Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2023 – 06:04 PM EST

PDB ID	:	8SOS
Title	:	Human CD1d presenting sphingomyelin C24:1 in complex with VHH nanobody 1D17
Authors	:	Shahine, A.; Rossjohn, J.
Deposited on	:	2023-04-29
Resolution	:	2.33 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

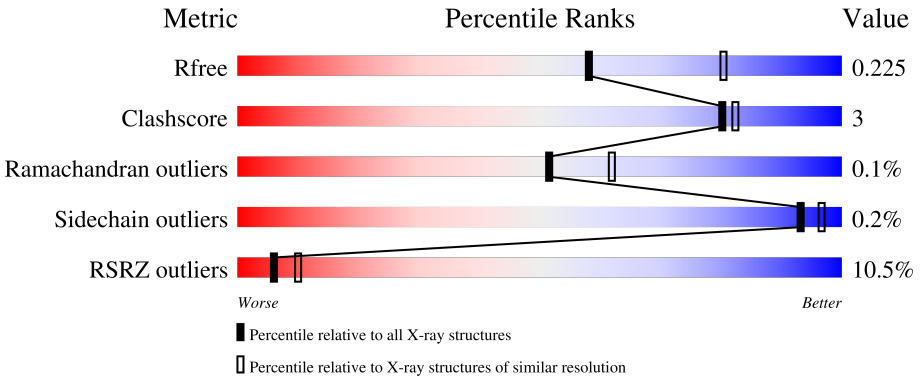
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 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 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	11% 69% 8% 22%
1	E	347	13% 71% 6% 23%
2	B	100	6% 94%
2	F	100	12% 93% 5%
3	D	127	2% 94% 6%

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Mol	Chain	Length	Quality of chain
3	G	127	2% 94% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8568 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	271	Total	C	N	O	S	0	2	0
			2164	1388	373	396	7			
1	E	268	Total	C	N	O	S	0	1	0
			2114	1355	362	390	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP P15813
E	4	MET	-	initiating methionine	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	2	0
			809	518	138	151	2			
2	F	98	Total	C	N	O	S	0	0	0
			800	510	136	152	2			

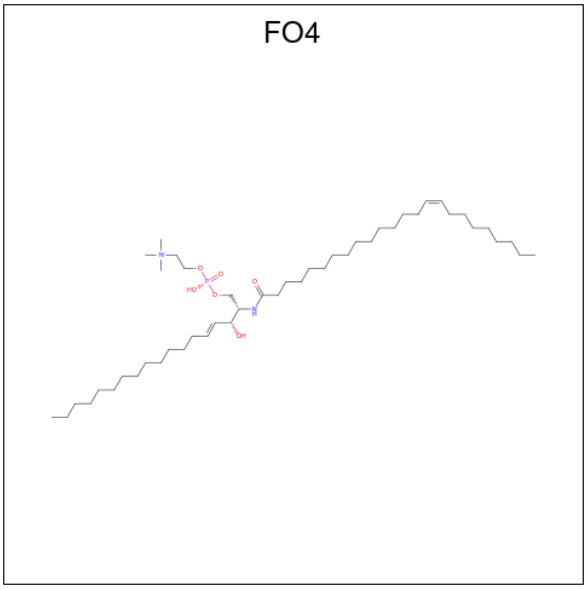
There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called Nanobody VHH ID17.

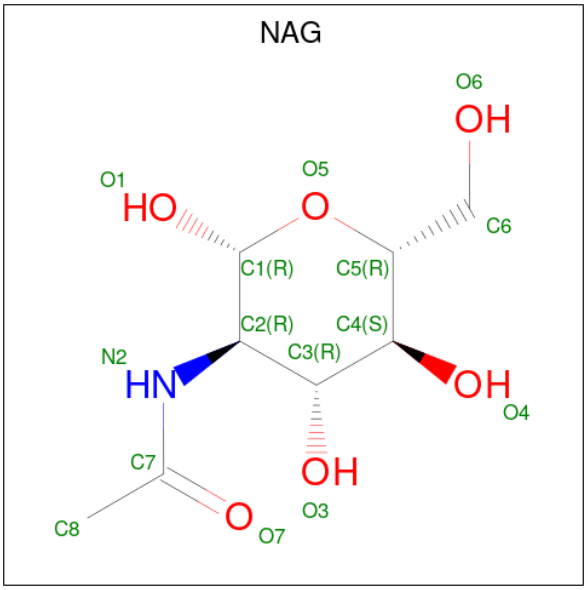
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	127	Total	C	N	O	S	0	0	0
			967	609	168	185	5			
3	G	127	Total	C	N	O	S	0	0	0
			974	613	170	186	5			

- Molecule 4 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
4	A	1	Total	C	N	O	P	0	0
			56	47	2	6	1		
4	E	1	Total	C	N	O	P	0	0
			56	47	2	6	1		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is water.

