



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:29 AM UTC

PDB ID : 4UUJ / pdb_00004uuJ
Title : POTASSIUM CHANNEL KCSA-FAB WITH TETRAHEXYLAMMONIUM
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Deposited on : 2014-07-29
Resolution : 2.40 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

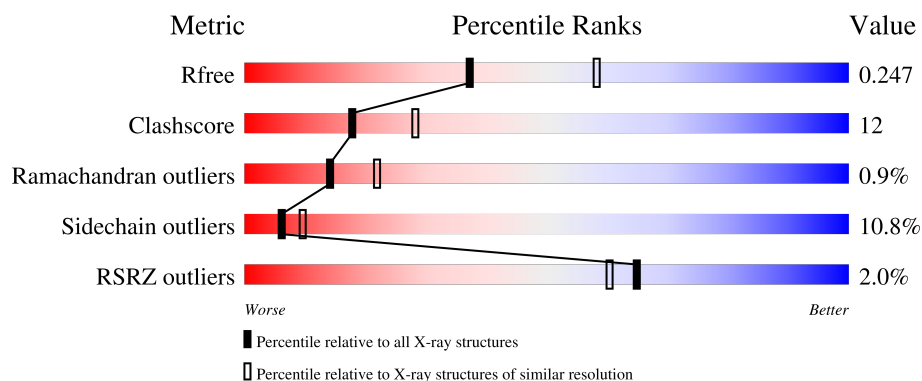
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	219	74% 22% .
2	B	212	2% 75% 21% .
3	C	111	4% 92% 8%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 4392 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 ANTIBODY FAB FRAGMENT LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1625	1030	271	318	6			

- Molecule 2 is a protein called ANTIBODY FAB FRAGMENT HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	4	0
			1682	1041	292	344	5			

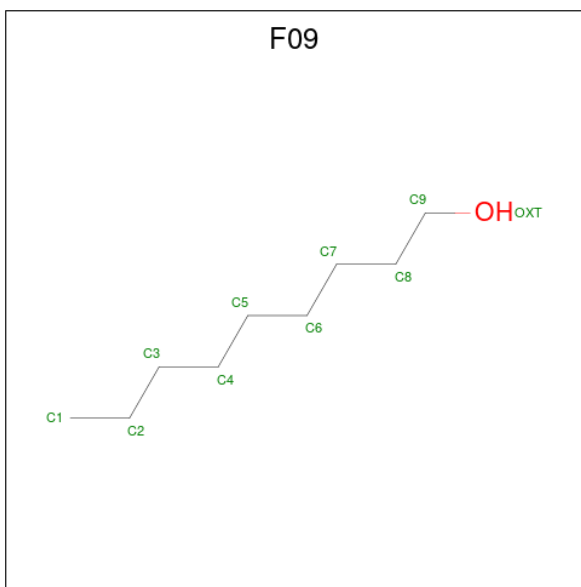
- Molecule 3 is a protein called VOLTAGE-GATED POTASSIUM CHANNEL KCSA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	111	Total	C	N	O	S	0	0	0
			820	538	140	140	2			

There are 9 discrepancies between the modelled and reference sequences:

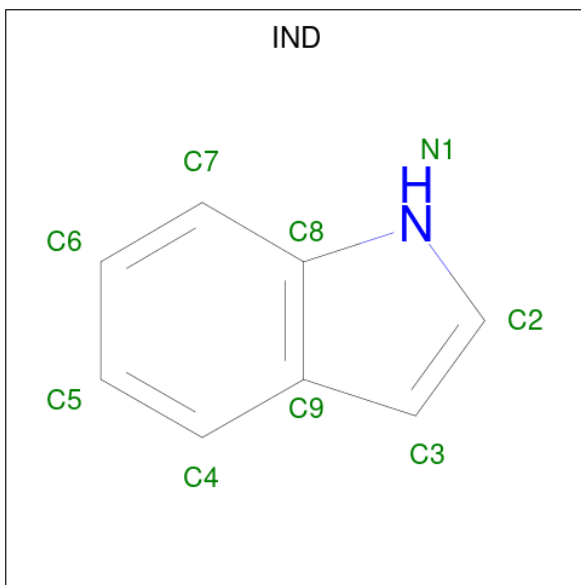
Chain	Residue	Modelled	Actual	Comment	Reference
C	11	ALA	-	expression tag	UNP P0A334
C	12	ALA	-	expression tag	UNP P0A334
C	13	VAL	-	expression tag	UNP P0A334
C	14	ALA	-	expression tag	UNP P0A334
C	15	LEU	-	expression tag	UNP P0A334
C	16	LEU	-	expression tag	UNP P0A334
C	17	LEU	-	expression tag	UNP P0A334
C	21	GLY	-	expression tag	UNP P0A334
C	90	CYS	LEU	conflict	UNP P0A334

- Molecule 4 is NONAN-1-OL (CCD ID: F09) (formula: C₉H₂₀O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 9 1	0	0
4	C	1	Total C 7 7	0	0
4	C	1	Total C 7 7	0	0
4	C	1	Total C 4 4	0	0

- Molecule 5 is INDOLE (CCD ID: IND) (formula: C_8H_7N).

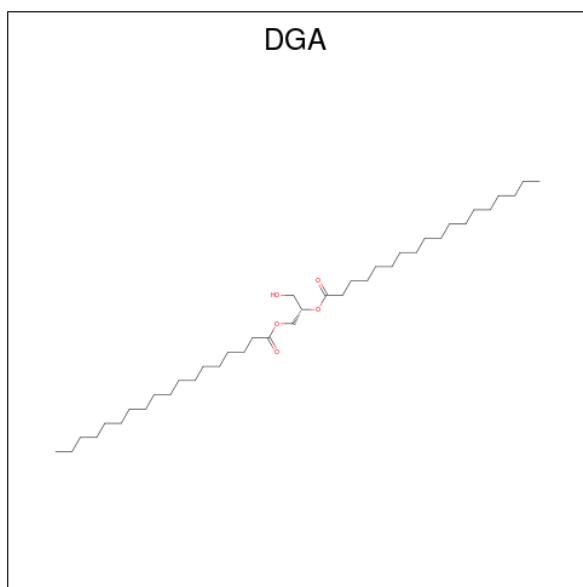


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	N	0	0
			9	8	1		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	4	Total	K		0	0
			4	4			

- Molecule 7 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C₃₉H₇₆O₅).

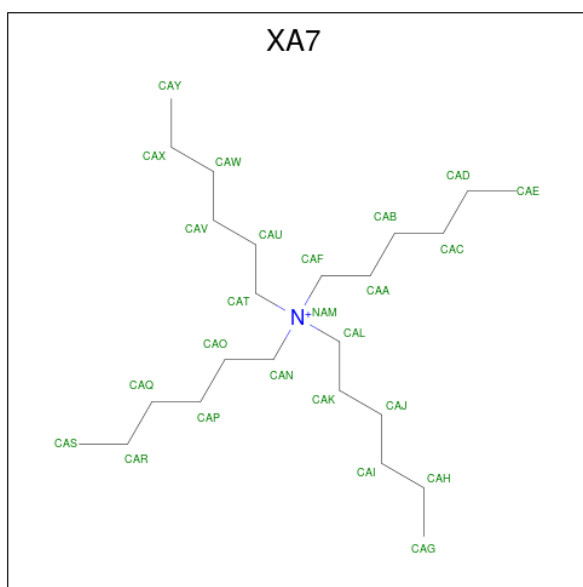


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			31	26	5		

- Molecule 8 is COBALT (II) ION (CCD ID: CO) (formula: Co).

