



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 09:20 pm BST

PDB ID : 6BH8
Title : Crystal structure of ZMPSTE24 in complex with phosphoramidon
Authors : Goblirsch, B.R.; Arachea, B.T.; Wiener, M.C.
Deposited on : 2017-10-30
Resolution : 3.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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	:	2.11
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)	:	2.11

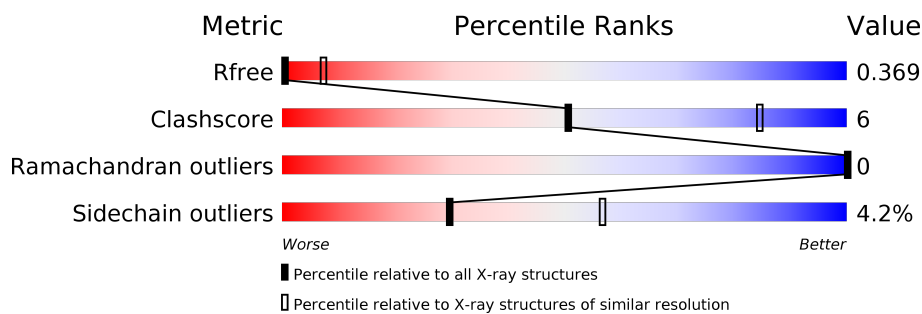
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.85 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	1048 (4.10-3.62)
Clashscore	141614	1015 (4.08-3.64)
Ramachandran outliers	138981	1069 (4.10-3.62)
Sidechain outliers	138945	1062 (4.10-3.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	483	
1	B	483	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12777 atoms, of which 6276 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 CAAX prenyl protease 1 homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	371	Total	C	H	N	O	S	0	0	0
			5986	2035	2952	477	512	10			
1	B	410	Total	C	H	N	O	S	0	0	0
			6605	2242	3256	523	574	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	ALA	THR	variant	UNP O75844
A	476	SER	-	expression tag	UNP O75844
A	477	GLY	-	expression tag	UNP O75844
A	478	LEU	-	expression tag	UNP O75844
A	479	GLU	-	expression tag	UNP O75844
A	480	VAL	-	expression tag	UNP O75844
A	481	LEU	-	expression tag	UNP O75844
A	482	PHE	-	expression tag	UNP O75844
A	483	GLN	-	expression tag	UNP O75844
B	137	ALA	THR	variant	UNP O75844
B	476	SER	-	expression tag	UNP O75844
B	477	GLY	-	expression tag	UNP O75844
B	478	LEU	-	expression tag	UNP O75844
B	479	GLU	-	expression tag	UNP O75844
B	480	VAL	-	expression tag	UNP O75844
B	481	LEU	-	expression tag	UNP O75844
B	482	PHE	-	expression tag	UNP O75844
B	483	GLN	-	expression tag	UNP O75844

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

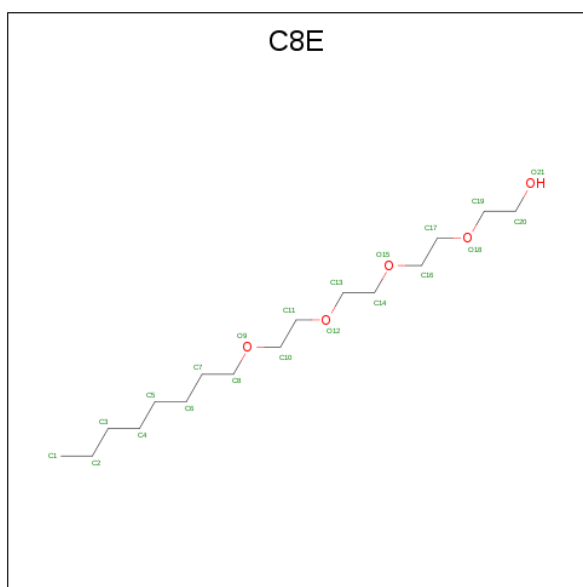
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0

- # RDF

- Molecule 4 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $\text{C}_{16}\text{H}_{34}\text{O}_5$).

