Full wwPDB X-ray Structure Validation Report

Dec 15, 2024 – 01:43 AM EST

PDB ID	:	1XXS
Title	:	Structural insights for fatty acid binding in a Lys49 phospholipase A2: crystal structure of myotoxin II from Bothrops moojeni complexed with stearic acid
Authors	:	Watanabe, L.; Soares, A.M.; Ward, R.J.; Fontes, M.R.; Arni, R.K.
Deposited on	:	2004-11-08
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:

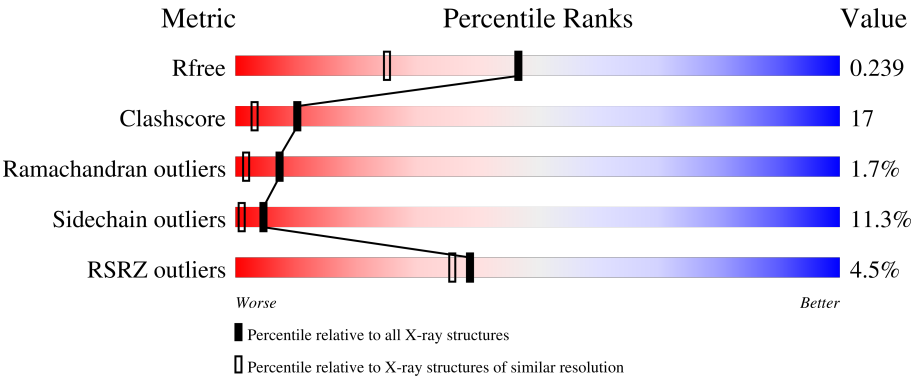
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (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 <=5%

Mol	Chain	Length	Quality of chain
1	A	122	5% 74% 20% 5% •
1	B	122	4% 66% 29% 5% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	STE	B	204	-	-	X	-
3	STE	B	206[B]	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2049 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

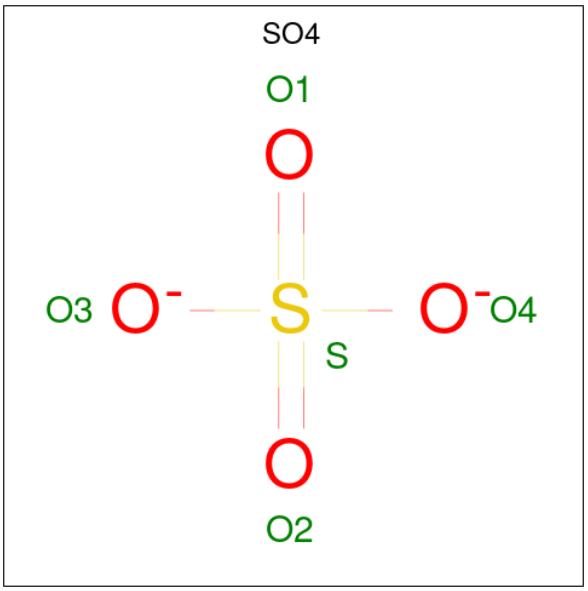
- Molecule 1 is a protein called Phospholipase A2 homolog 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	0	0	0
			958	597	167	179	15			
1	B	122	Total	C	N	O	S	7	0	0
			958	597	167	179	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	ALA	PHE	conflict	UNP Q9I834
B	126	ALA	PHE	conflict	UNP Q9I834

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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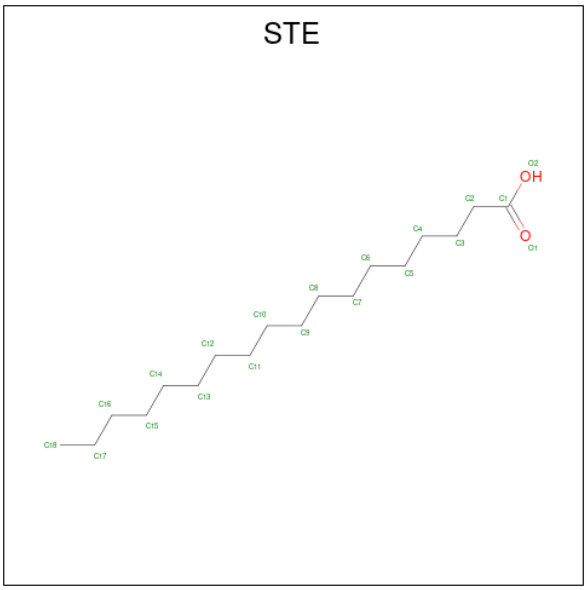
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$).



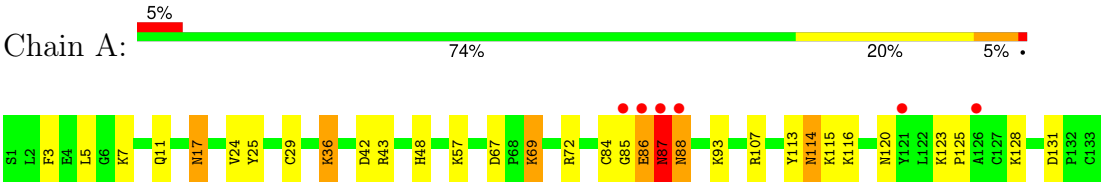
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 20 18 2	0	0
3	A	1	Total C O 17 15 2	0	0
3	A	1	Total C O 20 18 2	0	1
3	B	1	Total C O 20 18 2	0	0
3	B	1	Total C O 11 9 2	0	0
3	B	1	Total C O 20 18 2	0	1

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. 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.

