



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:15 PM UTC

PDB ID : 6BH8 / pdb_00006bh8
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 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

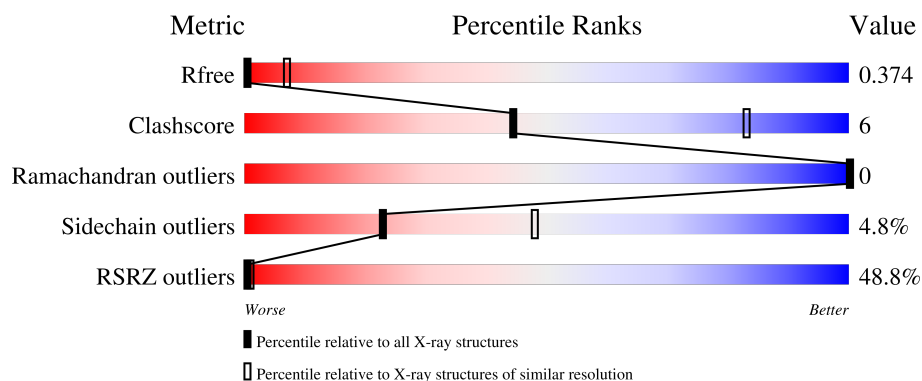
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1165 (4.02-3.70)
Clashscore	190562	1207 (4.02-3.70)
Ramachandran outliers	187476	1149 (4.02-3.70)
Sidechain outliers	187428	1142 (4.02-3.70)
RSRZ outliers	180081	1164 (4.02-3.70)

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	483	39% 68% 8% 23%
1	B	483	40% 75% 10% 15%

2 Entry composition [i](#)

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 (CCD ID: ZN) (formula: Zn).

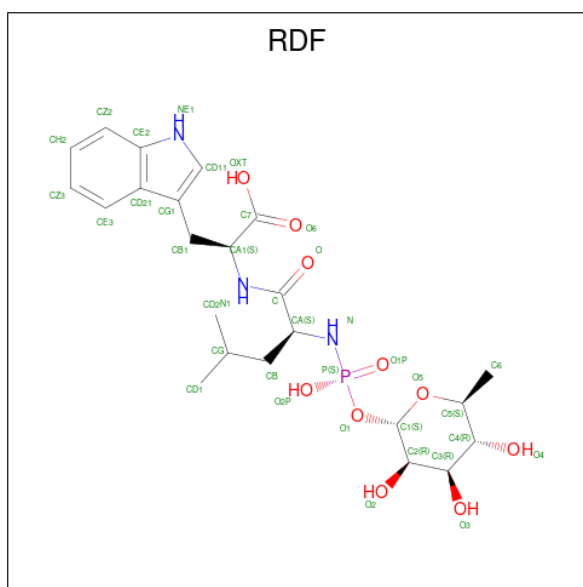
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

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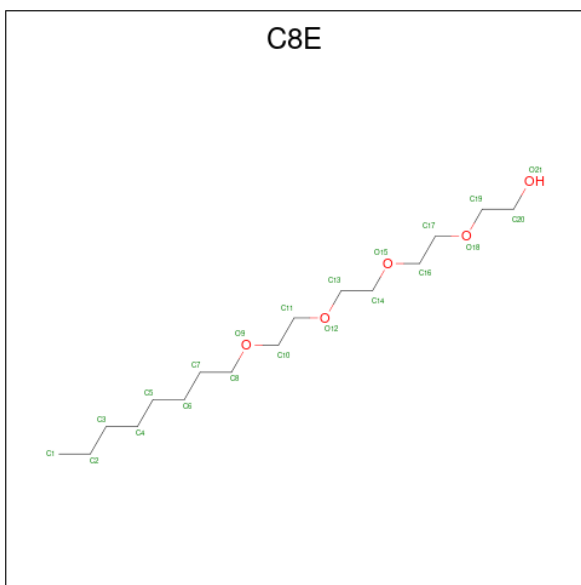
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0

- Molecule 3 is N-ALPHA-L-RHAMNOPYRANOSYLOXY(HYDROXYPHOSPHINYL)-L-L EUCYL-L-TRYPTOPHAN (CCD ID: RDF) (formula: $C_{23}H_{34}N_3O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 37	C 23	N 3	O 10	P 1	0	0
3	B	1	Total 37	C 23	N 3	O 10	P 1	0	0

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

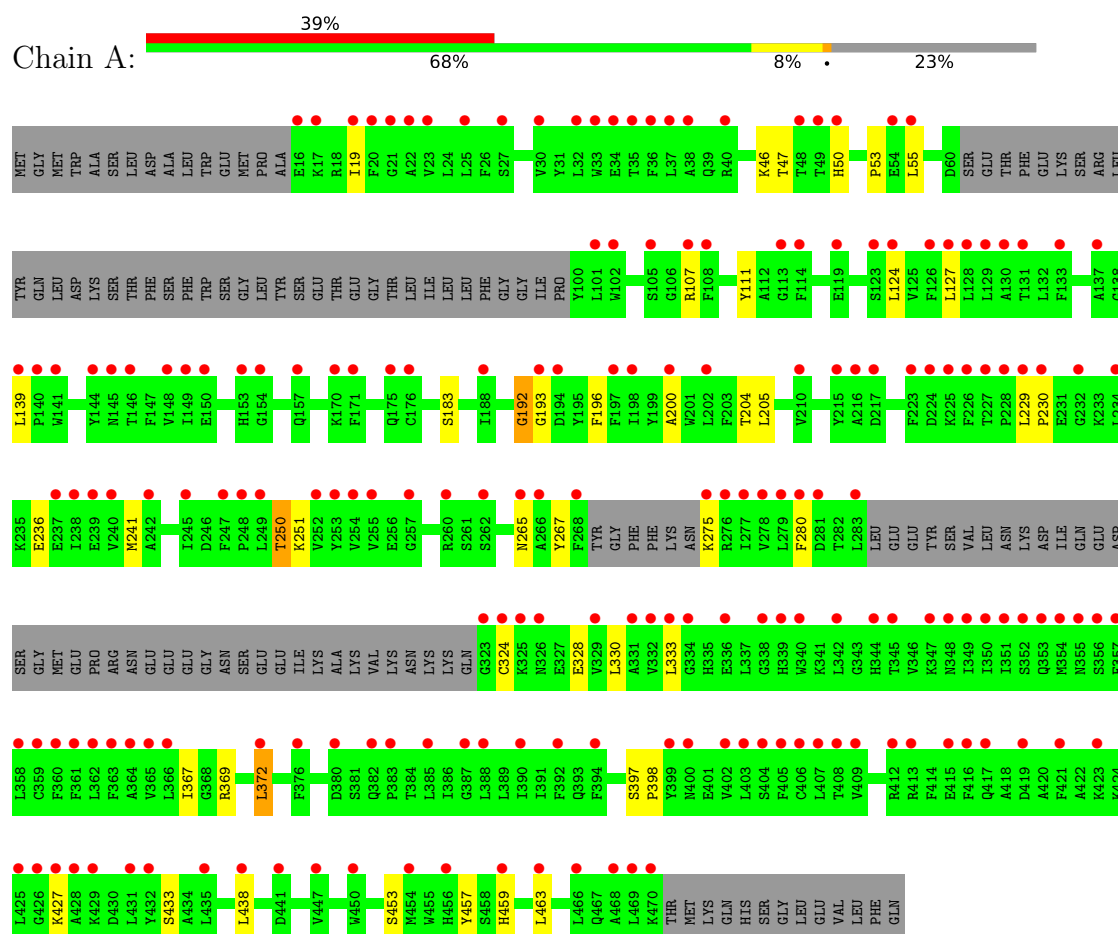


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 55	C 16	H 34	O 5	0	0
4	B	1	Total 55	C 16	H 34	O 5	0	0