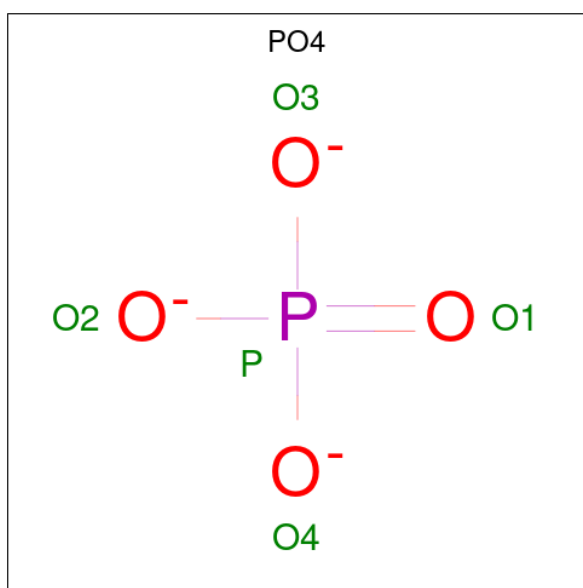
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	Co		0	0
			1	1			

- Molecule 9 is TETRAHEXYL AMMONNIUM (CCD ID: XA7) (formula: C₂₄H₅₂N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	N	0	1
			50	48	2		
9	C	1	Total	C	N	0	1
			50	48	2		

- Molecule 10 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	P	0	0
			5	4	1		

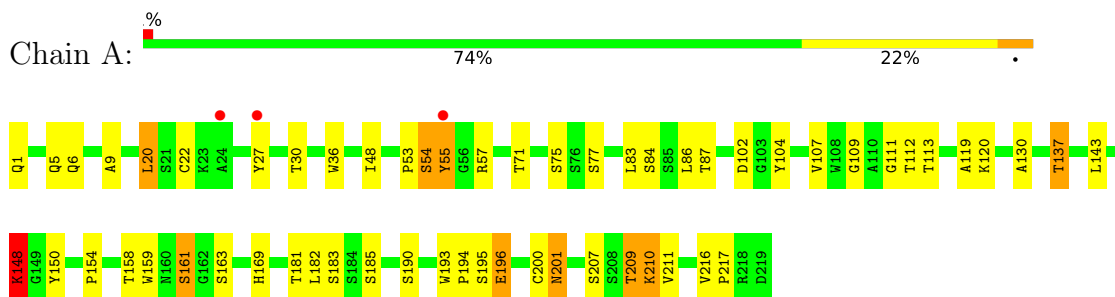
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	40	Total 40	O 40	0	0
11	B	35	Total 35	O 35	0	0
11	C	12	Total 12	O 12	0	0

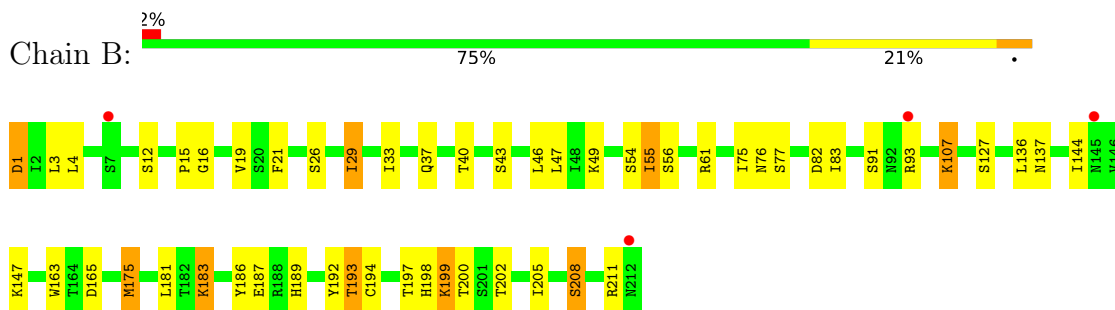
3 Residue-property plots [i](#)

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.

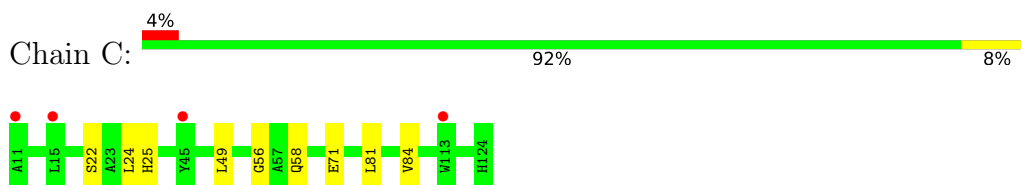
- Molecule 1: ANTIBODY FAB FRAGMENT LIGHT CHAIN



- Molecule 2: ANTIBODY FAB FRAGMENT HEAVY CHAIN



- Molecule 3: VOLTAGE-GATED POTASSIUM CHANNEL KCSA



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	154.62Å 154.62Å 75.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.64 – 2.40 28.64 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (28.64-2.40) 98.2 (28.64-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.191 , 0.248 0.197 , 0.247	Depositor DCC
R_{free} test set	1732 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	55.8	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.036 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4392	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XA7, IND, PO4, DGA, CO, F09, K

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	0.90	0/1669	1.03	7/2287 (0.3%)
2	B	0.95	1/1719 (0.1%)	1.00	5/2331 (0.2%)
3	C	1.12	0/839	1.15	2/1152 (0.2%)
All	All	0.97	1/4227 (0.0%)	1.04	14/5770 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	91	SER	CA-C	-5.20	1.46	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	43	SER	CA-C-N	-7.43	113.03	120.31
2	B	43	SER	C-N-CA	-7.43	113.03	120.31
3	C	84	VAL	CB-CA-C	-6.88	103.36	110.93
1	A	48	ILE	CB-CA-C	-6.50	104.07	111.55
1	A	169	HIS	CB-CA-C	-6.49	99.39	110.16
1	A	143	LEU	N-CA-C	-6.38	100.51	109.69
2	B	43	SER	N-CA-C	-6.29	102.76	110.31
1	A	148	LYS	N-CA-C	5.99	118.28	109.24
1	A	137	THR	N-CA-C	5.57	117.44	109.14
2	B	137	ASN	N-CA-C	5.48	117.83	108.90
1	A	130	ALA	N-CA-C	-5.36	103.38	110.40
1	A	9	ALA	N-CA-C	5.33	117.18	108.76
2	B	29	ILE	N-CA-C	5.14	120.03	109.34
3	C	22	SER	N-CA-C	5.01	117.63	109.86

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	1625	0	1563	26	0
2	B	1682	0	1606	33	0
3	C	820	0	837	10	0
4	A	10	0	19	0	0
4	C	18	0	33	2	0
5	B	9	0	7	0	0
6	C	4	0	0	0	0
7	C	31	0	44	0	0
8	C	1	0	0	0	0
9	C	100	0	208	40	0
10	C	5	0	0	0	0
11	A	40	0	0	2	0
11	B	35	0	0	3	0
11	C	12	0	0	3	0
All	All	4392	0	4317	104	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 12.