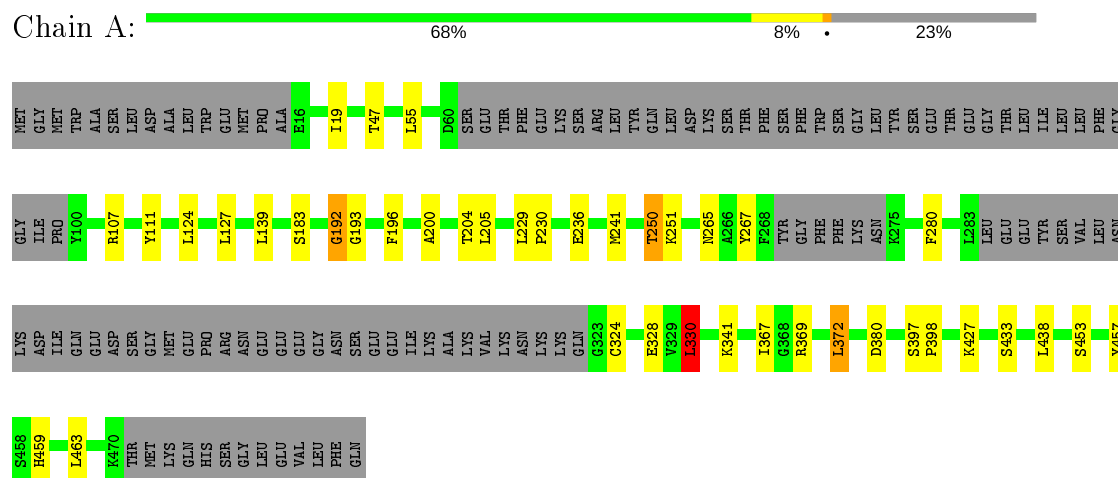


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 55	C 16	H 34	O 5	0	0
4	B	1	Total 55	C 16	H 34	O 5	0	0

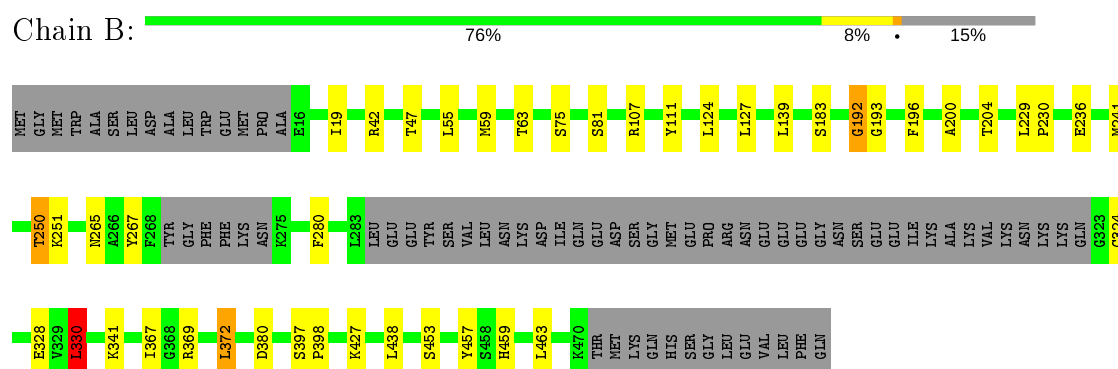
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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: CAAX prenyl protease 1 homolog



- Molecule 1: CAAX prenyl protease 1 homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.33Å 84.66Å 132.02Å 90.00° 96.26° 90.00°	Depositor
Resolution (Å)	47.03 – 3.85 47.03 – 3.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (47.03-3.85) 73.4 (47.03-3.80)	Depositor EDS
R_{merge}	0.51	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.44 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.338 , 0.371 0.338 , 0.369	Depositor DCC
R_{free} test set	1999 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	80.7	Xtriage
Anisotropy	0.801	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 103.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	12777	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, RDF, C8E

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	0.58	0/3121	0.66	2/4226 (0.0%)
1	B	0.59	0/3446	0.66	2/4667 (0.0%)
All	All	0.58	0/6567	0.66	4/8893 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	LEU	CA-CB-CG	5.79	128.62	115.30
1	B	330	LEU	CA-CB-CG	5.78	128.59	115.30
1	B	192	GLY	N-CA-C	5.04	125.70	113.10
1	A	192	GLY	N-CA-C	5.03	125.67	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3034	2952	3083	29	0
1	B	3349	3256	3388	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	37	0	32	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	37	0	32	11	0
4	A	21	34	34	0	0
4	B	21	34	34	0	0
All	All	6501	6276	6603	75	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 6.