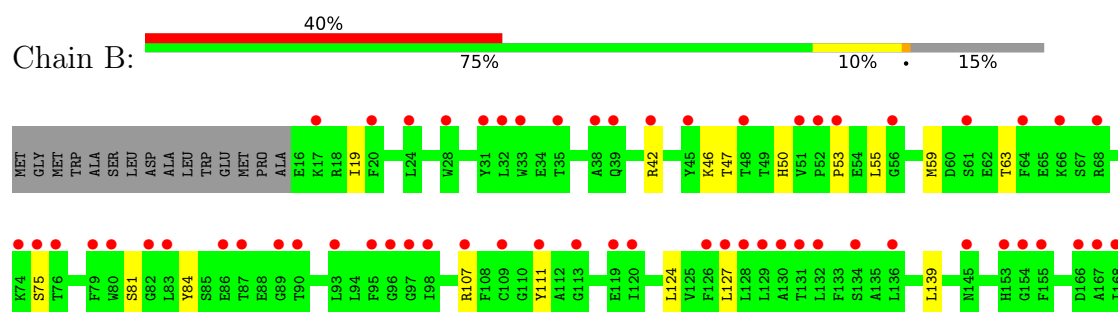
3 Residue-property plots

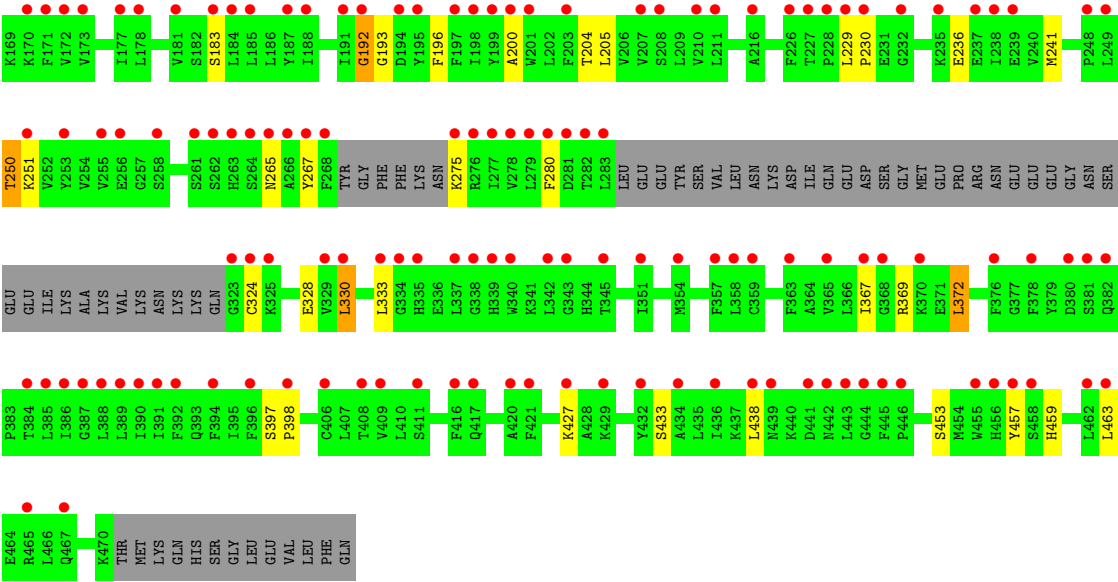
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 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 – 3.85	Depositor EDS
% Data completeness (in resolution range)	97.8 (47.03-3.85) 73.7 (47.03-3.85)	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 0.336 , 0.374	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 , 105.2	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	0.73	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	0.56	0/3121	0.67	1/4226 (0.0%)
1	B	0.56	0/3446	0.68	1/4667 (0.0%)
All	All	0.56	0/6567	0.68	2/8893 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	GLY	N-CA-C	5.28	125.70	113.18
1	A	192	GLY	N-CA-C	5.27	125.67	113.18

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	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	37	0	32	11	0
3	B	37	0	32	11	0
4	A	21	34	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	21	34	34	0	0
All	All	6501	6276	6603	78	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.

