Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2023 – 11:48 AM EDT

PDB ID	:	5A43
Title	:	Crystal structure of a dual topology fluoride ion channel.
Authors	:	Stockbridge, R.B.; Kolmakova-Partensky, L.; Shane, T.; Koide, A.; Koide, S.; Miller, C.; Newstead, S.
Deposited on	:	2015-06-04
Resolution	:	2.58 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 (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 (1)) were used in the production of this report:

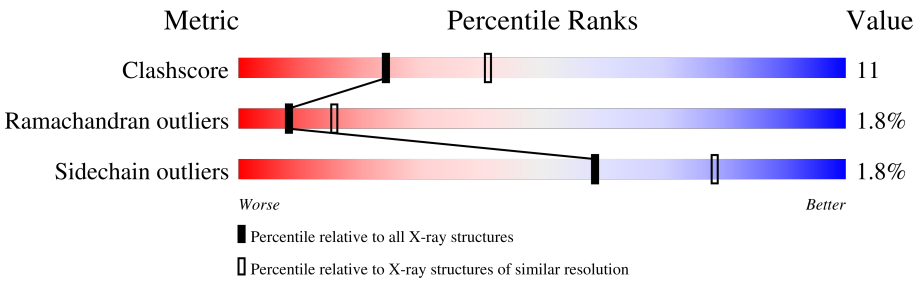
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.58 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))
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	126	72% 26% .
1	B	126	73% 26% .
2	C	96	79% 19% .
2	D	96	81% 18% .

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
4	DMU	A	1127	X	-	-	-
4	DMU	B	1129	X	-	-	-
4	DMU	C	1097	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3481 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 PUTATIVE FLUORIDE ION TRANSPORTER CRCB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	124	951	644	146	156	2	3	0	0	0
1	B	126	961	650	148	158	2	3	0	0	0

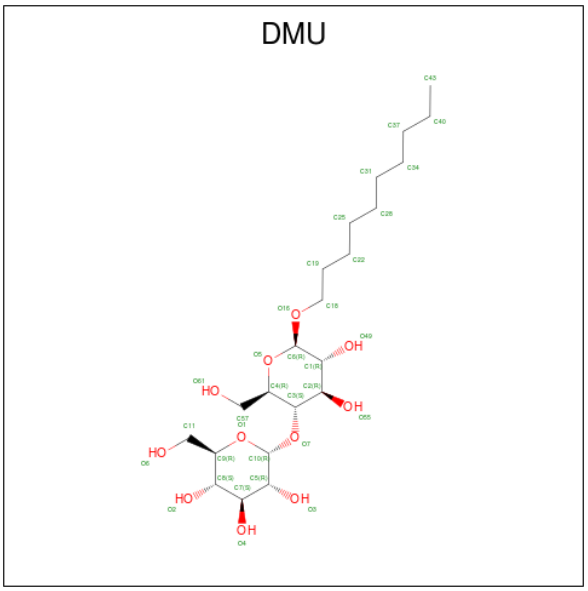
- Molecule 2 is a protein called MONOBODIES.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
2	C	96	728	470	108	149	1	0	0	0
2	D	96	728	470	108	149	1	0	0	0

- Molecule 3 is FLUORIDE ION (three-letter code: F) (formula: F).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	F		
3	A	1	1	1	0	0
3	B	1	1	1	0	0

- Molecule 4 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			33	22	11		
4	B	1	Total	C	O	0	0
			31	20	11		
4	C	1	Total	C	O	0	0
			27	16	11		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	B	2	Total	O	0	0
			2	2		
6	C	4	Total	O	0	0
			4	4		
6	D	11	Total	O	0	0
			11	11		

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.

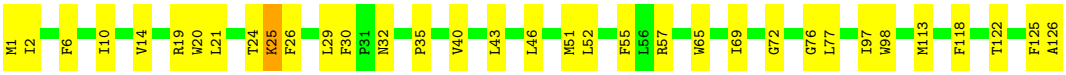
Note EDS failed to run properly.

