wwPDB X-ray Structure Validation Summary Report (i)

Nov 15, 2022 – 03:20 pm GMT

PDB ID	:	7QTV
Title	:	Beryllium fluoride form of the Na+,K+-ATPase (E2-BeFx)
Authors	:	Fruergaard, M.U.; Dach, I.; Andersen, J.L.; Ozol, M.; Shahsavar, A.; Quistgaard, E.M.; Poulsen, H.; Fedosova, N.U.; Nissen, P.
Deposited on	:	2022-01-16
Resolution	:	4.05 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

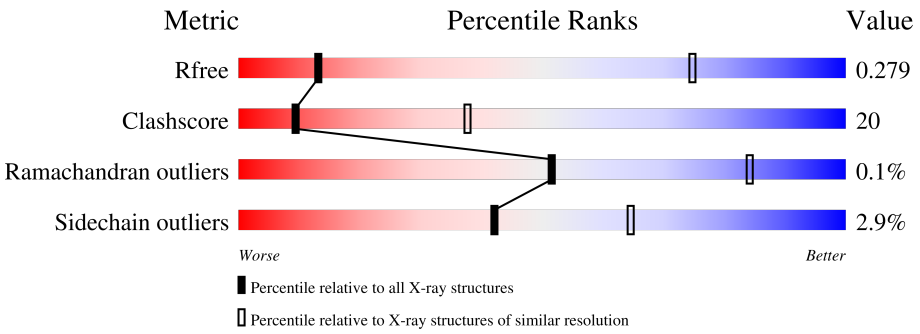
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1127 (4.42-3.70)
Clashscore	141614	1033 (4.40-3.72)
Ramachandran outliers	138981	1145 (4.42-3.70)
Sidechain outliers	138945	1133 (4.42-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	1021	63% 33% • •
1	C	1021	61% 36% • •
2	B	303	50% 44% • •
2	D	303	59% 36% • •
3	E	65	37% 11% • 51%
3	G	65	37% 12% 51%
4	F	2	50% 50%

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
5	BEF	C	1101	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 21017 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 Sodium/potassium-transporting ATPase subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	996	7726	4922	1301	1456	47	0	0	0
1	C	996	7726	4922	1301	1456	47	0	0	0

- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	291	2386	1546	390	437	13	0	0	0
2	D	291	2386	1546	390	437	13	0	0	0

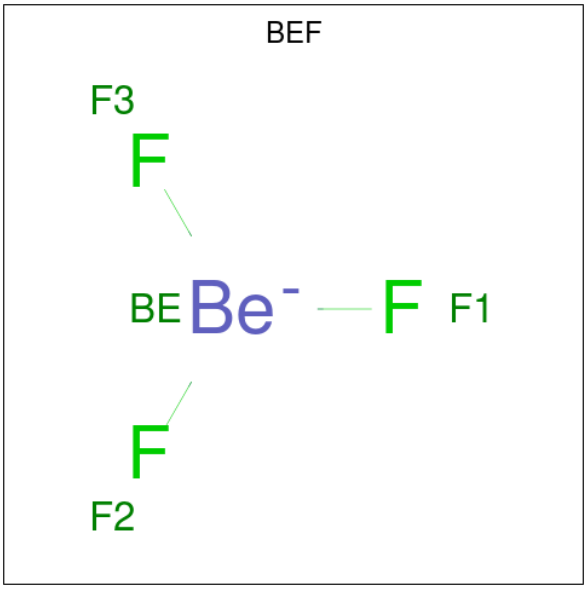
- Molecule 3 is a protein called FXYD domain-containing ion transport regulator.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	G	32	255	174	37	44	0	0	0
3	E	32	255	174	37	44	0	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

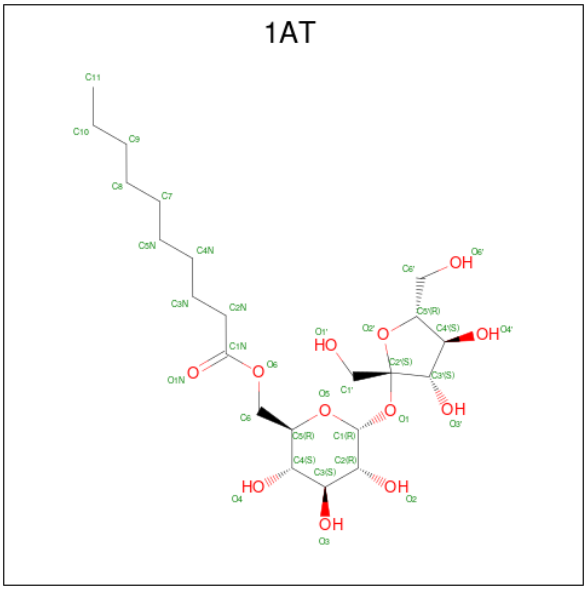
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	2	30	16	2	12	0	0	0

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



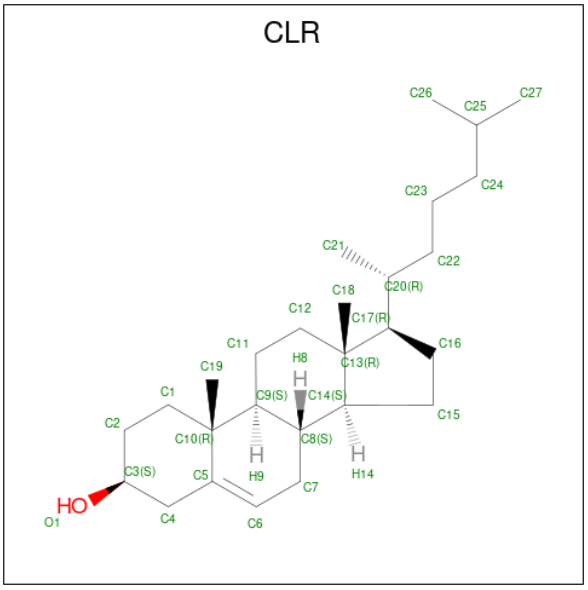
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Be	F		
5	A	1	4	1	3	0	0
			Total	Be	F		
5	C	1	4	1	3	0	0

- Molecule 6 is beta-D-fructofuranosyl 6-O-decanoyl-alpha-D-glucopyranoside (three-letter code: 1AT) (formula: $C_{22}H_{40}O_{12}$).



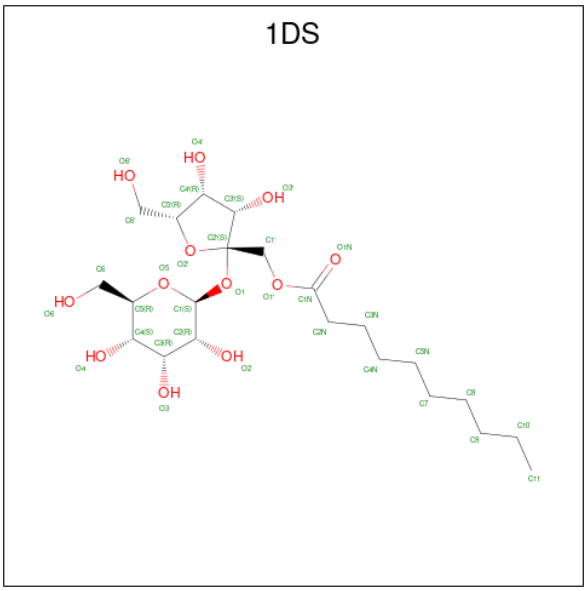
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	29	17	12	0	0

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	28	27	1	0	0
7	G	1	28	27	1	0	0
7	C	1	28	27	1	0	0
7	E	1	28	27	1	0	0

- Molecule 8 is 1-O-decanoyl-beta-D-tagatofuranosyl beta-D-allopyranoside (three-letter code: 1DS) (formula: $C_{22}H_{40}O_{12}$).

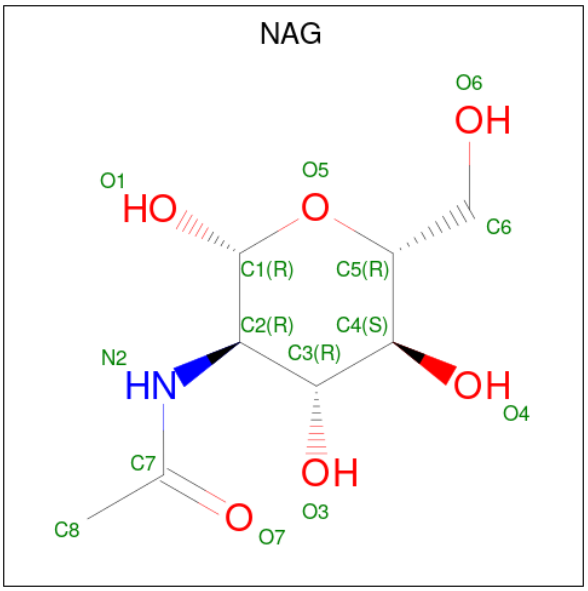


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	29	17	12	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
9	A	3	3	3	0	0
9	C	3	3	3	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	B	1	15	8	1	6	0	0
			Total	C	N	O		
10	B	1	15	8	1	6	0	0
			Total	C	N	O		
10	D	1	15	8	1	6	0	0
			Total	C	N	O		
10	D	1	15	8	1	6	0	0

- Molecule 11 is water.