All (78) 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:CG1	3:B:502:RDF:CE2	2.23	1.17
3:A:502:RDF:CG1	3:A:502:RDF:CE2	2.23	1.16
3:B:502:RDF:CD11	3:B:502:RDF:HD1	0.97	1.16
3:A:502:RDF:CD11	3:A:502:RDF:HD1	0.97	1.07
3:A:502:RDF:CG1	3:A:502:RDF:NE1	2.23	1.01
1:A:192:GLY:O	1:A:196:PHE:N	1.95	1.00
1:B:192:GLY:O	1:B:196:PHE:N	1.95	1.00
1:A:192:GLY:O	1:A:196:PHE:HA	1.67	0.93
1:B:192:GLY:O	1:B:196:PHE:HA	1.67	0.93
1:A:192:GLY:O	1:A:196:PHE:CB	2.20	0.89
1:B:192:GLY:O	1:B:196:PHE:CB	2.20	0.88
1:B:192:GLY:C	1:B:196:PHE:HB3	2.01	0.86
1:A:192:GLY:C	1:A:196:PHE:HB3	2.01	0.84
3:A:502:RDF:CG1	3:A:502:RDF:HD1	2.11	0.81
3:B:502:RDF:CG1	3:B:502:RDF:HD1	2.11	0.80
1:B:192:GLY:O	1:B:196:PHE:HB3	1.82	0.79
1:A:192:GLY:O	1:A:196:PHE:HB3	1.82	0.79
3:A:502:RDF:CG1	3:A:502:RDF:CE3	2.54	0.78
3:B:502:RDF:CG1	3:B:502:RDF:CE3	2.54	0.78
3:B:502:RDF:CG1	3:B:502:RDF:NE1	2.23	0.77
1:A:265:ASN:O	1:A:280:PHE:CD1	2.45	0.70
1:B:265:ASN:O	1:B:280:PHE:CD1	2.45	0.69
3:A:502:RDF:CE2	3:A:502:RDF:CE3	2.42	0.67
3:A:502:RDF:HD1	3:A:502:RDF:NE1	2.10	0.67
3:B:502:RDF:HD1	3:B:502:RDF:NE1	2.10	0.66
3:B:502:RDF:CE2	3:B:502:RDF:CE3	2.42	0.62
1:A:193:GLY:HA2	1:A:196:PHE:H	1.65	0.62
1:B:193:GLY:HA2	1:B:196:PHE:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ARG:HB2	1:A:372:LEU:HD22	1.82	0.60
1:B:369:ARG:HB2	1:B:372:LEU:HD22	1.82	0.60
1:A:397:SER:HB2	1:A:398:PRO:HD3	1.84	0.59
1:B:397:SER:HB2	1:B:398:PRO:HD3	1.84	0.59
1:B:438:LEU:CD1	3:B:502:RDF:HD11	2.34	0.58
1:B:192:GLY:C	1:B:196:PHE:CB	2.72	0.58
1:B:241:MET:HE2	1:B:427:LYS:HE3	1.87	0.57
1:A:438:LEU:CD1	3:A:502:RDF:HD11	2.34	0.57
1:A:241:MET:HE2	1:A:427:LYS:HE3	1.87	0.56
1:A:19:ILE:HD13	1:A:372:LEU:HD12	1.90	0.54
1:B:19:ILE:HD13	1:B:372:LEU:HD12	1.90	0.53
1:A:328:GLU:OE2	1:A:433:SER:OG	2.25	0.50
1:B:250:THR:HG22	1:B:251:LYS:N	2.27	0.50
1:A:250:THR:HG22	1:A:251:LYS:N	2.26	0.50
1:B:397:SER:CB	1:B:398:PRO:HD3	2.42	0.49
1:A:397:SER:CB	1:A:398:PRO:HD3	2.42	0.49
1:A:192:GLY:C	1:A:196:PHE:CB	2.72	0.49
1:B:250:THR:HG22	1:B:251:LYS:H	1.78	0.48
1:B:328:GLU:OE2	1:B:433:SER:OG	2.25	0.48
1:A:250:THR:CG2	1:A:251:LYS:N	2.76	0.48
1:A:250:THR:HG22	1:A:251:LYS:H	1.77	0.48
1:B:229:LEU:HD12	1:B:230:PRO:HD2	1.95	0.48
1:B:250:THR:CG2	1:B:251:LYS:N	2.77	0.48
1:A:438:LEU:HD13	3:A:502:RDF:CD1	2.44	0.47
1:A:229:LEU:HD12	1:A:230:PRO:HD2	1.95	0.47
1:B:438:LEU:HD13	3:B:502:RDF:CD1	2.44	0.47
1:A:438:LEU:HD13	3:A:502:RDF:HD11	1.96	0.47
1:A:324:CYS:HB3	1:A:328:GLU:HB2	1.98	0.46
1:B:438:LEU:HD13	3:B:502:RDF:HD11	1.96	0.46
1:B:200:ALA:O	1:B:204:THR:HG23	2.16	0.46
1:B:55:LEU:CD2	1:B:463:LEU:HD21	2.47	0.45
1:B:324:CYS:HB3	1:B:328:GLU:HB2	1.98	0.45
1:B:59:MET:HE3	1:B:63:THR:HG22	1.98	0.45
1:A:200:ALA:O	1:A:204:THR:HG23	2.17	0.45
1:B:205:LEU:C	1:B:205:LEU:HD23	2.42	0.45
1:A:55:LEU:CD2	1:A:463:LEU:HD21	2.47	0.45
1:A:205:LEU:C	1:A:205:LEU:HD23	2.42	0.45
1:B:53:PRO:C	1:B:55:LEU:H	2.25	0.44
1:A:53:PRO:C	1:A:55:LEU:H	2.25	0.44
1:B:453:SER:HB2	1:B:457:TYR:CD2	2.54	0.42
1:A:453:SER:HB2	1:A:457:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ARG:HD2	1:B:75:SER:OG	2.20	0.42
1:B:84:TYR:CD1	1:B:84:TYR:C	2.98	0.41
1:A:124:LEU:HD11	1:A:183:SER:HB3	2.04	0.40
1:B:241:MET:HE3	1:B:330:LEU:HD12	2.04	0.40
1:B:124:LEU:HD11	1:B:183:SER:HB3	2.04	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	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%)	311 (95%)	16 (5%)	22	48
1	B	362/426 (85%)	345 (95%)	17 (5%)	23	48
All	All	689/852 (81%)	656 (95%)	33 (5%)	23	48

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LYS
1	A	47	THR
1	A	50	HIS
1	A	107	ARG
1	A	111	TYR
1	A	127	LEU
1	A	139	LEU
1	A	236	GLU
1	A	250	THR
1	A	267	TYR
1	A	275	LYS
1	A	330	LEU
1	A	333	LEU
1	A	367	ILE
1	A	372	LEU
1	A	459	HIS
1	B	46	LYS
1	B	47	THR
1	B	50	HIS
1	B	81	SER
1	B	107	ARG
1	B	111	TYR
1	B	127	LEU
1	B	139	LEU
1	B	236	GLU
1	B	250	THR
1	B	267	TYR
1	B	275	LYS
1	B	330	LEU
1	B	333	LEU
1	B	367	ILE
1	B	372	LEU
1	B	459	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	353	GLN
1	A	400	ASN
1	B	353	GLN

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Mol	Chain	Res	Type
1	B	400	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	RDF	A	502	2	38,39,39	2.61	11 (28%)	53,57,57	1.29	8 (15%)
4	C8E	A	503	-	20,20,20	0.45	0	19,19,19	0.49	0
3	RDF	B	502	2	38,39,39	2.61	11 (28%)	53,57,57	1.30	8 (15%)
4	C8E	B	503	-	20,20,20	0.45	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
3	RDF	A	502	2	-	4/27/50/50	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	C8E	A	503	-	-	9/18/18/18	-
3	RDF	B	502	2	-	3/27/50/50	0/3/3/3
4	C8E	B	503	-	-	9/18/18/18	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	RDF	P-N	8.79	1.72	1.61
3	A	502	RDF	P-N	8.75	1.72	1.61
3	B	502	RDF	C-N1	8.06	1.51	1.34
3	A	502	RDF	C-N1	8.05	1.51	1.34
3	B	502	RDF	P-O2P	-4.47	1.44	1.56
3	A	502	RDF	P-O2P	-4.46	1.44	1.56
3	A	502	RDF	CB1-CG1	3.96	1.57	1.50
3	B	502	RDF	CB1-CG1	3.94	1.57	1.50
3	A	502	RDF	CD21-CG1	-3.65	1.38	1.44
3	B	502	RDF	CD21-CG1	-3.63	1.38	1.44
3	A	502	RDF	P-O1P	3.29	1.51	1.46
3	B	502	RDF	P-O1P	3.24	1.51	1.46
3	A	502	RDF	O5-C1	3.15	1.49	1.41
3	B	502	RDF	O5-C1	3.13	1.49	1.41
3	A	502	RDF	O4-C4	2.35	1.48	1.43
3	B	502	RDF	O4-C4	2.34	1.48	1.43
3	A	502	RDF	CD21-CE2	-2.17	1.38	1.41
3	B	502	RDF	CD21-CE2	-2.12	1.38	1.41
3	B	502	RDF	CA1-C7	2.12	1.58	1.52
3	A	502	RDF	P-O1	2.11	1.65	1.57
3	B	502	RDF	P-O1	2.11	1.65	1.57
3	A	502	RDF	CA1-C7	2.09	1.58	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	RDF	O1-P-O1P	-3.38	109.41	115.32
3	B	502	RDF	O1-P-O1P	-3.38	109.41	115.32
3	B	502	RDF	C6-C5-C4	-2.46	108.58	113.08
3	A	502	RDF	C6-C5-C4	-2.45	108.60	113.08
3	B	502	RDF	CZ2-CE2-CD21	-2.42	119.85	122.19
3	A	502	RDF	CG1-CD11-NE1	-2.40	107.68	110.31
3	B	502	RDF	CG1-CD11-NE1	-2.38	107.69	110.31
3	A	502	RDF	CZ2-CE2-CD21	-2.36	119.91	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	RDF	CG-CB-CA	-2.24	109.38	115.40
3	B	502	RDF	CG-CB-CA	-2.22	109.44	115.40
3	B	502	RDF	CD21-CG1-CD11	2.20	108.41	106.16
3	A	502	RDF	CD21-CG1-CD11	2.20	108.41	106.16
3	B	502	RDF	CA1-CB1-CG1	-2.16	109.36	113.44
3	A	502	RDF	CA1-CB1-CG1	-2.16	109.36	113.44
3	B	502	RDF	O1P-P-N	-2.06	109.50	112.75
3	A	502	RDF	O1P-P-N	-2.05	109.50	112.75