All (104) 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)
9:C:1131[B]:XA7:CAP	9:C:1131[B]:XA7:HAT1	1.78	1.12
9:C:1131[A]:XA7:CAP	9:C:1131[A]:XA7:HAT1	1.86	1.05
9:C:1131[A]:XA7:HAO2	9:C:1131[A]:XA7:HAU2	1.41	1.02
9:C:1131[A]:XA7:HAA1	9:C:1131[A]:XA7:HAP1	1.46	0.96
9:C:1131[B]:XA7:HAT1	9:C:1131[B]:XA7:HAP1	1.46	0.96
9:C:1131[B]:XA7:HAP1	9:C:1131[B]:XA7:HAA1	1.47	0.93
9:C:1131[B]:XA7:HAO2	9:C:1131[B]:XA7:HAU2	1.52	0.90
9:C:1131[A]:XA7:HAO2	9:C:1131[A]:XA7:CAU	1.98	0.88
9:C:1131[A]:XA7:HAT1	9:C:1131[A]:XA7:HAP1	1.53	0.88
4:C:1134:F09:H11	4:C:1135:F09:C7	2.06	0.85
2:B:189:HIS:O	2:B:211:ARG:NH2	2.12	0.82
9:C:1131[B]:XA7:HAT1	9:C:1131[B]:XA7:CAQ	2.11	0.79
9:C:1131[B]:XA7:HAO2	9:C:1131[B]:XA7:CAU	2.06	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:1131[B]:XA7:CAP	9:C:1131[B]:XA7:CAT	2.61	0.78
9:C:1131[A]:XA7:HAT1	9:C:1131[A]:XA7:CAQ	2.18	0.73
1:A:6:GLN:HE21	1:A:109:GLY:HA3	1.56	0.71
9:C:1131[A]:XA7:CAP	9:C:1131[A]:XA7:CAT	2.67	0.71
9:C:1131[B]:XA7:CAP	9:C:1131[B]:XA7:HAA1	2.19	0.71
9:C:1131[B]:XA7:HAT1	9:C:1131[B]:XA7:HAQ2	1.73	0.69
2:B:93[A]:ARG:HG2	3:C:58:GLN:HG2	1.76	0.67
9:C:1131[A]:XA7:HAT1	9:C:1131[A]:XA7:HAQ2	1.77	0.66
9:C:1131[A]:XA7:HAJ2	9:C:1131[A]:XA7:HAT2	1.77	0.66
9:C:1131[A]:XA7:HAQ2	9:C:1131[A]:XA7:HAW2	1.77	0.66
1:A:20:LEU:N	1:A:20:LEU:HD23	2.11	0.65
2:B:183:LYS:O	2:B:187:GLU:HG2	1.98	0.63
9:C:1131[A]:XA7:CAP	9:C:1131[A]:XA7:HAA1	2.22	0.63
9:C:1131[B]:XA7:CAU	9:C:1131[B]:XA7:CAO	2.77	0.63
2:B:163:TRP:CD1	2:B:175:MET:HG3	2.34	0.63
9:C:1131[B]:XA7:HAQ2	9:C:1131[B]:XA7:HAW2	1.81	0.61
1:A:207:SER:OG	1:A:209:THR:HG23	2.01	0.61
1:A:30:THR:O	1:A:54:SER:OG	2.16	0.59
4:C:1134:F09:C1	4:C:1135:F09:C7	2.78	0.58
2:B:93[B]:ARG:CG	3:C:56:GLY:HA2	2.34	0.57
1:A:193:TRP:CD1	1:A:194:PRO:HA	2.40	0.57
2:B:93[B]:ARG:HG2	3:C:56:GLY:HA2	1.87	0.56
1:A:27:TYR:HA	11:A:2008:HOH:O	2.05	0.55
2:B:163:TRP:HE1	2:B:175:MET:HE2	1.71	0.55
9:C:1131[A]:XA7:HAP1	9:C:1131[A]:XA7:CAT	2.33	0.54
1:A:182:LEU:C	1:A:182:LEU:HD12	2.32	0.54
9:C:1131[B]:XA7:HAJ2	9:C:1131[B]:XA7:HAT2	1.89	0.54
2:B:198:HIS:O	2:B:200:THR:N	2.41	0.54
2:B:15:PRO:HD3	2:B:107:LYS:O	2.07	0.54
2:B:46:LEU:HD23	2:B:55:ILE:HD12	1.89	0.53
1:A:150:TYR:OH	1:A:182:LEU:HD23	2.09	0.53
3:C:58:GLN:HB2	11:C:2003:HOH:O	2.10	0.51
2:B:163:TRP:NE1	2:B:175:MET:HE2	2.25	0.51
9:C:1131[B]:XA7:HAP1	9:C:1131[B]:XA7:CAT	2.25	0.50
2:B:93[A]:ARG:NH1	3:C:58:GLN:NE2	2.60	0.50
9:C:1131[A]:XA7:CAT	9:C:1131[A]:XA7:HAJ2	2.42	0.50
2:B:46:LEU:CD2	2:B:55:ILE:HD12	2.42	0.50
2:B:61:ARG:NH1	2:B:82:ASP:OD2	2.45	0.49
2:B:193:THR:HG22	2:B:208:SER:HB3	1.93	0.49
2:B:144:ILE:HG23	2:B:175:MET:HE3	1.95	0.49
2:B:93[A]:ARG:NH2	11:B:2027:HOH:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:1131[B]:XA7:HAJ2	9:C:1131[B]:XA7:HAV1	1.95	0.48
1:A:20:LEU:HD13	1:A:112:THR:HG21	1.94	0.48
2:B:16:GLY:O	2:B:77:SER:HA	2.14	0.48
1:A:20:LEU:N	1:A:20:LEU:CD2	2.77	0.48
2:B:21:PHE:HB3	11:B:2006:HOH:O	2.13	0.47
9:C:1131[B]:XA7:HAP1	9:C:1131[B]:XA7:CAA	2.32	0.47
9:C:1131[B]:XA7:HAK1	9:C:1131[B]:XA7:HAF1	1.47	0.47
1:A:53:PRO:O	1:A:55:TYR:N	2.43	0.47
1:A:83:LEU:HB3	1:A:86:LEU:HD21	1.96	0.47
2:B:93[A]:ARG:CG	3:C:58:GLN:HG2	2.44	0.47
9:C:1131[A]:XA7:HAG1	9:C:1131[A]:XA7:CAD	2.45	0.47
1:A:216:VAL:HG23	1:A:217:PRO:O	2.16	0.46
2:B:144:ILE:CG2	2:B:175:MET:HE3	2.45	0.46
9:C:1131[B]:XA7:HAU1	9:C:1131[B]:XA7:HAL2	1.46	0.46
1:A:159:TRP:CZ3	1:A:200:CYS:HB3	2.51	0.46
9:C:1131[A]:XA7:HAL2	9:C:1131[A]:XA7:HAU1	1.45	0.46
1:A:195:SER:OG	1:A:196:GLU:N	2.49	0.46
3:C:24:LEU:O	3:C:25:HIS:C	2.59	0.46
1:A:6:GLN:NE2	1:A:109:GLY:HA3	2.27	0.45
9:C:1131[A]:XA7:HAG1	9:C:1131[A]:XA7:HAE1	1.98	0.45
1:A:104:TYR:CE2	2:B:49:LYS:HD2	2.52	0.45
1:A:161:SER:HA	11:A:2037:HOH:O	2.17	0.45
1:A:161:SER:N	1:A:201:ASN:OD1	2.45	0.44
2:B:19:VAL:HG12	2:B:75:ILE:HB	2.00	0.44
1:A:6:GLN:NE2	1:A:111:GLY:H	2.15	0.44
1:A:148:LYS:HB3	1:A:181:THR:HG23	2.00	0.44
9:C:1131[A]:XA7:HAJ2	9:C:1131[A]:XA7:HAV1	1.99	0.44
1:A:22:CYS:HB2	1:A:36:TRP:CH2	2.53	0.43
2:B:1[A]:ASP:HA	11:B:2002:HOH:O	2.18	0.43
2:B:3:LEU:HB3	2:B:26:SER:HB3	2.01	0.43
2:B:46:LEU:CD2	2:B:55:ILE:CD1	2.96	0.43
1:A:182:LEU:HD12	1:A:183:SER:N	2.34	0.43
1:A:1:GLN:OE1	1:A:1:GLN:N	2.48	0.43
3:C:71:GLU:OE2	11:C:2007:HOH:O	2.21	0.42
2:B:186:TYR:HD1	2:B:192:TYR:HH	1.66	0.42
3:C:81:LEU:HB2	11:C:2007:HOH:O	2.18	0.42
1:A:113:THR:HB	1:A:154:PRO:HD3	2.02	0.42
9:C:1131[A]:XA7:HAF1	9:C:1131[A]:XA7:HAK1	1.51	0.42
2:B:187:GLU:O	2:B:211:ARG:NH2	2.53	0.42
2:B:37:GLN:HB2	2:B:47:LEU:HD11	2.01	0.42
9:C:1131[B]:XA7:HAF2	9:C:1131[B]:XA7:HAH2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93[B]:ARG:CD	3:C:56:GLY:HA2	2.50	0.41
2:B:16:GLY:C	2:B:77:SER:HA	2.45	0.41
2:B:61:ARG:HH12	2:B:82:ASP:CG	2.28	0.41
9:C:1131[B]:XA7:CAT	9:C:1131[B]:XA7:HAJ2	2.51	0.41
9:C:1131[B]:XA7:CAT	9:C:1131[B]:XA7:HAQ2	2.46	0.41
1:A:102:ASP:OD1	1:A:102:ASP:N	2.52	0.40
2:B:198:HIS:O	2:B:199:LYS:C	2.64	0.40
9:C:1131[A]:XA7:HAA2	9:C:1131[A]:XA7:HAN1	1.52	0.40
9:C:1131[A]:XA7:HAC1	9:C:1131[A]:XA7:HAS2	2.03	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	217/219 (99%)	206 (95%)	7 (3%)	4 (2%)	6	9
2	B	213/212 (100%)	202 (95%)	10 (5%)	1 (0%)	24	37
3	C	107/111 (96%)	105 (98%)	2 (2%)	0	100	100
All	All	537/542 (99%)	513 (96%)	19 (4%)	5 (1%)	14	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	199	LYS
1	A	55	TYR
1	A	54	SER
1	A	119	ALA
1	A	210	LYS

5.3.2 Protein sidechains ⓘ

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	176/185 (95%)	154 (88%)	22 (12%)	4	6
2	B	193/190 (102%)	167 (86%)	26 (14%)	4	5
3	C	78/79 (99%)	77 (99%)	1 (1%)	61	80
All	All	447/454 (98%)	398 (89%)	49 (11%)	6	9

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	20	LEU
1	A	57	ARG
1	A	71	THR
1	A	75	SER
1	A	77	SER
1	A	84	SER
1	A	87	THR
1	A	107	VAL
1	A	120	LYS
1	A	137	THR
1	A	148	LYS
1	A	158	THR
1	A	161	SER
1	A	163	SER
1	A	185	SER
1	A	190	SER
1	A	196	GLU
1	A	201	ASN
1	A	209	THR
1	A	210	LYS
1	A	211	VAL
2	B	1[A]	ASP
2	B	1[B]	ASP
2	B	4	LEU
2	B	12	SER