• Molecule 1: PUTATIVE FLUORIDE ION TRANSPORTER CRCB

Chain A:

• Molecule 1: PUTATIVE FLUORIDE ION TRANSPORTER CRCB

Chain B:

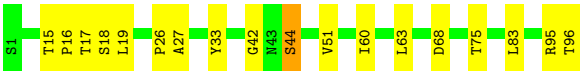


• Molecule 2: MONOBODIES

Chain C:

• Molecule 2: MONOBODIES

Chain D:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	87.42Å 87.42Å 146.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.25 – 2.58	Depositor
% Data completeness (in resolution range)	99.9 (24.25-2.58)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.57Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.224 , 0.264	Depositor
Wilson B-factor (Å^2)	62.6	Xtriage
Anisotropy	0.134	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
Total number of atoms	3481	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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: F, NA, DMU

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	0.44	0/973	0.62	0/1323
1	B	0.45	0/983	0.62	0/1337
2	C	0.52	0/747	0.75	2/1028 (0.2%)
2	D	0.53	0/747	0.73	1/1028 (0.1%)
All	All	0.48	0/3450	0.67	3/4716 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	76	MSE	CB-CG-SE	5.96	130.58	112.70
2	D	44	SER	C-N-CD	-5.40	108.72	120.60
2	C	76	MSE	CA-CB-CG	5.36	122.41	113.30