There are no chirality outliers.

All (25) torsion outliers are listed below:

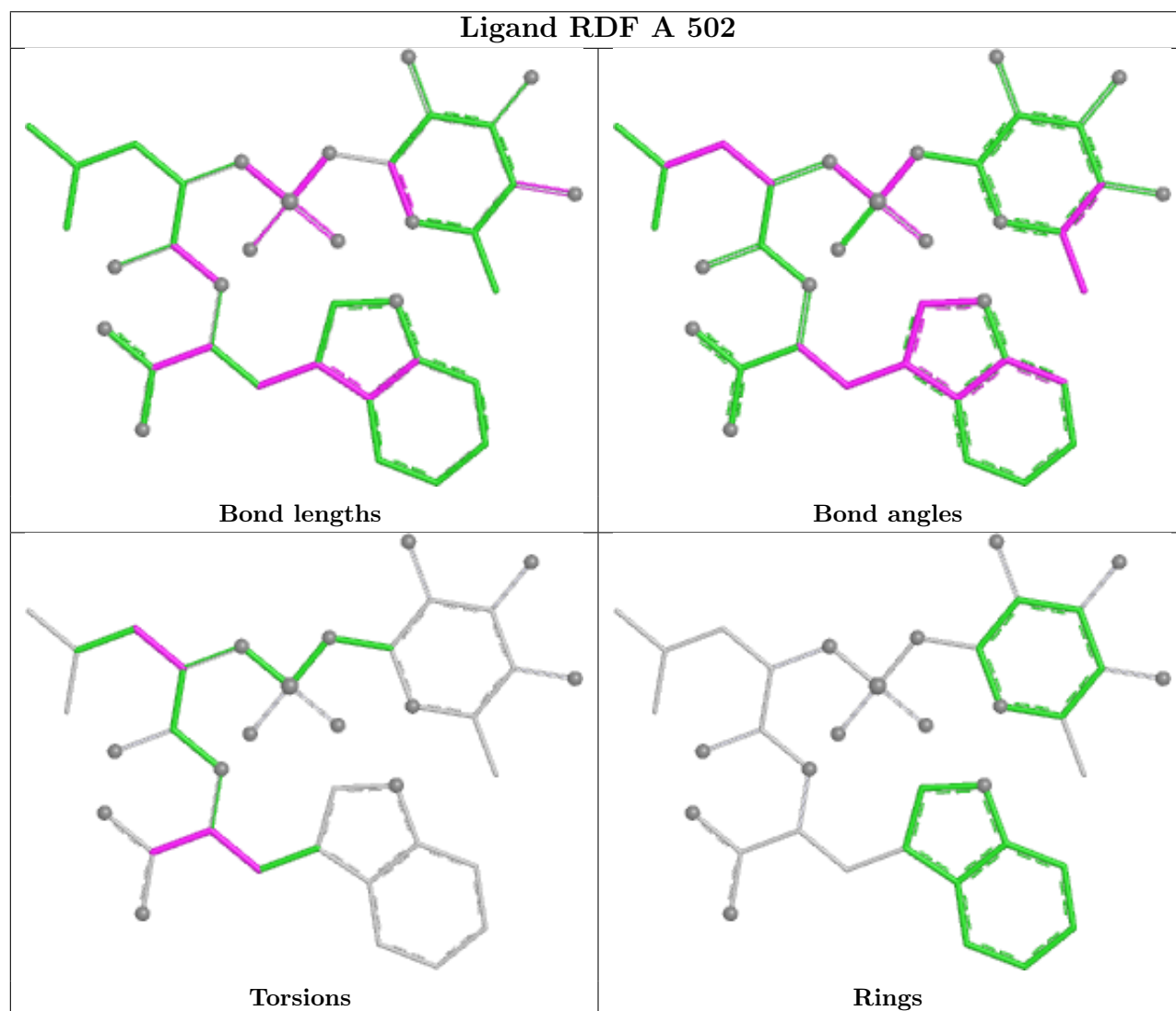
Mol	Chain	Res	Type	Atoms
4	A	503	C8E	O9-C10-C11-O12
4	B	503	C8E	O9-C10-C11-O12
4	B	503	C8E	C4-C5-C6-C7
4	A	503	C8E	C4-C5-C6-C7
4	A	503	C8E	C2-C3-C4-C5
4	B	503	C8E	C2-C3-C4-C5
4	A	503	C8E	C14-C13-O12-C11
4	B	503	C8E	C14-C13-O12-C11
4	A	503	C8E	O18-C19-C20-O21
4	B	503	C8E	O18-C19-C20-O21
3	A	502	RDF	OXT-C7-CA1-CB1
3	B	502	RDF	OXT-C7-CA1-CB1
4	A	503	C8E	C7-C8-O9-C10
4	B	503	C8E	C7-C8-O9-C10
3	A	502	RDF	O6-C7-CA1-CB1
3	B	502	RDF	O6-C7-CA1-CB1
4	B	503	C8E	C1-C2-C3-C4
4	A	503	C8E	C1-C2-C3-C4
3	A	502	RDF	C-CA-CB-CG
3	B	502	RDF	C-CA-CB-CG
4	A	503	C8E	C6-C7-C8-O9
4	B	503	C8E	C6-C7-C8-O9
4	B	503	C8E	C20-C19-O18-C17
4	A	503	C8E	C20-C19-O18-C17
3	A	502	RDF	C7-CA1-CB1-CG1