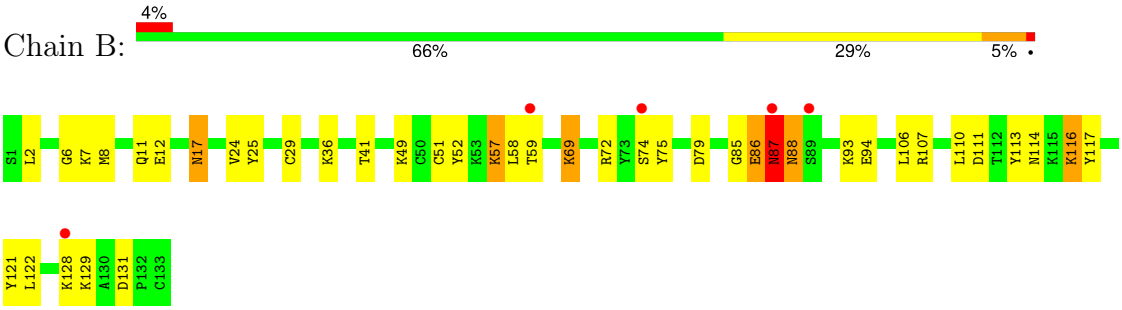
• Molecule 1: Phospholipase A2 homolog 2

Chain A:



• Molecule 1: Phospholipase A2 homolog 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.18Å 88.71Å 51.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.40 – 1.80 15.40 – 1.80	Depositor EDS
% Data completeness (in resolution range)	80.7 (15.40-1.80) 80.5 (15.40-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 1.63Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.166 , 0.247 0.215 , 0.239	Depositor DCC
R_{free} test set	1046 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2049	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, STE

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	1.02	1/976 (0.1%)	1.20	8/1305 (0.6%)
1	B	1.00	0/976	1.09	4/1305 (0.3%)
All	All	1.01	1/1952 (0.1%)	1.14	12/2610 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	CYS	CB-SG	-5.88	1.72	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	107	ARG	NE-CZ-NH2	-13.13	113.74	120.30
1	A	84	CYS	O-C-N	8.01	136.81	123.20
1	A	107	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	A	67	ASP	CB-CG-OD2	7.17	124.76	118.30
1	A	42	ASP	CB-CG-OD2	7.02	124.62	118.30
1	B	111	ASP	CB-CG-OD1	6.18	123.87	118.30
1	A	131	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	79	ASP	CB-CG-OD2	5.79	123.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	86	GLU	N-CA-C	5.18	124.99	111.00
1	B	86	GLU	N-CA-C	5.17	124.97	111.00
1	B	131	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	5	LEU	CB-CG-CD2	-5.05	102.42	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	GLY	Peptide
1	B	85	GLY	Peptide

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	958	0	945	18	1
1	B	958	0	945	47	1
2	A	15	0	0	0	0
2	B	10	0	0	0	0
3	A	57	0	84	9	0
3	B	51	0	76	26	0
All	All	2049	0	2050	69	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 17.

