Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2026 – 07:16 PM JST

PDB ID	:	9XII / pdb_00009xii
Title	:	Crystal structure of Macrobrachium rosenbergii lipocalin Y57F mutant in complex with astaxanthin
Authors	:	Guan, L.; Zhao, G.
Deposited on	:	2025-11-03
Resolution	:	2.99 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:

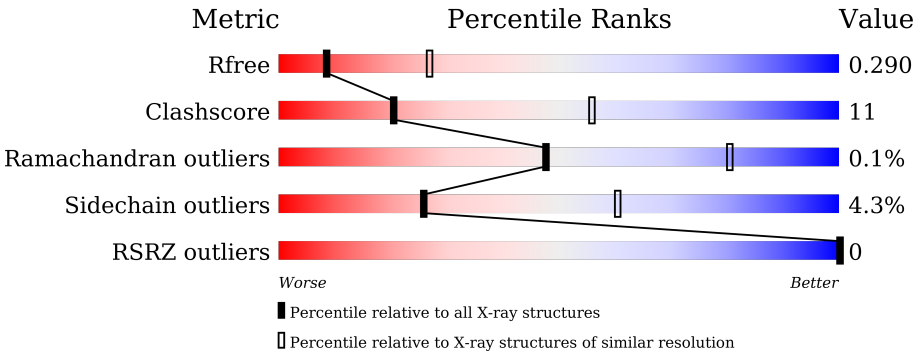
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.99 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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% 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	207	64% 24% 12%
1	C	207	67% 21% 12%
1	E	207	61% 27% 12%
1	G	207	62% 26% • 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6064 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 Crustacyanin-like lipocalin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1472	942	248	272	10			
1	C	183	Total	C	N	O	S	0	0	0
			1472	942	248	272	10			
1	E	183	Total	C	N	O	S	0	0	0
			1472	942	248	272	10			
1	G	183	Total	C	N	O	S	0	0	0
			1472	942	248	272	10			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A4Z4V4
A	-18	GLY	-	expression tag	UNP A4Z4V4
A	-17	SER	-	expression tag	UNP A4Z4V4
A	-16	SER	-	expression tag	UNP A4Z4V4
A	-15	HIS	-	expression tag	UNP A4Z4V4
A	-14	HIS	-	expression tag	UNP A4Z4V4
A	-13	HIS	-	expression tag	UNP A4Z4V4
A	-12	HIS	-	expression tag	UNP A4Z4V4
A	-11	HIS	-	expression tag	UNP A4Z4V4
A	-10	HIS	-	expression tag	UNP A4Z4V4
A	-9	SER	-	expression tag	UNP A4Z4V4
A	-8	SER	-	expression tag	UNP A4Z4V4
A	-7	GLY	-	expression tag	UNP A4Z4V4
A	-6	LEU	-	expression tag	UNP A4Z4V4
A	-5	VAL	-	expression tag	UNP A4Z4V4
A	-4	PRO	-	expression tag	UNP A4Z4V4
A	-3	ARG	-	expression tag	UNP A4Z4V4
A	-2	GLY	-	expression tag	UNP A4Z4V4
A	-1	SER	-	expression tag	UNP A4Z4V4
A	0	HIS	-	expression tag	UNP A4Z4V4
A	1	MET	-	expression tag	UNP A4Z4V4

