wwPDB X-ray Structure Validation Summary Report (i)

Apr 15, 2024 – 04:12 PM EDT

PDB ID	:	8SGB
Title	:	Crystal Structure of CD1d-lipid complexed with Beta-2-Microglobulin, TCR Alpha-Chain and TCR Beta-Chain
Authors	:	Chan Yew Poa, K.T.O.; Le Nours, J.; Rossjohn, J.
Deposited on	:	2023-04-12
Resolution	:	2.80 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:

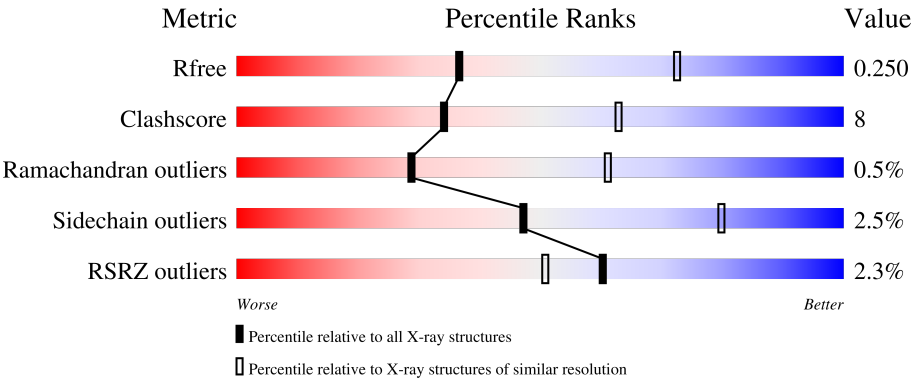
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	347	5%, 60%, 17%, 22%
2	B	100	89%, 7%
3	C	207	83%, 16%
4	D	243	83%, 15%
5	E	3	100%

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
7	FO4	A	403	X	-	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6439 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 Antigen-presenting glycoprotein CD1d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2105	1345	364	389	7			

There are 73 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP P15813
A	279	SER	-	expression tag	UNP P15813
A	280	LEU	-	expression tag	UNP P15813
A	281	VAL	-	expression tag	UNP P15813
A	282	PRO	-	expression tag	UNP P15813
A	283	ARG	-	expression tag	UNP P15813
A	284	GLY	-	expression tag	UNP P15813
A	285	SER	-	expression tag	UNP P15813
A	286	GLY	-	expression tag	UNP P15813
A	287	SER	-	expression tag	UNP P15813
A	288	ARG	-	expression tag	UNP P15813
A	289	ILE	-	expression tag	UNP P15813
A	290	ALA	-	expression tag	UNP P15813
A	291	ARG	-	expression tag	UNP P15813
A	292	LEU	-	expression tag	UNP P15813
A	293	GLU	-	expression tag	UNP P15813
A	294	GLU	-	expression tag	UNP P15813
A	295	LYS	-	expression tag	UNP P15813
A	296	VAL	-	expression tag	UNP P15813
A	297	LYS	-	expression tag	UNP P15813
A	298	THR	-	expression tag	UNP P15813
A	299	LEU	-	expression tag	UNP P15813
A	300	LYS	-	expression tag	UNP P15813
A	301	ALA	-	expression tag	UNP P15813
A	302	GLN	-	expression tag	UNP P15813
A	303	ASN	-	expression tag	UNP P15813
A	304	SER	-	expression tag	UNP P15813

