15,15,15	0.13	0	14,14,14	0.11	0
2	MYA	A	501	-	63,65,65	1.58	15 (23%)	85,91,91	1.41	13 (15%)
6	PG4	A	506	-	12,12,12	0.14	0	11,11,11	0.55	0
6	PG4	A	508	-	12,12,12	0.15	0	11,11,11	0.52	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	A1BHQ	A	502	-	-	2/16/24/24	0/5/5/5
5	1PE	B	505[B]	-	-	7/13/13/13	-
5	1PE	A	505[A]	-	-	6/13/13/13	-
6	PG4	B	506	-	-	5/10/10/10	-
6	PG4	A	509	-	-	1/10/10/10	-
2	MYA	B	501	-	-	0/64/80/80	0/3/3/3
5	1PE	A	507	-	-	3/13/13/13	-
2	MYA	A	501	-	-	1/64/80/80	0/3/3/3
6	PG4	A	506	-	-	5/10/10/10	-
6	PG4	A	508	-	-	4/10/10/10	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	A1BHQ	C26-S30	-7.05	1.62	1.73
3	A	502	A1BHQ	C26-N25	6.56	1.47	1.38
2	A	501	MYA	P2A-O3A	-5.55	1.53	1.59
3	A	502	A1BHQ	C05-C04	-5.32	1.35	1.40
2	B	501	MYA	P2A-O3A	-4.95	1.54	1.59
3	A	502	A1BHQ	C28-C29	4.94	1.42	1.34
3	A	502	A1BHQ	C26-N27	4.80	1.39	1.31
3	A	502	A1BHQ	C02-N25	4.71	1.45	1.37
3	A	502	A1BHQ	C28-N27	4.68	1.46	1.37
3	A	502	A1BHQ	C29-S30	-4.18	1.62	1.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	A1BHQ	C08-C07	3.88	1.54	1.47
2	B	501	MYA	C2M-S1	3.79	1.85	1.76
2	A	501	MYA	C2M-S1	3.47	1.84	1.76
3	A	502	A1BHQ	C09-N15	3.40	1.48	1.41
3	A	502	A1BHQ	C22-C05	3.37	1.45	1.39
2	B	501	MYA	C5A-C4A	3.33	1.45	1.39
2	B	501	MYA	O6A-C12	-3.32	1.33	1.43
2	B	501	MYA	C12-C11	3.27	1.58	1.52
2	A	501	MYA	C2A-N1A	3.20	1.39	1.33
2	A	501	MYA	C5A-C4A	3.11	1.44	1.39
2	B	501	MYA	C3M-C2M	-3.06	1.47	1.50
2	A	501	MYA	O6A-C12	-3.05	1.34	1.43
2	A	501	MYA	O3X-C3X	-3.02	1.33	1.44
2	B	501	MYA	C2A-N1A	2.96	1.39	1.33
2	B	501	MYA	O3X-C3X	-2.92	1.34	1.44
2	A	501	MYA	P3X-O3X	-2.86	1.54	1.59
2	A	501	MYA	P1A-O3A	-2.68	1.56	1.59
2	B	501	MYA	P1A-O3A	-2.64	1.56	1.59
2	B	501	MYA	C9-N8	2.59	1.39	1.33