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Mol	Chain	Res	Type
2	B	29	ILE
2	B	33	ILE
2	B	40	THR
2	B	54	SER
2	B	55	ILE
2	B	56	SER
2	B	76	ASN
2	B	83	ILE
2	B	107	LYS
2	B	127	SER
2	B	136	LEU
2	B	147	LYS
2	B	165	ASP
2	B	175	MET
2	B	181	LEU
2	B	183	LYS
2	B	193	THR
2	B	194	CYS
2	B	197	THR
2	B	202	THR
2	B	205	ILE
2	B	208	SER
3	C	49	LEU

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	6	GLN
2	B	27	GLN
2	B	138	ASN
3	C	25	HIS
3	C	58	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 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
9	XA7	C	1132[A]	-	24,24,24	0.72	0	26,26,26	0.84	2 (7%)
7	DGA	C	1129	-	30,30,43	1.45	3 (10%)	32,32,45	1.80	8 (25%)
4	F09	C	1134	-	6,6,9	0.48	0	5,5,8	0.23	0
4	F09	A	1220	-	9,9,9	1.28	1 (11%)	8,8,8	0.69	0
4	F09	C	1135	-	6,6,9	0.39	0	5,5,8	0.26	0
9	XA7	C	1131[B]	-	24,24,24	0.86	1 (4%)	26,26,26	0.76	0
10	PO4	C	1133	-	4,4,4	0.72	0	6,6,6	1.21	1 (16%)
5	IND	B	1213	-	10,10,10	1.10	0	13,13,13	0.65	0
4	F09	C	1136	-	3,3,9	0.53	0	2,2,8	0.50	0
9	XA7	C	1131[A]	-	24,24,24	0.87	1 (4%)	26,26,26	0.77	0
9	XA7	C	1132[B]	-	24,24,24	0.72	0	26,26,26	0.78	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
9	XA7	C	1132[A]	-	-	10/28/28/28	-
7	DGA	C	1129	-	-	17/32/32/45	-
4	F09	C	1134	-	-	2/4/4/7	-
4	F09	A	1220	-	-	4/7/7/7	-
4	F09	C	1135	-	-	1/4/4/7	-
9	XA7	C	1131[B]	-	-	20/28/28/28	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IND	B	1213	-	-	-	0/2/2/2
4	F09	C	1136	-	-	0/1/1/7	-
9	XA7	C	1131[A]	-	-	20/28/28/28	-
9	XA7	C	1132[B]	-	-	16/28/28/28	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1129	DGA	OG1-CA1	4.89	1.47	1.33
7	C	1129	DGA	OG2-CB1	3.96	1.45	1.34
4	A	1220	F09	OXT-C9	-3.44	1.24	1.42
7	C	1129	DGA	CB5-CB4	-3.38	1.35	1.51
9	C	1131[A]	XA7	CAE-CAD	-2.50	1.32	1.50
9	C	1131[B]	XA7	CAE-CAD	-2.50	1.32	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1129	DGA	OG1-CA1-CA2	5.55	128.76	111.83
7	C	1129	DGA	OG2-CB1-CB2	4.07	120.28	111.48
7	C	1129	DGA	OG1-CA1-OA1	-3.22	115.58	123.63
7	C	1129	DGA	OG1-CG1-CG2	3.06	117.22	108.40
7	C	1129	DGA	OG2-CB1-OB1	-2.69	117.42	123.70
10	C	1133	PO4	O4-P-O3	2.61	116.04	107.91
7	C	1129	DGA	CG2-OG2-CB1	-2.44	111.95	117.80
9	C	1132[A]	XA7	CAK-CAL-NAM	-2.09	108.07	115.97
9	C	1132[A]	XA7	CAU-CAT-NAM	-2.08	108.09	115.97
7	C	1129	DGA	OA1-CA1-CA2	-2.08	115.66	123.78
7	C	1129	DGA	CB5-CB4-CB3	2.02	124.57	114.37

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1129	DGA	CB2-CB1-OG2-CG2
7	C	1129	DGA	OG1-CG1-CG2-OG2
7	C	1129	DGA	OG2-CG2-CG3-OXT
9	C	1131[A]	XA7	CAO-CAN-NAM-CAT
9	C	1131[B]	XA7	CAO-CAN-NAM-CAT
9	C	1131[A]	XA7	CAO-CAN-NAM-CAL
9	C	1131[B]	XA7	CAO-CAN-NAM-CAL

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Mol	Chain	Res	Type	Atoms
9	C	1131[B]	XA7	CAO-CAN-NAM-CAF
9	C	1131[A]	XA7	CAO-CAN-NAM-CAF
9	C	1131[B]	XA7	NAM-CAN-CAO-CAP
7	C	1129	DGA	OB1-CB1-OG2-CG2
7	C	1129	DGA	CB3-CB4-CB5-CB6
9	C	1131[A]	XA7	NAM-CAN-CAO-CAP
9	C	1131[B]	XA7	CAA-CAF-NAM-CAL
9	C	1131[B]	XA7	CAA-CAF-NAM-CAN
9	C	1131[A]	XA7	CAA-CAF-NAM-CAL
9	C	1131[A]	XA7	CAA-CAF-NAM-CAN
9	C	1131[A]	XA7	CAJ-CAK-CAL-NAM
9	C	1131[B]	XA7	CAK-CAL-NAM-CAN
9	C	1131[B]	XA7	CAA-CAF-NAM-CAT
9	C	1131[B]	XA7	CAJ-CAK-CAL-NAM
9	C	1131[A]	XA7	CAA-CAF-NAM-CAT
9	C	1131[B]	XA7	CAK-CAL-NAM-CAF
9	C	1131[A]	XA7	CAK-CAL-NAM-CAN
9	C	1131[B]	XA7	CAK-CAL-NAM-CAT
9	C	1132[B]	XA7	NAM-CAN-CAO-CAP
9	C	1132[A]	XA7	CAB-CAA-CAF-NAM
9	C	1132[B]	XA7	CAB-CAA-CAF-NAM
4	C	1134	F09	C2-C3-C4-C5
9	C	1132[A]	XA7	NAM-CAN-CAO-CAP
9	C	1131[A]	XA7	CAK-CAL-NAM-CAF
9	C	1131[A]	XA7	CAK-CAL-NAM-CAT
9	C	1131[B]	XA7	NAM-CAT-CAU-CAV
7	C	1129	DGA	CA2-CA3-CA4-CA5
9	C	1131[A]	XA7	NAM-CAT-CAU-CAV
9	C	1132[A]	XA7	CAH-CAI-CAJ-CAK
9	C	1132[A]	XA7	CAU-CAV-CAW-CAX
9	C	1131[A]	XA7	CAH-CAI-CAJ-CAK
7	C	1129	DGA	CB4-CB5-CB6-CB7
9	C	1132[A]	XA7	CAT-CAU-CAV-CAW
9	C	1132[A]	XA7	CAI-CAJ-CAK-CAL
9	C	1131[B]	XA7	CAH-CAI-CAJ-CAK
9	C	1132[B]	XA7	CAT-CAU-CAV-CAW
9	C	1131[A]	XA7	CAU-CAV-CAW-CAX
9	C	1131[B]	XA7	CAU-CAV-CAW-CAX
9	C	1132[B]	XA7	CAU-CAV-CAW-CAX
4	A	1220	F09	C4-C5-C6-C7
9	C	1132[B]	XA7	CAH-CAI-CAJ-CAK
9	C	1132[B]	XA7	CAI-CAJ-CAK-CAL