The worst 5 of 75 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)
3:B:502:RDF:CD11	3:B:502:RDF:CG1	1.39	1.21
1:A:192:GLY:O	1:A:196:PHE:CA	1.89	1.20
3:A:502:RDF:CD11	3:A:502:RDF:CG1	1.39	1.20
1:B:192:GLY:O	1:B:196:PHE:CA	1.89	1.19
3:B:502:RDF:CE2	3:B:502:RDF:CG1	2.23	1.17

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	363/483 (75%)	354 (98%)	9 (2%)	0	100	100
1	B	404/483 (84%)	395 (98%)	9 (2%)	0	100	100
All	All	767/966 (79%)	749 (98%)	18 (2%)	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	327/426 (77%)	313 (96%)	14 (4%)	29	56
1	B	362/426 (85%)	347 (96%)	15 (4%)	30	57
All	All	689/852 (81%)	660 (96%)	29 (4%)	30	57

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	459	HIS
1	B	107	ARG
1	B	372	LEU
1	B	47	THR
1	B	111	TYR

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

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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$
4	C8E	A	503	-	20,20,20	0.44	0	19,19,19	0.49	0
3	RDF	A	502	2	34,39,39	2.74	9 (26%)	44,57,57	1.20	5 (11%)
3	RDF	B	502	2	34,39,39	2.75	9 (26%)	44,57,57	1.20	5 (11%)
4	C8E	B	503	-	20,20,20	0.44	0	19,19,19	0.49	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
4	C8E	A	503	-	-	9/18/18/18	-
3	RDF	A	502	2	-	4/22/50/50	0/3/3/3
3	RDF	B	502	2	-	4/22/50/50	0/3/3/3
4	C8E	B	503	-	-	9/18/18/18	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	RDF	P-N	10.17	1.72	1.61
3	A	502	RDF	P-N	10.13	1.72	1.61
3	B	502	RDF	C-N1	7.85	1.51	1.34
3	A	502	RDF	C-N1	7.83	1.51	1.34
3	B	502	RDF	P-O2P	-4.39	1.44	1.56

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	RDF	O1-P-O1P	-3.37	109.41	115.36
3	A	502	RDF	O1-P-O1P	-3.37	109.41	115.36
3	B	502	RDF	C6-C5-C4	-2.43	108.58	113.07
3	A	502	RDF	C6-C5-C4	-2.42	108.60	113.07
3	B	502	RDF	CA1-N1-C	-2.28	119.77	123.19

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

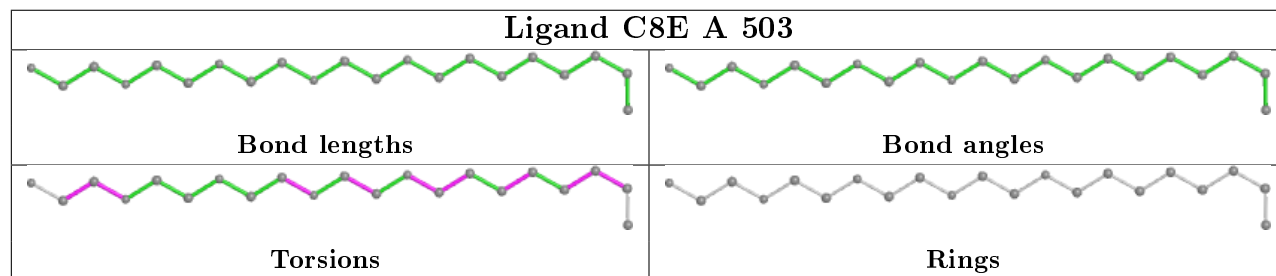
Mol	Chain	Res	Type	Atoms
3	B	502	RDF	C7-CA1-CB1-CG1
3	A	502	RDF	C7-CA1-CB1-CG1
4	A	503	C8E	O9-C10-C11-O12
4	B	503	C8E	O9-C10-C11-O12
3	B	502	RDF	C7-CA1-N1-C