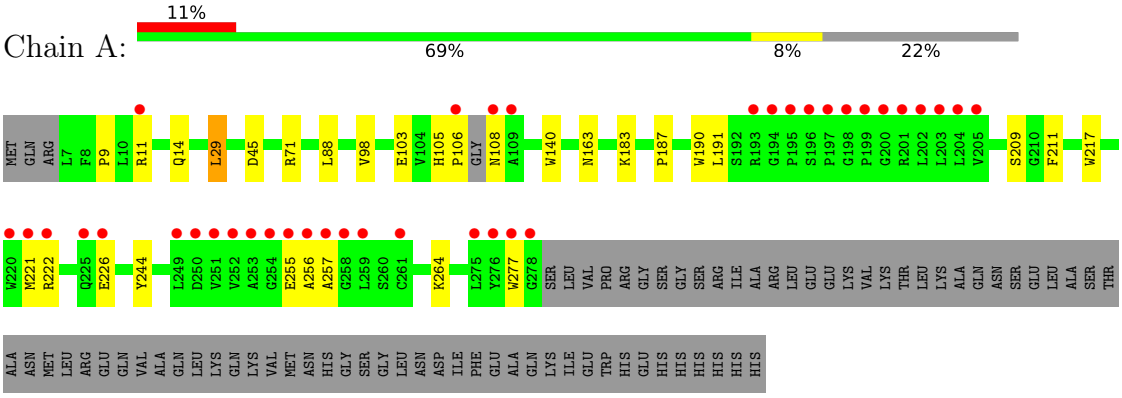
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	135	Total O 135 135	0	0
6	B	89	Total O 89 89	0	0
6	D	57	Total O 57 57	0	0
6	E	166	Total O 166 166	0	0
6	F	39	Total O 39 39	0	0
6	G	86	Total O 86 86	0	0

3 Residue-property plots

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.

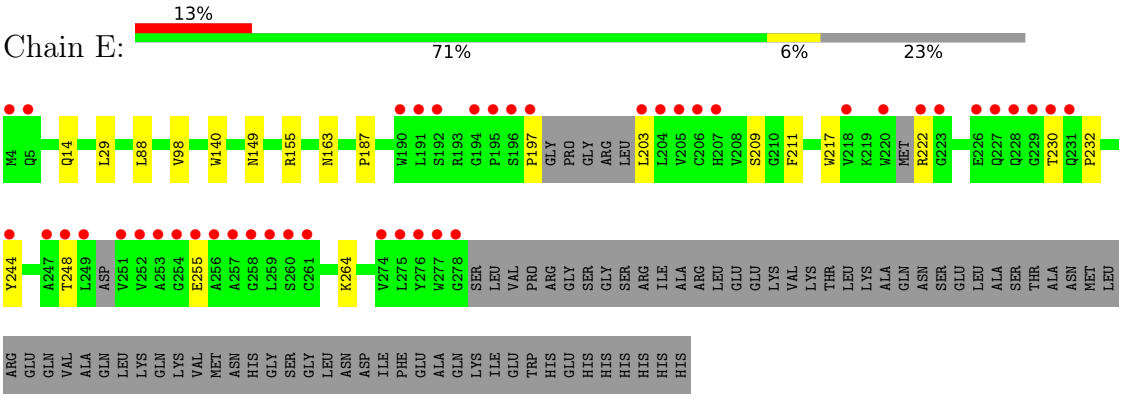
• Molecule 1: Antigen-presenting glycoprotein CD1d

Chain A:



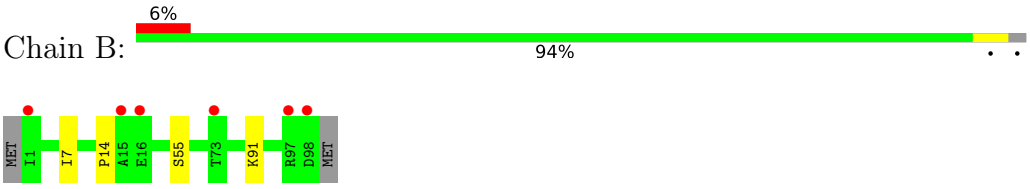
• Molecule 1: Antigen-presenting glycoprotein CD1d

Chain E:



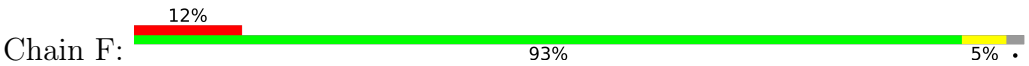
• Molecule 2: Beta-2-microglobulin

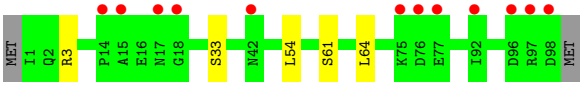
Chain B:



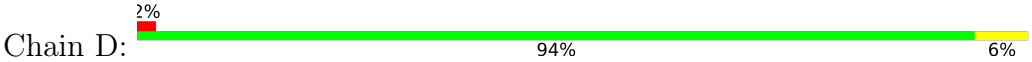
• Molecule 2: Beta-2-microglobulin

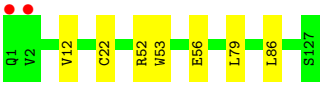
Chain F:



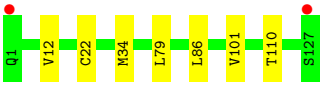


• Molecule 3: Nanobody VHH ID17





• Molecule 3: Nanobody VHH ID17



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	136.45Å 136.45Å 166.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.66 – 2.33 44.66 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.66-2.33) 99.9 (44.66-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487)	Depositor
R, R_{free}	0.209 , 0.230 0.205 , 0.225	Depositor DCC
R_{free} test set	3991 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	42.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8568	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: NAG, FO4

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	0.24	0/2234	0.46	0/3045
1	E	0.24	0/2178	0.47	0/2966
2	B	0.24	0/838	0.48	0/1140
2	F	0.24	0/823	0.48	0/1120
3	D	0.24	0/988	0.52	0/1339
3	G	0.25	0/995	0.52	0/1347
All	All	0.24	0/8056	0.48	0/10957

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2164	0	2078	18	0
1	E	2114	0	1994	12	0
2	B	809	0	763	3	0
2	F	800	0	744	3	0
3	D	967	0	949	4	0
3	G	974	0	964	4	0
4	A	56	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	56	0	0	0	0
5	A	28	0	26	0	0
5	E	28	0	26	0	0
6	A	135	0	0	4	0
6	B	89	0	0	0	0
6	D	57	0	0	0	0
6	E	166	0	0	2	0
6	F	39	0	0	0	0
6	G	86	0	0	0	0
All	All	8568	0	7544	42	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 3.