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Chain	Residue	Modelled	Actual	Comment	Reference
A	305	GLU	-	expression tag	UNP P15813
A	306	LEU	-	expression tag	UNP P15813
A	307	ALA	-	expression tag	UNP P15813
A	308	SER	-	expression tag	UNP P15813
A	309	THR	-	expression tag	UNP P15813
A	310	ALA	-	expression tag	UNP P15813
A	311	ASN	-	expression tag	UNP P15813
A	312	MET	-	expression tag	UNP P15813
A	313	LEU	-	expression tag	UNP P15813
A	314	ARG	-	expression tag	UNP P15813
A	315	GLU	-	expression tag	UNP P15813
A	316	GLN	-	expression tag	UNP P15813
A	317	VAL	-	expression tag	UNP P15813
A	318	ALA	-	expression tag	UNP P15813
A	319	GLN	-	expression tag	UNP P15813
A	320	LEU	-	expression tag	UNP P15813
A	321	LYS	-	expression tag	UNP P15813
A	322	GLN	-	expression tag	UNP P15813
A	323	LYS	-	expression tag	UNP P15813
A	324	VAL	-	expression tag	UNP P15813
A	325	MET	-	expression tag	UNP P15813
A	326	ASN	-	expression tag	UNP P15813
A	327	HIS	-	expression tag	UNP P15813
A	328	GLY	-	expression tag	UNP P15813
A	329	SER	-	expression tag	UNP P15813
A	330	GLY	-	expression tag	UNP P15813
A	331	LEU	-	expression tag	UNP P15813
A	332	ASN	-	expression tag	UNP P15813
A	333	ASP	-	expression tag	UNP P15813
A	334	ILE	-	expression tag	UNP P15813
A	335	PHE	-	expression tag	UNP P15813
A	336	GLU	-	expression tag	UNP P15813
A	337	ALA	-	expression tag	UNP P15813
A	338	GLN	-	expression tag	UNP P15813
A	339	LYS	-	expression tag	UNP P15813
A	340	ILE	-	expression tag	UNP P15813
A	341	GLU	-	expression tag	UNP P15813
A	342	TRP	-	expression tag	UNP P15813
A	343	HIS	-	expression tag	UNP P15813
A	344	GLU	-	expression tag	UNP P15813
A	345	HIS	-	expression tag	UNP P15813
A	346	HIS	-	expression tag	UNP P15813

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Chain	Residue	Modelled	Actual	Comment	Reference
A	347	HIS	-	expression tag	UNP P15813
A	348	HIS	-	expression tag	UNP P15813
A	349	HIS	-	expression tag	UNP P15813
A	350	HIS	-	expression tag	UNP P15813

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			808	514	136	156	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

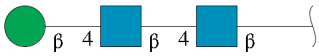
- Molecule 3 is a protein called Natural Killer T cell receptor TRAV26A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	205	Total	C	N	O	S	0	0	0
			1550	970	265	306	9			

- Molecule 4 is a protein called Natural Killer T cell receptor TRBV19 beta chain.

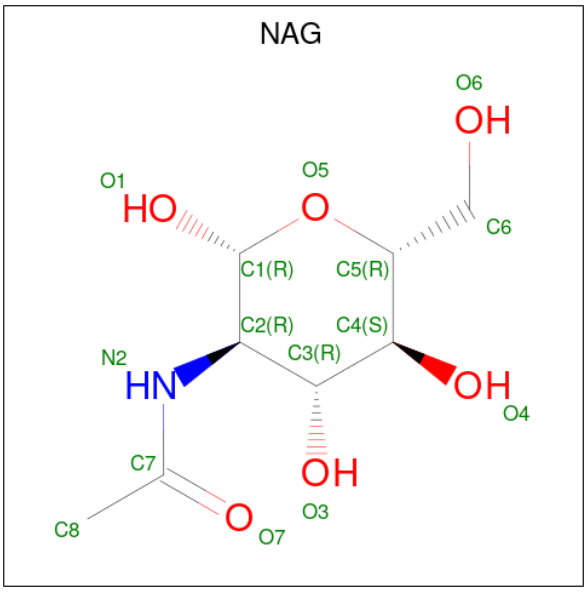
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1833	1161	318	348	6			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



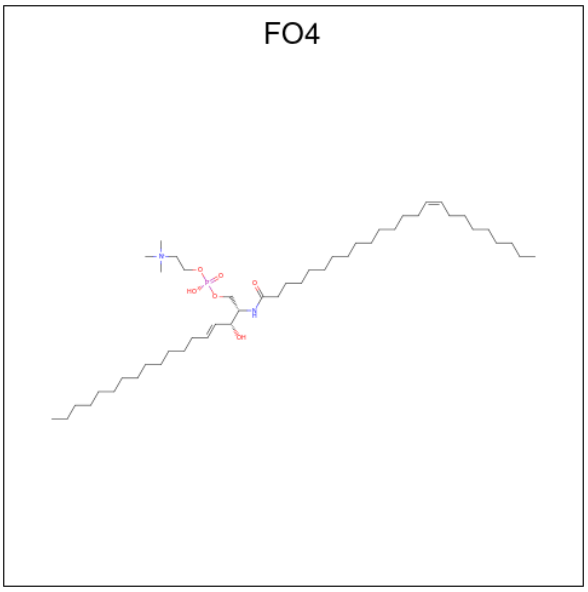
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is sphingomyelin (three-letter code: FO4) (formula: $C_{47}H_{94}N_2O_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			56	47	2	6	1		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Na 1 1	0	0

- Molecule 9 is water.