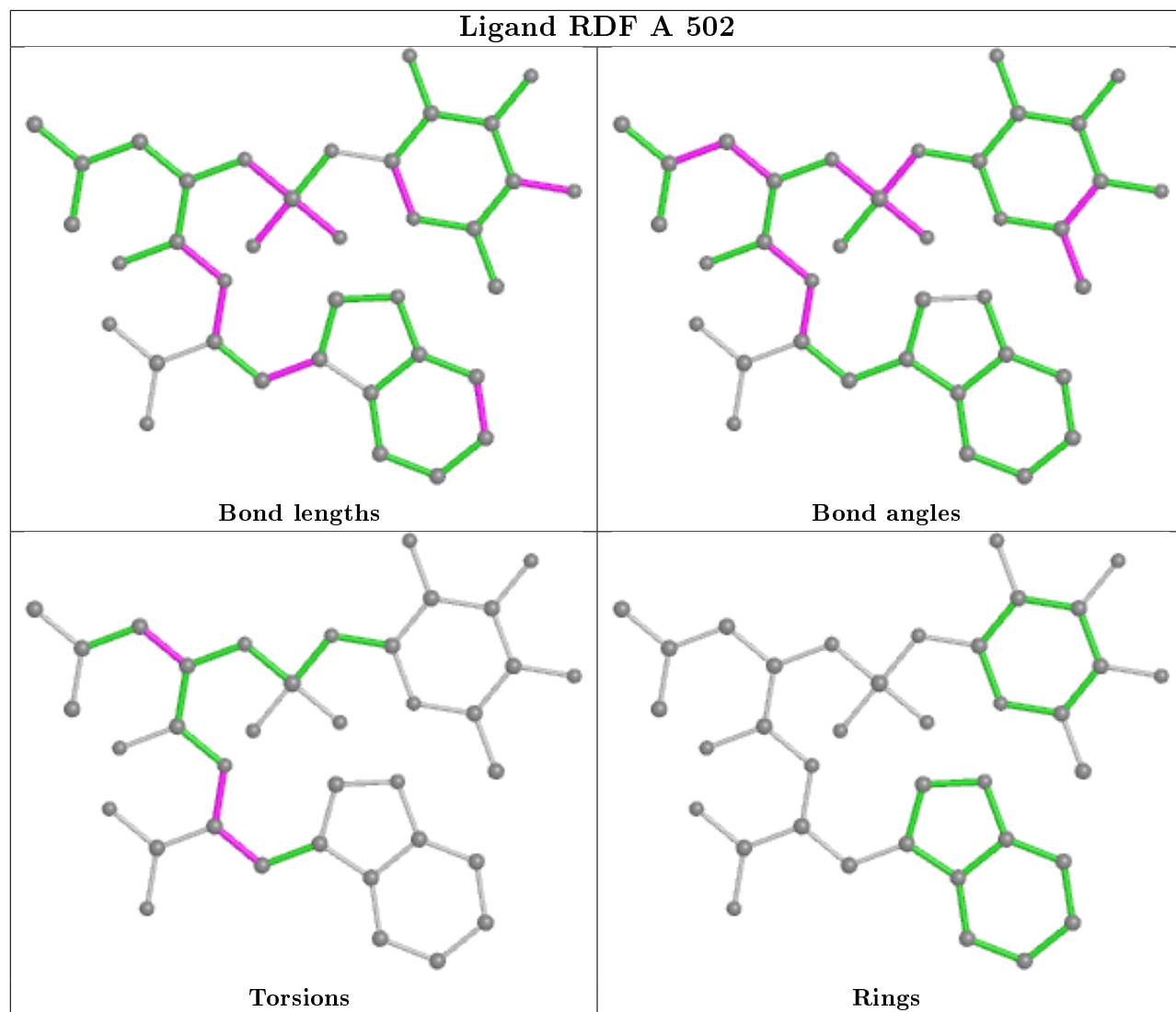
There are no ring outliers.