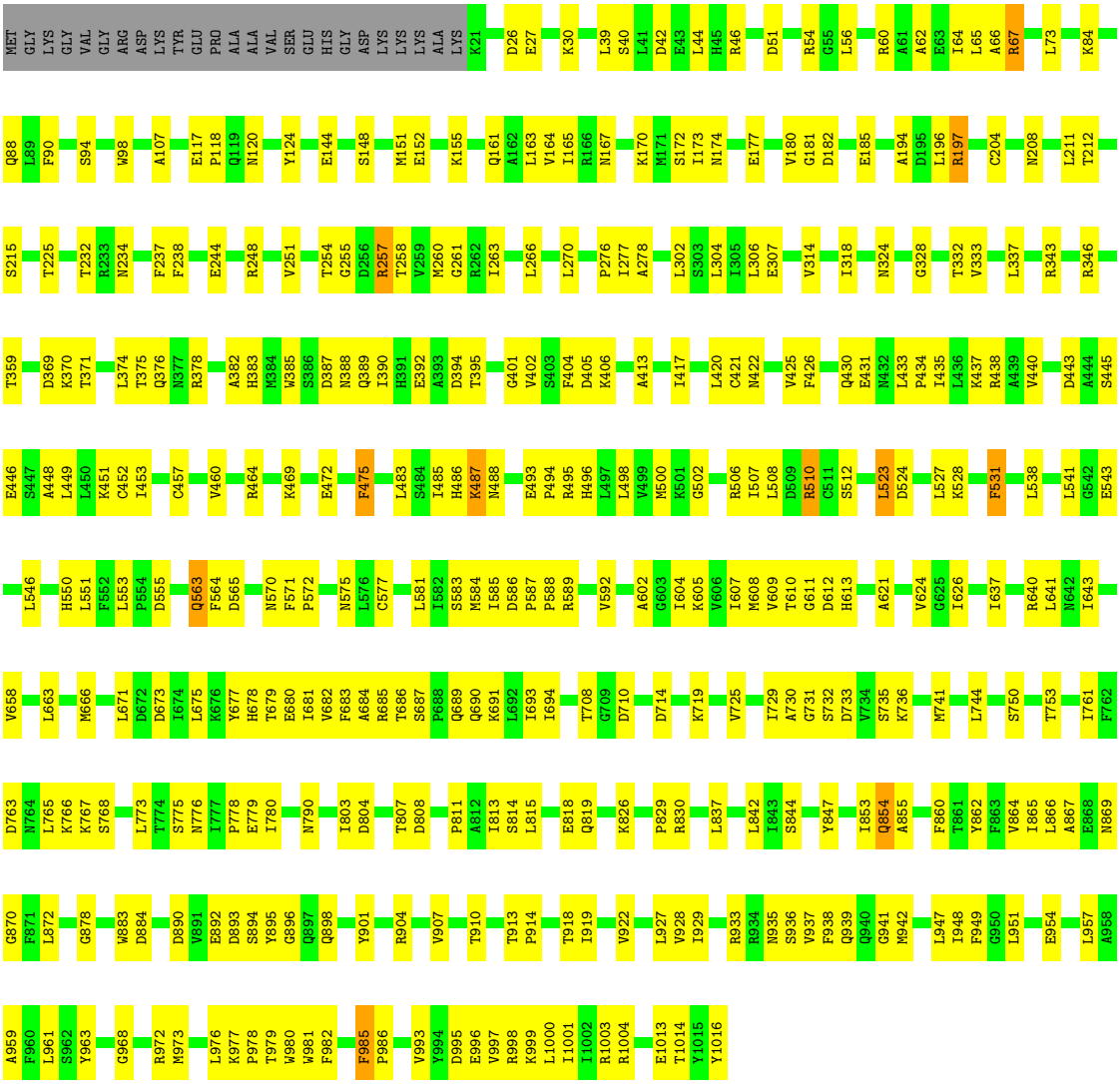
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	5	5	5	0	0
			Total	O		
11	C	4	4	4	0	0

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. 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: Sodium/potassium-transporting ATPase subunit alpha-1

Chain A: 63% 33% ••



- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

Chain C: 61% 36% ••

MET GLY LYS GLY VAL GLY ARG ASP LYS TYR GLU PRO ALA ALA VAL SER GLU HIS GLY ASP LYS LYS LYS ALA LYS K21 E22 M25 D26 D35 L39 D42 E43 L44 K47 Y48 L56 T57 P58 A59 R60 A61 A62 E63 R67 D68 N71 T74 E81

M95 L96 I99 A112 E117 P118 Q119 Y124 L129 S130 A131 I134 C138 S147 I150 M151 E152 K155 I173 N174 A175 E176 E177 V180 G181 E185 V186 K187 G188 G189 D190 R191 I192 L196 R197 I198 I199 S200 A201 C204 K205 V206 D207 N208

T219 R220 S221 P222 D223 F224 N228 P229 L230 E231 T232 R233 N234 I235 F238 S239 T240 N241 C242 V243 E244 R248 G249 I250 V251 G255 D256 R257 T258 V259 M260 G261 R262 I263 A264 T265 L266 L270 I277 A278 A279 E280 I281 E282 H283 P284 I285 H286 I287 I288 A292 L302

I305 A313 F316 L317 I318 V322 A323 N324 E327 G328 T332 C336 R343 R346 K347 N348 C349 L350 E355 L360 G361 S362 T363 C367 S368 D369 K370 T371 G372 T373 L374 T375 G376 N377 R378 V381 A382 H383 M384 W385 S386 D387 N388 Q389 I390 H391 E392

A393 D394 T395 G401 D405 K406 T407 T410 R416 I417 A418 N422 Q430 P434 I435 L436 K437 R438 D443 A444 S445 L449 L450 K451 C452 I453 C457 G458 S459 V460 K461 E462 M463 R464 Y467 T468 K469 E472 F475 N476 N479 K480 Y481 Q482 L483

H486 K487 E493 P494 R495 H496 M500 K501 C511 S512 S513 I514 L515 Q521 P522 L523 D524 E525 K528 D529 A530 N533 L538 E543 R544 V545 L546 G547 F548 L553 E560 F564 D565 T566 D567 D574 N575 L576 C577 F578 L581 I582 S583 M584 I585 D586 P587

P588 V592 V596 G597 S601 A602 G603 I604 K605 V606 I607 M608 V609 T610 G611 D612 A621 V624 G625 I626 E632 D636 L641 N642 I643 P644 Q647 G660 L671 D672 D673 I674 L675 K676 Y677 H678 I681 V682 F683 A684 R685 T686 S687 P688 Q689 Q690 K691 L692

I693 I694 I704 T708 G709 D710 D714 I723 G724 V725 A726 M727 G731 S732 D733 K736 D740 M741 I742 L743 L744 T753 G754 V755 E756 E757 G758 R759 L760 I761 F762 D763 N764 L765 K766 K767 S768 T774 S775 N776 I777 P778 E779 I780 N790 L793 I803 D804

T807 D808 S814 L815 K826 P829 R830 K836 L837 V838 Q841 M845 A846 Y847 Q854 A855 Y862 F863 V864 I865 N869 G870 F871 L872 G878 W883 D884 D885 I888 V891 E892 D893 S894 Y895 W899 T900 Y901 E902 Q903 R904 K905 I906 V907 E908 F909

T910 C911 P914 V917 T918 I919 V922 I929 C930 K931 T932 S936 V937 F938 G941 M942 K943 I946 L947 I948 L951 E954 L961 S962 Y963 G968 M973 L976 K977 P978 T979 W980 W981 A984 F985 P986 Y987 S988 V993 Y994 D995 E996 V997 R998 K999

L1000 I1001 I1002 R1003 G1008 W1009 K1012 E1013 T1014 Y1015 Y1016

- Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain B: 50% 44%

MET ALA ARG GLY LYS ALA LYS GLU GLU GLY SER TRP K13 K14 F15 I16 W17 N18 K21 K22 E23 F24 L25 G26 R27 S31 I35 Y39 L46 I49 T53 I54 Q55 V56 M57 I61 K65 P66 T67 Y68 T78 Q79 I80 P81 Q82 E87 I88 S89 F90

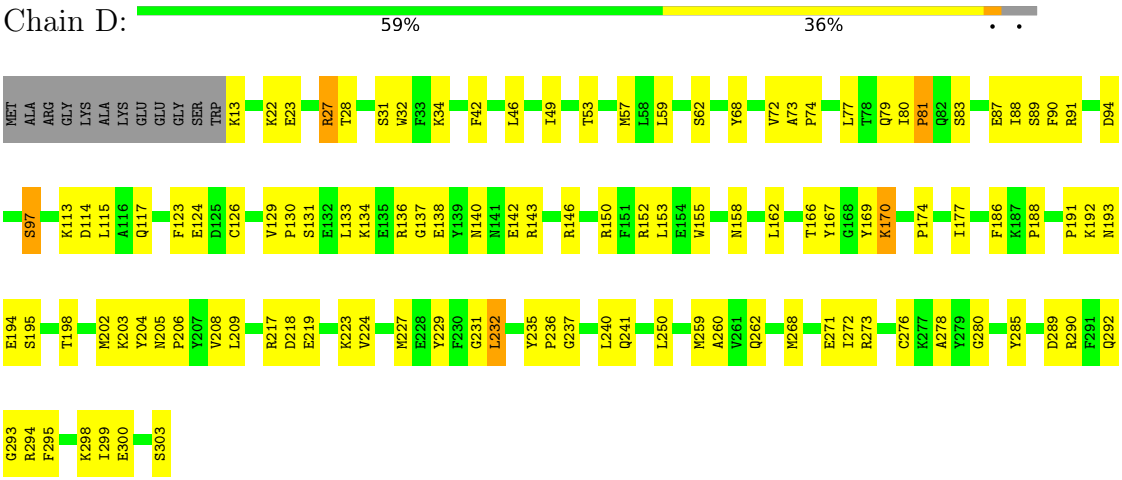
R91 P92 N93 D94 S97 Y98 E99 S100 Y101 V102 V103 S104 I105 V106 R107 F108 L109 E110 K113 D114 L115 A116 Q117 K118 D119 F123 E124 D125 C126 S131 E132 L133 R136 G137 E138 R143 R146 R150 F151 R152 L153 E154 W155 L156 G157 N158 C159 S160 E165 G168

Y169 K170 D171 G172 K173 I177 L180 N181 R182 K187 P188 K189 P190 P191 K192 N193 E194 S195 L196 V201 M202 K203 Y204 N205 P206 Y207 V208 L209 P210 V211 H212 R217 D218 E219 D220 K221 V224 G225 T226 M227 E228 Y229 F230 G231 L232 P236 G237 Q241 Y242 Y245 Y246