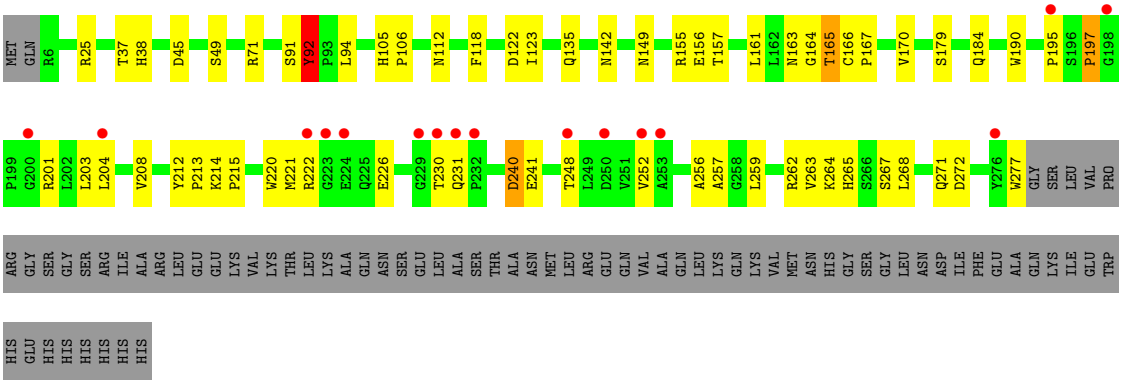
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	5	Total O 5 5	0	0
9	B	4	Total O 4 4	0	0
9	C	8	Total O 8 8	0	0
9	D	2	Total O 2 2	0	0

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.

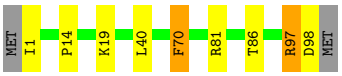
• Molecule 1: Antigen-presenting glycoprotein CD1d

Chain A:



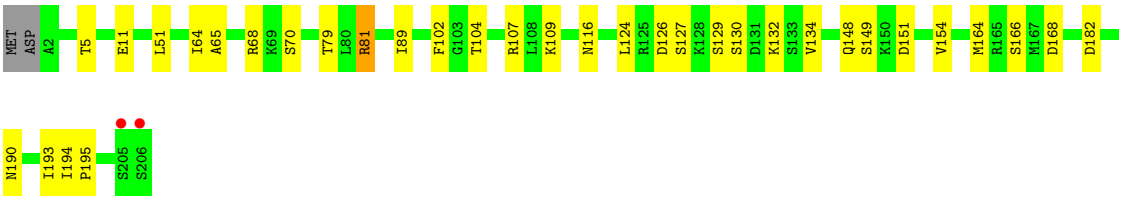
• Molecule 2: Beta-2-microglobulin

Chain B:



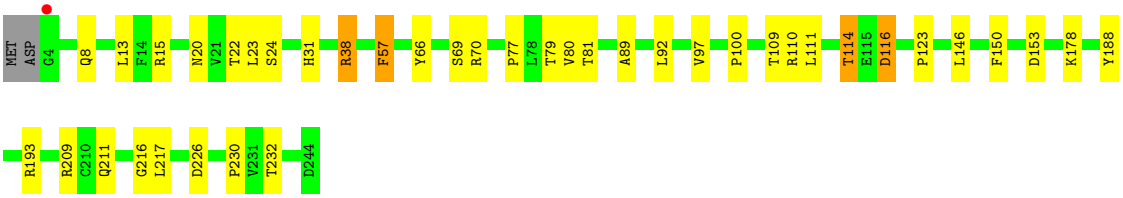
• Molecule 3: Natural Killer T cell receptor TRAV26A-2 alpha chain

Chain C:



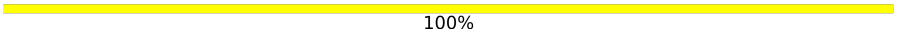
• Molecule 4: Natural Killer T cell receptor TRBV19 beta chain

Chain D:



• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	136.78Å 136.78Å 69.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.36 – 2.80 48.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.36-2.80) 99.9 (48.36-2.80)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155, PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.208 , 0.249 0.209 , 0.250	Depositor DCC
R_{free} test set	1643 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	71.6	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6439	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 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FO4, BMA, NA, NAG

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	0.33	0/2170	0.51	0/2969
2	B	0.33	0/831	0.51	0/1130
3	C	0.33	0/1587	0.52	0/2170
4	D	0.39	1/1887 (0.1%)	0.51	0/2585
All	All	0.35	1/6475 (0.0%)	0.51	0/8854

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	57	PHE	CG-CD1	-5.22	1.30	1.38

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2105	0	1939	50	1
2	B	808	0	752	6	1
3	C	1550	0	1411	20	0
4	D	1833	0	1636	29	0
5	E	39	0	34	1	0
6	A	28	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	56	0	0	0	0
8	A	1	0	0	0	0
9	A	5	0	0	2	0
9	B	4	0	0	0	0
9	C	8	0	0	4	0
9	D	2	0	0	0	0
All	All	6439	0	5798	103	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 8.

The worst 5 of 103 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)
3:C:51:LEU:O	3:C:68:ARG:NH1	1.84	1.11
1:A:268:LEU:HD22	1:A:271:GLN:O	1.49	1.10
3:C:126:ASP:OD2	3:C:127:SER:N	2.08	0.86
4:D:209:ARG:NH1	4:D:211:GLN:OE1	2.08	0.86
3:C:116:ASN:OD1	9:C:301:HOH:O	1.95	0.82

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:135:GLN:O	2:B:19:LYS:NZ[4_544]	2.16	0.04

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	270/347 (78%)	248 (92%)	20 (7%)	2 (1%)	22 53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	96/100 (96%)	89 (93%)	7 (7%)	0	100	100
3	C	203/207 (98%)	184 (91%)	18 (9%)	1 (0%)	29	61
4	D	239/243 (98%)	214 (90%)	24 (10%)	1 (0%)	34	66
All	All	808/897 (90%)	735 (91%)	69 (8%)	4 (0%)	29	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	116	ASP
1	A	197	PRO
3	C	168	ASP
1	A	92	TYR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/302 (72%)	211 (98%)	5 (2%)	50	82
2	B	90/95 (95%)	88 (98%)	2 (2%)	52	83
3	C	164/185 (89%)	159 (97%)	5 (3%)	41	75
4	D	181/212 (85%)	177 (98%)	4 (2%)	52	83
All	All	651/794 (82%)	635 (98%)	16 (2%)	47	80

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	114	THR
4	D	38	ARG
3	C	70	SER
4	D	15	ARG
3	C	5	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
4	D	8	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

3 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	$\#\|Z\| > 2$
5	NAG	E	1	5,1	14,14,15	0.44	0	17,19,21	0.48	0
5	NAG	E	2	5	14,14,15	0.45	0	17,19,21	1.07	1 (5%)
5	BMA	E	3	5	11,11,12	1.32	2 (18%)	15,15,17	1.20	2 (13%)

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
5	NAG	E	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	3	BMA	C4-C5	2.61	1.58	1.53
5	E	3	BMA	O5-C5	2.25	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	2	NAG	C1-O5-C5	3.03	116.30	112.19
5	E	3	BMA	O5-C1-C2	-2.59	106.77	110.77
5	E	3	BMA	C1-C2-C3	-2.18	106.98	109.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