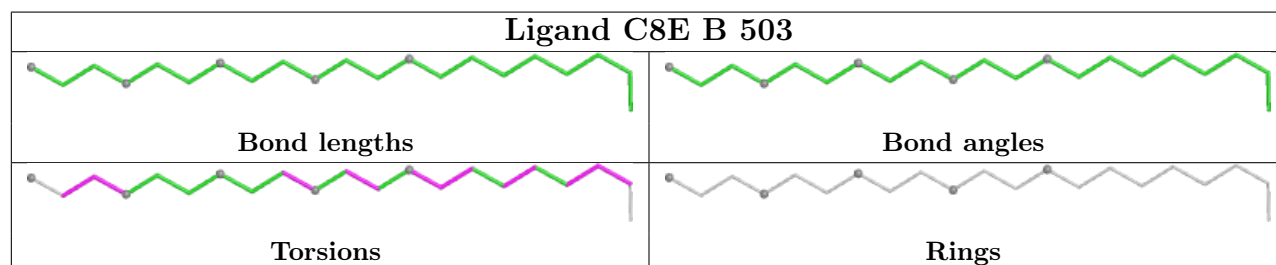
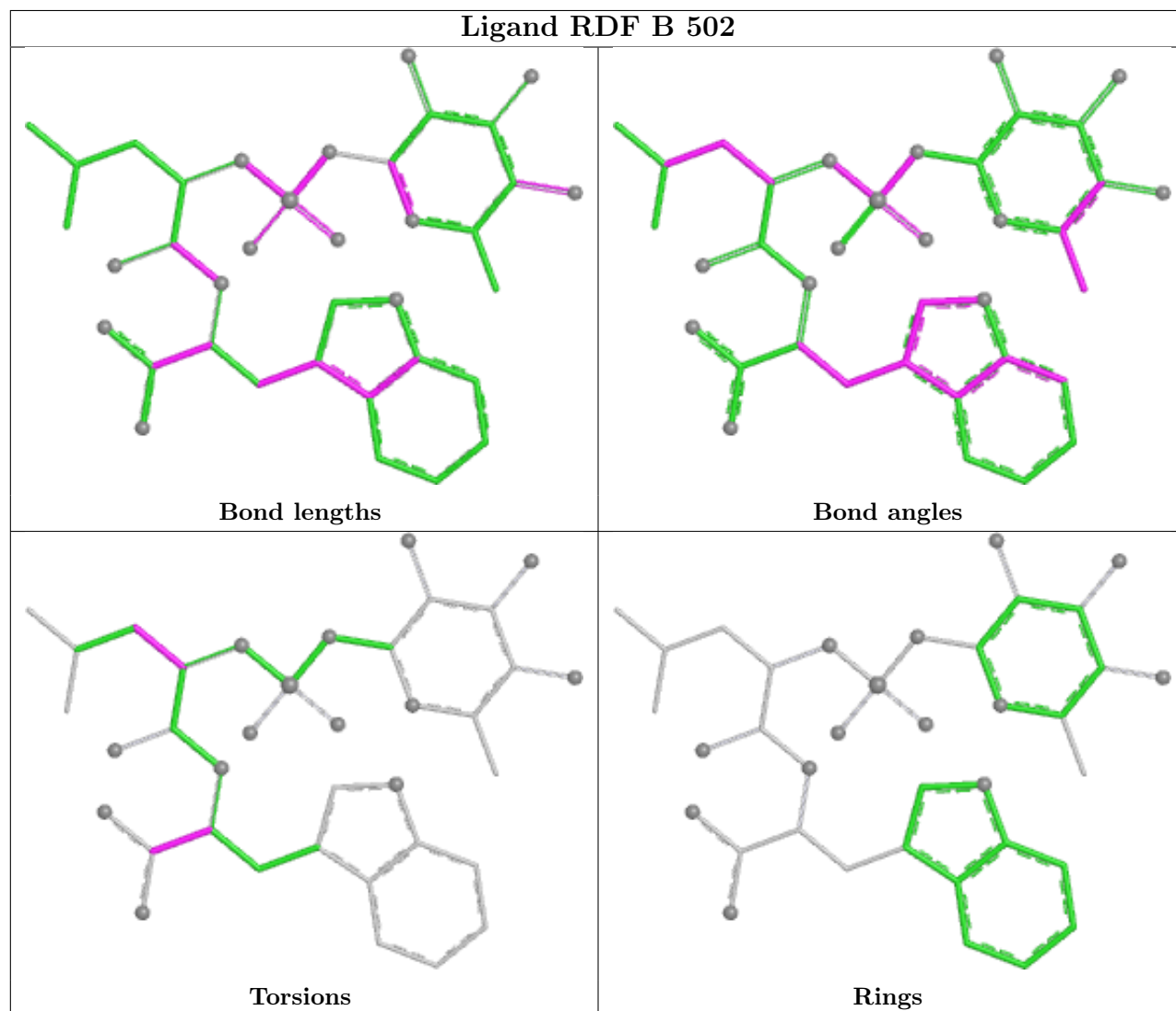
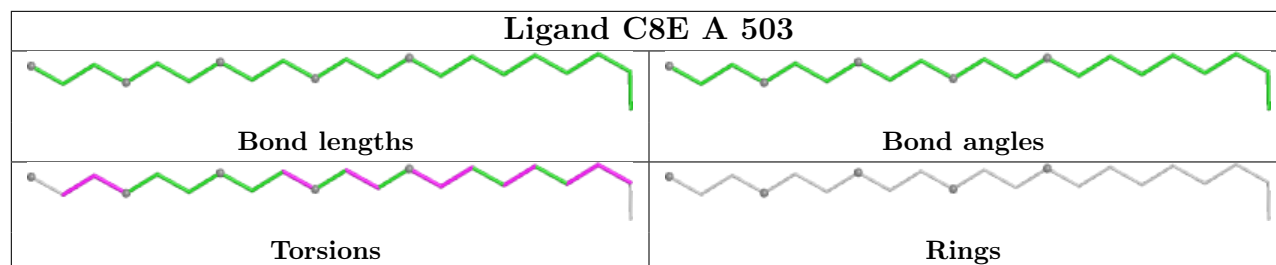
There are no ring outliers.

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

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	371/483 (76%)	2.50	190 (51%) 0 1	62, 139, 201, 300	0
1	B	410/483 (84%)	2.40	191 (46%) 0 1	58, 141, 200, 274	0
All	All	781/966 (80%)	2.45	381 (48%) 0 1	58, 140, 200, 300	0