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	951	0	1006	26	0
1	B	961	0	1016	28	0
2	C	728	0	716	12	0
2	D	728	0	716	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	33	0	42	1	0
4	B	31	0	35	2	0
4	C	27	0	27	1	0
5	B	1	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	1	0
6	C	4	0	0	0	0
6	D	11	0	0	0	0
All	All	3481	0	3558	77	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 (77) 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:A:46:LEU:HB2	1:A:113:MSE:HE3	1.69	0.74
1:A:4:SER:HB2	1:A:67:LEU:HD23	1.72	0.71
1:A:57:ARG:HG2	1:A:57:ARG:HH11	1.55	0.70
1:B:51:MSE:HE3	1:B:55:PHE:HE1	1.57	0.68
1:A:2:ILE:HD11	1:B:20:TRP:HH2	1.58	0.67
1:B:57:ARG:HH11	1:B:125:PHE:HD2	1.41	0.67
1:B:51:MSE:HE2	1:B:69:ILE:HG21	1.76	0.66
1:A:59:PRO:O	1:A:60:HIS:HB3	1.95	0.66
1:A:27:ASN:HD21	1:A:37:THR:HG23	1.59	0.65
1:A:64:PHE:HD2	1:A:65:TRP:CD1	2.19	0.61
4:A:1127:DMU:H20	4:A:1127:DMU:H12	1.82	0.60
1:B:51:MSE:HE3	1:B:55:PHE:CE1	2.36	0.60
2:C:65:PRO:HA	2:C:96:THR:HG21	1.84	0.60
2:D:33:TYR:HB2	2:D:51:VAL:HG22	1.85	0.59
2:C:81:SER:O	2:C:81:SER:OG	2.19	0.58
1:A:2:ILE:HD11	1:B:20:TRP:CH2	2.38	0.57
2:C:44:SER:H	2:C:45:PRO:HA	1.70	0.56
1:B:30:PHE:HB3	1:B:35:PRO:HD3	1.87	0.56
4:C:1097:DMU:O49	4:C:1097:DMU:H7	2.06	0.55
1:A:70:THR:O	1:A:74:CYS:HB2	2.07	0.55
1:B:51:MSE:CE	1:B:69:ILE:HD13	2.37	0.55
1:A:37:THR:HG21	1:A:82:THR:HG21	1.88	0.54
1:B:19:ARG:NH1	1:B:76:GLY:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:SER:HB2	1:A:67:LEU:CD2	2.38	0.54
1:B:1:MSE:O	1:B:2:ILE:HD13	2.08	0.54
2:C:23:TRP:CE2	2:C:56:SER:HA	2.42	0.53
2:D:26:PRO:HG3	2:D:75:THR:HG21	1.91	0.53
1:B:21:LEU:O	1:B:25:LYS:HG3	2.09	0.53
1:A:10:ILE:O	1:A:14:VAL:HG23	2.09	0.53
1:B:6:PHE:CZ	1:B:10:ILE:HD11	2.44	0.52
1:A:64:PHE:HB3	1:A:65:TRP:HD1	1.75	0.52
2:D:15:THR:HG22	2:D:17:THR:H	1.75	0.50
1:B:19:ARG:HG3	1:B:40:VAL:HG21	1.93	0.50
1:B:51:MSE:HE2	1:B:69:ILE:HD13	1.93	0.49
1:B:43:LEU:HD23	1:B:77:LEU:HD21	1.94	0.49
1:A:65:TRP:CD1	1:A:65:TRP:N	2.80	0.49
2:C:65:PRO:HA	2:C:96:THR:CG2	2.42	0.48
1:B:6:PHE:O	1:B:10:ILE:HD12	2.14	0.48
1:A:109:GLY:O	1:A:113:MSE:HG2	2.13	0.48
1:B:52:LEU:HD23	2:D:83:LEU:HB3	1.96	0.47
2:D:60:ILE:HG22	2:D:63:LEU:HD21	1.97	0.47
1:A:32:ASN:HB3	1:A:98:TRP:CD2	2.50	0.47
2:D:95:ARG:O	2:D:96:THR:HB	2.14	0.47
1:B:46:LEU:N	1:B:113:MSE:HB3	2.30	0.47
1:A:124:LEU:HD22	1:A:125:PHE:HD1	1.80	0.46
1:A:2:ILE:HD12	1:A:5:LEU:H	1.80	0.46
2:C:67:VAL:H	2:C:96:THR:HB	1.81	0.45
2:C:64:LYS:HB2	2:C:67:VAL:HG21	1.98	0.45
2:D:15:THR:HG23	2:D:16:PRO:HD2	1.98	0.45
1:B:26:PHE:HA	1:B:29:LEU:HD13	1.99	0.45
2:C:72:THR:HG22	2:C:91:SER:OG	2.16	0.44
1:A:57:ARG:HG2	1:A:57:ARG:NH1	2.26	0.44
1:B:57:ARG:HH12	1:B:126:ALA:HB3	1.83	0.44
1:B:32:ASN:HB3	1:B:98:TRP:CD2	2.52	0.44
4:B:1129:DMU:O1	4:B:1129:DMU:H29	2.17	0.44
4:B:1129:DMU:H35	2:C:52:PRO:HB3	2.00	0.44
1:B:65:TRP:O	1:B:69:ILE:HD12	2.18	0.43
2:C:39:GLU:HB2	2:C:44:SER:HB2	1.99	0.43
1:A:3:LYS:O	1:A:64:PHE:HE1	2.01	0.43
1:B:55:PHE:HB2	6:B:2002:HOH:O	2.18	0.42
1:B:6:PHE:CE1	1:B:10:ILE:HD11	2.54	0.42
2:D:16:PRO:HA	2:D:96:THR:HG22	2.02	0.42
1:A:79:THR:CG2	1:A:82:THR:H	2.32	0.42
1:B:10:ILE:O	1:B:14:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:O	1:A:51:MSE:HG2	2.18	0.42
2:C:23:TRP:NE1	2:C:56:SER:HA	2.35	0.42
1:B:46:LEU:HA	1:B:113:MSE:O	2.19	0.42
1:A:64:PHE:HB3	1:A:65:TRP:CD1	2.54	0.41
1:B:118:PHE:O	1:B:122:THR:HG23	2.20	0.41
2:D:18:SER:O	2:D:19:LEU:HD23	2.21	0.41
1:B:20:TRP:O	1:B:24:THR:HG23	2.21	0.41
2:D:68:ASP:HA	2:D:95:ARG:HA	2.03	0.41
1:A:7:ALA:HB1	1:A:68:MSE:HB2	2.02	0.41
2:C:16:PRO:O	2:C:96:THR:HG21	2.20	0.41
2:D:26:PRO:O	2:D:27:ALA:HB3	2.20	0.41
1:A:79:THR:HG22	1:A:82:THR:H	1.86	0.40
1:A:120:ILE:O	1:A:124:LEU:HB2	2.21	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	122/126 (97%)	115 (94%)	5 (4%)	2 (2%)	9 18
1	B	124/126 (98%)	117 (94%)	6 (5%)	1 (1%)	19 37
2	C	94/96 (98%)	86 (92%)	5 (5%)	3 (3%)	4 6
2	D	94/96 (98%)	88 (94%)	4 (4%)	2 (2%)	7 12
All	All	434/444 (98%)	406 (94%)	20 (5%)	8 (2%)	8 16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	82	ASP
2	D	42	GLY