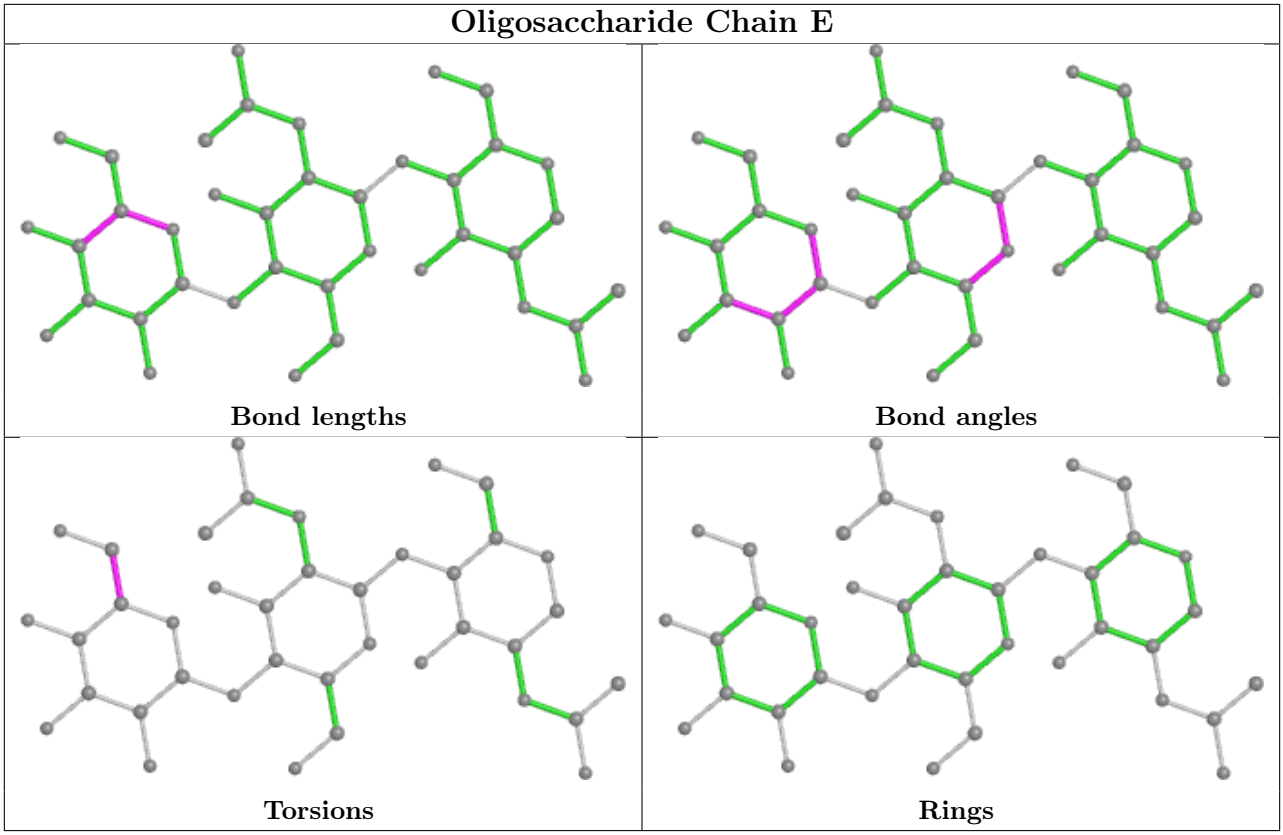
Mol	Chain	Res	Type	Atoms
5	E	3	BMA	C4-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	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.



5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
7	FO4	A	403	-	54,55,55	2.29	7 (12%)	60,63,63	1.18	7 (11%)
6	NAG	A	401	1	14,14,15	0.39	0	17,19,21	0.66	0
6	NAG	A	402	1	14,14,15	0.53	0	17,19,21	0.61	1 (5%)

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
6	NAG	A	401	1	-	3/6/23/26	0/1/1/1
7	FO4	A	403	-	1/1/5/10	24/60/60/60	-
6	NAG	A	402	1	-	2/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	403	FO4	O-C	-13.26	1.18	1.43
7	A	403	FO4	C17-N	6.78	1.48	1.34
7	A	403	FO4	C-C1	3.24	1.55	1.50
7	A	403	FO4	C18-C17	2.71	1.56	1.51
7	A	403	FO4	P-O2	2.27	1.68	1.59

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	403	FO4	O-C-C16	4.73	120.49	107.93
7	A	403	FO4	O-C-C1	3.31	119.71	110.85
7	A	403	FO4	C16-N-C17	-3.20	118.08	123.48
7	A	403	FO4	C18-C17-N	2.43	120.04	115.83
7	A	403	FO4	O1-C17-N	-2.28	119.11	122.95

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	403	FO4	C

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	403	FO4	O-C-C1-C2
7	A	403	FO4	C42-O4-P-O2
7	A	403	FO4	O4-C42-C43-N1
7	A	403	FO4	C1-C-C16-N
7	A	403	FO4	C1-C-C16-C41