2	B	501	MYA	C5-N4	2.59	1.39	1.33
2	B	501	MYA	C2X-C3X	2.50	1.58	1.53
2	A	501	MYA	C9-N8	2.50	1.39	1.33
3	A	502	A1BHQ	C03-C04	2.39	1.44	1.41
2	A	501	MYA	C5-N4	2.31	1.38	1.33
3	A	502	A1BHQ	C20-N15	2.30	1.50	1.46
2	A	501	MYA	C3X-C4X	2.30	1.58	1.52
2	B	501	MYA	C8A-N7A	2.20	1.35	1.31
3	A	502	A1BHQ	C08-C09	-2.17	1.37	1.41
2	A	501	MYA	C8A-N7A	2.17	1.35	1.31
2	B	501	MYA	C6A-N6A	2.17	1.39	1.34
2	A	501	MYA	C12-C11	2.14	1.56	1.52
2	A	501	MYA	C3M-C2M	-2.06	1.48	1.50
2	A	501	MYA	C4A-N3A	2.06	1.38	1.34

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	A1BHQ	C29-S30-C26	10.94	97.38	89.32
3	A	502	A1BHQ	C29-C28-N27	-6.31	110.61	117.12
3	A	502	A1BHQ	C04-C05-N06	5.20	108.09	105.13
3	A	502	A1BHQ	C05-C04-N21	-4.85	106.11	110.31
2	B	501	MYA	C3M-C2M-S1	4.80	119.13	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	A1BHQ	C31-C29-C28	-4.80	124.48	129.10
2	A	501	MYA	C3M-C2M-S1	4.77	119.09	113.40
2	A	501	MYA	C7-C6-C5	4.07	119.18	112.39
2	A	501	MYA	C6-C5-N4	3.45	122.63	116.34
2	B	501	MYA	C6-C5-N4	3.44	122.62	116.34
2	B	501	MYA	C7-C6-C5	3.42	118.10	112.39
3	A	502	A1BHQ	S30-C26-N27	-3.14	112.14	115.58
2	B	501	MYA	O5A-P2A-O3A	3.07	115.56	107.27
2	A	501	MYA	O5-C5-N4	-2.98	117.19	123.03
2	A	501	MYA	O5A-P2A-O3A	2.88	115.07	107.27
2	B	501	MYA	O2M-C2M-S1	-2.77	119.16	122.68
2	A	501	MYA	C5A-C4A-N3A	-2.76	122.91	126.72
2	A	501	MYA	C2X-C3X-C4X	-2.75	98.42	103.24
2	A	501	MYA	O2M-C2M-S1	-2.74	119.19	122.68
2	B	501	MYA	C5A-C4A-N3A	-2.73	122.95	126.72
3	A	502	A1BHQ	C22-C05-C04	-2.73	120.00	122.57
2	A	501	MYA	C2-S1-C2M	2.60	109.53	101.84
2	B	501	MYA	O5-C5-N4	-2.55	118.02	123.03
2	B	501	MYA	O3X-P3X-O9A	-2.38	100.84	109.33
2	B	501	MYA	C2X-C3X-C4X	-2.32	99.18	103.24