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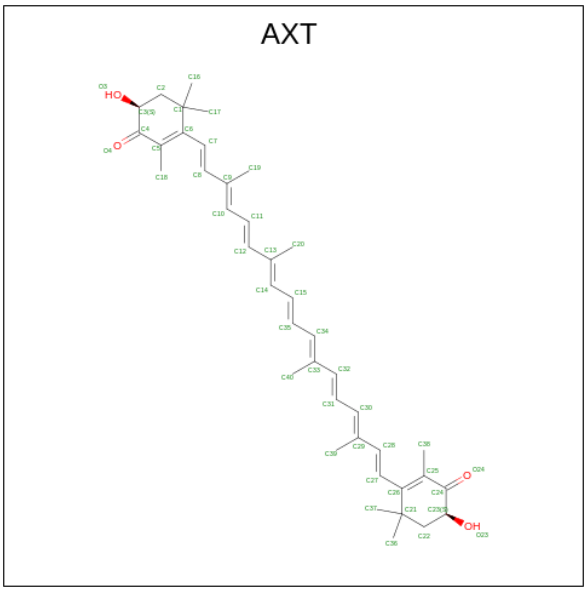
Chain	Residue	Modelled	Actual	Comment	Reference
A	57	PHE	TYR	engineered mutation	UNP A4Z4V4
C	-19	MET	-	initiating methionine	UNP A4Z4V4
C	-18	GLY	-	expression tag	UNP A4Z4V4
C	-17	SER	-	expression tag	UNP A4Z4V4
C	-16	SER	-	expression tag	UNP A4Z4V4
C	-15	HIS	-	expression tag	UNP A4Z4V4
C	-14	HIS	-	expression tag	UNP A4Z4V4
C	-13	HIS	-	expression tag	UNP A4Z4V4
C	-12	HIS	-	expression tag	UNP A4Z4V4
C	-11	HIS	-	expression tag	UNP A4Z4V4
C	-10	HIS	-	expression tag	UNP A4Z4V4
C	-9	SER	-	expression tag	UNP A4Z4V4
C	-8	SER	-	expression tag	UNP A4Z4V4
C	-7	GLY	-	expression tag	UNP A4Z4V4
C	-6	LEU	-	expression tag	UNP A4Z4V4
C	-5	VAL	-	expression tag	UNP A4Z4V4
C	-4	PRO	-	expression tag	UNP A4Z4V4
C	-3	ARG	-	expression tag	UNP A4Z4V4
C	-2	GLY	-	expression tag	UNP A4Z4V4
C	-1	SER	-	expression tag	UNP A4Z4V4
C	0	HIS	-	expression tag	UNP A4Z4V4
C	1	MET	-	expression tag	UNP A4Z4V4
C	57	PHE	TYR	engineered mutation	UNP A4Z4V4
E	-19	MET	-	initiating methionine	UNP A4Z4V4
E	-18	GLY	-	expression tag	UNP A4Z4V4
E	-17	SER	-	expression tag	UNP A4Z4V4
E	-16	SER	-	expression tag	UNP A4Z4V4
E	-15	HIS	-	expression tag	UNP A4Z4V4
E	-14	HIS	-	expression tag	UNP A4Z4V4
E	-13	HIS	-	expression tag	UNP A4Z4V4
E	-12	HIS	-	expression tag	UNP A4Z4V4
E	-11	HIS	-	expression tag	UNP A4Z4V4
E	-10	HIS	-	expression tag	UNP A4Z4V4
E	-9	SER	-	expression tag	UNP A4Z4V4
E	-8	SER	-	expression tag	UNP A4Z4V4
E	-7	GLY	-	expression tag	UNP A4Z4V4
E	-6	LEU	-	expression tag	UNP A4Z4V4
E	-5	VAL	-	expression tag	UNP A4Z4V4
E	-4	PRO	-	expression tag	UNP A4Z4V4
E	-3	ARG	-	expression tag	UNP A4Z4V4
E	-2	GLY	-	expression tag	UNP A4Z4V4
E	-1	SER	-	expression tag	UNP A4Z4V4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP A4Z4V4
E	1	MET	-	expression tag	UNP A4Z4V4
E	57	PHE	TYR	engineered mutation	UNP A4Z4V4
G	-19	MET	-	initiating methionine	UNP A4Z4V4
G	-18	GLY	-	expression tag	UNP A4Z4V4
G	-17	SER	-	expression tag	UNP A4Z4V4
G	-16	SER	-	expression tag	UNP A4Z4V4
G	-15	HIS	-	expression tag	UNP A4Z4V4
G	-14	HIS	-	expression tag	UNP A4Z4V4
G	-13	HIS	-	expression tag	UNP A4Z4V4
G	-12	HIS	-	expression tag	UNP A4Z4V4
G	-11	HIS	-	expression tag	UNP A4Z4V4
G	-10	HIS	-	expression tag	UNP A4Z4V4
G	-9	SER	-	expression tag	UNP A4Z4V4
G	-8	SER	-	expression tag	UNP A4Z4V4
G	-7	GLY	-	expression tag	UNP A4Z4V4
G	-6	LEU	-	expression tag	UNP A4Z4V4
G	-5	VAL	-	expression tag	UNP A4Z4V4
G	-4	PRO	-	expression tag	UNP A4Z4V4
G	-3	ARG	-	expression tag	UNP A4Z4V4
G	-2	GLY	-	expression tag	UNP A4Z4V4
G	-1	SER	-	expression tag	UNP A4Z4V4
G	0	HIS	-	expression tag	UNP A4Z4V4
G	1	MET	-	expression tag	UNP A4Z4V4
G	57	PHE	TYR	engineered mutation	UNP A4Z4V4

- Molecule 2 is ASTAXANTHIN (CCD ID: AXT) (formula: $C_{40}H_{52}O_4$) (labeled as "Ligand of Interest" by depositor).



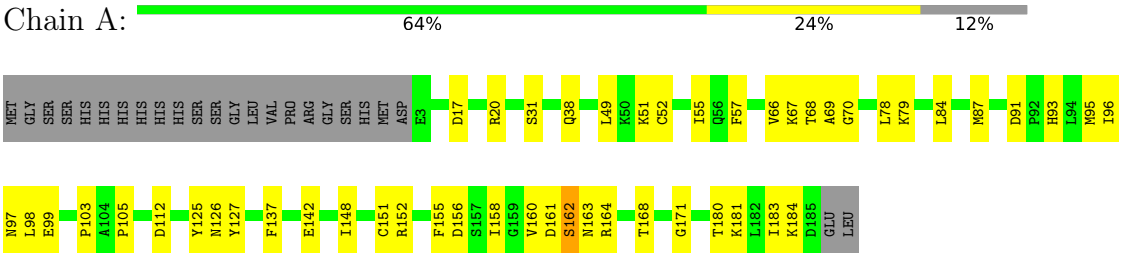
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 44 40 4	0	0
2	A	1	Total C O 44 40 4	0	0
2	E	1	Total C O 44 40 4	0	0
2	G	1	Total C O 44 40 4	0	0

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.