G247 K248 L249 L250 Y254 L255 Q256 P257 L258 M259 A260 T264 N265 L266 I274 E275 C276 K277 A278 Y285 S286 D289 R290 F291 Q292 G293 R294 F295 D296 V297 K298 I299 E300 V301 K302 S303

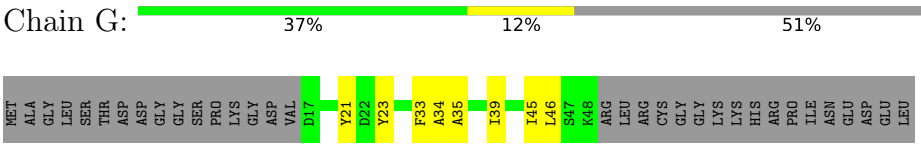
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain D:



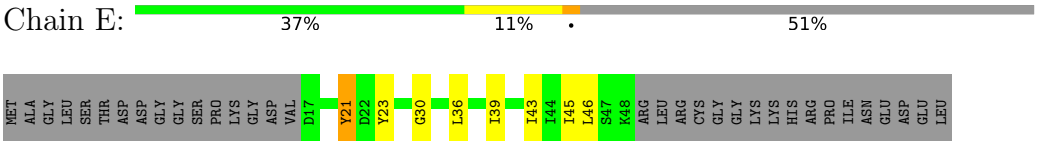
• Molecule 3: FXYD domain-containing ion transport regulator

Chain G:



• Molecule 3: FXYD domain-containing ion transport regulator

Chain E:



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.47Å 118.08Å 494.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.67 – 4.05 29.67 – 4.05	Depositor EDS
% Data completeness (in resolution range)	68.9 (29.67-4.05) 68.9 (29.67-4.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 4.11Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.246 , 0.281 0.247 , 0.279	Depositor DCC
R_{free} test set	1928 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	147.7	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.065 for k,h,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	21017	wwPDB-VP
Average B, all atoms (Å^2)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: NAG, 1DS, MG, 1AT, CLR, BEF

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	0.31	0/7876	0.56	2/10688 (0.0%)
1	C	0.32	1/7876 (0.0%)	0.59	5/10688 (0.0%)
2	B	0.34	0/2449	0.63	0/3301
2	D	0.34	0/2449	0.63	2/3301 (0.1%)
3	E	0.26	0/261	0.48	0/354
3	G	0.32	0/261	0.47	0/354
All	All	0.32	1/21172 (0.0%)	0.59	9/28686 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	564	PHE	CE1-CZ	5.77	1.48	1.37

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	565	ASP	CB-CG-OD1	6.90	124.51	118.30
1	C	566	THR	OG1-CB-CG2	-6.32	95.46	110.00
1	A	487	LYS	CA-CB-CG	5.46	125.42	113.40
1	C	565	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	C	59	ALA	N-CA-CB	5.39	117.65	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7726	0	7776	303	1
1	C	7726	0	7776	285	0
2	B	2386	0	2360	138	0
2	D	2386	0	2363	108	0
3	E	255	0	259	7	0
3	G	255	0	259	8	0
4	F	30	0	29	1	0
5	A	4	0	0	1	0
5	C	4	0	0	4	0
6	A	29	0	25	6	0
7	A	28	0	46	8	0
7	C	28	0	46	4	0
7	E	28	0	46	4	0
7	G	28	0	46	6	0
8	A	29	0	27	9	0
9	A	3	0	0	0	0
9	C	3	0	0	0	0
10	B	30	0	29	3	0
10	D	30	0	28	4	0
11	A	5	0	0	2	0
11	C	4	0	0	3	0
All	All	21017	0	21115	828	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 20.

The worst 5 of 828 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)
2:D:193:ASN:ND2	10:D:401:NAG:O3	1.87	1.08
1:C:845:MET:SD	1:C:998:ARG:NH1	2.31	1.03
1:A:487:LYS:NZ	1:A:494:PRO:O	1.92	1.01
2:B:208:VAL:HG22	2:B:237:GLY:HA3	1.40	0.99
2:B:80:ILE:HG13	2:B:81:PRO:HD3	1.45	0.98

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:172:SER:OG	1:A:640:ARG:O[4_445]	1.85	0.35

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	994/1021 (97%)	935 (94%)	59 (6%)	0	100	100
1	C	994/1021 (97%)	936 (94%)	58 (6%)	0	100	100
2	B	289/303 (95%)	267 (92%)	20 (7%)	2 (1%)	22	61
2	D	289/303 (95%)	272 (94%)	17 (6%)	0	100	100
3	E	30/65 (46%)	28 (93%)	2 (7%)	0	100	100
3	G	30/65 (46%)	27 (90%)	3 (10%)	0	100	100
All	All	2626/2778 (94%)	2465 (94%)	159 (6%)	2 (0%)	51	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	169	TYR
2	B	205	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	847/865 (98%)	825 (97%)	22 (3%)	46	67

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Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	847/865 (98%)	824 (97%)	23 (3%)	44	66
2	B	261/269 (97%)	255 (98%)	6 (2%)	50	70
2	D	261/269 (97%)	249 (95%)	12 (5%)	27	54
3	E	26/52 (50%)	24 (92%)	2 (8%)	13	40
3	G	26/52 (50%)	26 (100%)	0	100	100
All	All	2268/2372 (96%)	2203 (97%)	65 (3%)	42	64

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	158	ASN
2	D	186	PHE
2	B	126	CYS
2	B	93	ASN
2	D	218	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	193	ASN
2	D	205	ASN
2	B	79	GLN
2	B	212	HIS
1	C	488	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)

2 monosaccharides 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	$\#\|Z\| > 2$
4	NAG	F	1	2,4	15,15,15	1.34	2 (13%)	21,21,21	1.58	4 (19%)
4	NAG	F	2	4	15,15,15	1.08	1 (6%)	21,21,21	0.94	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1	2,4	-	0/6/26/26	0/1/1/1
4	NAG	F	2	4	-	1/6/26/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	NAG	O5-C1	-4.71	1.31	1.42
4	F	2	NAG	C1-C2	-3.57	1.48	1.52
4	F	1	NAG	C1-C2	-2.02	1.50	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	1	NAG	O1-C1-O5	-4.57	96.67	110.38
4	F	1	NAG	C4-C3-C2	2.99	114.72	110.34
4	F	1	NAG	O1-C1-C2	-2.63	103.76	109.22
4	F	2	NAG	C1-C2-C3	-2.50	107.14	110.54
4	F	1	NAG	C3-C4-C5	2.45	114.61	110.24

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	2	NAG	O5-C5-C6-O6

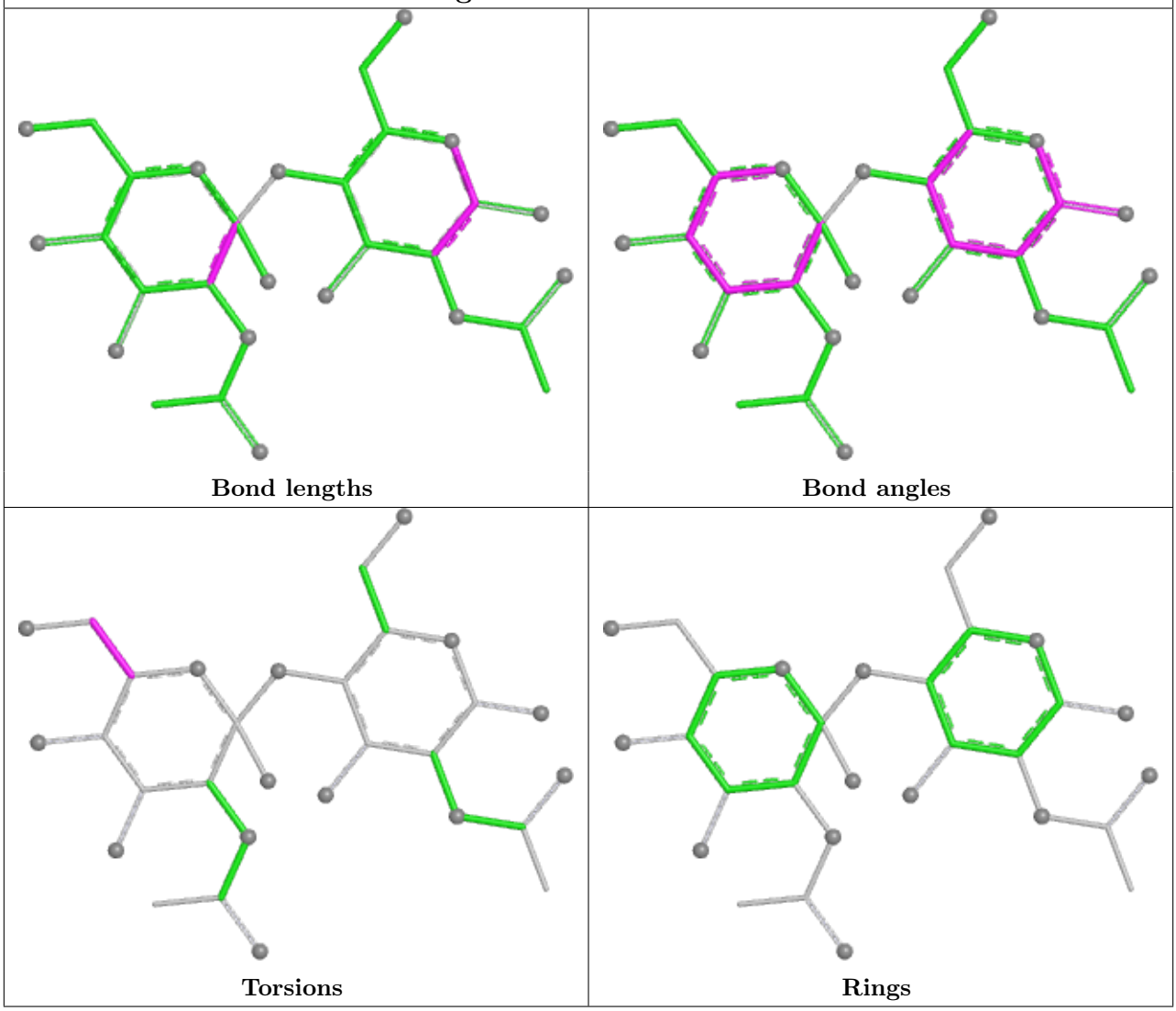
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	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 oligosaccharide.