2	B	501	MYA	C4A-N9A-C8A	2.30	108.15	105.74
3	A	502	A1BHQ	C08-C09-N15	-2.25	116.26	120.80
2	B	501	MYA	O2M-C2M-C3M	-2.24	121.39	123.98
2	A	501	MYA	C13-C11-C10	2.23	112.58	108.77
2	B	501	MYA	C2-S1-C2M	2.23	108.44	101.84
2	A	501	MYA	O2M-C2M-C3M	-2.23	121.41	123.98
2	B	501	MYA	N3A-C4A-N9A	2.17	130.85	127.17
3	A	502	A1BHQ	C31-C29-S30	2.12	125.40	121.03
2	A	501	MYA	N3A-C4A-N9A	2.12	130.77	127.17
2	A	501	MYA	O1A-P1A-O2A	2.09	122.18	112.44
3	A	502	A1BHQ	C04-N21-C07	2.07	108.48	105.09
2	B	501	MYA	C7-N8-C9	2.06	126.24	122.55
3	A	502	A1BHQ	C14-C08-C07	-2.04	114.67	119.27

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	508	PG4	O2-C3-C4-O3
6	B	506	PG4	O4-C7-C8-O5
5	B	505[B]	1PE	OH7-C16-C26-OH6
6	A	508	PG4	O4-C7-C8-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	505[B]	1PE	OH5-C14-C24-OH4
6	A	509	PG4	O2-C3-C4-O3
5	A	505[A]	1PE	OH4-C13-C23-OH3
5	B	505[B]	1PE	OH6-C15-C25-OH5
6	A	506	PG4	O3-C5-C6-O4
5	B	505[B]	1PE	C23-C13-OH4-C24
5	B	505[B]	1PE	C16-C26-OH6-C15
5	B	505[B]	1PE	C12-C22-OH3-C23
6	A	508	PG4	C1-C2-O2-C3
6	A	506	PG4	C6-C5-O3-C4
6	B	506	PG4	O1-C1-C2-O2
5	B	505[B]	1PE	OH4-C13-C23-OH3
5	A	505[A]	1PE	C12-C22-OH3-C23
5	A	505[A]	1PE	C13-C23-OH3-C22
3	A	502	A1BHQ	O01-C02-C03-C04
5	A	505[A]	1PE	C23-C13-OH4-C24
6	A	506	PG4	O2-C3-C4-O3
6	A	506	PG4	C1-C2-O2-C3
5	A	505[A]	1PE	OH2-C12-C22-OH3
5	A	507	1PE	C13-C23-OH3-C22
3	A	502	A1BHQ	N25-C02-C03-C04
6	B	506	PG4	C4-C3-O2-C2
6	B	506	PG4	C5-C6-O4-C7
2	A	501	MYA	C3M-C2M-S1-C2
6	A	508	PG4	O3-C5-C6-O4
5	A	507	1PE	OH2-C12-C22-OH3
6	B	506	PG4	O2-C3-C4-O3
6	A	506	PG4	O1-C1-C2-O2
5	A	507	1PE	OH4-C13-C23-OH3
5	A	505[A]	1PE	C24-C14-OH5-C25

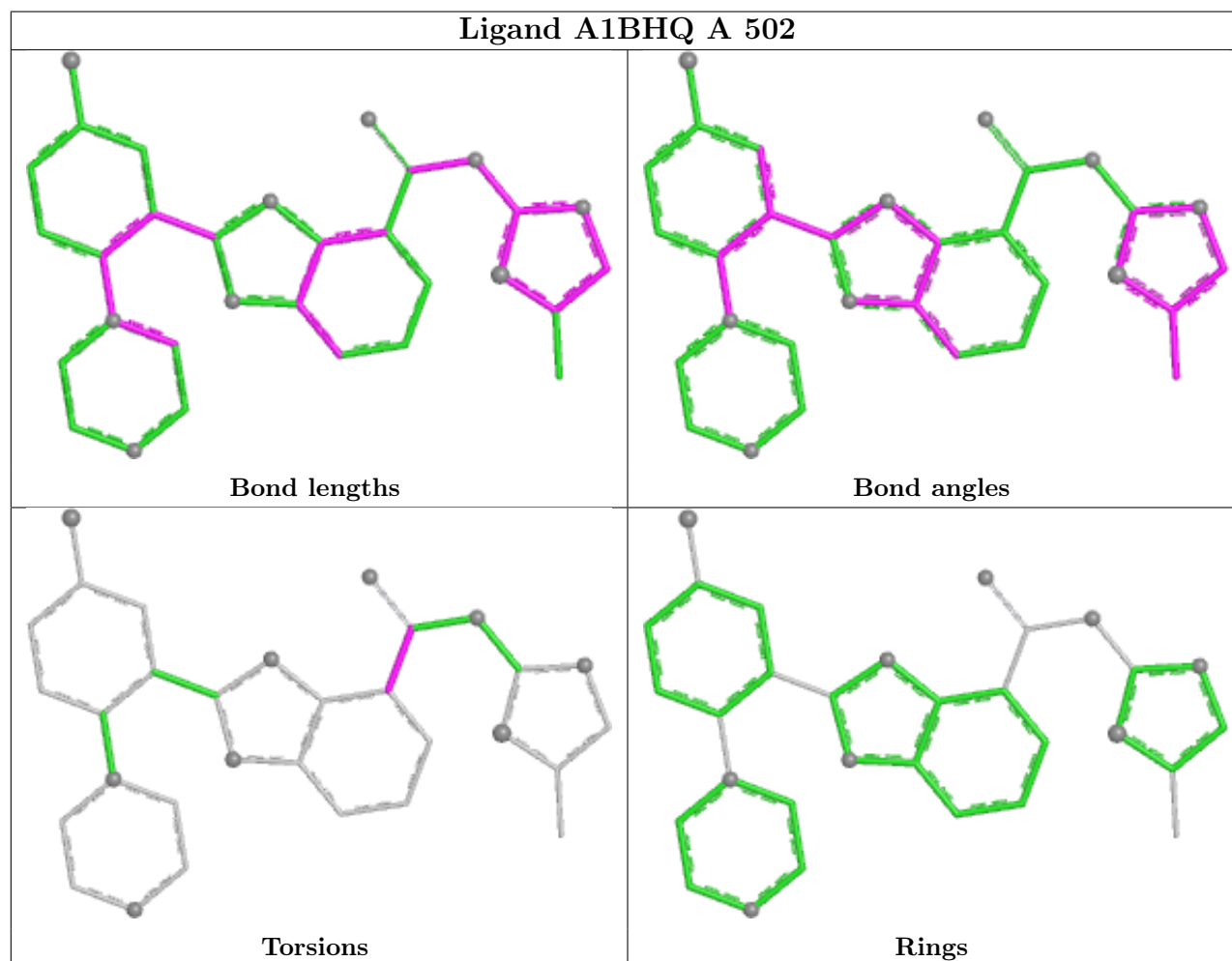
There are no ring outliers.