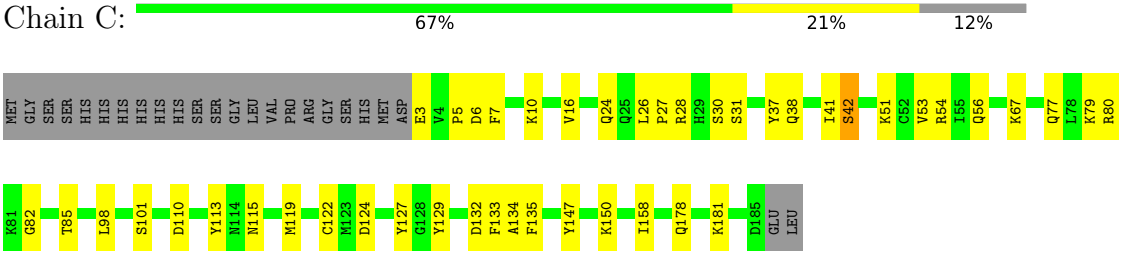
• Molecule 1: Crustacyanin-like lipocalin

Chain A:



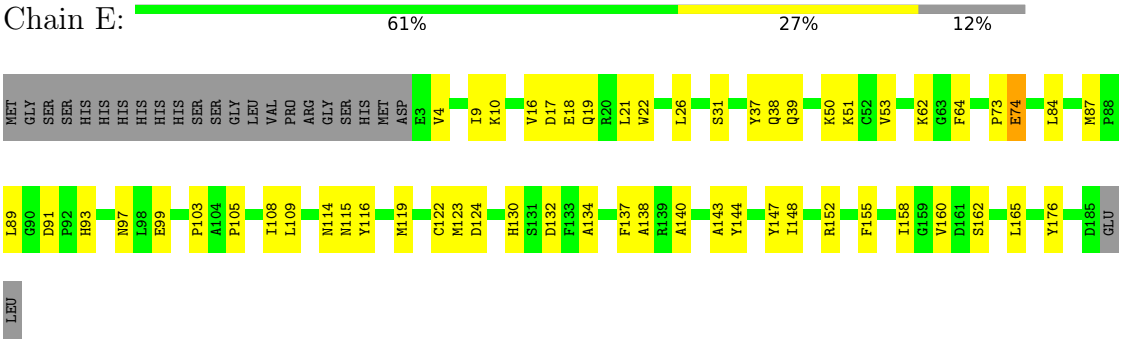
• Molecule 1: Crustacyanin-like lipocalin

Chain C:



• Molecule 1: Crustacyanin-like lipocalin

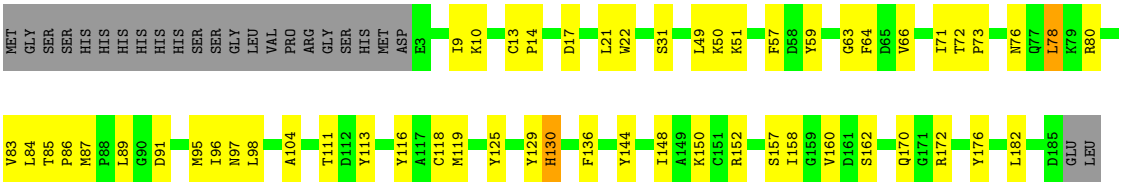
Chain E:



• Molecule 1: Crustacyanin-like lipocalin

Chain G:




MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ASP E3 I9 K10 C13 P14 D17 L21 W22 S31 L49 K50 K51 F57 D58 Y59 G63 F64 D65 V66 I71 T72 P73 N76 Q77 L78 K79 R80
V83 L84 T85 P86 M87 P88 L89 G90 D91 M95 I96 N97 L98 A104 T111 D112 Y113 Y116 A117 C118 M119 Y125 Y129 H130 F136 Y144 I148 A149 K150 C151 R152 S157 I158 G159 V160 D161 S162 Q170 G171 R172 Y176 L182 D185 GLU LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.16Å 120.26Å 78.91Å 90.00° 103.08° 90.00°	Depositor
Resolution (Å)	76.87 – 2.99 76.87 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (76.87-2.99) 92.1 (76.87-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.198 , 0.291 0.197 , 0.290	Depositor DCC
R_{free} test set	1602 reflections (9.88%)	wwPDB-VP
Wilson B-factor (Å^2)	38.5	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6064	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AXT

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	0.39	0/1511	0.58	0/2045
1	C	0.37	0/1511	0.55	0/2045
1	E	0.37	0/1511	0.56	0/2045
1	G	0.38	0/1511	0.54	0/2045
All	All	0.38	0/6044	0.56	0/8180

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	1472	0	1421	37	0
1	C	1472	0	1421	24	0
1	E	1472	0	1421	36	0
1	G	1472	0	1421	34	0
2	A	88	0	104	11	0
2	E	44	0	52	5	0
2	G	44	0	52	1	0
All	All	6064	0	5892	134	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 11.