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
10	NAG	D	401	-	15,15,15	0.24	0	21,21,21	0.49	0
7	CLR	E	101	-	31,31,31	0.74	1 (3%)	48,48,48	1.21	6 (12%)
5	BEF	A	1101	1	0,3,3	-	-	-		
7	CLR	G	101	-	31,31,31	0.70	1 (3%)	48,48,48	1.28	9 (18%)
7	CLR	C	1102	-	31,31,31	0.72	1 (3%)	48,48,48	1.37	7 (14%)
6	1AT	A	1102	-	30,30,35	1.49	3 (10%)	43,43,48	2.47	15 (34%)
7	CLR	A	1103	-	31,31,31	0.68	0	48,48,48	1.58	8 (16%)
8	1DS	A	1104	-	30,30,35	1.33	5 (16%)	42,43,48	2.88	18 (42%)
10	NAG	D	402	2	15,15,15	0.90	1 (6%)	21,21,21	0.71	0
10	NAG	B	401	2	15,15,15	0.42	0	21,21,21	0.60	1 (4%)
10	NAG	B	402	2	15,15,15	0.86	1 (6%)	21,21,21	1.46	2 (9%)
5	BEF	C	1101	-	0,3,3	-	-	-		

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
10	NAG	D	401	-	-	2/6/26/26	0/1/1/1
7	CLR	E	101	-	-	5/10/68/68	0/4/4/4
7	CLR	G	101	-	-	2/10/68/68	0/4/4/4
7	CLR	C	1102	-	-	4/10/68/68	0/4/4/4
6	1AT	A	1102	-	-	10/19/58/63	0/2/2/2
7	CLR	A	1103	-	-	9/10/68/68	0/4/4/4
8	1DS	A	1104	-	-	7/19/58/63	0/2/2/2
10	NAG	B	401	2	-	2/6/26/26	0/1/1/1
10	NAG	B	402	2	-	0/6/26/26	0/1/1/1
10	NAG	D	402	2	-	2/6/26/26	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1102	1AT	O6-C1N	4.65	1.46	1.33
8	A	1104	1DS	O1'-C1N	3.01	1.42	1.33
10	B	402	NAG	O5-C1	-2.86	1.35	1.42
10	D	402	NAG	C1-C2	2.85	1.56	1.52
6	A	1102	1AT	C4'-C5'	-2.73	1.46	1.53

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1102	1AT	O2-C2-C3	-6.92	94.36	110.35
8	A	1104	1DS	C1'-O1'-C1N	6.92	128.87	116.88
8	A	1104	1DS	O2-C2-C3	6.22	124.72	110.35
6	A	1102	1AT	O1-C1-C2	5.94	125.76	108.29
8	A	1104	1DS	O1-C2'-C3'	5.86	126.47	108.08

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1102	1AT	O1'-C1'-C2'-O1
6	A	1102	1AT	O1'-C1'-C2'-C3'
8	A	1104	1DS	O1'-C1'-C2'-O1
8	A	1104	1DS	O1'-C1'-C2'-C3'
8	A	1104	1DS	O1'-C1'-C2'-O2'

There are no ring outliers.

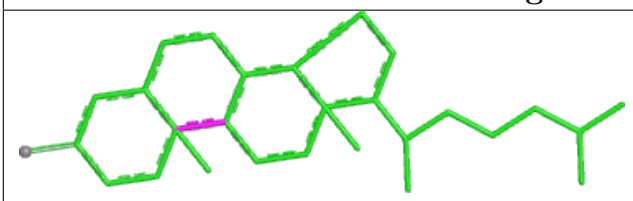
11 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	401	NAG	4	0
7	E	101	CLR	4	0
5	A	1101	BEF	1	0
7	G	101	CLR	6	0
7	C	1102	CLR	4	0
6	A	1102	1AT	6	0
7	A	1103	CLR	8	0
8	A	1104	1DS	9	0
10	B	401	NAG	2	0
10	B	402	NAG	1	0
5	C	1101	BEF	4	0

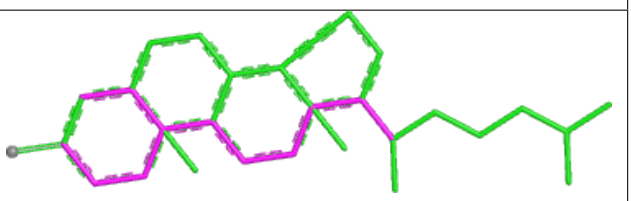
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

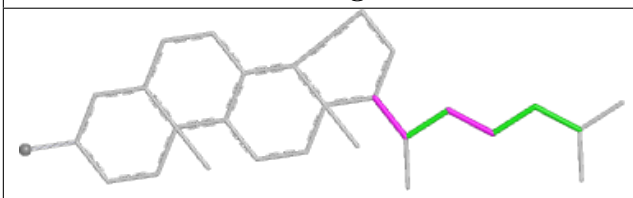
Ligand CLR E 101



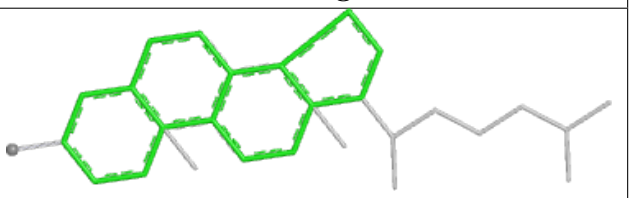
Bond lengths



Bond angles

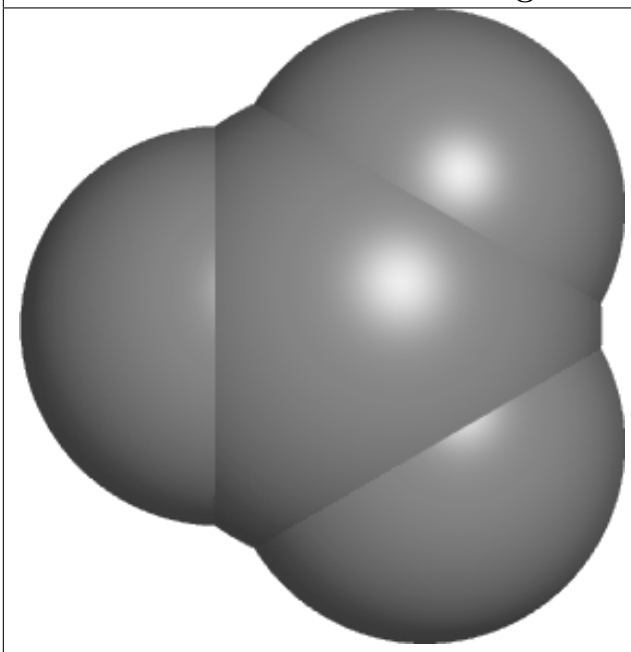


Torsions



Rings

Ligand BEF A 1101



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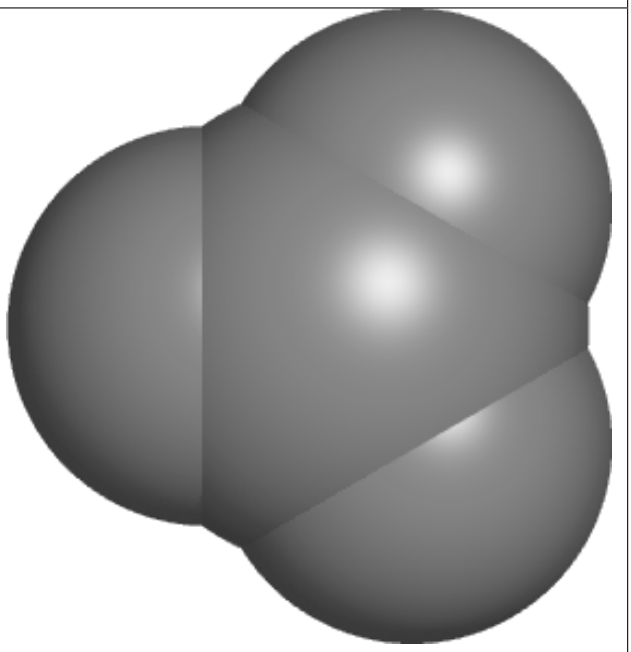

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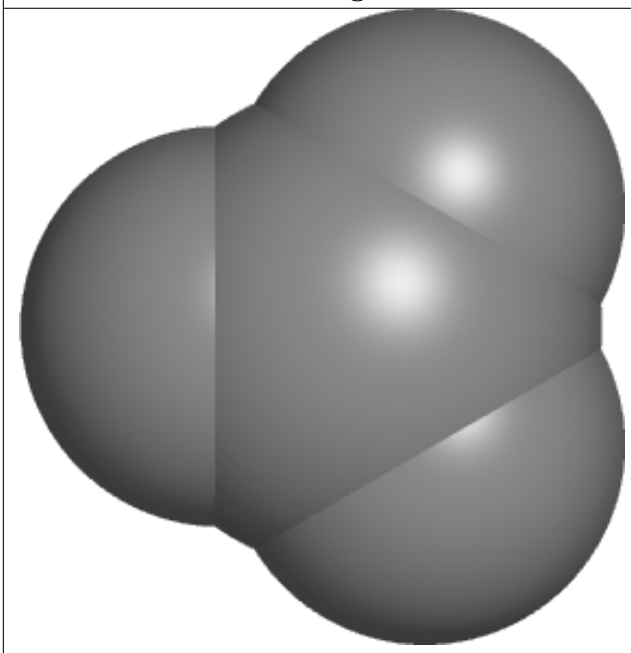