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Mol	Chain	Res	Type
2	D	44	SER
1	A	62	ASP
2	C	41	GLY
2	C	44	SER
1	B	72	GLY
1	A	34	PRO

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	105/102 (103%)	104 (99%)	1 (1%)	76	89
1	B	105/102 (103%)	103 (98%)	2 (2%)	57	77
2	C	85/84 (101%)	81 (95%)	4 (5%)	26	48
2	D	85/84 (101%)	85 (100%)	0	100	100
All	All	380/372 (102%)	373 (98%)	7 (2%)	59	78

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	VAL
1	B	25	LYS
1	B	97	ILE
2	C	28	VAL
2	C	43	ASN
2	C	54	SER
2	C	76	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
4	DMU	C	1097	-	28,28,34	0.58	1 (3%)	39,39,45	1.14	2 (5%)
4	DMU	B	1129	-	32,32,34	0.48	1 (3%)	43,43,45	0.80	0
4	DMU	A	1127	-	34,34,34	0.46	1 (2%)	45,45,45	0.60	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
4	DMU	C	1097	-	2/2/10/10	5/13/53/59	0/2/2/2
4	DMU	B	1129	-	1/1/10/10	4/17/57/59	1/2/2/2
4	DMU	A	1127	-	2/2/10/10	5/19/59/59	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1097	DMU	O16-C6	2.51	1.44	1.40
4	B	1129	DMU	O16-C6	2.20	1.44	1.40
4	A	1127	DMU	O16-C6	2.16	1.43	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1097	DMU	O7-C3-C2	3.87	117.59	107.28
4	C	1097	DMU	O5-C6-O16	-2.24	104.67	109.97

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1127	DMU	C5
4	A	1127	DMU	C9
4	B	1129	DMU	C9
4	C	1097	DMU	C5
4	C	1097	DMU	C9

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1127	DMU	C19-C18-O16-C6
4	C	1097	DMU	O5-C6-O16-C18
4	C	1097	DMU	C2-C3-O7-C10
4	C	1097	DMU	C1-C6-O16-C18
4	A	1127	DMU	O16-C18-C19-C22
4	B	1129	DMU	C18-C19-C22-C25
4	B	1129	DMU	O16-C18-C19-C22
4	C	1097	DMU	O6-C11-C9-O1
4	B	1129	DMU	O6-C11-C9-O1
4	A	1127	DMU	O5-C6-O16-C18
4	A	1127	DMU	C18-C19-C22-C25
4	A	1127	DMU	C25-C28-C31-C34
4	C	1097	DMU	C4-C3-O7-C10
4	B	1129	DMU	C19-C22-C25-C28

All (1) ring outliers are listed below:

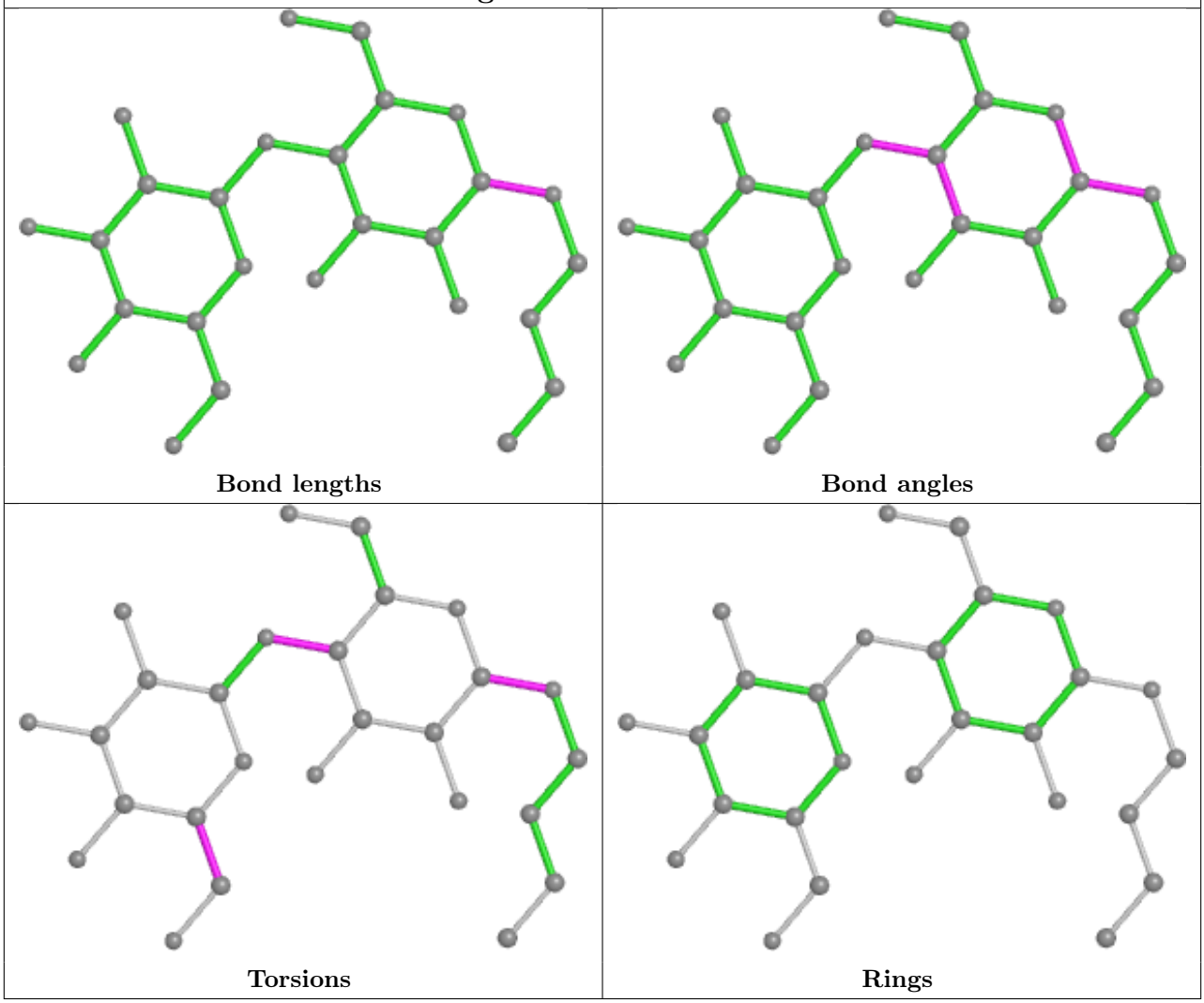
Mol	Chain	Res	Type	Atoms
4	B	1129	DMU	C10-C5-C7-C8-C9-O1

3 monomers are involved in 4 short contacts:

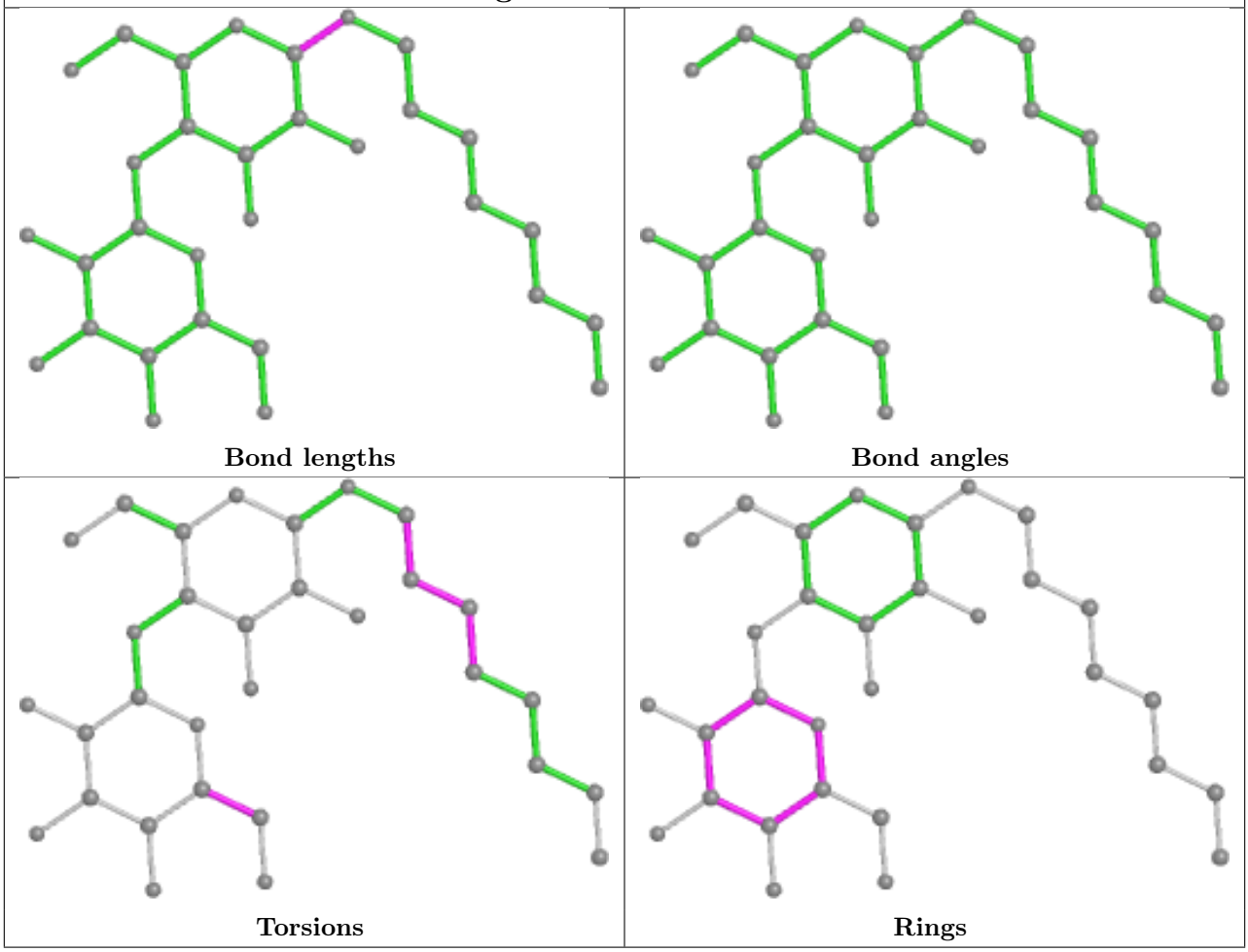
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1097	DMU	1	0
4	B	1129	DMU	2	0
4	A	1127	DMU	1	0