All (134) 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:E:87:MET:HG2	1:E:91:ASP:HB2	1.62	0.81
1:A:158:ILE:HG13	1:A:160:VAL:HG23	1.71	0.71
1:G:84:LEU:HD13	1:G:96:ILE:HB	1.71	0.71
1:A:183:ILE:HG23	1:A:184:LYS:HE2	1.74	0.69
2:A:202:AXT:H31	1:C:5:PRO:HG2	1.73	0.69
1:A:105:PRO:HD3	2:A:202:AXT:H382	1.75	0.66
1:G:87:MET:HE3	1:G:89:LEU:H	1.59	0.66
1:A:148:ILE:HG13	1:A:152:ARG:HD2	1.80	0.64
1:G:158:ILE:HG13	1:G:160:VAL:HG23	1.79	0.64
1:C:24:GLN:O	1:C:27:PRO:HD2	1.99	0.63
1:C:147:TYR:HA	1:C:150:LYS:HD3	1.80	0.63
1:A:95:MET:HE2	2:A:202:AXT:H383	1.84	0.59
1:G:87:MET:HG2	1:G:91:ASP:HB2	1.85	0.59
1:C:38:GLN:HB3	1:C:53:VAL:HB	1.84	0.58
1:E:87:MET:HE3	1:E:89:LEU:HB2	1.84	0.57
1:G:148:ILE:HD11	1:G:152:ARG:NH1	2.19	0.57
1:G:50:LYS:HD2	1:G:73:PRO:HB3	1.86	0.57
1:E:152:ARG:HG2	1:E:162:SER:HB2	1.85	0.57
1:A:97:ASN:HB3	1:A:103:PRO:HA	1.88	0.56
1:C:10:LYS:HD3	1:C:129:TYR:CZ	2.41	0.55
1:E:144:TYR:CE1	1:E:148:ILE:HD13	2.41	0.55
2:E:201:AXT:H8	2:E:201:AXT:H161	1.88	0.55
1:G:57:PHE:HD1	1:G:66:VAL:HG22	1.72	0.55
1:C:42:SER:HB3	1:C:134:ALA:H	1.74	0.53
1:A:79:LYS:HD2	1:A:183:ILE:HA	1.91	0.53
2:A:202:AXT:H161	2:A:202:AXT:H8	1.90	0.53
1:G:80:ARG:NE	1:G:98:LEU:HD23	2.24	0.52
1:C:82:GLY:HA3	1:C:98:LEU:HD23	1.91	0.52
1:A:51:LYS:HG3	1:A:52:CYS:SG	2.50	0.52
1:A:156:ASP:HB3	1:E:10:LYS:NZ	2.25	0.51
1:C:119:MET:HB2	1:C:135:PHE:HB2	1.92	0.51
1:C:31:SER:HB2	1:C:113:TYR:CD2	2.46	0.51
1:E:122:CYS:SG	1:E:132:ASP:HB3	2.50	0.51
1:C:133:PHE:HB3	1:C:135:PHE:CZ	2.46	0.51
1:E:39:GLN:NE2	1:E:138:ALA:HB3	2.26	0.51
1:G:125:TYR:OH	2:G:201:AXT:H34	2.12	0.50
1:A:95:MET:CE	2:A:202:AXT:H383	2.42	0.50
1:A:126:ASN:HB3	1:C:124:ASP:OD1	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:GLN:HB3	1:E:53:VAL:HB	1.92	0.50
1:A:17:ASP:OD2	1:A:20:ARG:HD3	2.12	0.49
1:E:17:ASP:O	1:E:21:LEU:HD12	2.11	0.49
1:A:180:THR:O	1:A:183:ILE:HG22	2.12	0.49
1:E:4:VAL:HG22	2:E:201:AXT:H393	1.93	0.49
1:E:124:ASP:HA	1:E:130:HIS:HA	1.94	0.49
1:E:105:PRO:HD2	1:E:123:MET:HE3	1.95	0.48
1:G:72:THR:OG1	1:G:76:ASN:HB3	2.13	0.48
1:E:140:ALA:HB3	1:E:143:ALA:HB2	1.94	0.48
1:A:156:ASP:HB3	1:E:10:LYS:HZ2	1.78	0.48
1:E:16:VAL:HG22	1:E:158:ILE:HG21	1.94	0.48
1:C:37:TYR:CE1	1:C:54:ARG:HG3	2.49	0.48
1:E:50:LYS:HB2	1:E:73:PRO:HG3	1.96	0.48
1:G:17:ASP:O	1:G:21:LEU:HD13	2.14	0.47
1:G:51:LYS:HG3	1:G:71:ILE:HB	1.97	0.47
1:A:67:LYS:HB3	1:A:183:ILE:HG12	1.97	0.47
1:G:57:PHE:CD1	1:G:66:VAL:HG22	2.50	0.47
1:G:87:MET:HG2	1:G:91:ASP:H	1.80	0.47
1:E:108:ILE:HG12	1:E:119:MET:HG2	1.96	0.47
1:C:41:ILE:HG22	1:C:135:PHE:HD1	1.80	0.47
1:G:59:TYR:HD1	1:G:64:PHE:CE2	2.32	0.47
1:A:84:LEU:HD12	1:A:96:ILE:HB	1.97	0.47
1:E:37:TYR:HE2	1:E:176:TYR:CE1	2.33	0.46
1:E:87:MET:CE	1:E:89:LEU:HB2	2.43	0.46
1:A:55:ILE:HD13	1:A:137:PHE:CZ	2.50	0.46
1:G:50:LYS:HB2	1:G:73:PRO:HD3	1.97	0.46
1:E:119:MET:HE3	1:E:119:MET:HB2	1.72	0.46
1:G:116:TYR:CE2	1:G:150:LYS:HG2	2.51	0.46
1:E:109:LEU:HD12	1:E:155:PHE:CD1	2.51	0.45
1:A:20:ARG:HE	1:A:20:ARG:HB3	1.36	0.45
1:A:55:ILE:HD13	1:A:137:PHE:CE2	2.51	0.45
1:E:93:HIS:NE2	1:E:105:PRO:HB3	2.30	0.45
1:G:49:LEU:HD21	1:G:78:LEU:HB3	1.98	0.45