All (381) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	324	CYS	12.9
1	B	388	LEU	12.5
1	A	224	ASP	11.3
1	B	441	ASP	10.5
1	B	265	ASN	10.4
1	B	86	GLU	10.3
1	A	403	LEU	9.9
1	B	438	LEU	9.7
1	B	420	ALA	9.6
1	A	353	GLN	9.5
1	A	266	ALA	9.0
1	A	332	VAL	8.6
1	B	442	ASN	8.6
1	A	150	GLU	8.6
1	B	109	CYS	8.5
1	A	37	LEU	8.3
1	A	21	GLY	8.3
1	A	48	THR	8.1
1	B	394	PHE	8.0
1	A	400	ASN	7.8
1	B	389	LEU	7.7
1	A	30	VAL	7.5
1	B	386	ILE	7.5
1	B	90	THR	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	149	ILE	7.4
1	A	426	GLY	7.2
1	B	282	THR	7.2
1	B	20	PHE	7.1
1	B	263	HIS	7.0
1	B	283	LEU	6.9
1	B	249	LEU	6.8
1	A	338	GLY	6.8
1	B	367	ILE	6.7
1	B	185	LEU	6.6
1	A	16	GLU	6.6
1	A	350	ILE	6.4
1	A	257	GLY	6.4
1	A	466	LEU	6.3
1	B	436	ILE	6.2
1	A	355	ASN	6.2
1	B	443	LEU	6.1
1	A	351	ILE	6.1
1	B	75	SER	6.0
1	A	469	LEU	6.0
1	A	268	PHE	6.0
1	B	281	ASP	6.0
1	B	429	LYS	6.0
1	A	283	LEU	5.9
1	B	264	SER	5.9
1	B	329	VAL	5.8
1	B	385	LEU	5.8
1	A	223	PHE	5.8
1	A	124	LEU	5.7
1	A	129	LEU	5.6
1	A	146	THR	5.6
1	A	154	GLY	5.4
1	B	439	ASN	5.4
1	A	226	PHE	5.3
1	B	98	ILE	5.3
1	A	416	PHE	5.2
1	B	181	VAL	5.2
1	A	470	LYS	5.2
1	B	184	LEU	5.2
1	B	155	PHE	5.2
1	A	359	CYS	5.2
1	B	380	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	409	VAL	5.1
1	B	31	TYR	5.1
1	B	79	PHE	5.0
1	A	265	ASN	5.0
1	A	450	TRP	5.0
1	B	463	LEU	5.0
1	B	230	PRO	5.0
1	A	364	ALA	5.0
1	A	431	LEU	5.0
1	B	267	TYR	5.0
1	B	268	PHE	4.9
1	A	33	TRP	4.9
1	B	24	LEU	4.9
1	A	229	LEU	4.8
1	B	456	HIS	4.8
1	A	372	LEU	4.8
1	A	145	ASN	4.7
1	A	133	PHE	4.7
1	B	266	ALA	4.7
1	B	211	LEU	4.7
1	A	254	VAL	4.7
1	A	435	LEU	4.6
1	A	101	LEU	4.6
1	B	253	TYR	4.6
1	A	459	HIS	4.5
1	A	423	LYS	4.5
1	A	345	THR	4.5
1	B	390	ILE	4.5
1	B	323	GLY	4.5
1	A	421	PHE	4.4
1	B	278	VAL	4.4
1	A	404	SER	4.4
1	A	144	TYR	4.4
1	A	408	THR	4.3
1	B	93	LEU	4.3
1	B	280	PHE	4.3
1	A	238	ILE	4.3
1	A	230	PRO	4.3
1	B	276	ARG	4.3
1	B	391	ILE	4.2
1	B	335	HIS	4.2
1	B	136	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	167	ALA	4.1
1	B	216	ALA	4.1
1	A	349	ILE	4.1
1	B	354	MET	4.1
1	B	177	ILE	4.1
1	B	238	ILE	4.1
1	B	210	VAL	4.1
1	B	445	PHE	4.0
1	B	262	SER	4.0
1	A	228	PRO	4.0
1	A	252	VAL	4.0
1	B	444	GLY	4.0
1	A	358	LEU	3.9
1	B	279	LEU	3.9
1	B	387	GLY	3.9
1	A	176	CYS	3.9
1	B	227	THR	3.9
1	A	130	ALA	3.9
1	B	228	PRO	3.9
1	B	28	TRP	3.9
1	B	145	ASN	3.9
1	A	276	ARG	3.9
1	A	342	LEU	3.9
1	A	405	PHE	3.9
1	B	458	SER	3.9
1	A	148	VAL	3.8
1	A	55	LEU	3.8
1	A	253	TYR	3.8
1	A	357	PHE	3.8
1	B	457	TYR	3.8
1	A	340	TRP	3.8
1	B	343	GLY	3.8
1	A	278	VAL	3.8
1	A	331	ALA	3.8
1	B	131	THR	3.8
1	A	175	GLN	3.7
1	A	102	TRP	3.7
1	B	153	HIS	3.7
1	B	261	SER	3.7
1	A	363	PHE	3.7
1	A	376	PHE	3.7
1	B	201	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	89	GLY	3.7
1	B	345	THR	3.7
1	A	392	PHE	3.7
1	A	54	GLU	3.7
1	A	354	MET	3.7
1	A	326	ASN	3.6
1	B	255	VAL	3.6
1	A	339	HIS	3.6
1	A	352	SER	3.6
1	B	188	ILE	3.6
1	A	428	ALA	3.6
1	A	333	LEU	3.6
1	A	141	TRP	3.5
1	A	128	LEU	3.5
1	A	387	GLY	3.5
1	B	208	SER	3.5
1	B	107	ARG	3.5
1	B	237	GLU	3.5
1	B	168	ILE	3.5
1	A	402	VAL	3.5
1	B	203	PHE	3.5
1	A	225	LYS	3.4
1	A	210	VAL	3.4
1	B	56	GLY	3.4
1	B	229	LEU	3.4
1	B	198	ILE	3.4
1	B	235	LYS	3.4
1	B	384	THR	3.4
1	B	76	THR	3.3
1	B	129	LEU	3.3
1	A	194	ASP	3.3
1	A	277	ILE	3.3
1	A	390	ILE	3.3
1	B	178	LEU	3.3
1	A	348	ASN	3.3
1	A	323	GLY	3.3
1	B	96	GLY	3.3
1	A	113	GLY	3.2
1	B	199	TYR	3.2
1	A	227	THR	3.2
1	A	255	VAL	3.2
1	B	82	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	432	TYR	3.2
1	B	200	ALA	3.2
1	B	378	PHE	3.2
1	B	173	VAL	3.2
1	A	281	ASP	3.2
1	A	242	ALA	3.2
1	A	425	LEU	3.2
1	B	363	PHE	3.1
1	A	324	CYS	3.1
1	A	275	LYS	3.1
1	A	234	LEU	3.1
1	A	407	LEU	3.1
1	B	417	GLN	3.1
1	A	38	ALA	3.1
1	B	239	GLU	3.1
1	B	127	LEU	3.1
1	B	120	ILE	3.0
1	B	455	TRP	3.0
1	A	383	PRO	3.0
1	B	80	TRP	3.0
1	B	333	LEU	3.0
1	B	126	PHE	3.0
1	B	171	PHE	3.0
1	B	166	ASP	3.0
1	B	376	PHE	3.0
1	B	187	TYR	3.0
1	B	256	GLU	3.0
1	A	365	VAL	3.0
1	A	454	MET	3.0
1	B	42	ARG	3.0
1	A	22	ALA	3.0
1	B	325	LYS	2.9
1	A	140	PRO	2.9
1	B	172	VAL	2.9
1	B	398	PRO	2.9
1	A	27	SER	2.9
1	A	232	GLY	2.9
1	A	123	SER	2.9
1	A	35	THR	2.9
1	A	447	VAL	2.9
1	B	408	THR	2.9
1	A	280	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	358	LEU	2.8
1	A	248	PRO	2.8
1	B	39	GLN	2.8
1	B	368	GLY	2.8
1	B	95	PHE	2.8
1	A	260	ARG	2.8
1	A	347	LYS	2.8
1	A	139	LEU	2.8
1	B	365	VAL	2.8
1	B	197	PHE	2.8
1	A	153	HIS	2.8
1	B	191	ILE	2.8
1	B	195	TYR	2.8
1	A	25	LEU	2.7
1	B	45	TYR	2.7
1	B	275	LYS	2.7
1	A	239	GLU	2.7
1	A	200	ALA	2.7
1	B	462	LEU	2.7
1	B	277	ILE	2.7
1	B	351	ILE	2.7
1	B	357	PHE	2.7
1	B	411	SER	2.7
1	A	32	LEU	2.7
1	B	132	LEU	2.7
1	A	388	LEU	2.7
1	B	207	VAL	2.7
1	B	248	PRO	2.7
1	B	382	GLN	2.7
1	B	416	PHE	2.7
1	B	226	PHE	2.6
1	A	19	ILE	2.6
1	A	412	ARG	2.6
1	A	249	LEU	2.6
1	A	394	PHE	2.6
1	B	337	LEU	2.6
1	A	385	LEU	2.6
1	B	119	GLU	2.6
1	A	429	LYS	2.6
1	B	434	ALA	2.6
1	B	32	LEU	2.6
1	B	342	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	216	ALA	2.6
1	B	113	GLY	2.6
1	A	406	CYS	2.5
1	B	406	CYS	2.5
1	B	432	TYR	2.5
1	B	465	ARG	2.5
1	A	114	PHE	2.5
1	A	356	SER	2.5
1	A	215	TYR	2.5
1	A	417	GLN	2.5
1	A	245	ILE	2.5
1	B	251	LYS	2.5
1	B	97	GLY	2.5
1	B	66	LYS	2.5
1	A	279	LEU	2.4
1	A	413	ARG	2.4
1	B	338	GLY	2.4
1	A	49	THR	2.4
1	A	131	THR	2.4
1	B	61	SER	2.4
1	B	87	THR	2.4
1	B	258	SER	2.4
1	A	193	GLY	2.4
1	A	427	LYS	2.4
1	B	427	LYS	2.4
1	A	344	HIS	2.4
1	A	240	VAL	2.4
1	B	111	TYR	2.4
1	B	192	GLY	2.4
1	B	232	GLY	2.4
1	B	83	LEU	2.4
1	A	34	GLU	2.4
1	B	392	PHE	2.3
1	B	330	LEU	2.3
1	A	329	VAL	2.3
1	A	137	ALA	2.3
1	A	336	GLU	2.3
1	A	36	PHE	2.3
1	A	456	HIS	2.3
1	A	23	VAL	2.3
1	B	381	SER	2.3
1	A	438	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	128	LEU	2.3
1	A	198	ILE	2.3
1	A	380	ASP	2.3
1	A	334	GLY	2.3
1	B	48	THR	2.3
1	B	33	TRP	2.3
1	A	127	LEU	2.3
1	A	362	LEU	2.3
1	B	183	SER	2.3
1	B	339	HIS	2.3
1	B	370	LYS	2.3
1	A	40	ARG	2.3
1	A	202	LEU	2.3
1	B	334	GLY	2.2
1	B	35	THR	2.2
1	A	108	PHE	2.2
1	B	340	TRP	2.2
1	B	130	ALA	2.2
1	A	107	ARG	2.2
1	A	20	PHE	2.2
1	A	157	GLN	2.2
1	B	446	PRO	2.2
1	B	467	GLN	2.2
1	B	64	PHE	2.2
1	A	325	LYS	2.2
1	B	17	LYS	2.2
1	B	359	CYS	2.1
1	A	126	PHE	2.1
1	B	154	GLY	2.1
1	A	105	SER	2.1
1	A	50	HIS	2.1
1	A	188	ILE	2.1
1	A	468	ALA	2.1
1	A	382	GLN	2.1
1	A	170	LYS	2.1
1	A	419	ASP	2.1
1	A	441	ASP	2.1
1	A	399	TYR	2.1
1	B	52	PRO	2.1
1	A	237	GLU	2.1
1	A	360	PHE	2.1
1	B	53	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	361	PHE	2.1
1	A	197	PHE	2.1
1	A	247	PHE	2.1
1	B	396	PHE	2.1
1	B	409	VAL	2.1
1	B	74	LYS	2.0
1	B	170	LYS	2.0
1	A	171	PHE	2.0
1	B	421	PHE	2.0
1	A	366	LEU	2.0
1	A	17	LYS	2.0
1	A	119	GLU	2.0
1	A	217	ASP	2.0
1	A	415	GLU	2.0
1	B	194	ASP	2.0
1	A	262	SER	2.0
1	B	38	ALA	2.0
1	B	68	ARG	2.0
1	A	463	LEU	2.0
1	B	134	SER	2.0
1	B	51	VAL	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.