All (69) 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:69:LYS:NZ	3:B:204:STE:O2	1.83	1.12
1:A:7:LYS:HE2	3:A:205[A]:STE:H152	1.42	1.01
3:A:202:STE:H102	3:A:202:STE:H142	1.39	1.01
1:B:69:LYS:HZ1	3:B:204:STE:C3	1.78	0.96
1:B:69:LYS:HZ1	3:B:204:STE:H32	1.31	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:202:STE:H142	3:A:202:STE:C10	2.02	0.87
1:B:69:LYS:NZ	3:B:204:STE:H32	1.93	0.83
1:B:87:ASN:HA	1:B:93:LYS:NZ	1.98	0.78
1:B:12:GLU:OE1	1:B:107:ARG:HD3	1.87	0.75
1:B:7:LYS:HE2	3:B:206[B]:STE:H142	1.70	0.73
1:A:114:ASN:OD1	1:A:116:LYS:HE3	1.89	0.73
1:B:11:GLN:HA	3:B:206[B]:STE:C3	2.19	0.73
1:B:69:LYS:HZ1	3:B:204:STE:C1	2.05	0.69
3:A:205[A]:STE:H21	1:B:11:GLN:HG2	1.73	0.69
1:B:69:LYS:HZ1	3:B:204:STE:C2	2.05	0.69
1:B:87:ASN:HA	1:B:93:LYS:HZ2	1.60	0.65
1:B:7:LYS:NZ	3:B:206[B]:STE:H161	2.12	0.65
1:B:114:ASN:ND2	1:B:116:LYS:HD3	2.13	0.64
1:A:11:GLN:HG2	3:A:205[A]:STE:C7	2.28	0.64
1:B:17:ASN:HD22	1:B:17:ASN:C	2.01	0.64
1:A:3:PHE:CD2	1:A:72:ARG:NH1	2.67	0.63
1:B:69:LYS:HE3	3:B:204:STE:H42	1.84	0.60
1:B:7:LYS:HZ3	3:B:206[B]:STE:H111	1.67	0.58
3:A:202:STE:H102	3:A:202:STE:C14	2.24	0.58
1:B:7:LYS:CE	3:B:206[B]:STE:H161	2.35	0.56
1:B:87:ASN:HA	1:B:93:LYS:HZ1	1.68	0.56
1:B:87:ASN:O	1:B:88:ASN:C	2.44	0.56
1:A:87:ASN:O	1:A:88:ASN:C	2.44	0.56
1:B:69:LYS:NZ	3:B:204:STE:C3	2.58	0.56
1:A:17:ASN:C	1:A:17:ASN:HD22	2.10	0.54
1:B:52:TYR:HE2	3:B:204:STE:H32	1.72	0.53
1:B:8:MET:HA	1:B:11:GLN:HE21	1.73	0.52
1:B:25:TYR:O	1:B:29:CYS:HB2	2.10	0.52
1:B:11:GLN:HG2	3:B:206[B]:STE:C7	2.40	0.52
1:A:114:ASN:OD1	1:A:116:LYS:CE	2.57	0.51
1:B:11:GLN:OE1	3:B:206[B]:STE:H71	2.11	0.51
1:A:120:ASN:O	1:A:123:LYS:HG3	2.09	0.51
1:A:7:LYS:O	1:A:11:GLN:HG3	2.11	0.50
1:A:7:LYS:CE	3:A:205[A]:STE:H152	2.28	0.49
1:B:11:GLN:HG2	3:B:206[B]:STE:H71	1.95	0.48
1:A:25:TYR:O	1:A:29:CYS:HB2	2.14	0.48
1:A:69:LYS:CB	1:A:69:LYS:NZ	2.77	0.48
1:B:49:LYS:HG2	3:B:204:STE:H22	1.96	0.48
1:B:57:LYS:O	1:B:57:LYS:HG2	2.15	0.47
1:B:6:GLY:HA3	3:B:203:STE:H102	1.97	0.46
1:B:49:LYS:HE2	3:B:204:STE:H22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:TYR:CE2	1:B:113:TYR:CE2	3.05	0.45
1:B:7:LYS:NZ	3:B:206[B]:STE:H111	2.31	0.45
1:A:48:HIS:HD1	3:A:201:STE:C1	2.26	0.45
1:B:58:LEU:CD2	1:B:94:GLU:HB3	2.46	0.45
1:B:24:VAL:O	1:B:24:VAL:HG12	2.17	0.45
1:B:57:LYS:HB3	1:B:57:LYS:HE2	1.45	0.45
1:B:58:LEU:HD21	1:B:94:GLU:HB3	1.99	0.44
1:B:69:LYS:HZ2	1:B:69:LYS:HG2	1.74	0.44
1:B:11:GLN:NE2	1:B:75:TYR:OH	2.51	0.44
1:A:3:PHE:HB2	3:A:201:STE:H151	2.00	0.43
1:B:52:TYR:CE2	3:B:204:STE:H32	2.53	0.43
3:B:206[B]:STE:H122	3:B:206[B]:STE:H92	1.35	0.43
1:B:116:LYS:HE2	1:B:117:TYR:CE1	2.54	0.42
1:B:7:LYS:NZ	3:B:206[B]:STE:C16	2.82	0.42
1:A:69:LYS:CB	1:A:69:LYS:HZ3	2.33	0.42
1:B:2:LEU:HD21	3:B:204:STE:H62	2.01	0.41
1:A:25:TYR:CE2	1:A:113:TYR:CE2	3.08	0.41
1:A:123:LYS:N	1:A:125:PRO:CD	2.83	0.41
1:B:51:CYS:O	1:B:57:LYS:HE2	2.21	0.41
1:B:7:LYS:HZ3	3:B:206[B]:STE:C16	2.33	0.41
1:B:110:LEU:HA	1:B:110:LEU:HD23	1.84	0.41
1:B:41:THR:HG23	1:B:106:LEU:HD22	2.03	0.40
1:A:36:LYS:HB3	1:A:128:LYS:HB3	2.03	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:17:ASN:ND2	1:B:121:TYR:OH[4_556]	1.72	0.48

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	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	7 2
1	B	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	7 2
All	All	240/244 (98%)	228 (95%)	8 (3%)	4 (2%)	7 2

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	B	87	ASN
1	A	88	ASN
1	B	88	ASN

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	106/106 (100%)	95 (90%)	11 (10%)	5 1
1	B	106/106 (100%)	93 (88%)	13 (12%)	4 1
All	All	212/212 (100%)	188 (89%)	24 (11%)	4 1

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	24	VAL
1	A	36	LYS
1	A	43	ARG
1	A	57	LYS
1	A	69	LYS
1	A	86	GLU
1	A	87	ASN
1	A	93	LYS
1	A	114	ASN
1	A	115	LYS
1	B	17	ASN

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Mol	Chain	Res	Type
1	B	36	LYS
1	B	57	LYS
1	B	59	THR
1	B	69	LYS
1	B	72	ARG
1	B	74	SER
1	B	86	GLU
1	B	87	ASN
1	B	116	LYS
1	B	122	LEU
1	B	128	LYS
1	B	129	LYS