1:G:31:SER:HB2	1:G:113:TYR:HD2	1.80	0.45
1:G:118:CYS:C	1:G:119:MET:HG3	2.42	0.45
1:A:142:GLU:CD	1:A:171:GLY:HA3	2.42	0.45
2:E:201:AXT:H7	2:E:201:AXT:H181	1.76	0.44
1:G:111:THR:HG23	1:G:113:TYR:CE1	2.51	0.44
1:E:4:VAL:HG22	2:E:201:AXT:H27	1.98	0.44
1:G:10:LYS:HE2	1:G:129:TYR:CZ	2.52	0.44
1:A:69:ALA:HA	1:A:78:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:ALA:HB1	1:E:155:PHE:CZ	2.53	0.44
1:E:97:ASN:HB3	1:E:103:PRO:HA	1.98	0.44
1:A:93:HIS:CE1	1:C:127:TYR:CE2	3.06	0.44
2:A:201:AXT:H181	2:A:201:AXT:H7	1.80	0.44
1:G:96:ILE:HG23	1:G:96:ILE:O	2.18	0.44
1:A:87:MET:SD	1:A:91:ASP:HB2	2.58	0.44
1:A:49:LEU:HD13	1:A:70:GLY:N	2.33	0.43
1:C:98:LEU:O	1:C:101:SER:HB2	2.18	0.43
2:A:202:AXT:H181	2:A:202:AXT:H7	1.72	0.43
1:G:152:ARG:HG3	1:G:162:SER:HB2	2.00	0.43
1:G:170:GLN:HB3	1:G:176:TYR:OH	2.18	0.43
2:A:202:AXT:H193	1:C:135:PHE:HE2	1.84	0.43
1:A:161:ASP:HB3	1:A:164:ARG:HG3	2.00	0.43
1:C:115:ASN:HB3	1:C:147:TYR:CZ	2.54	0.43
1:G:136:PHE:C	1:G:136:PHE:CD1	2.96	0.43
1:A:125:TYR:OH	2:A:201:AXT:H34	2.19	0.42
1:A:127:TYR:CD2	2:A:201:AXT:H23	2.53	0.42
1:A:161:ASP:O	1:A:164:ARG:HB2	2.19	0.42
1:C:28:ARG:HB2	1:C:113:TYR:OH	2.20	0.42
1:G:22:TRP:HH2	1:G:86:PRO:HB3	1.83	0.42
1:G:63:GLY:HA3	1:G:85:THR:HA	2.01	0.42
1:G:84:LEU:HA	1:G:95:MET:O	2.20	0.42
1:A:38:GLN:HG2	1:A:168:THR:OG1	2.19	0.42
1:G:83:VAL:O	1:G:96:ILE:HA	2.20	0.42
2:A:201:AXT:H27	2:A:201:AXT:H381	1.71	0.42
1:C:77:GLN:HE22	1:C:178:GLN:HG2	1.84	0.42
1:E:74:GLU:H	1:E:74:GLU:HG3	1.46	0.42
1:G:9:ILE:HG13	1:G:130:HIS:CE1	2.55	0.42
1:G:13:CYS:HA	1:G:14:PRO:HD3	1.87	0.42
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.82	0.41
1:A:181:LYS:HD3	1:A:181:LYS:HA	1.81	0.41
1:C:56:GLN:HB3	1:C:67:LYS:HB2	2.02	0.41
1:E:16:VAL:HG12	1:E:18:GLU:HG2	2.01	0.41
1:A:67:LYS:HB3	1:A:183:ILE:CG1	2.50	0.41
1:A:162:SER:C	1:A:164:ARG:H	2.28	0.41
1:E:9:ILE:HG13	1:E:130:HIS:NE2	2.35	0.41
1:A:112:ASP:OD1	1:A:112:ASP:C	2.63	0.41
1:C:16:VAL:HG22	1:C:158:ILE:HG21	2.01	0.41
1:G:31:SER:HB2	1:G:113:TYR:CD2	2.55	0.41
1:C:122:CYS:SG	1:C:132:ASP:HB3	2.61	0.41
1:C:5:PRO:HB3	1:C:7:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LYS:C	1:C:80:ARG:HG3	2.46	0.41
1:E:22:TRP:CZ2	1:E:26:LEU:HD13	2.56	0.41
1:E:115:ASN:HB3	1:E:147:TYR:CZ	2.56	0.41
1:E:155:PHE:HB3	1:E:160:VAL:HB	2.03	0.41
1:G:95:MET:HA	1:G:104:ALA:O	2.21	0.41
1:A:151:CYS:HB3	1:A:155:PHE:HE2	1.86	0.40
1:E:38:GLN:HA	1:E:137:PHE:CD1	2.56	0.40
1:E:116:TYR:CD1	1:E:116:TYR:C	3.00	0.40
2:E:201:AXT:H3	2:E:201:AXT:H173	1.81	0.40
1:A:52:CYS:O	1:A:70:GLY:HA2	2.22	0.40
1:A:57:PHE:CD1	1:A:66:VAL:HG22	2.56	0.40
1:E:64:PHE:HB2	1:E:84:LEU:HB3	2.04	0.40
1:E:109:LEU:HD23	1:E:109:LEU:HA	1.90	0.40
1:E:155:PHE:HE2	1:E:165:LEU:HD11	1.87	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	181/207 (87%)	168 (93%)	13 (7%)	0	100	100
1	C	181/207 (87%)	172 (95%)	9 (5%)	0	100	100
1	E	181/207 (87%)	169 (93%)	12 (7%)	0	100	100
1	G	181/207 (87%)	165 (91%)	15 (8%)	1 (1%)	21	56
All	All	724/828 (87%)	674 (93%)	49 (7%)	1 (0%)	48	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	144	TYR