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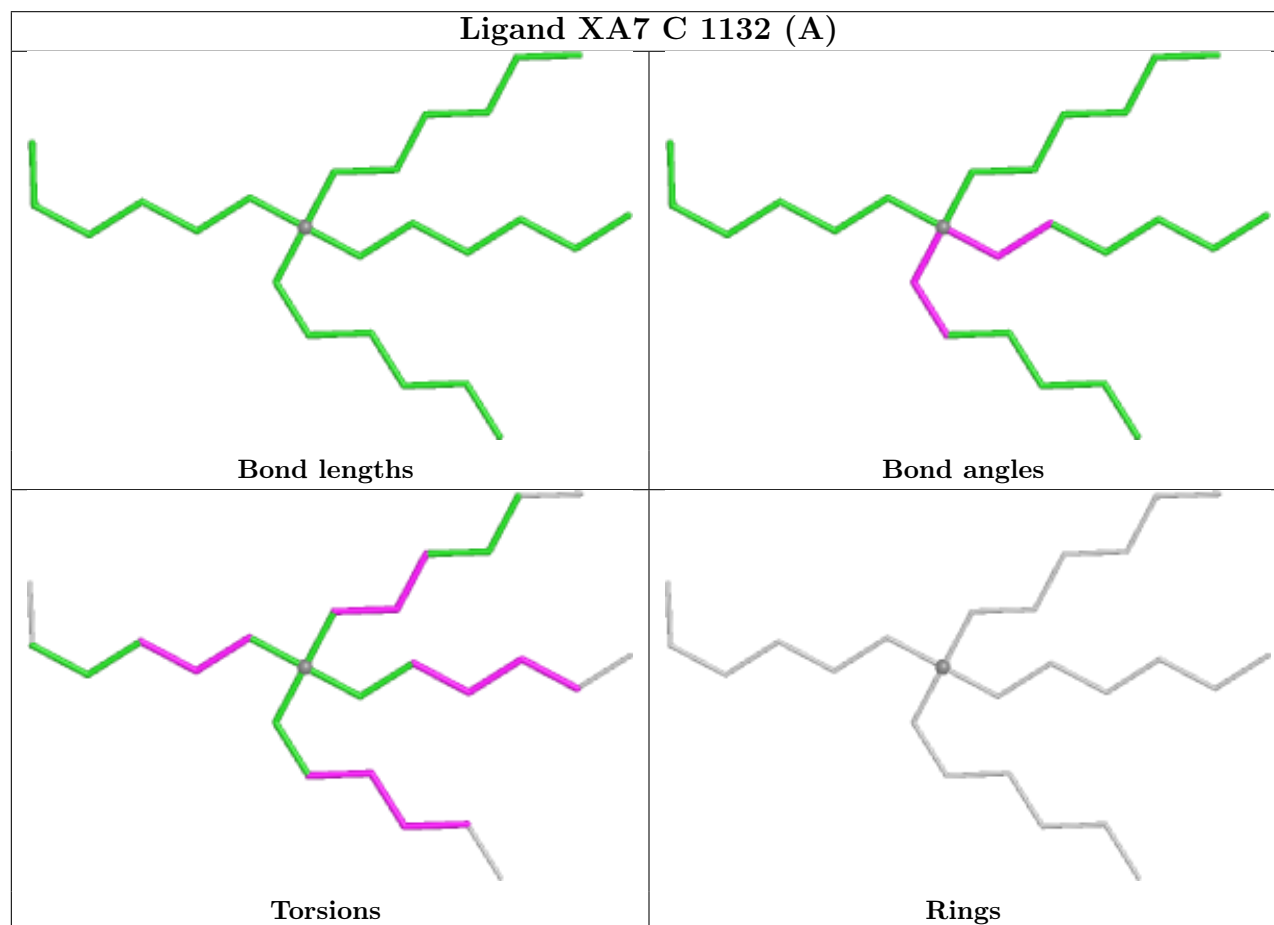
Mol	Chain	Res	Type	Atoms
9	C	1132[A]	XA7	CAN-CAO-CAP-CAQ
9	C	1132[A]	XA7	CAF-CAA-CAB-CAC
9	C	1131[A]	XA7	CAA-CAB-CAC-CAD
7	C	1129	DGA	CB1-CB2-CB3-CB4
7	C	1129	DGA	CA6-CA7-CA8-CA9
9	C	1131[B]	XA7	CAV-CAW-CAX-CAY
9	C	1131[A]	XA7	CAV-CAW-CAX-CAY
9	C	1132[B]	XA7	CAG-CAH-CAI-CAJ
9	C	1131[B]	XA7	CAA-CAB-CAC-CAD
9	C	1132[B]	XA7	CAA-CAF-NAM-CAL
9	C	1132[B]	XA7	CAV-CAW-CAX-CAY
9	C	1131[B]	XA7	CAN-CAO-CAP-CAQ
7	C	1129	DGA	OG1-CG1-CG2-CG3
7	C	1129	DGA	CG1-CG2-CG3-OXT
9	C	1131[A]	XA7	CAN-CAO-CAP-CAQ
9	C	1131[A]	XA7	CAF-CAA-CAB-CAC
4	C	1135	F09	C4-C5-C6-C7
9	C	1132[B]	XA7	CAA-CAF-NAM-CAN
4	C	1134	F09	C4-C5-C6-C7
9	C	1131[B]	XA7	CAF-CAA-CAB-CAC
9	C	1132[A]	XA7	CAV-CAW-CAX-CAY
7	C	1129	DGA	OG1-CA1-CA2-CA3
9	C	1132[A]	XA7	CAG-CAH-CAI-CAJ
9	C	1132[B]	XA7	CAA-CAF-NAM-CAT
9	C	1132[B]	XA7	CAF-CAA-CAB-CAC
9	C	1131[A]	XA7	CAG-CAH-CAI-CAJ
4	A	1220	F09	C7-C8-C9-OXT
9	C	1131[B]	XA7	CAG-CAH-CAI-CAJ
9	C	1132[B]	XA7	CAO-CAN-NAM-CAT
7	C	1129	DGA	CB6-CB7-CB8-CB9
4	A	1220	F09	C5-C6-C7-C8
7	C	1129	DGA	CB9-CAB-CBB-CCB
9	C	1131[A]	XA7	CAI-CAJ-CAK-CAL
9	C	1131[B]	XA7	CAI-CAJ-CAK-CAL
9	C	1132[B]	XA7	CAO-CAN-NAM-CAF
9	C	1132[B]	XA7	CAN-CAO-CAP-CAQ
9	C	1132[B]	XA7	CAO-CAN-NAM-CAL
7	C	1129	DGA	CBB-CCB-CDB-CEB
7	C	1129	DGA	OA1-CA1-CA2-CA3
4	A	1220	F09	C2-C3-C4-C5
7	C	1129	DGA	CB2-CB3-CB4-CB5