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	11	GLN
1	A	17	ASN
1	B	11	GLN
1	B	17	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)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	305	-	4,4,4	0.29	0	6,6,6	0.21	0
3	STE	A	201	-	19,19,19	0.48	0	19,19,19	1.00	1 (5%)
2	SO4	B	301	-	4,4,4	0.29	0	6,6,6	0.44	0
3	STE	B	204	3	10,10,19	0.46	0	10,10,19	1.13	2 (20%)
3	STE	B	206[B]	-	19,19,19	0.38	0	19,19,19	1.40	2 (10%)
2	SO4	A	304	-	4,4,4	0.35	0	6,6,6	0.27	0
3	STE	A	202	3	16,16,19	0.39	0	16,16,19	1.22	2 (12%)
3	STE	A	205[A]	-	19,19,19	0.56	0	19,19,19	1.43	3 (15%)
3	STE	B	203	-	19,19,19	0.35	0	19,19,19	1.41	3 (15%)
2	SO4	B	303	-	4,4,4	0.35	0	6,6,6	0.29	0
2	SO4	A	302	-	4,4,4	0.32	0	6,6,6	0.45	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	STE	A	201	-	-	8/17/17/17	-
3	STE	B	204	3	-	6/8/8/17	-
3	STE	B	206[B]	-	-	10/17/17/17	-
3	STE	A	202	3	-	10/14/14/17	-
3	STE	B	203	-	-	10/17/17/17	-
3	STE	A	205[A]	-	-	14/17/17/17	-

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	206[B]	STE	O2-C1-C2	4.02	126.70	114.00
3	A	205[A]	STE	O2-C1-C2	3.41	124.78	114.00
3	B	203	STE	C3-C2-C1	-3.27	105.96	114.51
3	A	205[A]	STE	O2-C1-O1	-3.18	115.16	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	203	STE	O2-C1-C2	2.83	122.95	114.00
3	B	206[B]	STE	O1-C1-C2	-2.68	114.60	123.09
3	A	202	STE	C3-C2-C1	-2.58	107.78	114.51
3	A	205[A]	STE	C3-C2-C1	2.42	120.82	114.51
3	B	204	STE	O2-C1-C2	2.33	121.36	114.00
3	A	202	STE	O2-C1-O1	-2.23	117.59	123.33
3	A	201	STE	O2-C1-O1	-2.15	117.81	123.33
3	B	204	STE	O2-C1-O1	-2.10	117.94	123.33
3	B	203	STE	O1-C1-C2	-2.04	116.63	123.09

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	204	STE	C2-C3-C4-C5
3	B	206[B]	STE	C9-C10-C11-C12
3	A	202	STE	C11-C12-C13-C14
3	A	205[A]	STE	C10-C11-C12-C13
3	B	204	STE	C1-C2-C3-C4
3	B	203	STE	C13-C14-C15-C16
3	A	205[A]	STE	C3-C4-C5-C6
3	B	204	STE	C4-C5-C6-C7
3	B	206[B]	STE	C3-C4-C5-C6
3	A	201	STE	C6-C7-C8-C9
3	A	205[A]	STE	C13-C14-C15-C16
3	A	201	STE	C13-C14-C15-C16
3	A	205[A]	STE	C12-C13-C14-C15
3	A	202	STE	C7-C8-C9-C10
3	A	205[A]	STE	C5-C6-C7-C8
3	B	204	STE	C6-C7-C8-C9
3	A	205[A]	STE	C1-C2-C3-C4
3	A	205[A]	STE	C4-C5-C6-C7
3	B	203	STE	C12-C13-C14-C15
3	B	206[B]	STE	C11-C12-C13-C14
3	B	206[B]	STE	C7-C8-C9-C10
3	A	202	STE	C5-C6-C7-C8
3	A	201	STE	C9-C10-C11-C12
3	B	203	STE	C15-C16-C17-C18
3	B	206[B]	STE	C13-C14-C15-C16
3	B	203	STE	C11-C12-C13-C14
3	B	203	STE	C3-C4-C5-C6
3	B	203	STE	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	B	206[B]	STE	C2-C3-C4-C5
3	A	202	STE	C12-C13-C14-C15
3	A	205[A]	STE	C15-C16-C17-C18
3	A	205[A]	STE	C11-C12-C13-C14
3	B	206[B]	STE	C5-C6-C7-C8
3	B	206[B]	STE	C10-C11-C12-C13
3	A	201	STE	C5-C6-C7-C8
3	B	203	STE	C4-C5-C6-C7
3	B	206[B]	STE	C12-C13-C14-C15
3	A	202	STE	C2-C3-C4-C5
3	A	201	STE	C11-C10-C9-C8
3	A	202	STE	C11-C10-C9-C8
3	A	205[A]	STE	O2-C1-C2-C3
3	A	202	STE	C9-C10-C11-C12
3	A	205[A]	STE	O1-C1-C2-C3
3	B	203	STE	C10-C11-C12-C13
3	A	205[A]	STE	C6-C7-C8-C9
3	A	205[A]	STE	C11-C10-C9-C8
3	B	204	STE	O1-C1-C2-C3
3	A	205[A]	STE	C2-C3-C4-C5
3	A	201	STE	C15-C16-C17-C18
3	A	201	STE	C4-C5-C6-C7
3	A	202	STE	C1-C2-C3-C4
3	A	202	STE	O1-C1-C2-C3
3	B	203	STE	C7-C8-C9-C10
3	B	204	STE	O2-C1-C2-C3
3	A	202	STE	O2-C1-C2-C3
3	A	201	STE	C1-C2-C3-C4
3	B	203	STE	C2-C3-C4-C5
3	B	206[B]	STE	O2-C1-C2-C3