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	158/179 (88%)	153 (97%)	5 (3%)	34	67
1	C	158/179 (88%)	149 (94%)	9 (6%)	18	52
1	E	158/179 (88%)	151 (96%)	7 (4%)	25	60
1	G	158/179 (88%)	152 (96%)	6 (4%)	29	63
All	All	632/716 (88%)	605 (96%)	27 (4%)	26	60

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	68	THR
1	A	99	GLU
1	A	162	SER
1	A	163	ASN
1	C	3	GLU
1	C	6	ASP
1	C	26	LEU
1	C	30	SER
1	C	42	SER
1	C	51	LYS
1	C	85	THR
1	C	110	ASP
1	C	181	LYS
1	E	19	GLN
1	E	31	SER
1	E	51	LYS
1	E	62	LYS
1	E	74	GLU
1	E	99	GLU
1	E	114	ASN
1	G	78	LEU
1	G	97	ASN
1	G	130	HIS

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Mol	Chain	Res	Type
1	G	157	SER
1	G	172	ARG
1	G	182	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	115	ASN
1	C	38	GLN
1	C	47	GLN
1	C	77	GLN
1	E	163	ASN
1	G	39	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	AXT	G	201	-	45,45,45	0.73	0	52,64,64	1.32	6 (11%)
2	AXT	A	201	-	45,45,45	0.74	0	52,64,64	1.44	12 (23%)
2	AXT	E	201	-	45,45,45	0.75	1 (2%)	52,64,64	1.42	7 (13%)
2	AXT	A	202	-	45,45,45	0.76	0	52,64,64	1.69	8 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AXT	G	201	-	-	6/29/75/75	0/2/2/2
2	AXT	A	201	-	-	1/29/75/75	0/2/2/2
2	AXT	E	201	-	-	2/29/75/75	0/2/2/2
2	AXT	A	202	-	-	6/29/75/75	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	AXT	C34-C33	2.19	1.38	1.35

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	202	AXT	C38-C25-C26	-5.85	114.70	124.11
2	G	201	AXT	C15-C14-C13	3.90	132.87	127.31
2	E	201	AXT	C16-C1-C6	3.88	116.60	110.30
2	A	202	AXT	C7-C8-C9	3.84	132.04	126.23
2	A	201	AXT	C37-C21-C26	3.75	116.39	110.30
2	A	202	AXT	O24-C24-C25	3.65	127.47	121.44
2	A	202	AXT	C16-C1-C6	3.58	116.11	110.30
2	E	201	AXT	C11-C10-C9	3.45	132.24	127.31
2	A	202	AXT	C31-C30-C29	2.94	131.50	127.31
2	A	201	AXT	C11-C10-C9	2.92	131.47	127.31
2	A	201	AXT	C28-C29-C30	-2.87	114.53	118.94
2	A	202	AXT	C27-C28-C29	-2.86	121.92	126.23
2	E	201	AXT	C40-C33-C34	2.81	126.86	122.92
2	E	201	AXT	C1-C6-C7	2.79	123.66	115.78
2	G	201	AXT	O4-C4-C5	2.65	125.83	121.44
2	G	201	AXT	C1-C6-C7	2.65	123.28	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	202	AXT	O4-C4-C5	2.48	125.55	121.44
2	G	201	AXT	O24-C24-C25	2.45	125.48	121.44
2	A	201	AXT	C20-C13-C14	-2.44	119.51	122.92
2	G	201	AXT	C35-C34-C33	2.42	130.77	127.31
2	A	201	AXT	C31-C30-C29	2.42	130.76	127.31
2	A	202	AXT	C39-C29-C30	2.42	126.31	122.92
2	A	201	AXT	C8-C7-C6	2.31	133.70	127.20
2	A	201	AXT	C38-C25-C24	-2.31	111.76	116.13
2	E	201	AXT	C8-C7-C6	2.28	133.62	127.20
2	G	201	AXT	C39-C29-C30	2.22	126.04	122.92
2	E	201	AXT	C17-C1-C6	-2.19	106.75	110.30
2	A	201	AXT	C38-C25-C26	-2.13	120.68	124.11
2	A	201	AXT	C1-C6-C7	2.11	121.76	115.78
2	A	201	AXT	C2-C3-C4	-2.11	104.82	109.57
2	E	201	AXT	C35-C34-C33	2.10	130.30	127.31
2	A	201	AXT	C39-C29-C30	2.07	125.82	122.92
2	A	201	AXT	C21-C26-C27	2.03	121.52	115.78

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	202	AXT	C21-C26-C27-C28
2	E	201	AXT	C21-C26-C27-C28
2	E	201	AXT	C25-C26-C27-C28
2	G	201	AXT	C27-C28-C29-C39
2	G	201	AXT	C27-C28-C29-C30
2	A	201	AXT	C21-C26-C27-C28
2	G	201	AXT	C1-C6-C7-C8
2	G	201	AXT	C5-C6-C7-C8
2	G	201	AXT	C21-C26-C27-C28
2	G	201	AXT	C25-C26-C27-C28
2	A	202	AXT	C25-C26-C27-C28
2	A	202	AXT	C31-C32-C33-C40
2	A	202	AXT	C31-C32-C33-C34
2	A	202	AXT	C27-C28-C29-C30
2	A	202	AXT	C27-C28-C29-C39