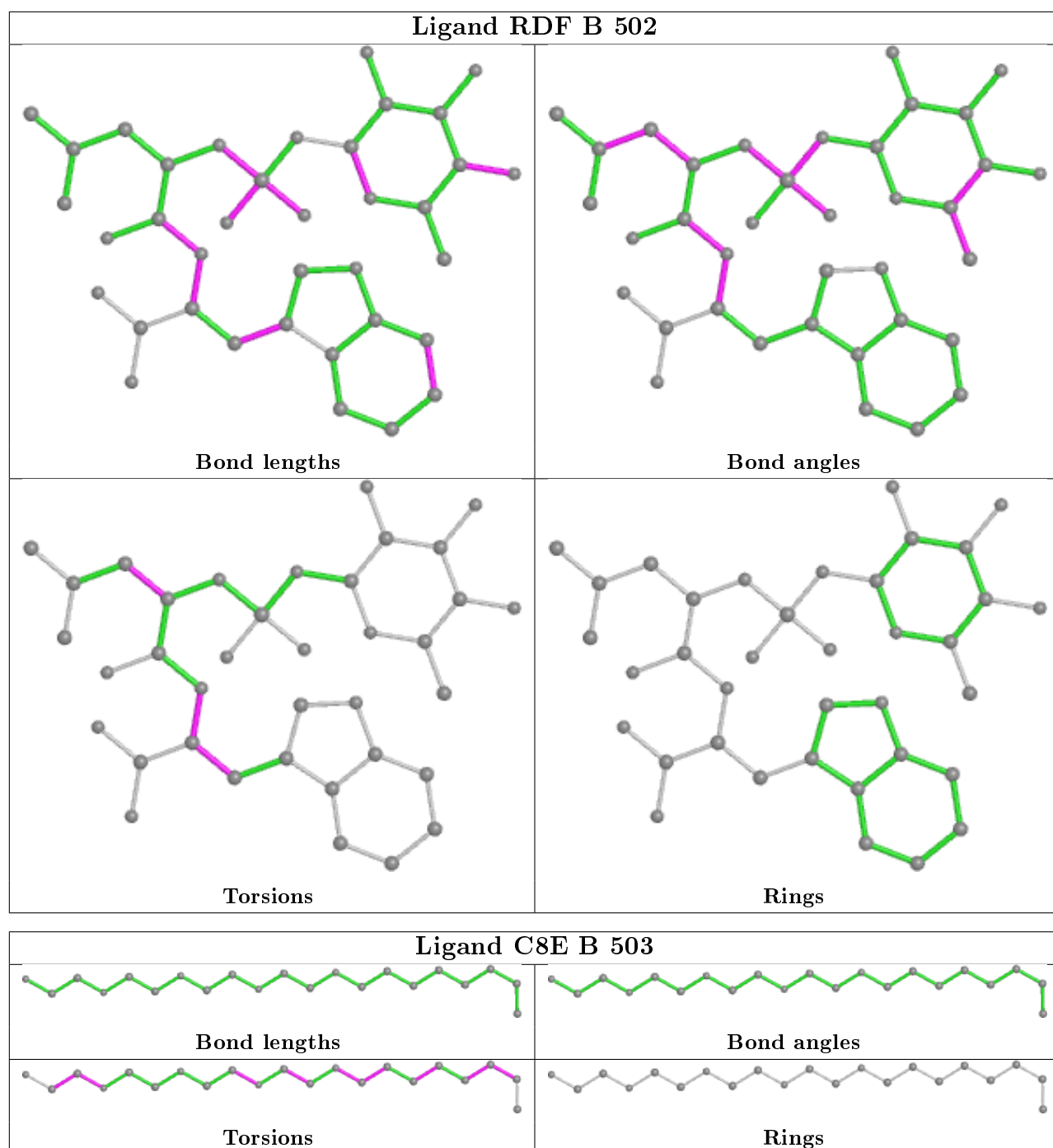
2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	RDF	11	0
3	B	502	RDF	11	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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