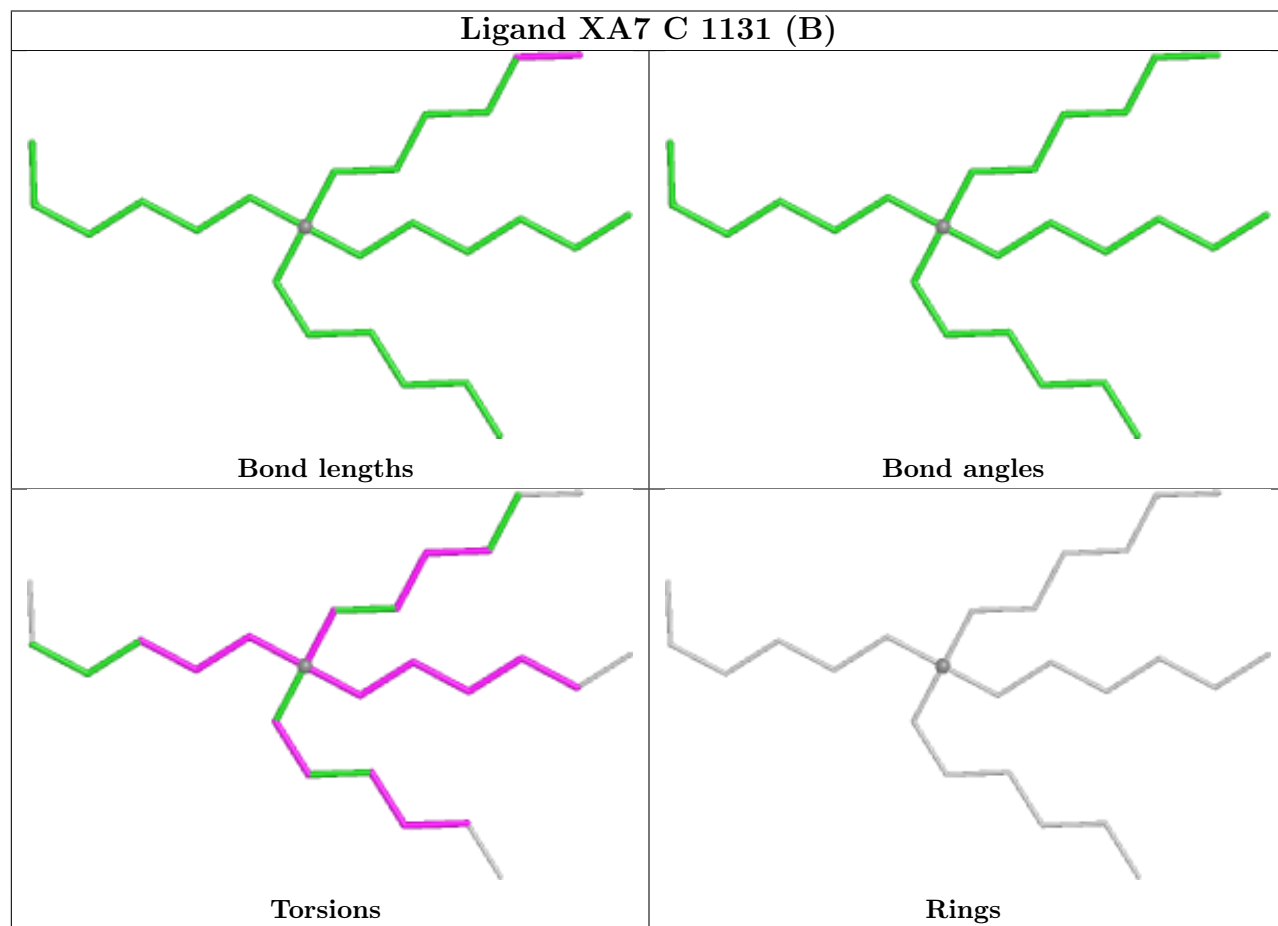
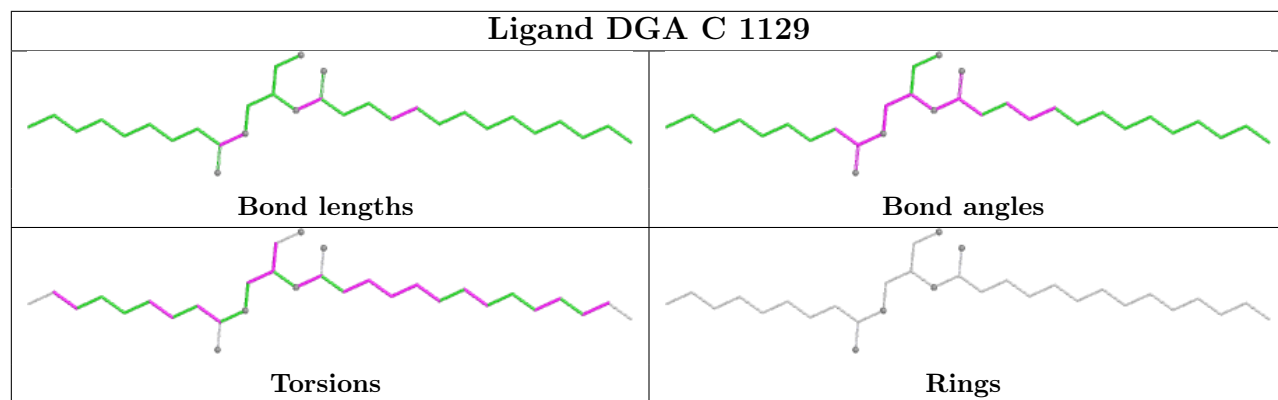
There are no ring outliers.

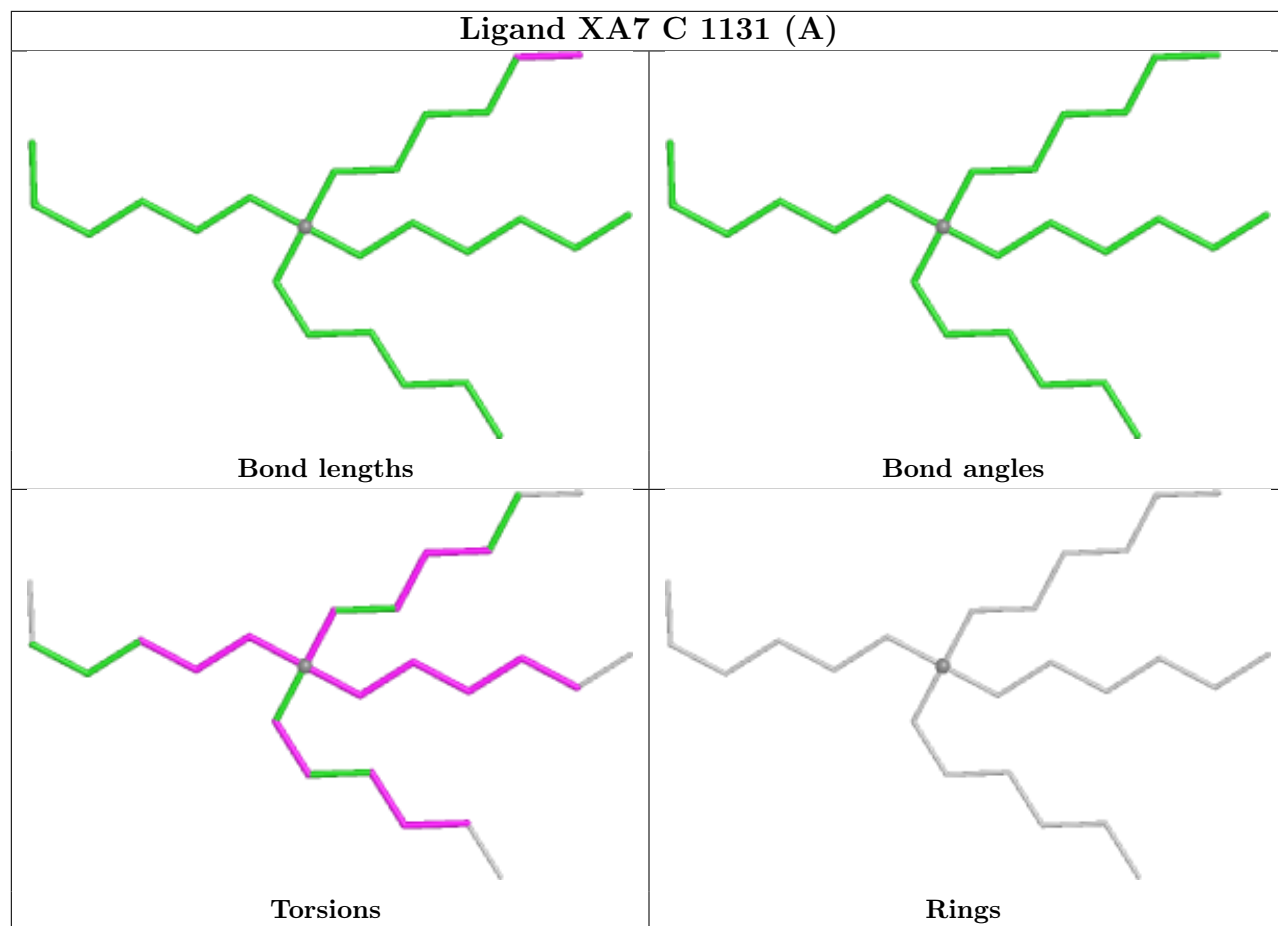
4 monomers are involved in 42 short contacts:

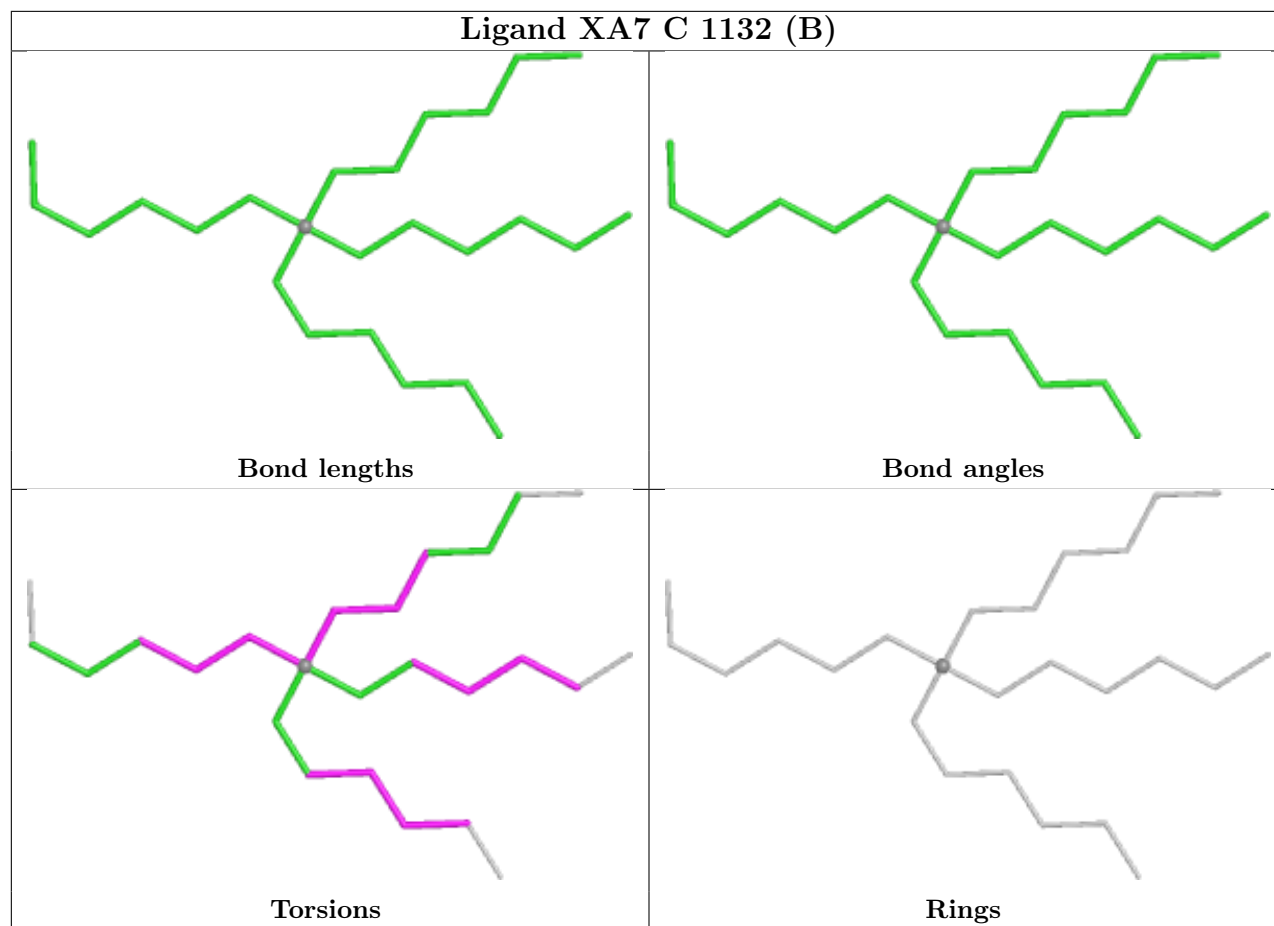
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1134	F09	2	0
4	C	1135	F09	2	0
9	C	1131[B]	XA7	20	0
9	C	1131[A]	XA7	20	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	17:LEU	C	21:GLY	N	7.82

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	219/219 (100%)	0.13	3 (1%) 73 69	45, 81, 111, 128	0
2	B	212/212 (100%)	-0.06	4 (1%) 66 62	23, 74, 113, 158	4 (1%)
3	C	111/111 (100%)	-0.14	4 (3%) 46 42	36, 51, 104, 124	0
All	All	542/542 (100%)	0.00	11 (2%) 65 60	23, 73, 111, 158	4 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	11	ALA	3.3
2	B	7[A]	SER	3.2
3	C	45	TYR	3.1
2	B	212	ASN	3.0
1	A	55	TYR	2.9
3	C	15	LEU	2.9
1	A	27	TYR	2.8
2	B	145	ASN	2.4
1	A	24	ALA	2.3
3	C	113	TRP	2.2
2	B	93[A]	ARG	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 ⓘ

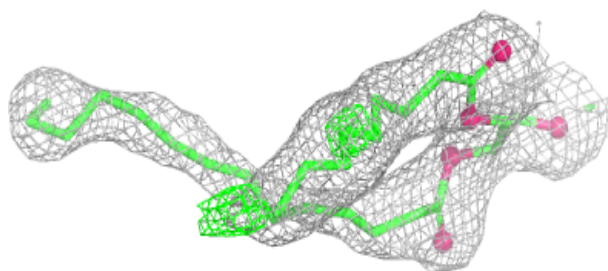
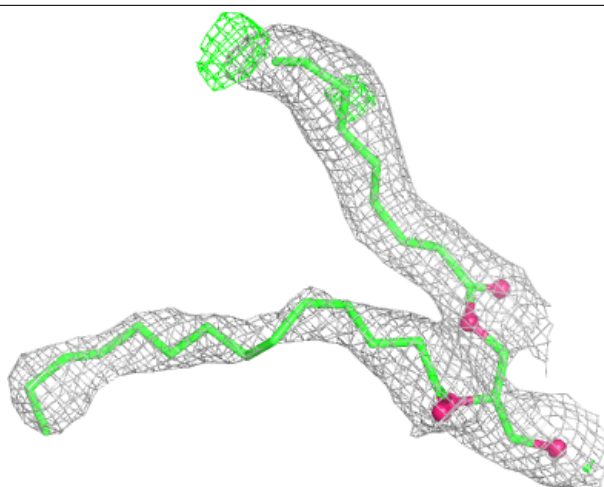
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	IND	B	1213	9/9	0.71	0.22	100,112,124,127	0
4	F09	C	1136	4/10	0.85	0.33	72,74,74,79	0
4	F09	C	1135	7/10	0.88	0.25	83,101,118,125	0
7	DGA	C	1129	31/44	0.90	0.15	51,90,98,104	0
4	F09	A	1220	10/10	0.91	0.16	70,79,84,86	0
10	PO4	C	1133	5/5	0.93	0.08	69,70,102,114	0
4	F09	C	1134	7/10	0.95	0.14	62,66,77,86	0
9	XA7	C	1132[B]	25/25	0.96	0.18	36,36,37,37	25
9	XA7	C	1132[A]	25/25	0.96	0.18	11,11,12,12	25
9	XA7	C	1131[B]	25/25	0.97	0.19	92,96,99,100	25
9	XA7	C	1131[A]	25/25	0.97	0.19	73,77,82,83	25
6	K	C	1125	1/1	0.98	0.04	39,39,39,39	1
6	K	C	1126	1/1	0.99	0.04	35,35,35,35	1
6	K	C	1127	1/1	0.99	0.05	36,36,36,36	1
6	K	C	1128	1/1	0.99	0.03	44,44,44,44	1
8	CO	C	1130	1/1	1.00	0.04	51,51,51,51	1

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.

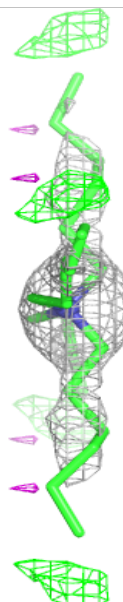
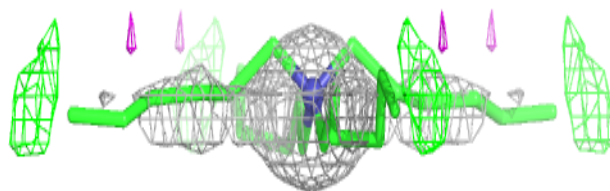
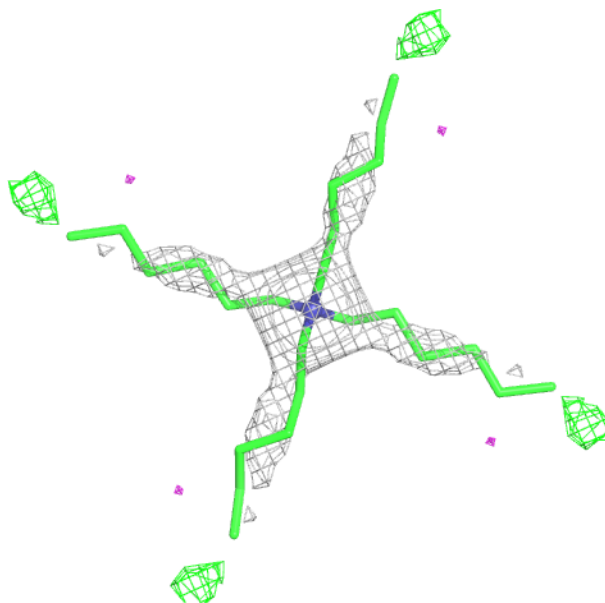
Electron density around DGA C 1129:

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



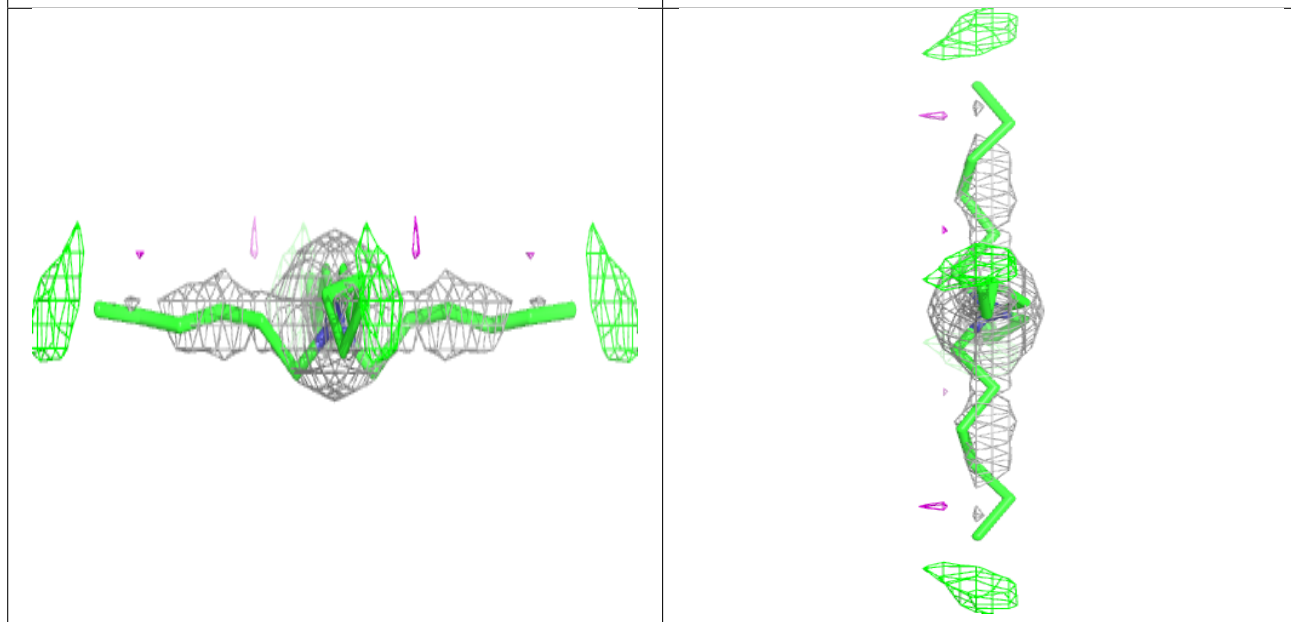
Electron density around XA7 C 1132 (B):

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



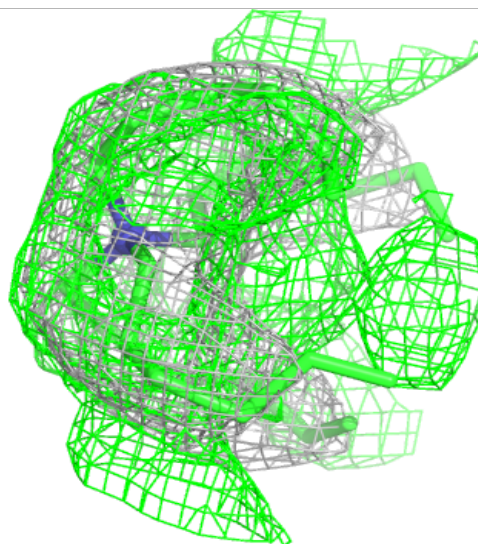
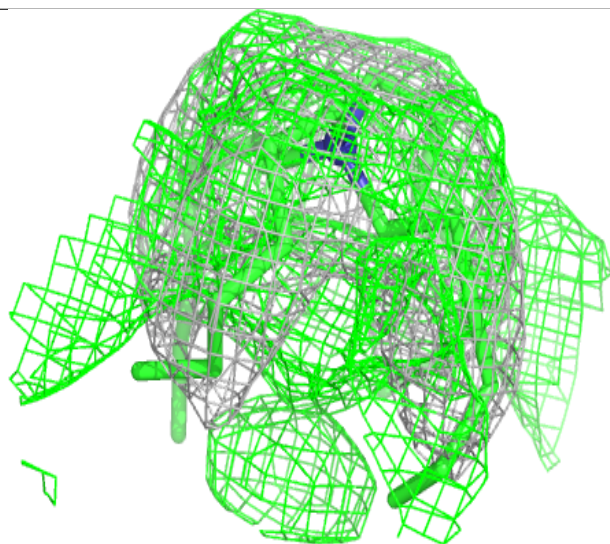
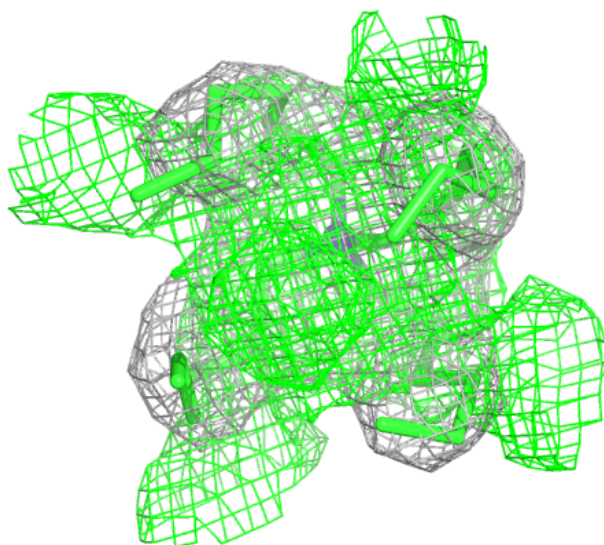
Electron density around XA7 C 1132 (A):

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



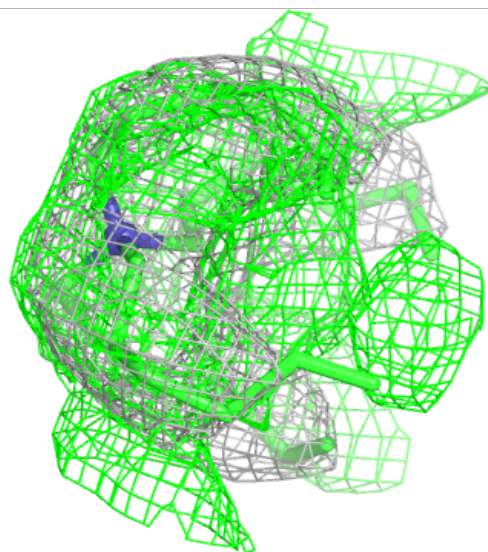
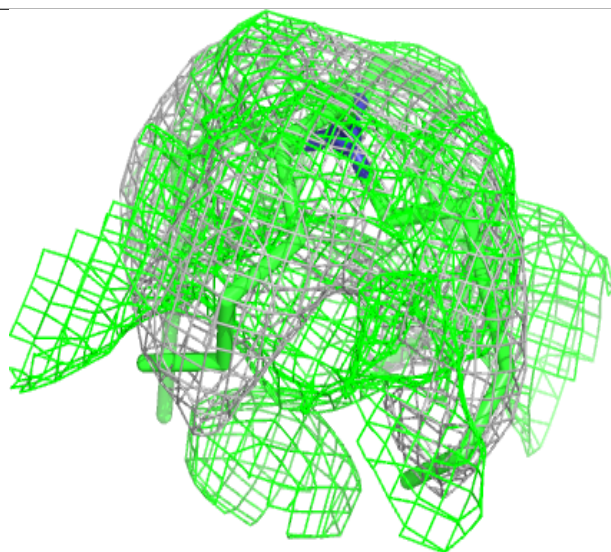
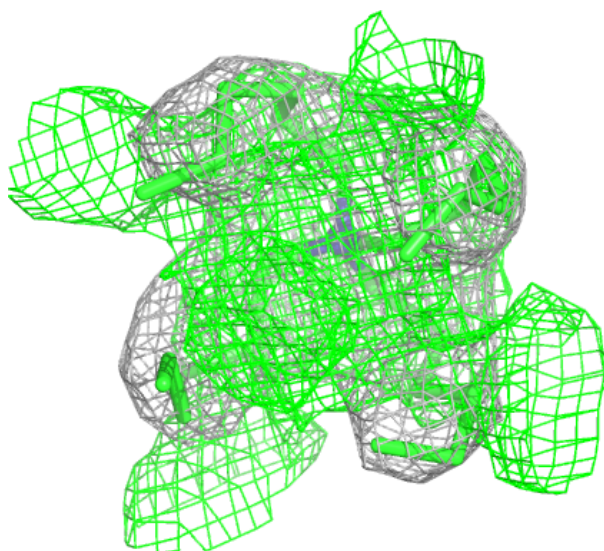
Electron density around XA7 C 1131 (B):

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



Electron density around XA7 C 1131 (A):

$2mF_o-DF_c$ (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.