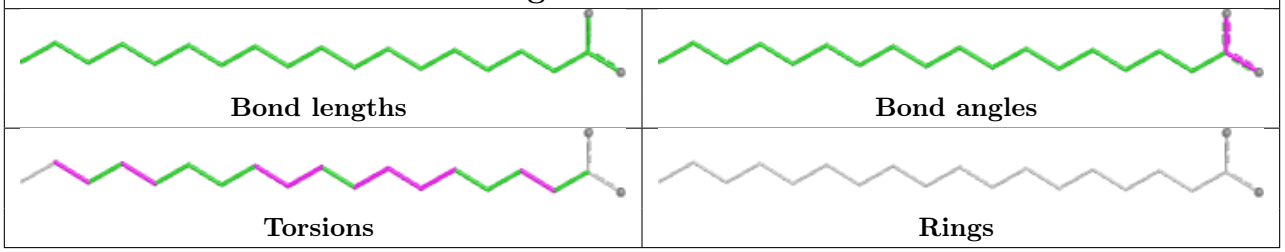
There are no ring outliers.

6 monomers are involved in 35 short contacts:

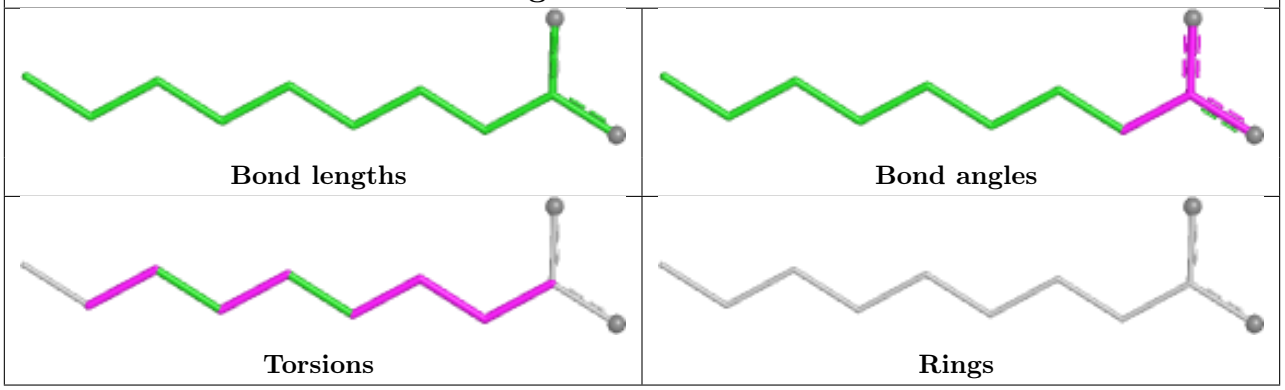
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	STE	2	0
3	B	204	STE	13	0
3	B	206[B]	STE	12	0
3	A	202	STE	3	0
3	A	205[A]	STE	4	0
3	B	203	STE	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