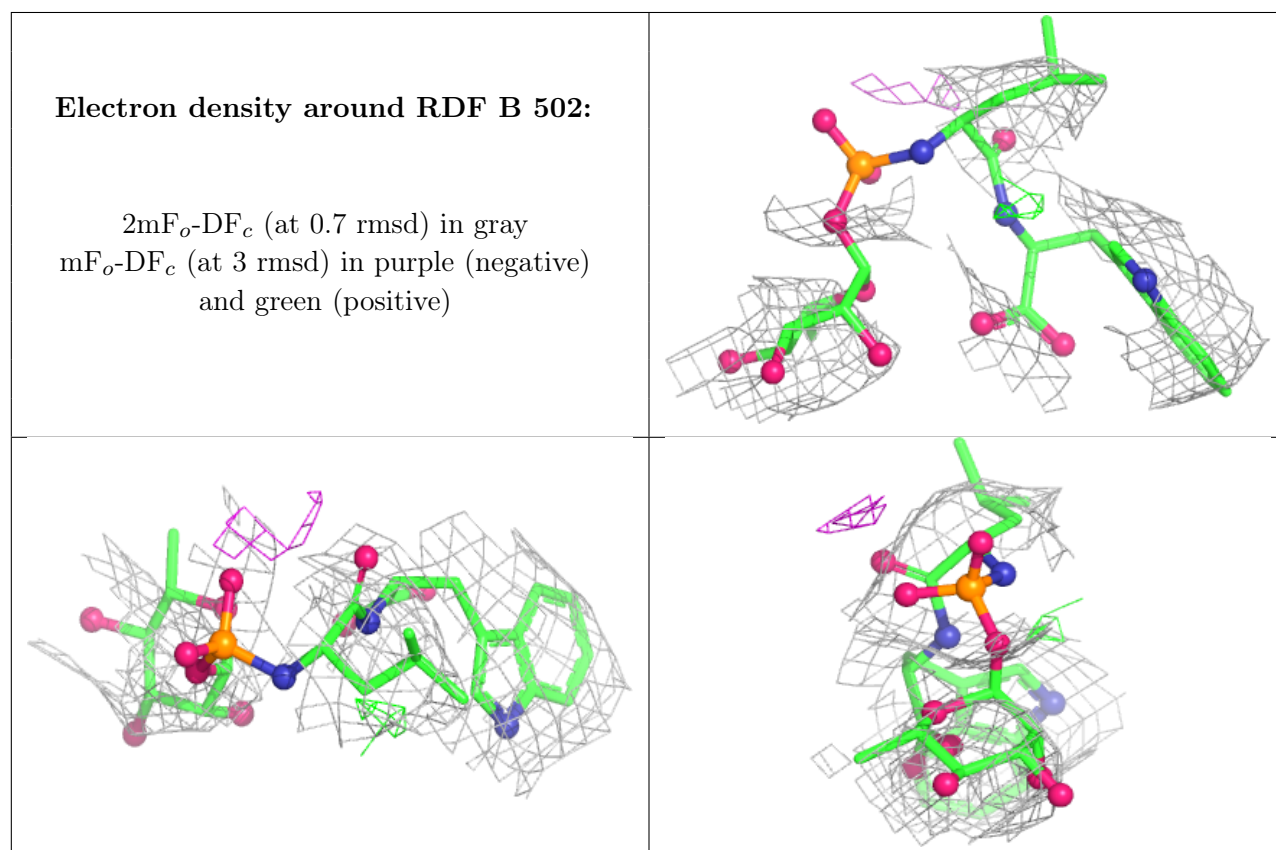
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	RDF	B	502	37/37	0.80	0.22	50,133,186,206	0
4	C8E	B	503	21/21	0.82	0.44	51,157,236,241	0