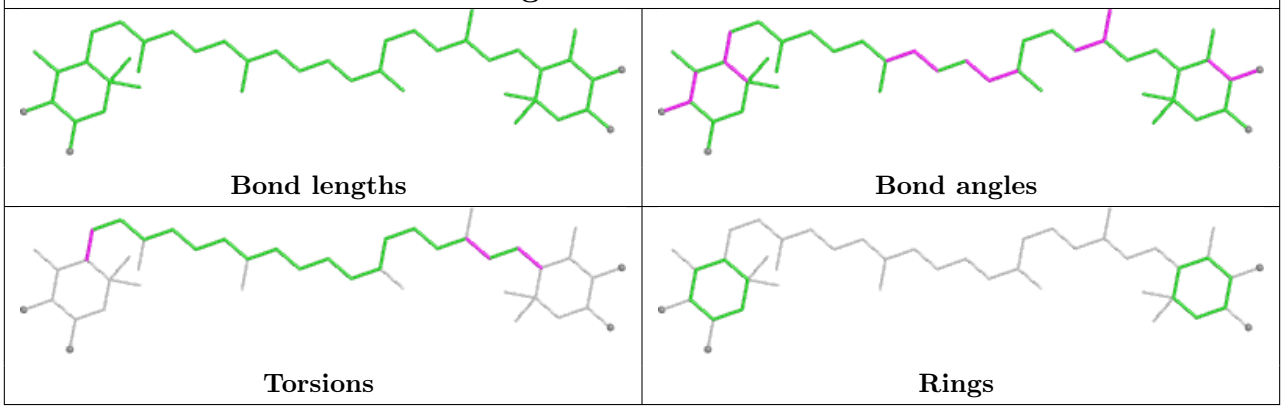
There are no ring outliers.

4 monomers are involved in 17 short contacts:

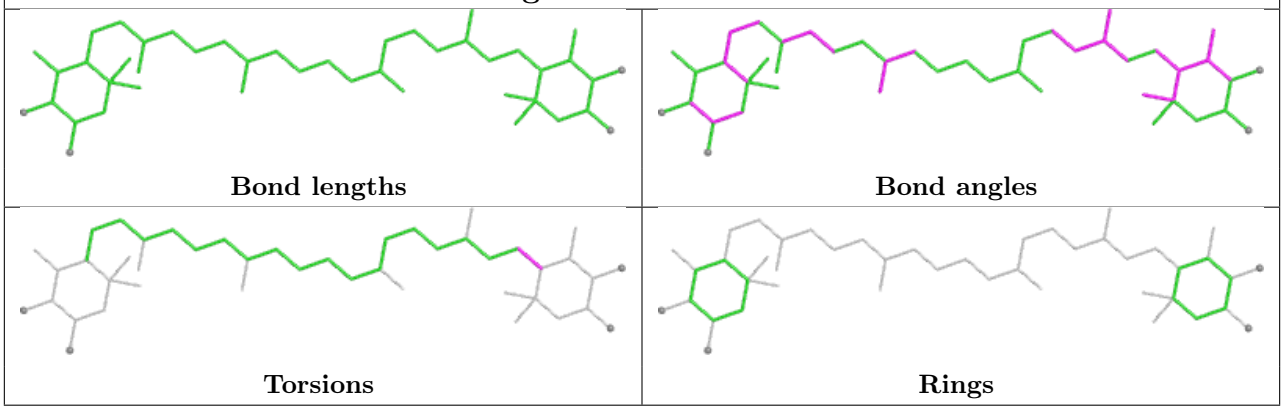
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	201	AXT	1	0
2	A	201	AXT	4	0
2	E	201	AXT	5	0
2	A	202	AXT	7	0

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.