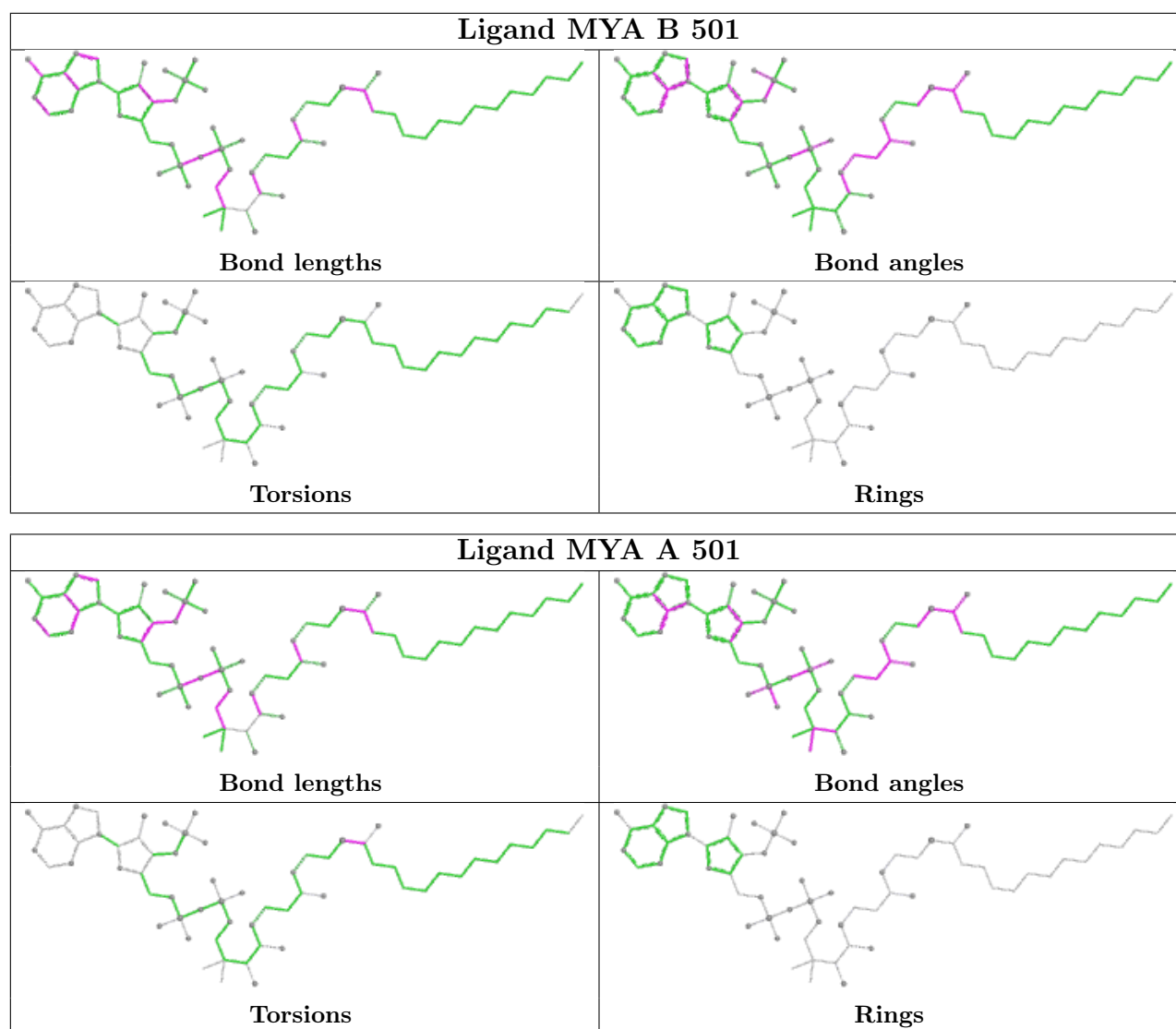
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	A1BHQ	1	0
6	A	509	PG4	3	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	426/431 (98%)	0.11	15 (3%)	47 47	13, 38, 72, 107	34 (7%)
1	B	426/431 (98%)	0.06	10 (2%)	61 61	15, 38, 73, 119	30 (7%)
All	All	852/862 (98%)	0.08	25 (2%)	53 53	13, 38, 73, 119	64 (7%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	383[A]	PHE	5.0
1	B	58	SER	4.4
1	B	225[A]	TYR	4.1
1	A	246	ASN	3.6
1	A	379[A]	ASN	3.3
1	A	386[A]	ILE	3.0
1	B	383	PHE	3.0
1	B	323	ILE	3.0
1	B	382	ARG	2.8
1	A	58	SER	2.8
1	A	264	ILE	2.8
1	A	247	MET	2.8
1	A	385[A]	THR	2.7
1	B	55	ASP	2.6
1	A	465	LEU	2.6
1	B	59	GLU	2.6
1	B	56	SER	2.5
1	A	57	SER	2.4
1	A	317[A]	TYR	2.3