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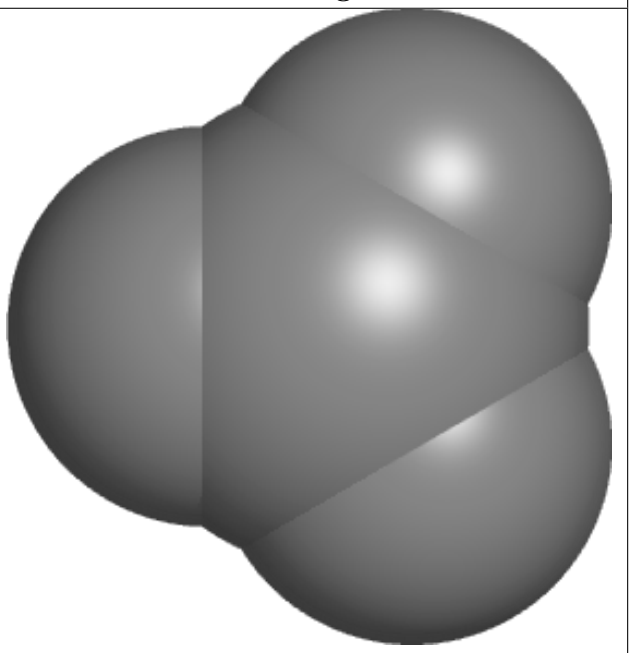
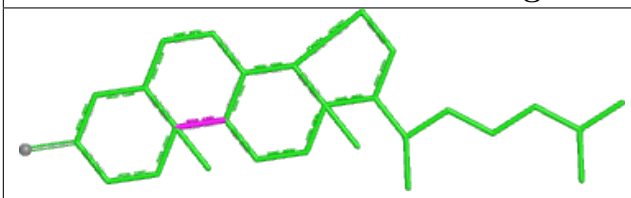
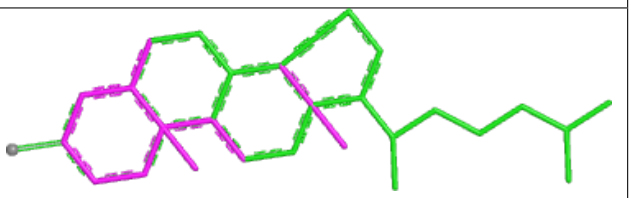
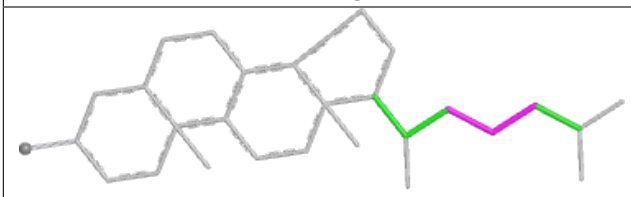
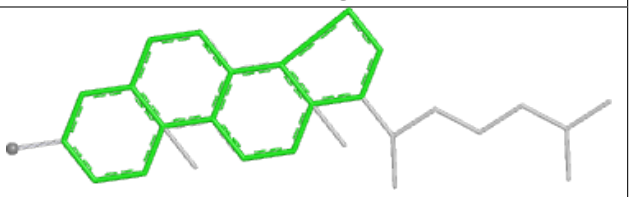


Rings

Ligand CLR G 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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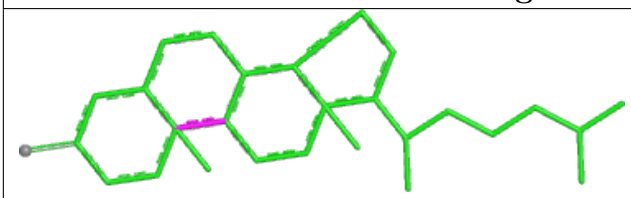
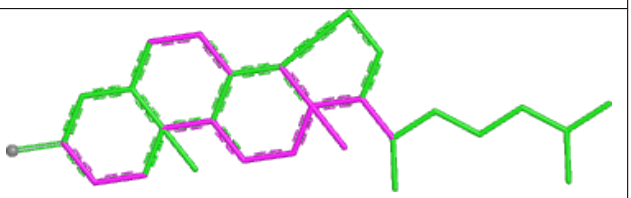
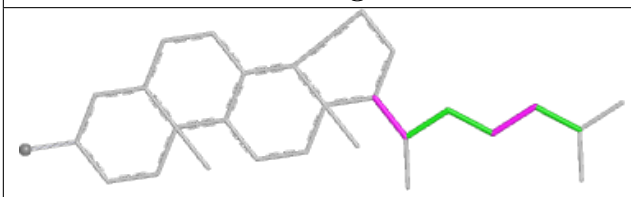
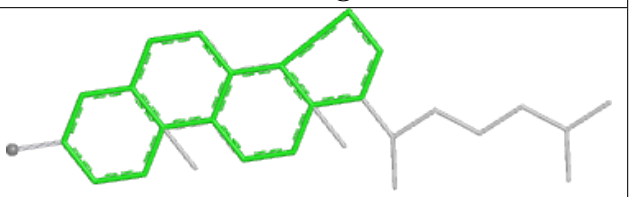
 Bond lengths	 Bond angles
 Torsions	 Rings

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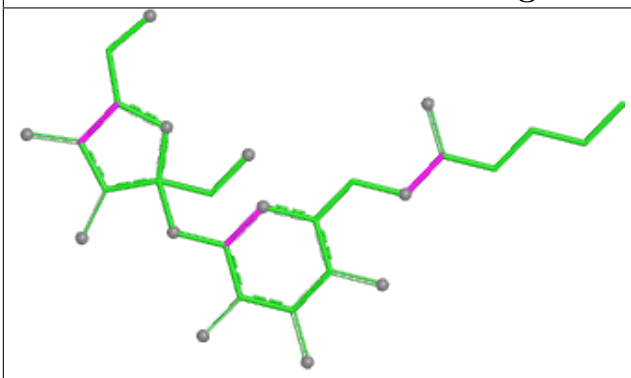
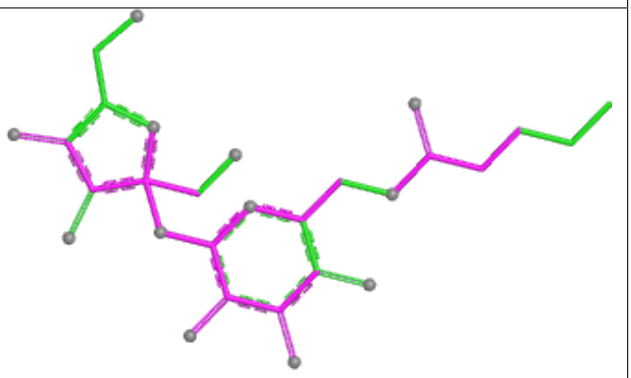
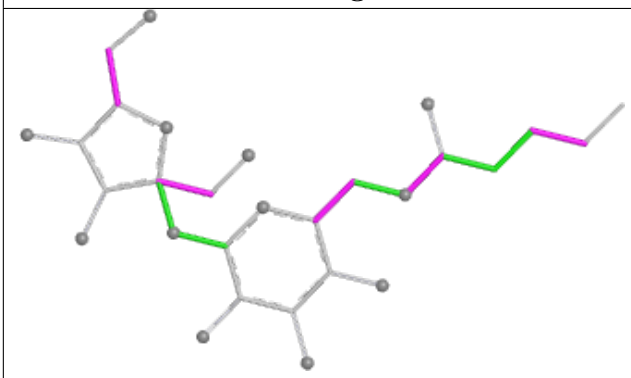
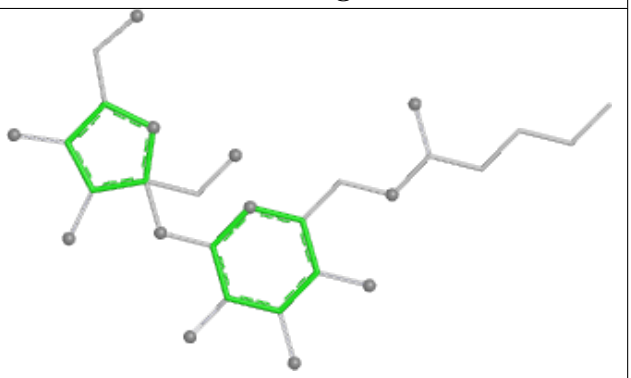
 Bond lengths	 Bond angles
 Torsions	 Rings