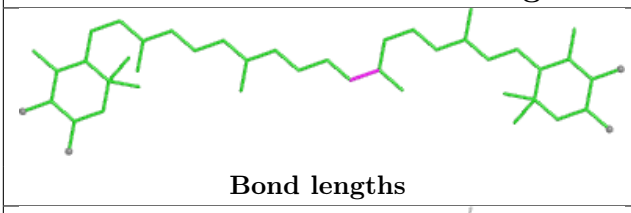
Ligand AXT G 201



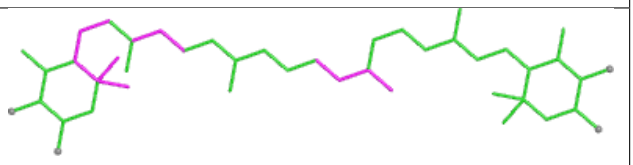
Ligand AXT A 201



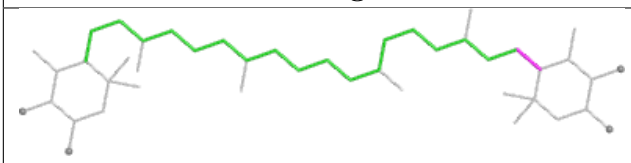
Ligand AXT E 201



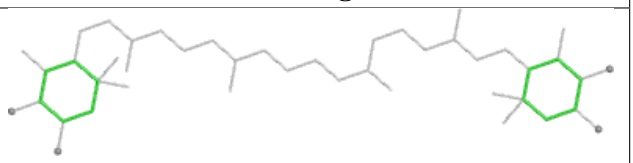
Bond lengths



Bond angles

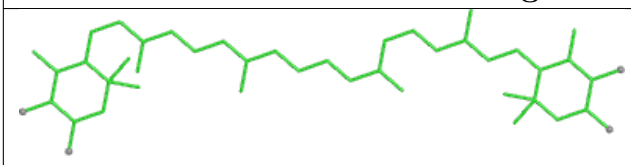


Torsions

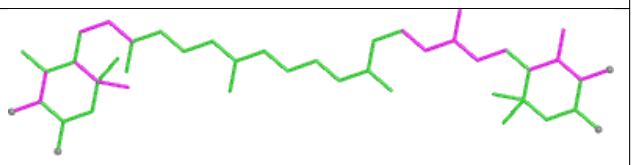


Rings

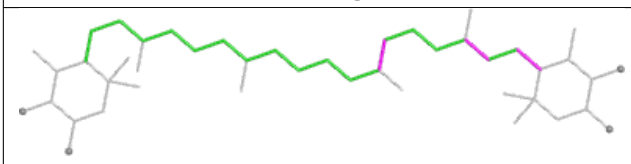
Ligand AXT A 202



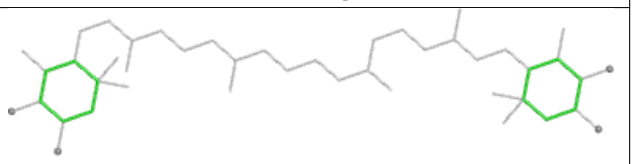
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	183/207 (88%)	-0.04	0	100	100	17, 33, 51, 72	0
1	C	183/207 (88%)	-0.19	0	100	100	14, 34, 49, 66	0
1	E	183/207 (88%)	-0.11	0	100	100	18, 33, 56, 79	0
1	G	183/207 (88%)	0.15	0	100	100	23, 42, 61, 66	0
All	All	732/828 (88%)	-0.05	0	100	100	14, 36, 57, 79	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands

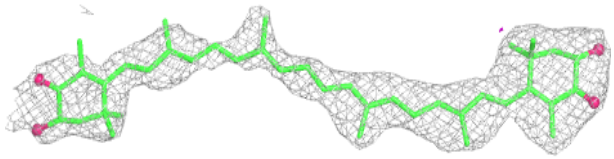
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

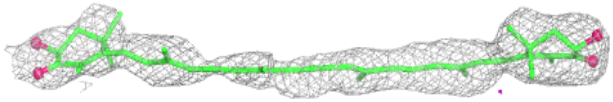
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AXT	E	201	44/44	0.92	0.12	13,31,48,53	0
2	AXT	G	201	44/44	0.92	0.11	25,32,39,44	0
2	AXT	A	201	44/44	0.93	0.11	13,24,34,37	0
2	AXT	A	202	44/44	0.94	0.09	16,24,29,34	0

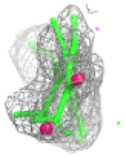
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AXT E 201:

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

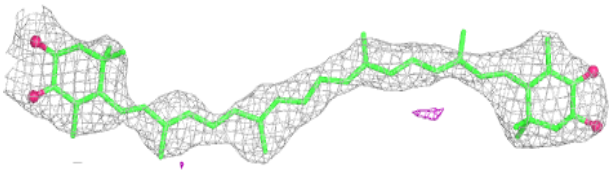


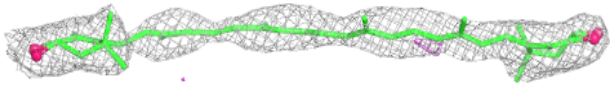


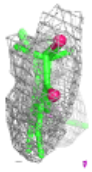


Electron density around AXT G 201:

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

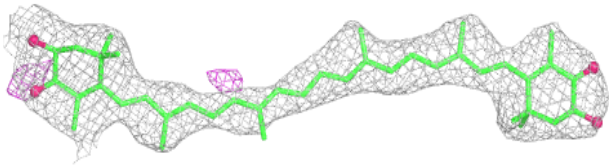


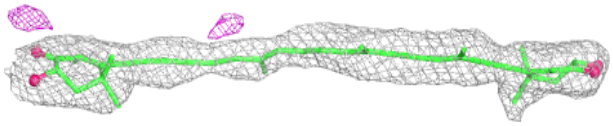




Electron density around AXT A 201:

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

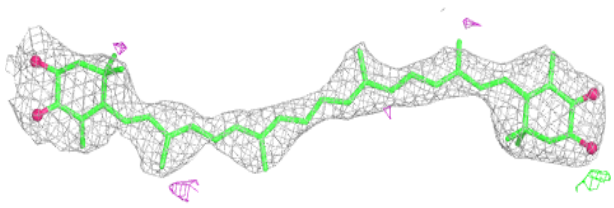


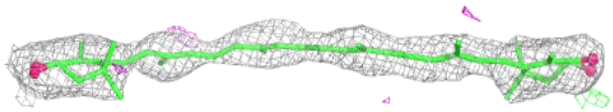


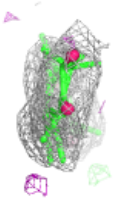


Electron density around AXT A 202:

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







6.5 Other polymers

There are no such residues in this entry.