1	A	384[A]	PRO	2.2
1	A	116[A]	GLN	2.2
1	B	114	ASP	2.1
1	A	434	ASP	2.1
1	B	245[A]	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	262	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

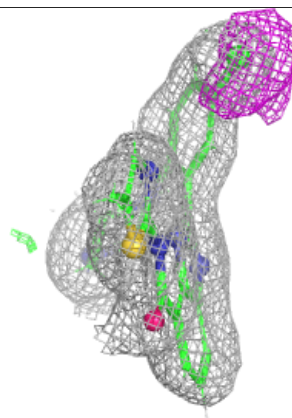
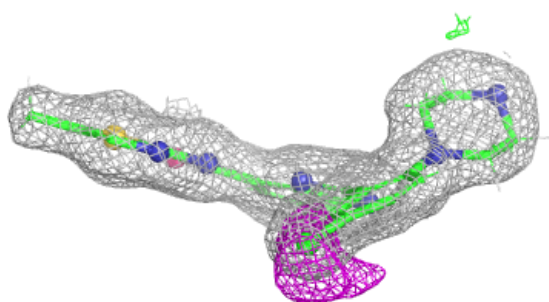
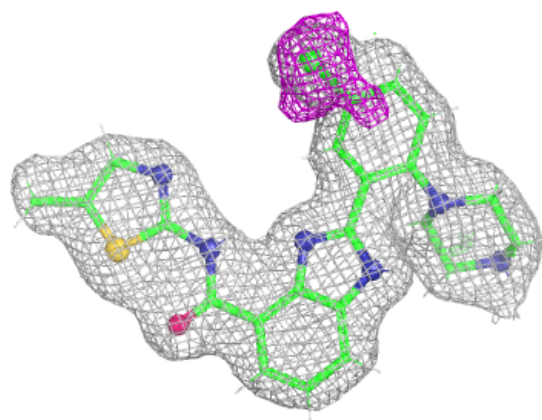
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PG4	A	509	13/13	0.58	0.17	85,116,131,134	0
6	PG4	B	506	13/13	0.73	0.13	71,93,105,109	0
6	PG4	A	508	13/13	0.75	0.12	70,89,111,112	0
5	1PE	A	507	16/16	0.85	0.11	41,57,77,79	0
5	1PE	B	505[B]	16/16	0.85	0.14	41,56,70,71	38
6	PG4	A	506	13/13	0.85	0.11	54,76,99,102	0
5	1PE	A	505[A]	16/16	0.88	0.13	41,50,58,59	38
4	CL	B	504	1/1	0.93	0.20	56,56,56,56	0