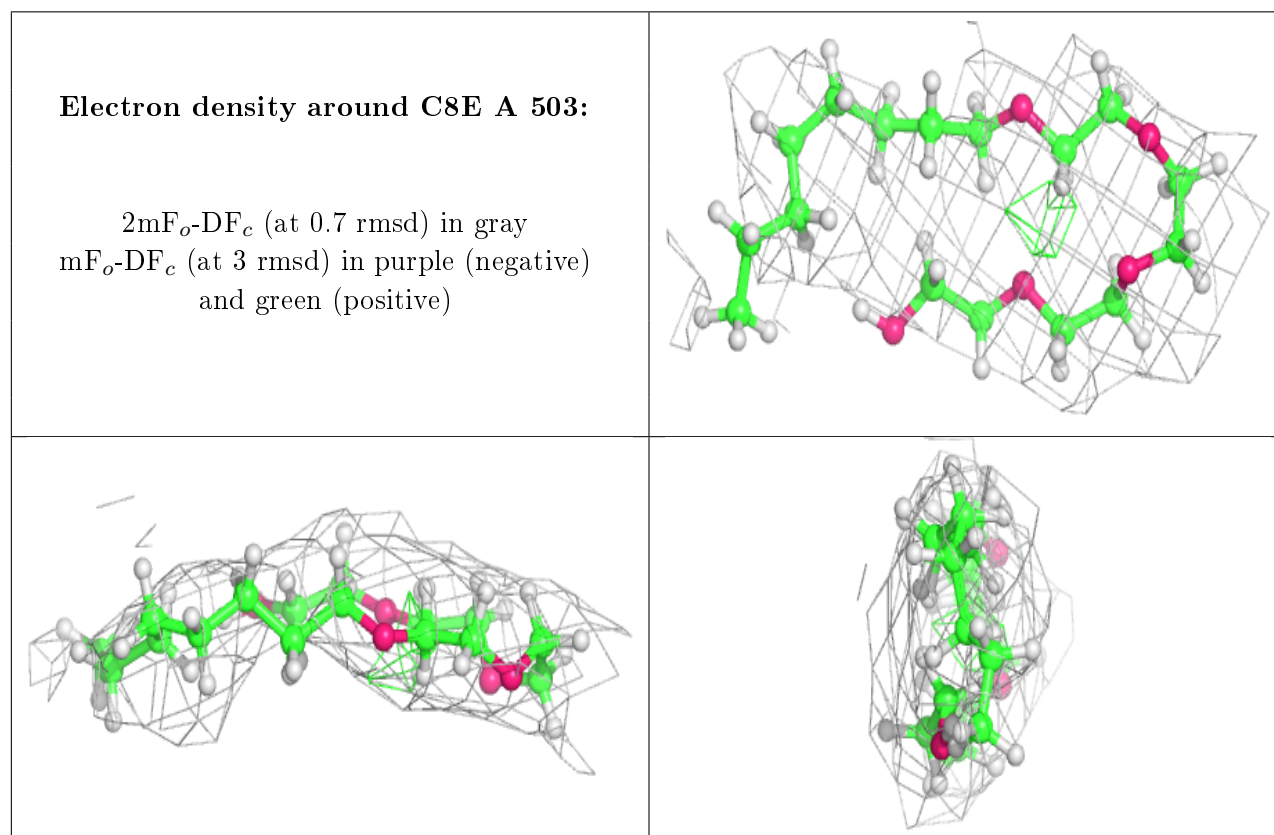
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

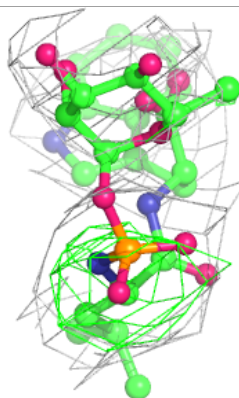
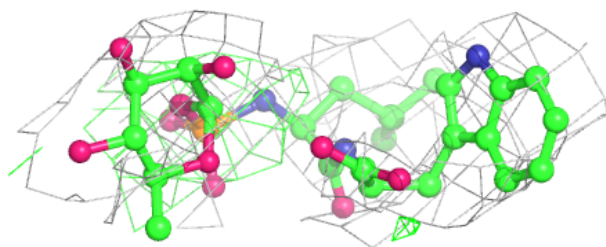
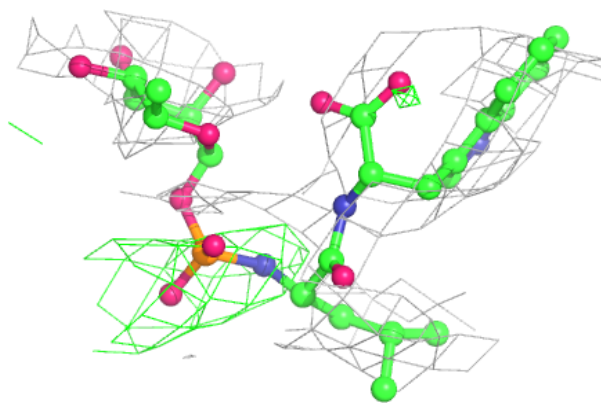
Unable to reproduce the depositors R factor - this section is therefore empty.