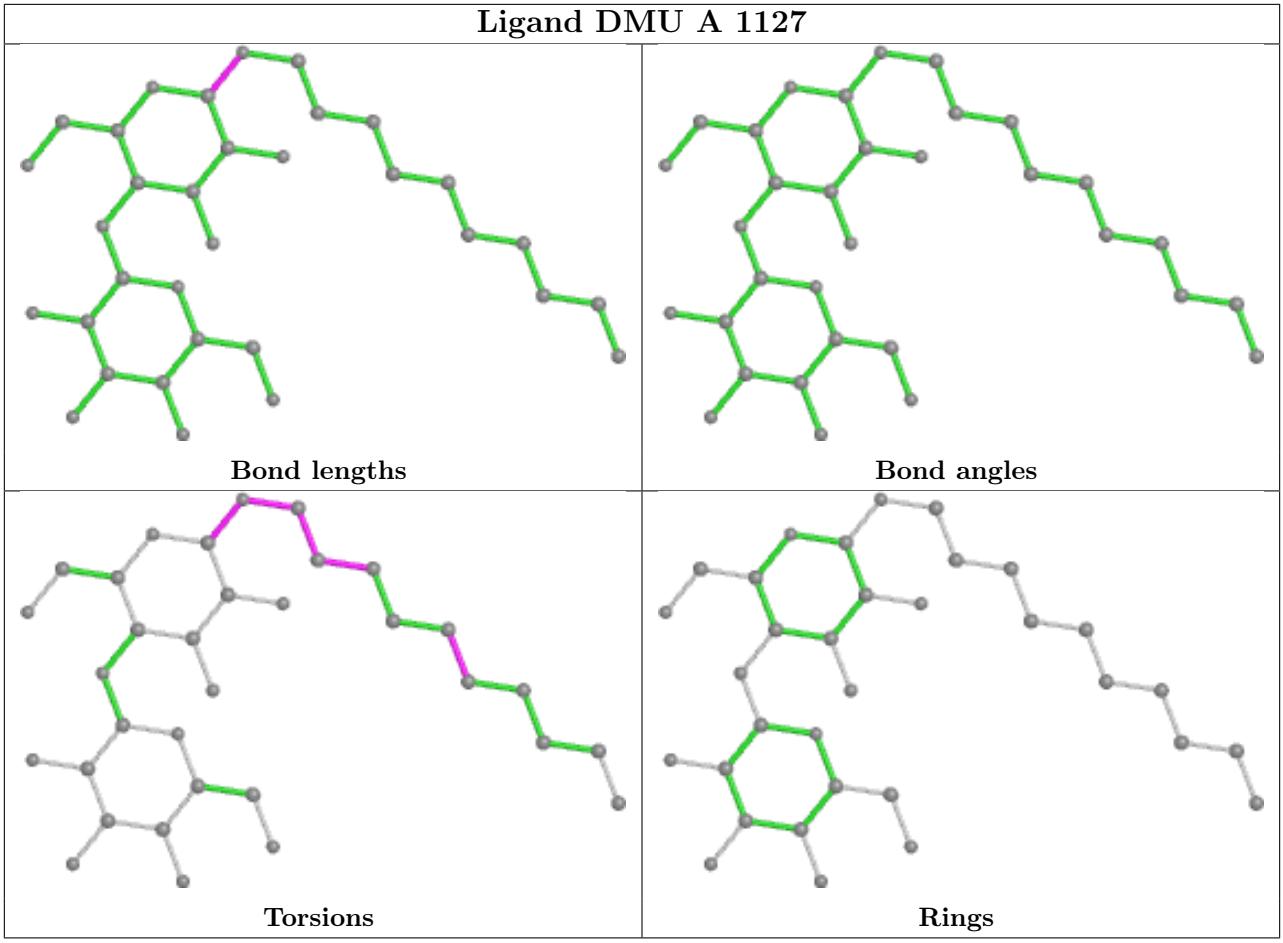
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand DMU C 1097



Ligand DMU B 1129





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)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.