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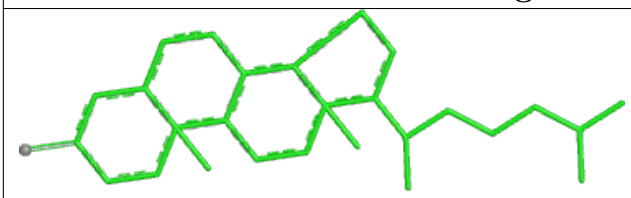
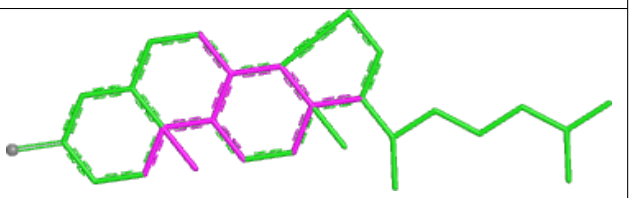
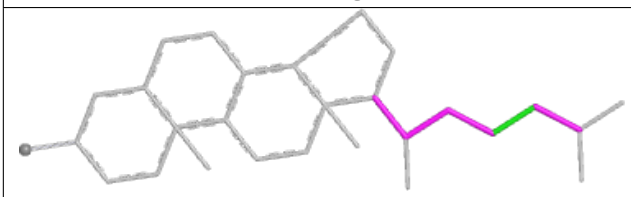
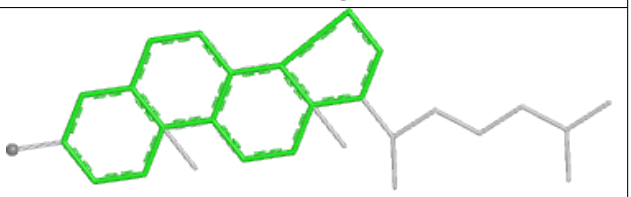
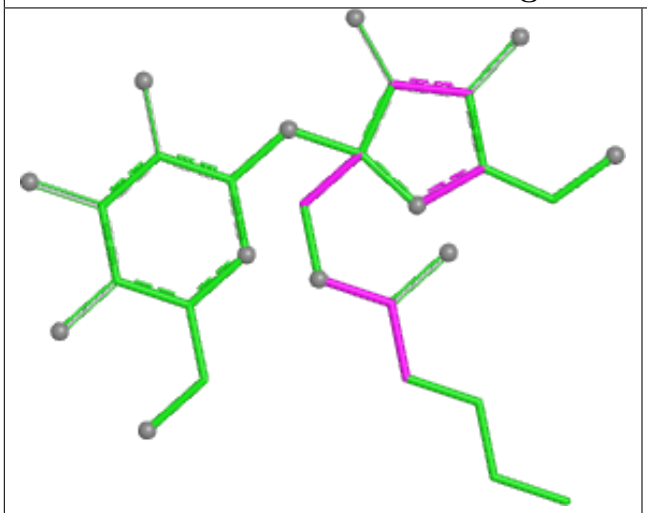
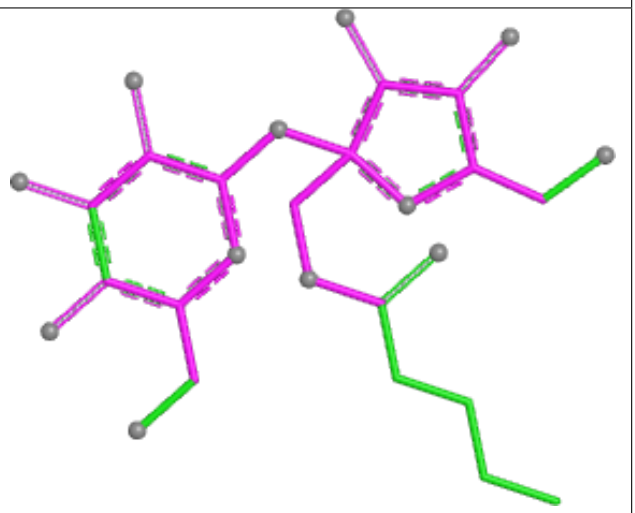
 Bond lengths	 Bond angles
 Torsions	 Rings

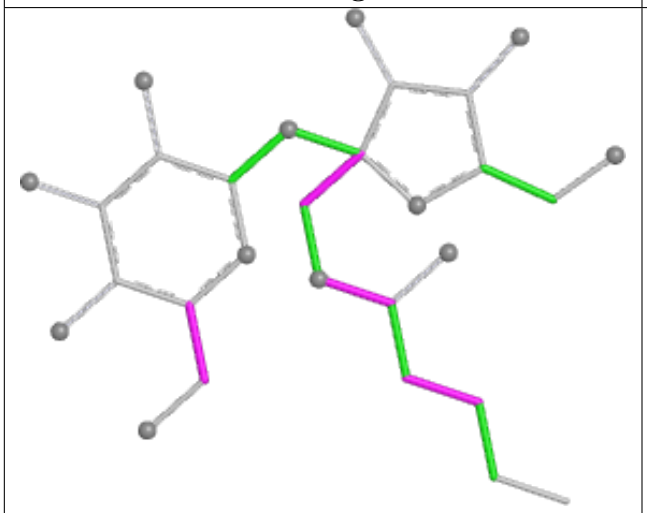
Ligand 1DS A 1104



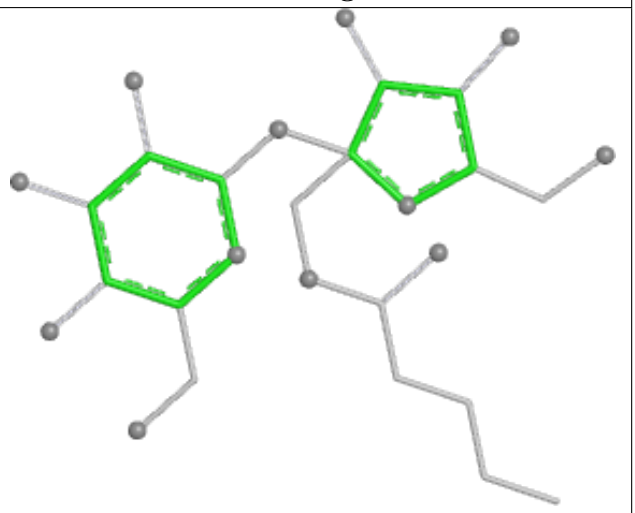
Bond lengths



Bond angles

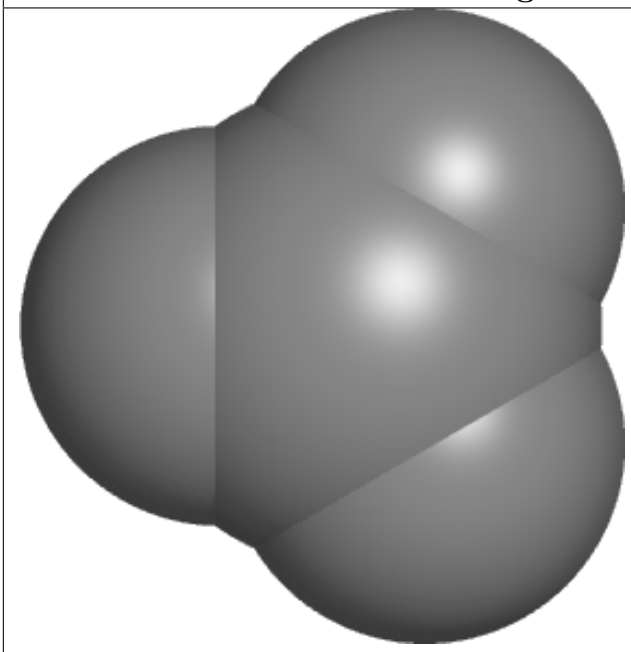


Torsions



Rings

Ligand BEF C 1101



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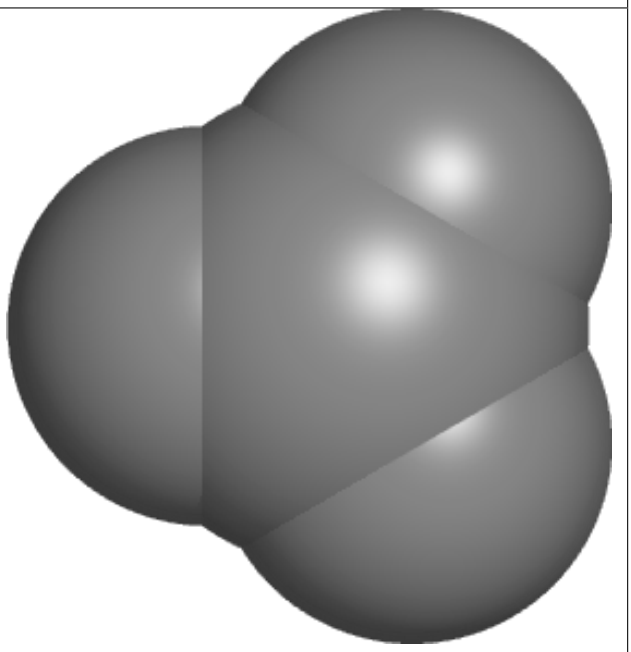
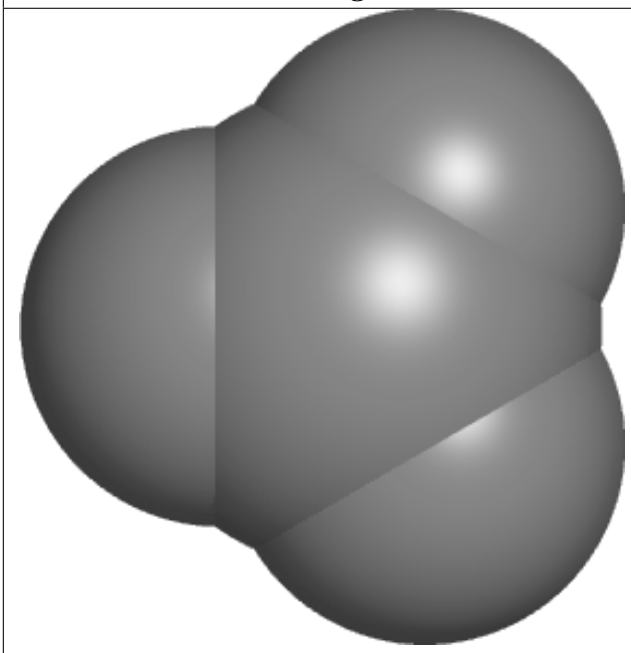
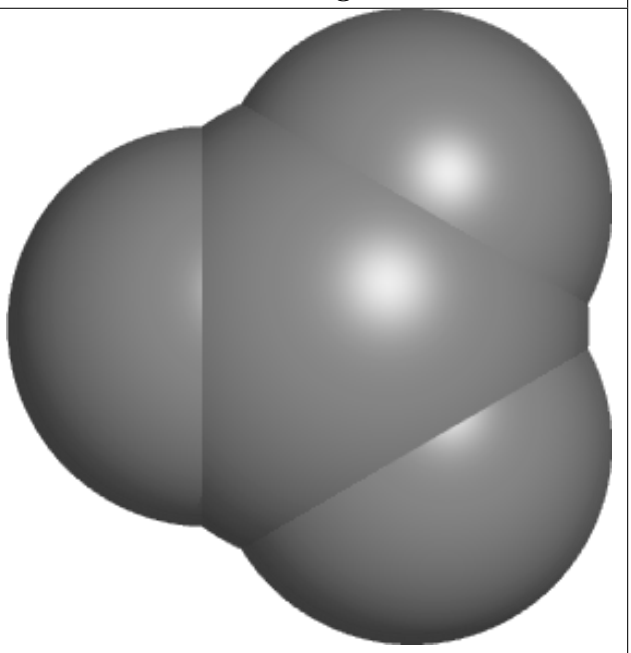