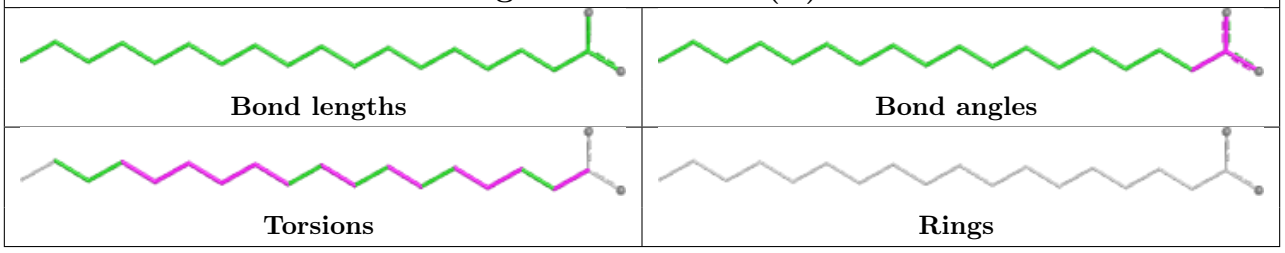
Ligand STE A 201

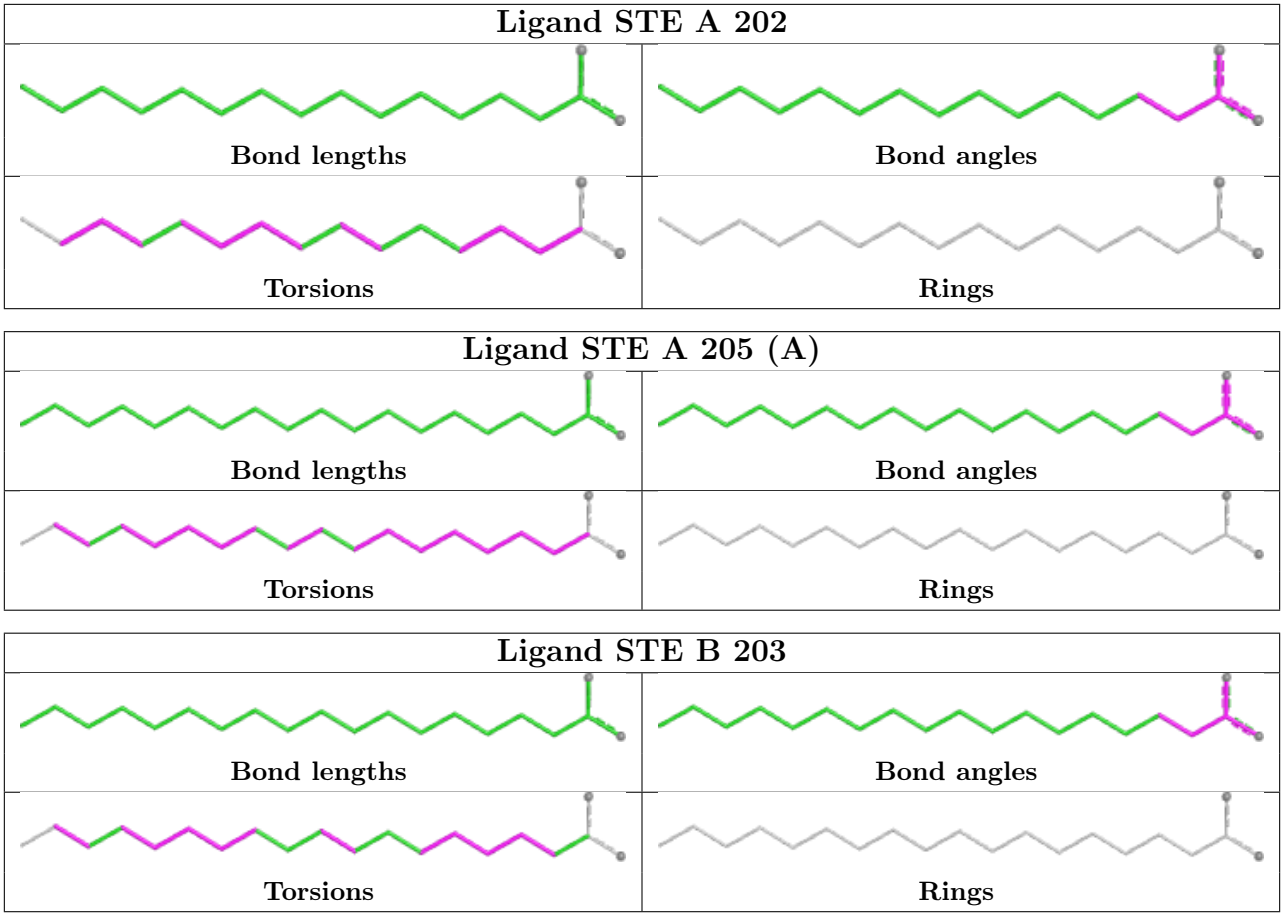


Ligand STE B 204



Ligand STE B 206 (B)





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

Warning: The R factor obtained from EDS is 0.2229, which does not match the depositor's R factor of 0.166. Please interpret the results in this section carefully.

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^{th} 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	122/122 (100%)	0.20	6 (4%)	36	33	21, 29, 55, 69	0
1	B	122/122 (100%)	0.16	5 (4%)	42	39	18, 32, 51, 69	1 (0%)
All	All	244/244 (100%)	0.18	11 (4%)	39	36	18, 30, 55, 69	1 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	ASN	5.5
1	A	88	ASN	5.3
1	A	85	GLY	3.6
1	A	86	GLU	3.1
1	A	121	TYR	3.0
1	B	87	ASN	3.0
1	B	89	SER	2.6
1	B	128	LYS	2.4
1	A	126	ALA	2.4
1	B	74	SER	2.2
1	B	59	THR	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

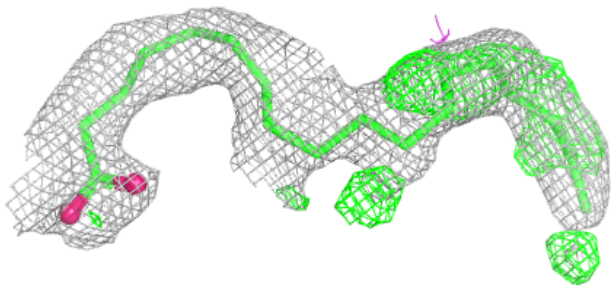
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