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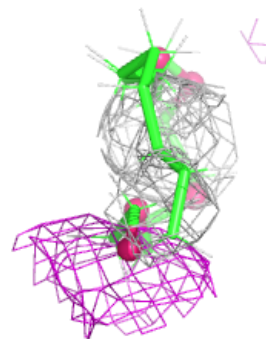
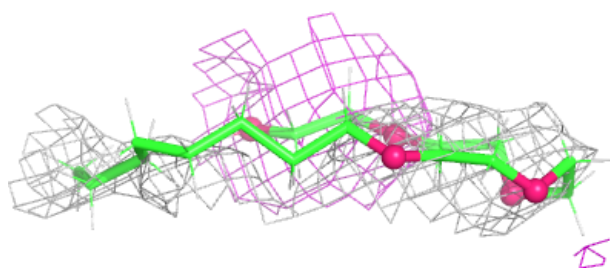
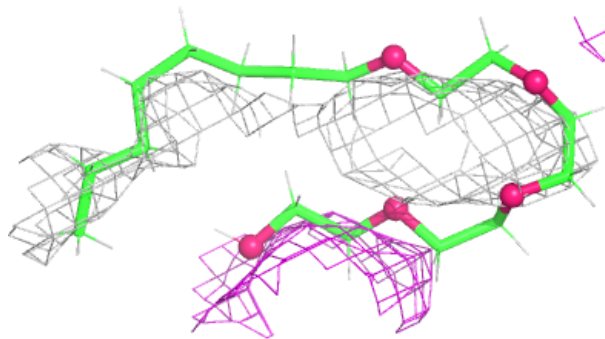
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	501	1/1	0.83	0.13	174,174,174,174	0
3	RDF	A	502	37/37	0.83	0.31	49,130,184,201	0
4	C8E	A	503	21/21	0.85	0.27	33,108,163,171	0
2	ZN	A	501	1/1	0.96	0.07	169,169,169,169	0

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.



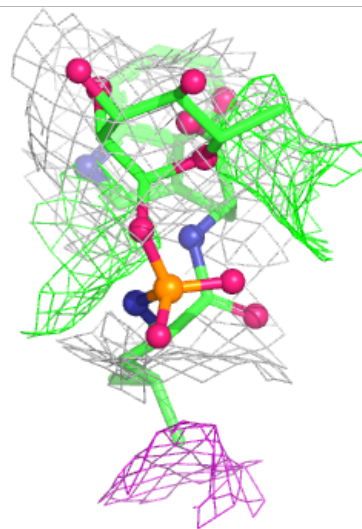
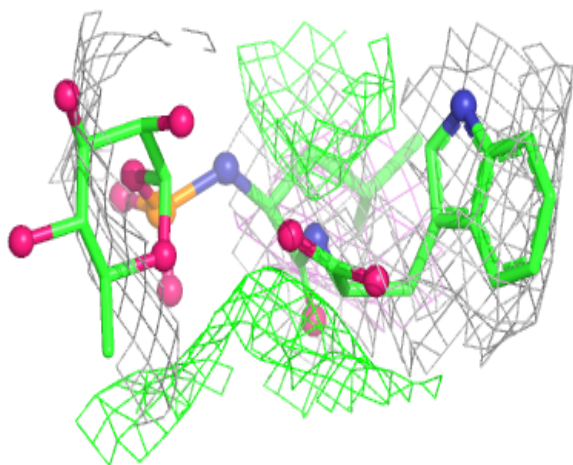
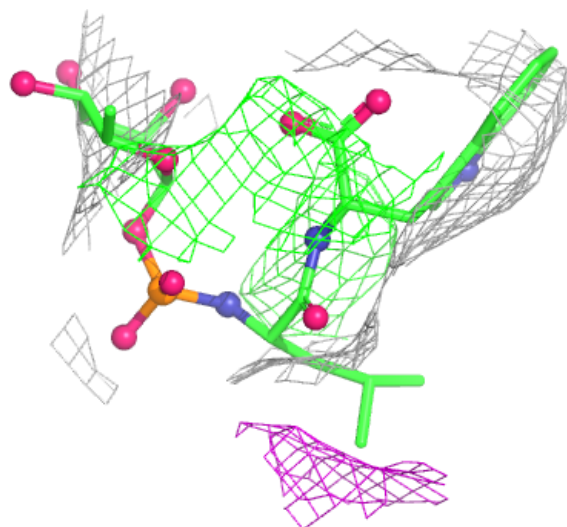
Electron density around C8E B 503:

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



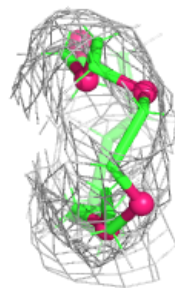
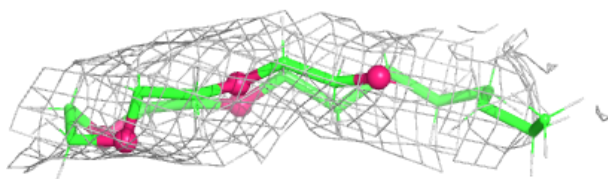
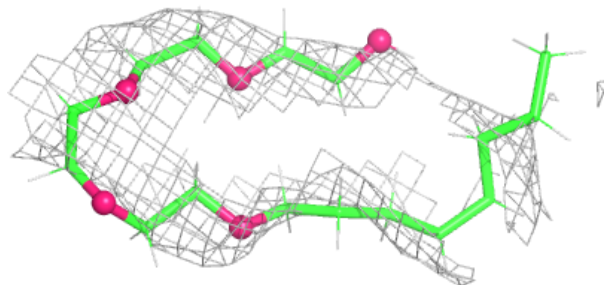
Electron density around RDF A 502:

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



Electron density around C8E A 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](#)

There are no such residues in this entry.