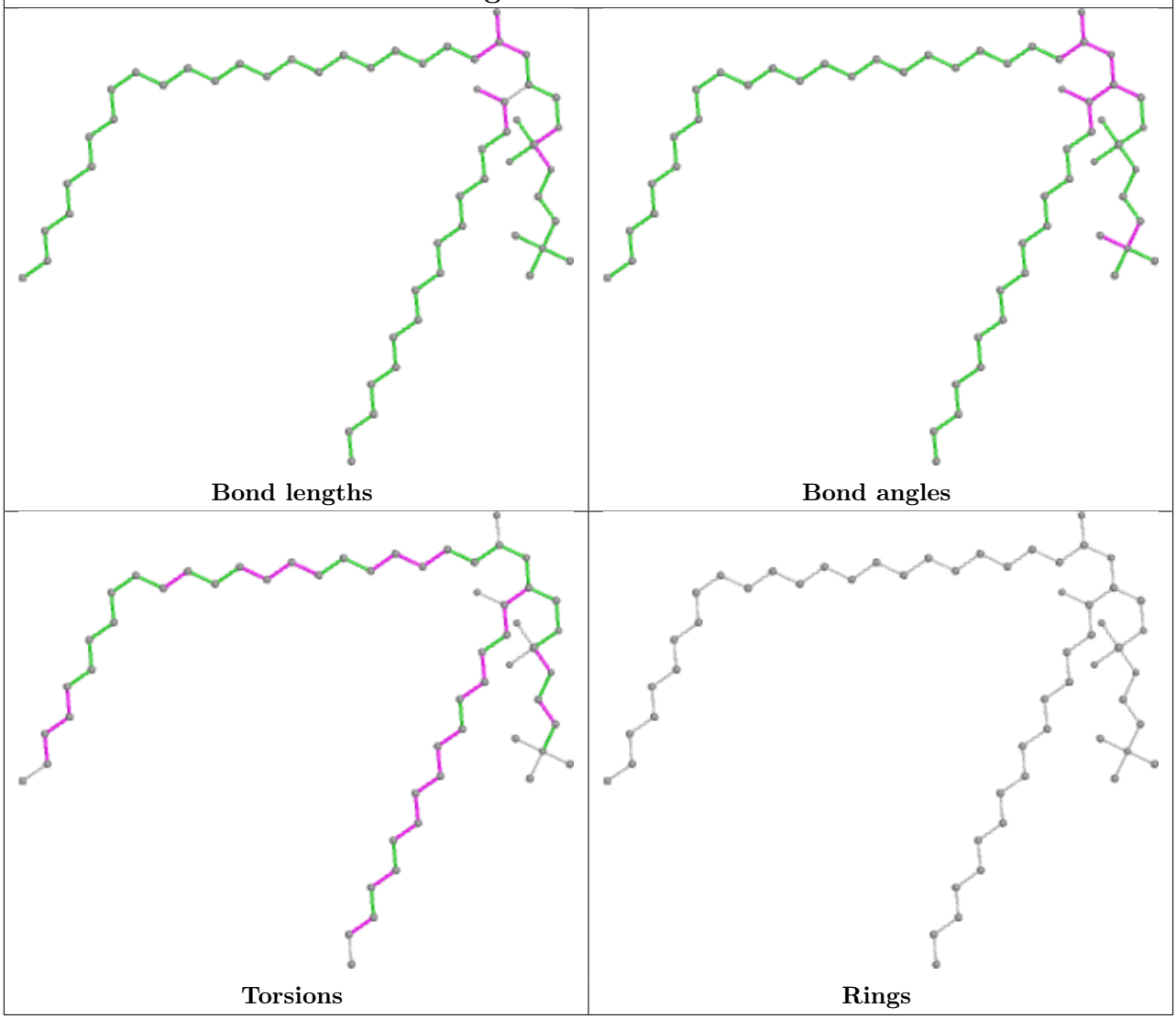
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	402	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 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 FO4 A 403



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	272/347 (78%)	-0.01	16 (5%) 22 14	48, 71, 129, 167	0
2	B	98/100 (98%)	-0.46	0 100 100	44, 56, 83, 117	0
3	C	205/207 (99%)	-0.20	2 (0%) 82 77	41, 60, 106, 131	0
4	D	241/243 (99%)	-0.36	1 (0%) 92 91	43, 85, 116, 127	0
All	All	816/897 (90%)	-0.22	19 (2%) 60 51	41, 68, 118, 167	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	GLY	9.4
1	A	229	GLY	6.2
1	A	231	GLN	5.0
1	A	232	PRO	4.0
1	A	198	GLY	3.9