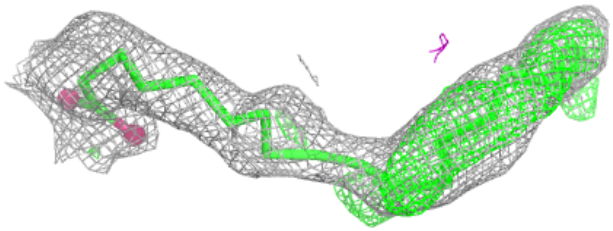
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	302	5/5	0.64	0.16	96,97,97,97	0
3	STE	A	205[A]	20/20	0.64	0.24	25,30,37,38	20
3	STE	B	204	11/20	0.64	0.16	76,76,78,79	0
2	SO4	B	303	5/5	0.67	0.18	95,95,95,96	0
3	STE	B	206[B]	20/20	0.71	0.20	26,29,34,36	20
2	SO4	A	304	5/5	0.75	0.14	101,102,102,102	0
3	STE	A	202	17/20	0.76	0.14	58,59,65,65	0
2	SO4	A	305	5/5	0.83	0.11	68,70,71,71	0
3	STE	B	203	20/20	0.86	0.11	33,46,53,54	0
2	SO4	B	301	5/5	0.91	0.08	63,64,65,65	0
3	STE	A	201	20/20	0.92	0.11	31,46,56,56	0

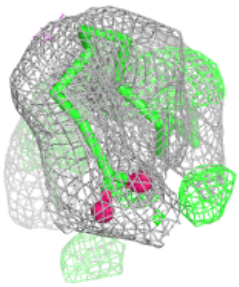
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE A 205 (A):

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

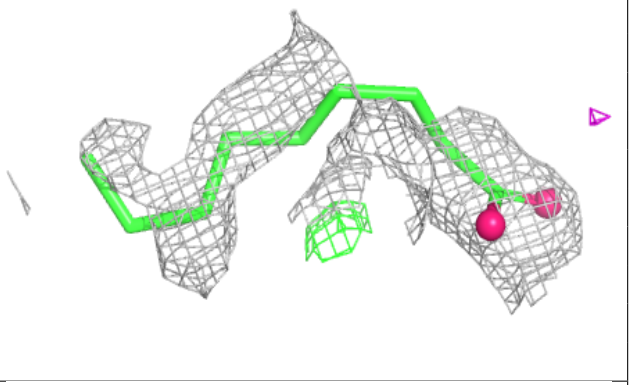


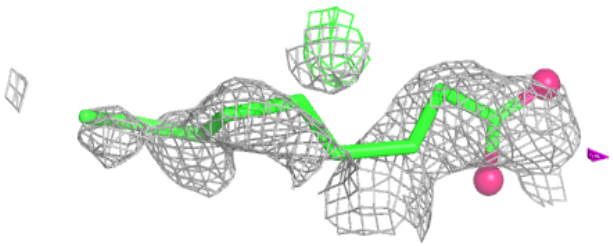


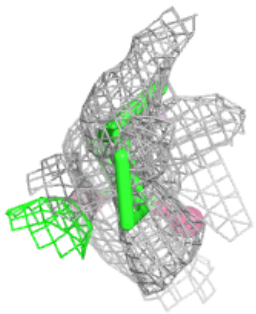


Electron density around STE B 204:

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

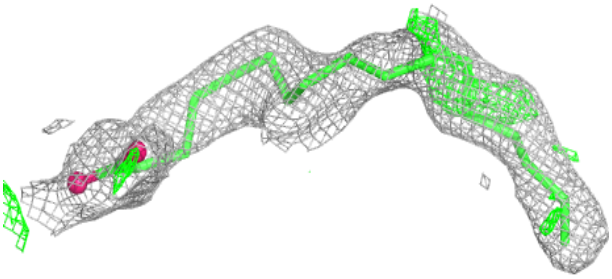


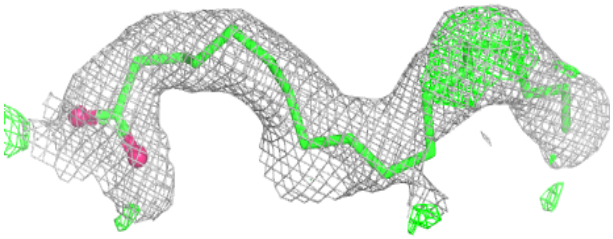


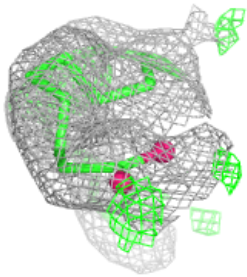


Electron density around STE B 206 (B):

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

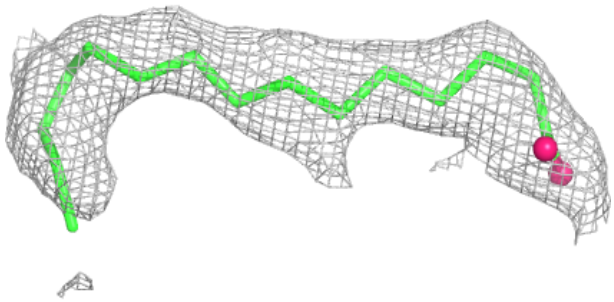


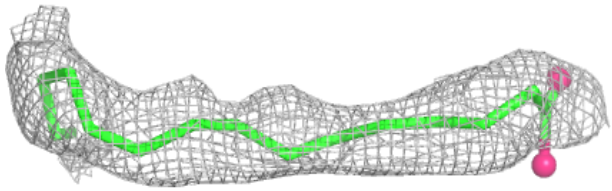


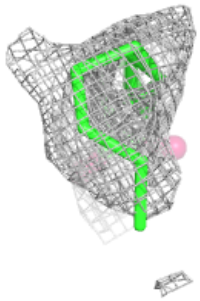


Electron density around STE A 202:

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

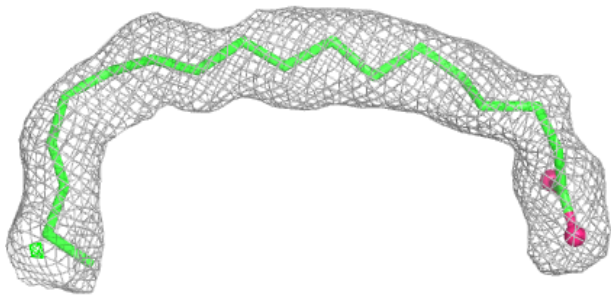


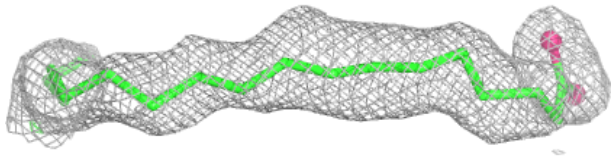


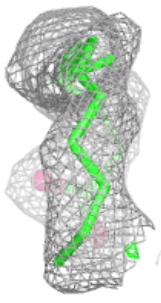


Electron density around STE B 203:

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

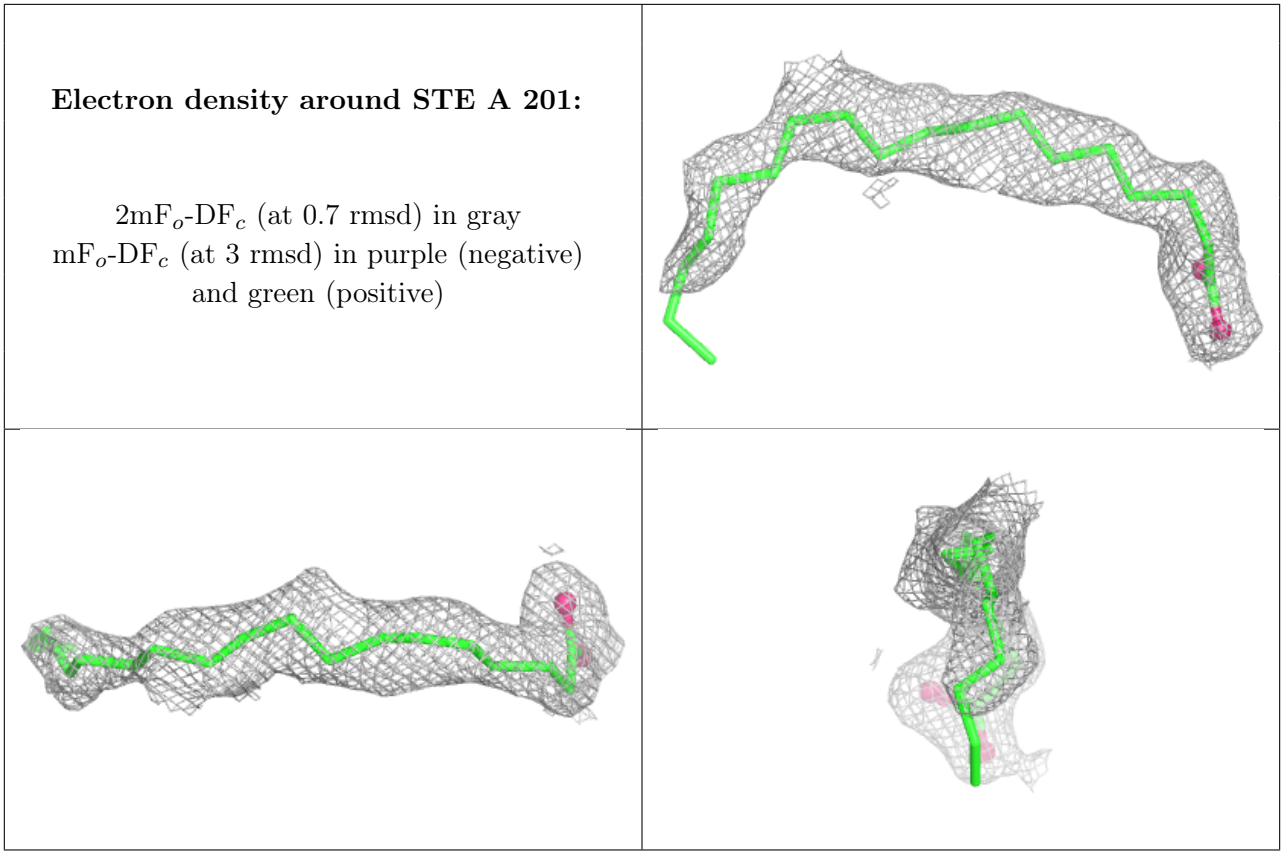






Electron density around STE A 201:

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



6.5 Other polymers

There are no such residues in this entry.