Bond angles



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

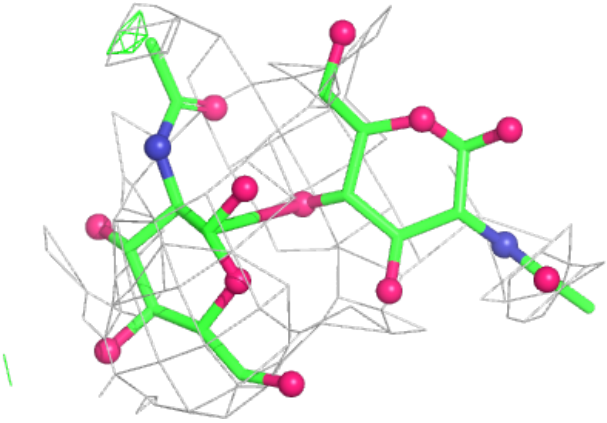
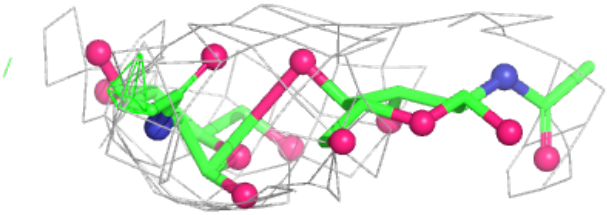
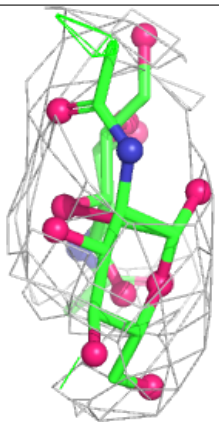
6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

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

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain F: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

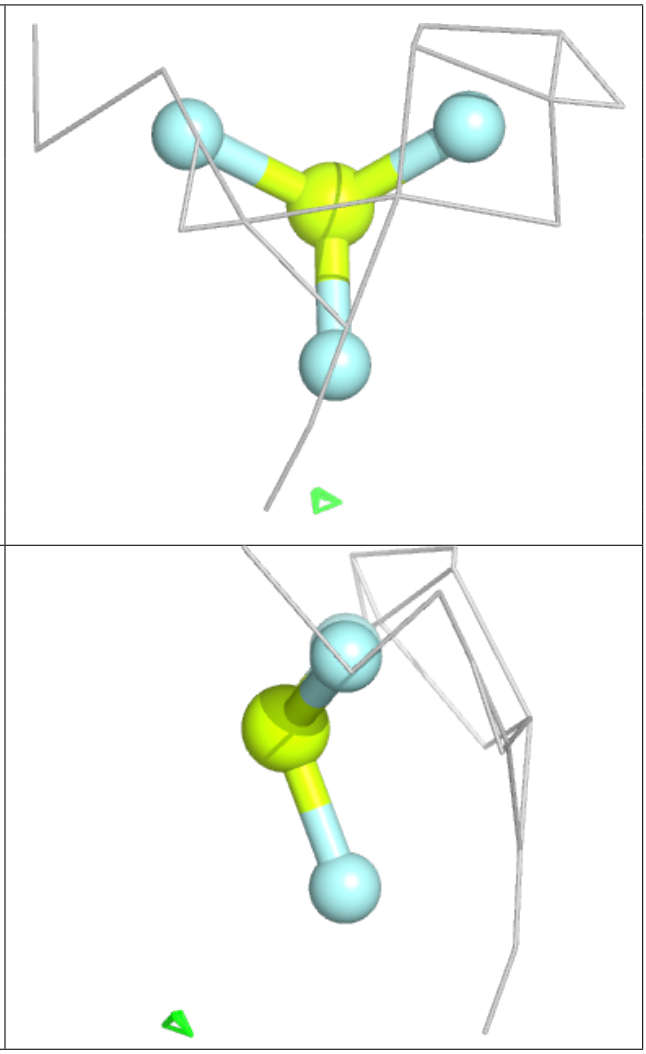
6.4 Ligands (i)

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

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

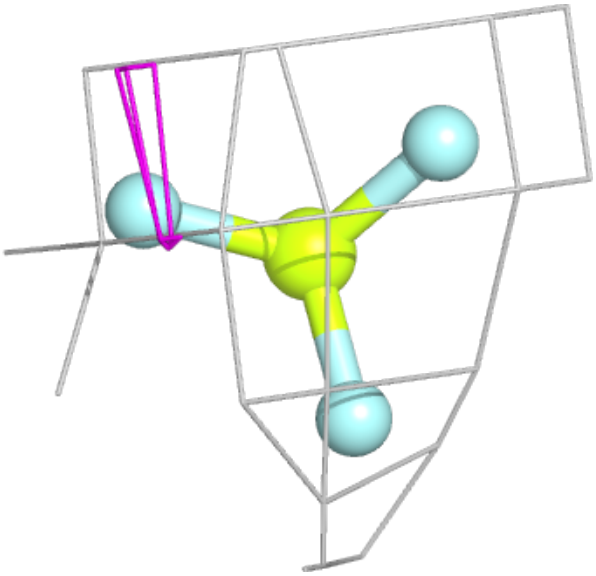
Electron density around BEF A 1101:

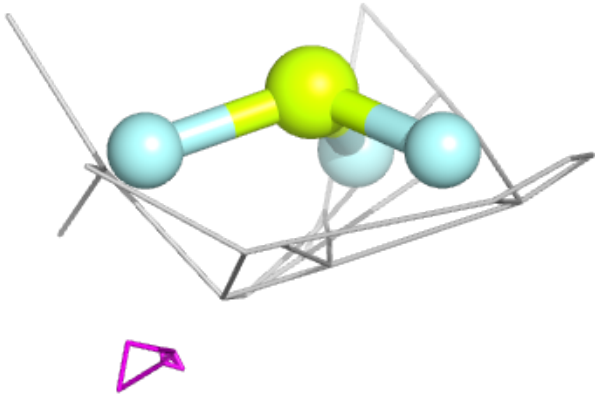
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

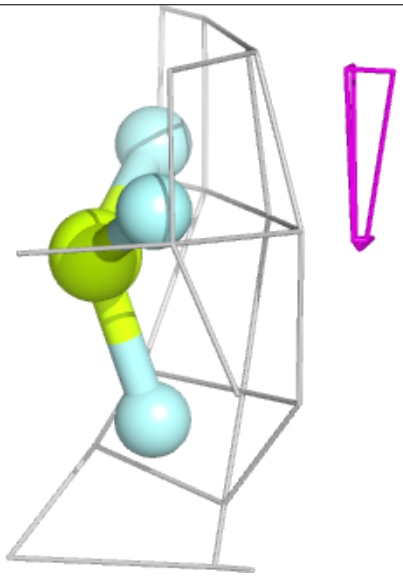


Electron density around BEF C 1101:

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

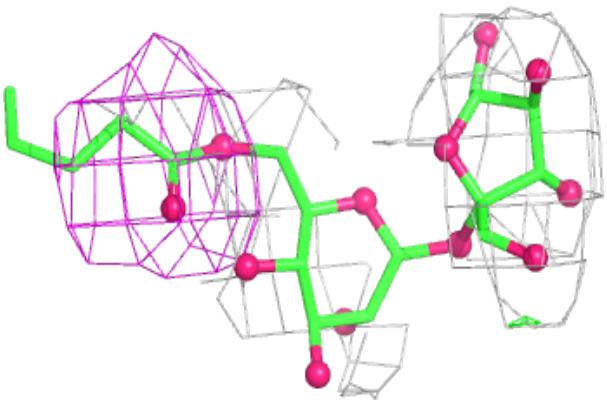


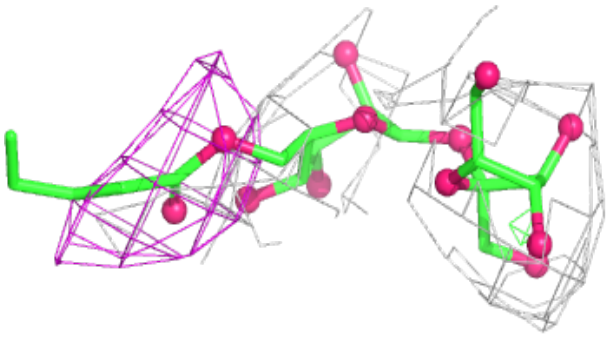


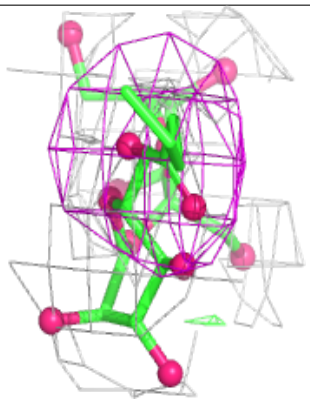


Electron density around 1AT A 1102:

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

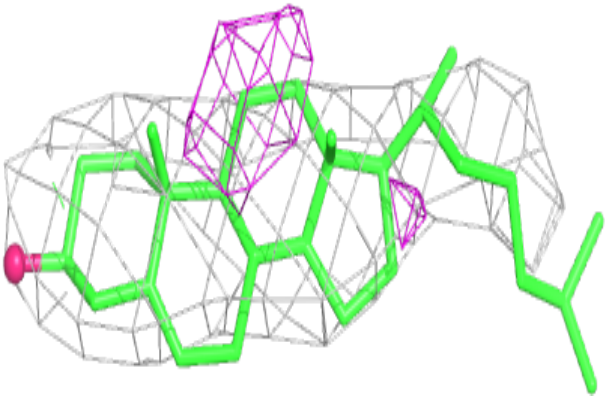


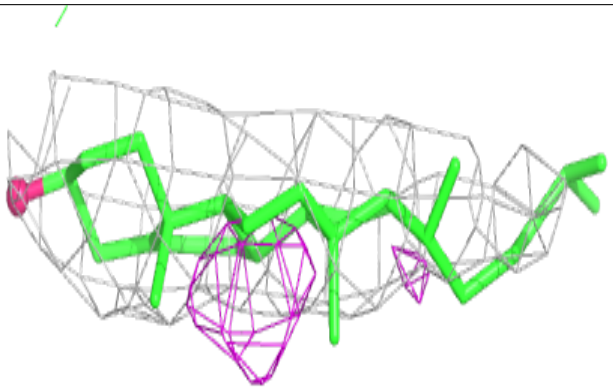


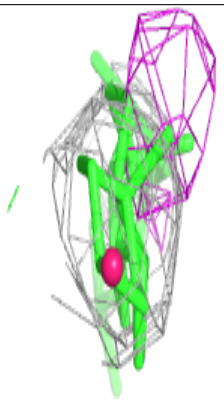


Electron density around CLR A 1103:

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

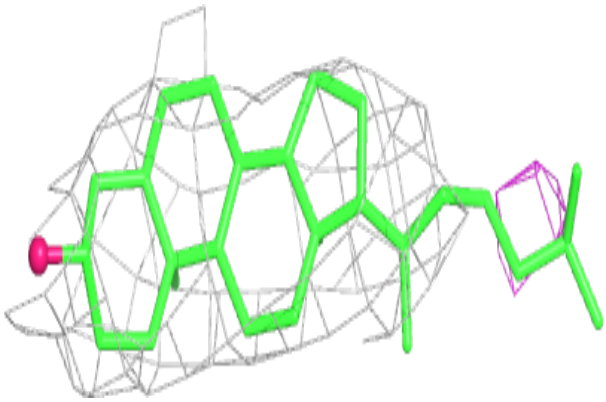


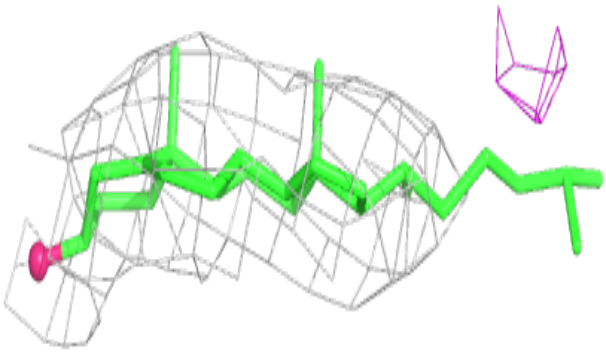




Electron density around CLR G 101:

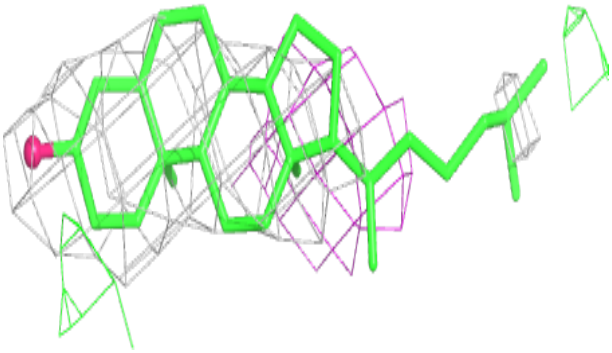
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

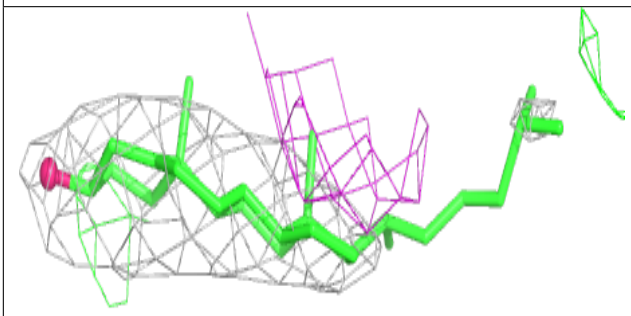


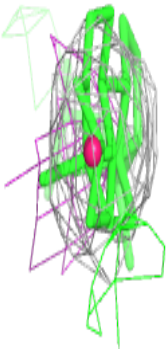


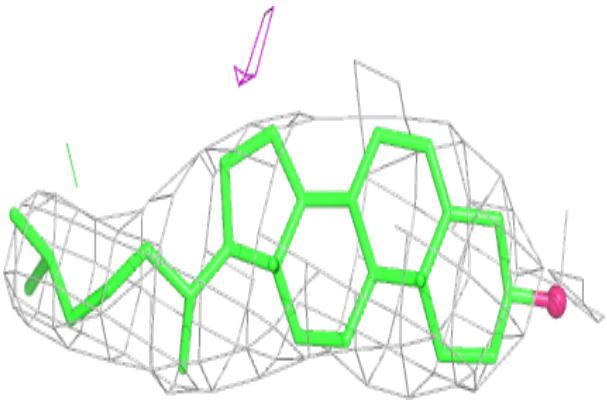
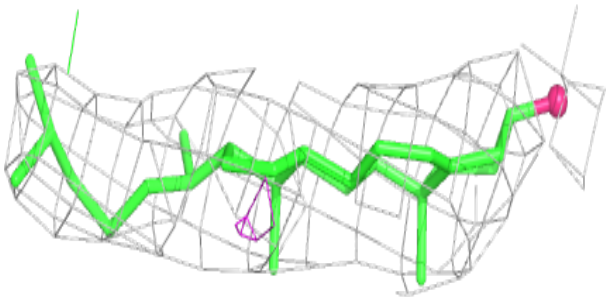
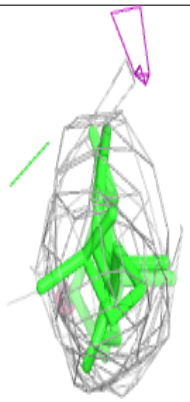
Electron density around CLR C 1102:

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



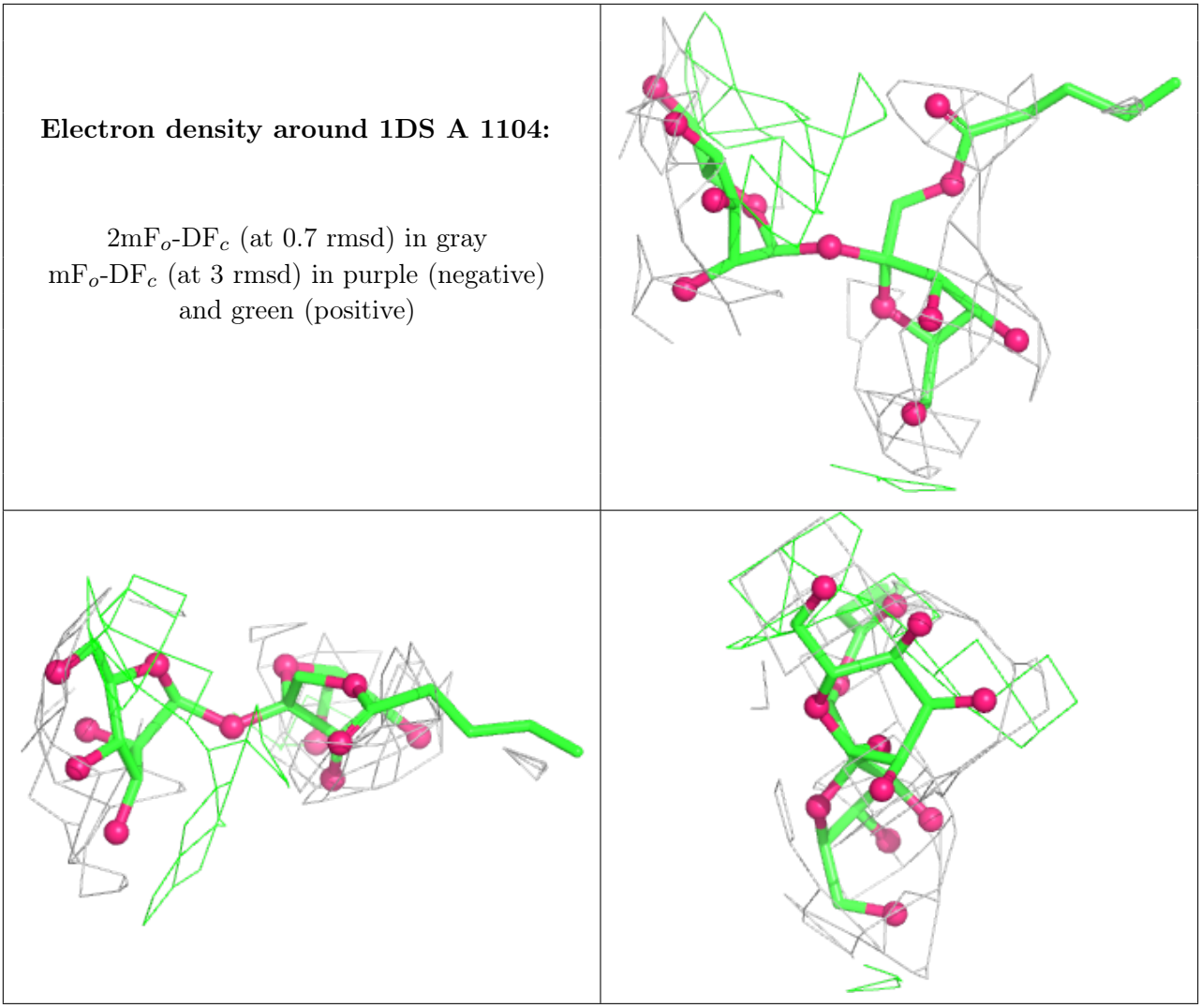




Electron density around CLR E 101: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around 1DS A 1104:

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



6.5 Other polymers (i)

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