4	CL	B	503[A]	1/1	0.94	0.10	45,45,45,45	1
3	A1BHQ	A	502	31/31	0.94	0.07	26,33,46,47	0
4	CL	A	503	1/1	0.94	0.13	50,50,50,50	0
4	CL	B	502	1/1	0.95	0.10	47,47,47,47	0
4	CL	A	504	1/1	0.95	0.13	51,51,51,51	0
2	MYA	B	501	63/63	0.96	0.06	22,31,42,44	0
2	MYA	A	501	63/63	0.96	0.07	22,30,41,50	0

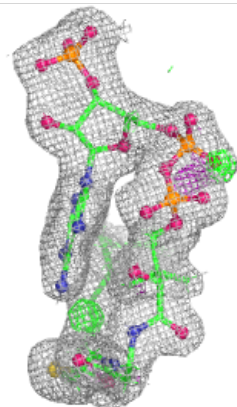
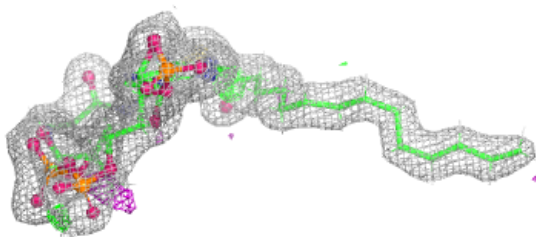
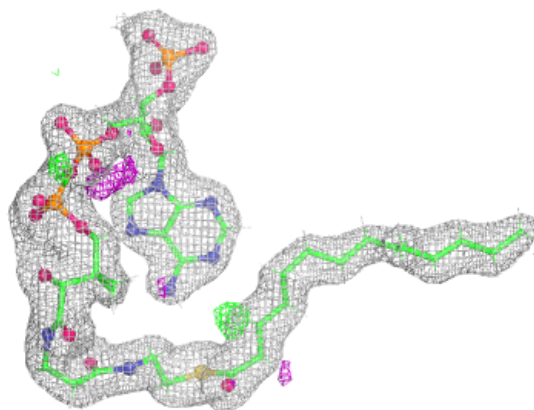
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

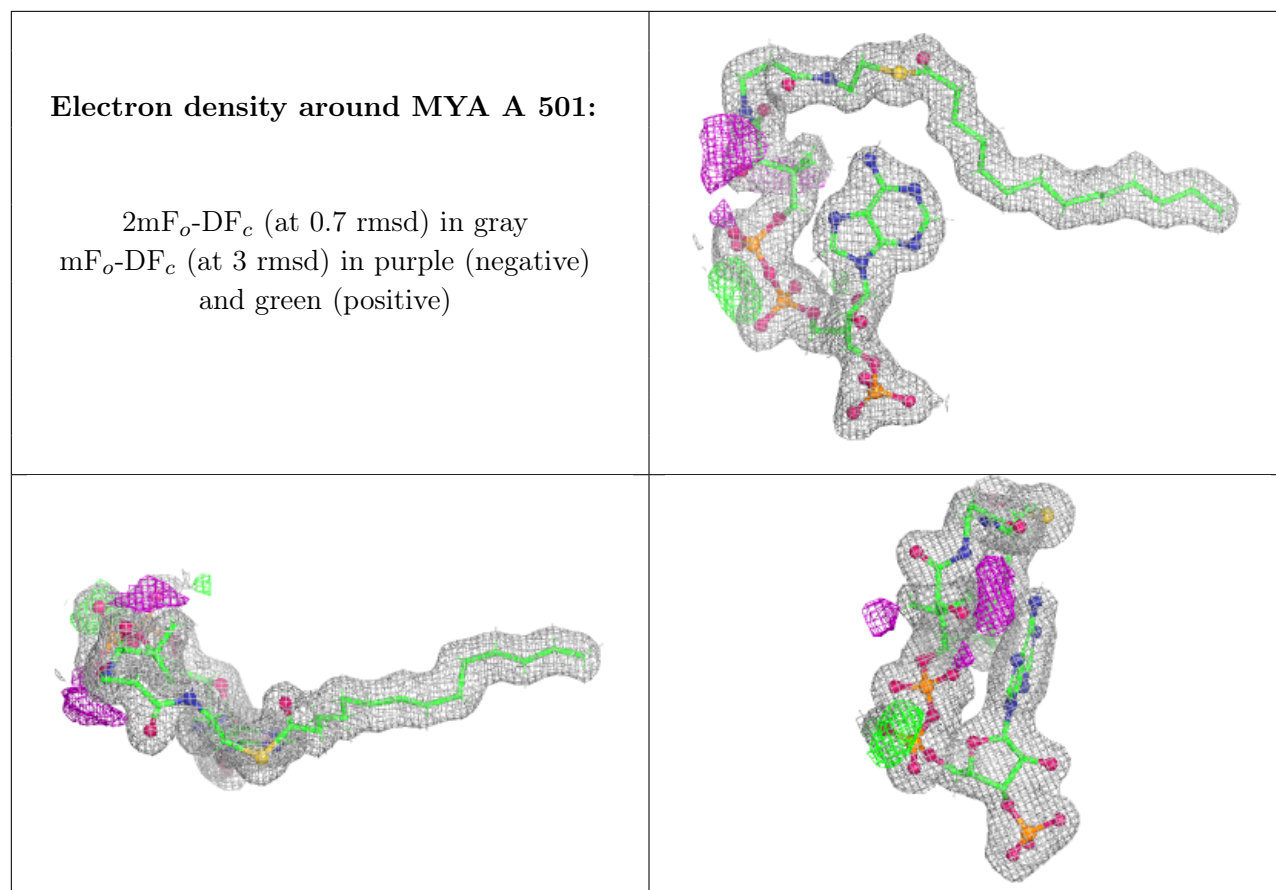
Electron density around A1BHQ A 502:

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

**Electron density around MYA B 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 ⓘ

There are no such residues in this entry.