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

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

6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	E	3	11/12	0.66	0.24	98,106,118,121	0
5	NAG	E	2	14/15	0.92	0.15	74,84,90,92	0

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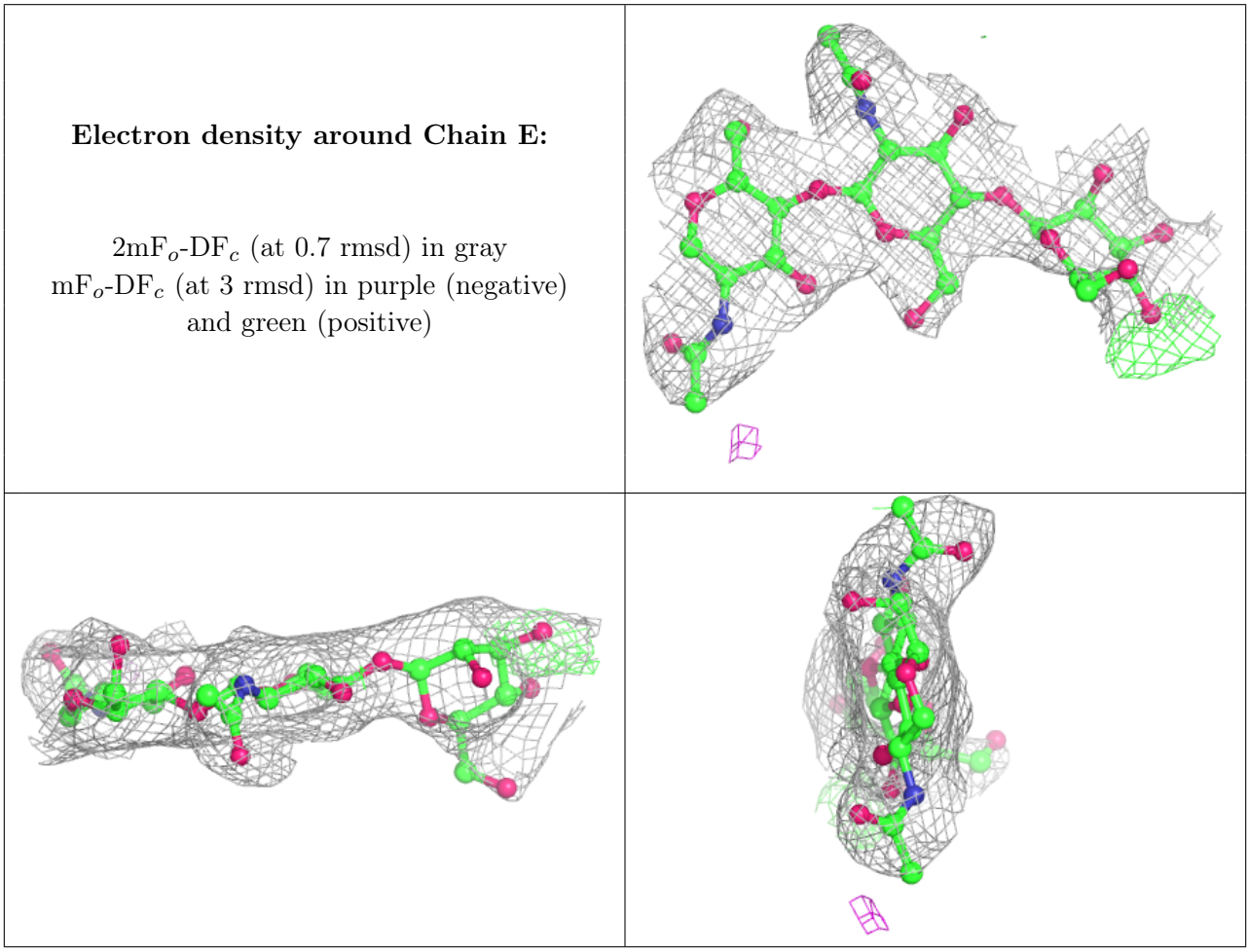
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	E	1	14/15	0.96	0.14	59,70,82,92	0

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 E:

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



6.4 Ligands

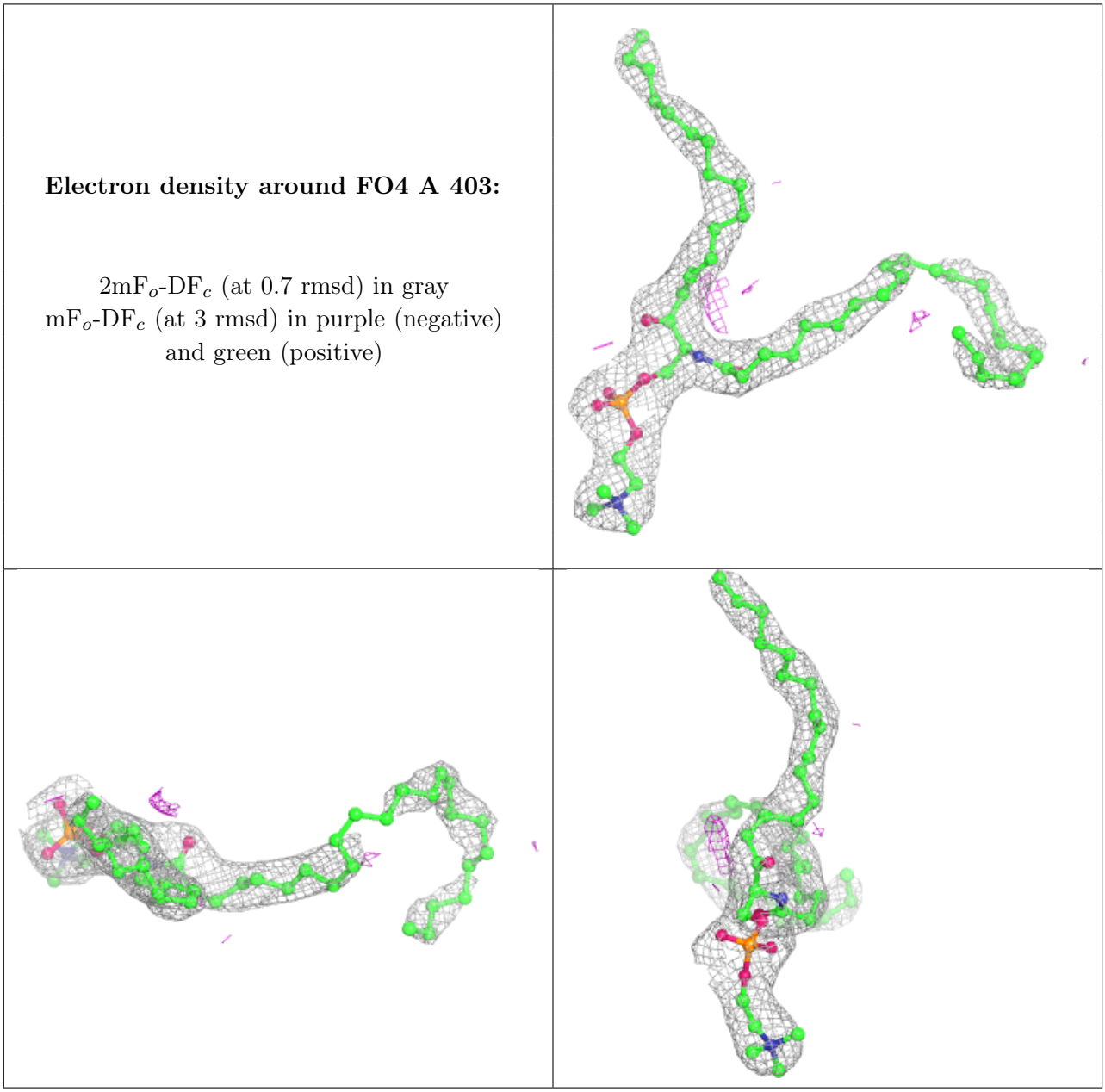
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	A	401	14/15	0.88	0.14	86,105,110,112	0
6	NAG	A	402	14/15	0.90	0.17	86,94,106,107	0
8	NA	A	404	1/1	0.94	0.12	67,67,67,67	0
7	FO4	A	403	56/56	0.96	0.27	54,66,89,97	0

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

Electron density around FO4 A 403:

$2mF_o$-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.