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.



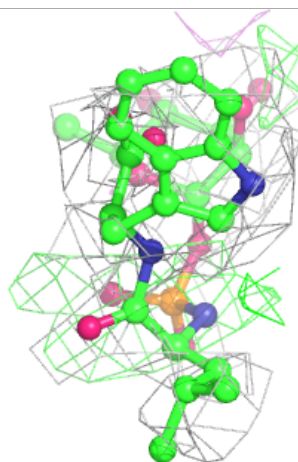
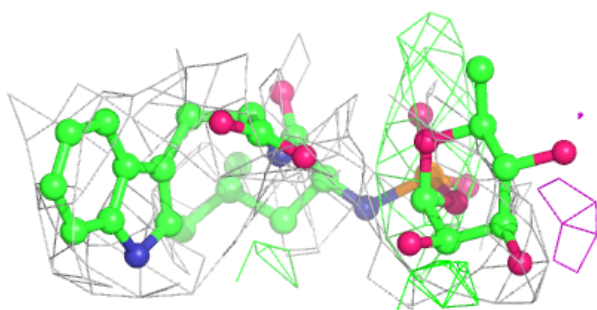
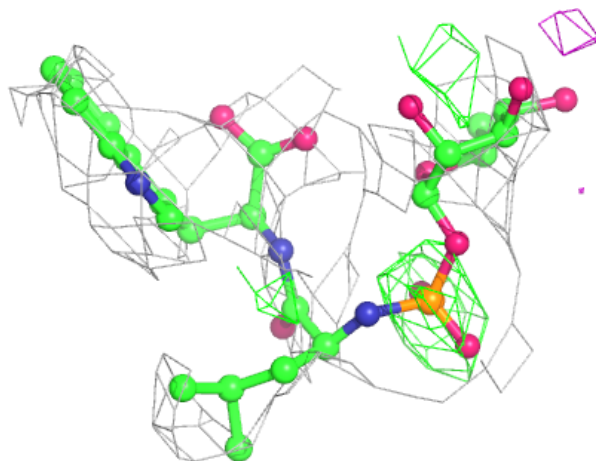
Electron density around RDF B 502:

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



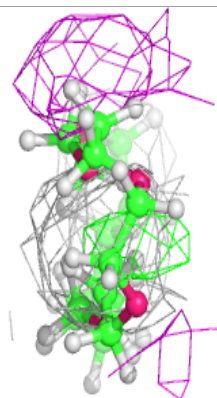
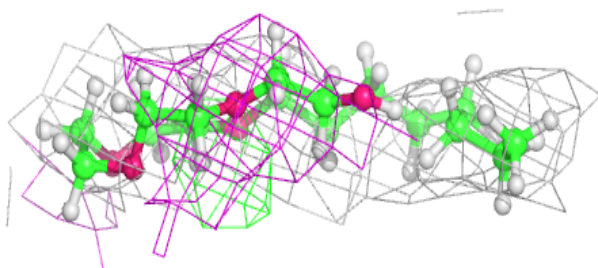
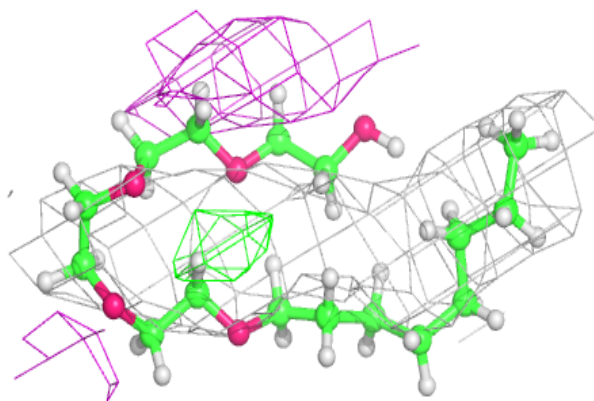
Electron density around RDF A 502:

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



Electron density around C8E B 503:

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



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.