All (42) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:PRO:HB3	1:E:211:PHE:HB3	1.74	0.69
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.75	0.69
1:E:222:ARG:NH2	1:E:255:GLU:O	2.23	0.67
1:E:217:TRP:HB3	1:E:264:LYS:HB2	1.78	0.66
1:E:209:SER:HB2	1:E:244:TYR:HD1	1.66	0.61
1:E:163:ASN:ND2	6:E:503:HOH:O	2.34	0.60
2:B:7:ILE:HD12	2:B:91:LYS:HD3	1.82	0.60
1:A:163:ASN:ND2	6:A:507:HOH:O	2.37	0.58
1:A:217:TRP:HB3	1:A:264:LYS:HB2	1.87	0.57
1:A:14:GLN:HB3	1:A:98:VAL:HB	1.87	0.57
2:F:33:SER:HB2	2:F:54:LEU:HD21	1.88	0.55
1:A:209:SER:HB2	1:A:244:TYR:HD1	1.73	0.53
1:A:221:MET:HG2	1:A:226:GLU:HA	1.90	0.53
1:A:9:PRO:HB3	1:A:103:GLU:HB3	1.91	0.51
1:A:183:LYS:NZ	6:A:512:HOH:O	2.43	0.51
1:A:255:GLU:O	1:A:257:ALA:N	2.39	0.50
1:E:14:GLN:HB3	1:E:98:VAL:HB	1.93	0.50
1:E:149:ASN:HA	1:E:155:ARG:HD2	1.96	0.47
1:E:230:THR:O	1:E:232:PRO:HD3	2.14	0.47
1:A:11:ARG:NH1	6:A:510:HOH:O	2.40	0.46
3:G:34:MET:HB3	3:G:79:LEU:HD22	1.98	0.46
3:G:12:VAL:HG11	3:G:86:LEU:HD13	1.98	0.46
2:F:54:LEU:HA	2:F:64:LEU:HD13	1.99	0.45
3:D:12:VAL:HG21	3:D:86:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:52:ARG:HD2	3:D:53:TRP:CE3	2.53	0.43
1:A:45:ASP:O	1:A:71:ARG:HD3	2.19	0.43
1:A:29:LEU:HD11	2:B:55:SER:HB2	2.00	0.43
1:A:105:HIS:ND1	6:A:506:HOH:O	2.37	0.42
1:E:203:LEU:HD11	1:E:248:THR:HB	2.01	0.42
1:A:190:TRP:CZ3	2:B:14:PRO:HD3	2.54	0.42
1:A:88:LEU:HD13	1:A:140:TRP:CE3	2.55	0.41
1:E:88:LEU:HD13	1:E:140:TRP:CE3	2.55	0.41
1:A:106:PRO:O	1:A:108:ASN:ND2	2.42	0.41
1:A:191:LEU:HD13	1:A:277:TRP:HE3	1.85	0.41
1:E:197:PRO:HD3	1:E:203:LEU:HB2	2.02	0.41
2:F:3:ARG:HH11	2:F:61:SER:HB3	1.86	0.41
3:D:52:ARG:HB3	3:D:56:GLU:OE1	2.21	0.41
1:E:163:ASN:ND2	6:E:517:HOH:O	2.54	0.41
3:D:22:CYS:HB3	3:D:79:LEU:HB3	2.02	0.40
1:A:222:ARG:NH1	1:A:257:ALA:O	2.53	0.40
3:G:22:CYS:HB3	3:G:79:LEU:HB3	2.03	0.40
3:G:101:VAL:HG11	3:G:110:THR:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	269/347 (78%)	261 (97%)	7 (3%)	1 (0%)	34 38
1	E	261/347 (75%)	255 (98%)	6 (2%)	0	100 100
2	B	98/100 (98%)	98 (100%)	0	0	100 100
2	F	96/100 (96%)	96 (100%)	0	0	100 100
3	D	125/127 (98%)	122 (98%)	3 (2%)	0	100 100
3	G	125/127 (98%)	122 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	974/1148 (85%)	954 (98%)	19 (2%)	1 (0%)	51 62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	ALA

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	233/302 (77%)	232 (100%)	1 (0%)	91 95
1	E	223/302 (74%)	222 (100%)	1 (0%)	91 95
2	B	89/95 (94%)	89 (100%)	0	100 100
2	F	88/95 (93%)	88 (100%)	0	100 100
3	D	102/104 (98%)	102 (100%)	0	100 100
3	G	104/104 (100%)	104 (100%)	0	100 100
All	All	839/1002 (84%)	837 (100%)	2 (0%)	93 96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	E	29	LEU

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)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	403	1	14,14,15	0.26	0	17,19,21	0.41	0
5	NAG	E	403	1	14,14,15	0.24	0	17,19,21	0.39	0
5	NAG	A	402	1	14,14,15	0.19	0	17,19,21	0.57	0
4	FO4	E	401	-	54,55,55	0.32	0	60,63,63	0.42	0
4	FO4	A	401	-	54,55,55	0.33	0	60,63,63	0.37	0
5	NAG	E	402	1	14,14,15	0.26	0	17,19,21	0.41	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
5	NAG	A	403	1	-	2/6/23/26	0/1/1/1
5	NAG	E	403	1	-	2/6/23/26	0/1/1/1
5	NAG	A	402	1	-	1/6/23/26	0/1/1/1
4	FO4	E	401	-	-	7/60/60/60	-
4	FO4	A	401	-	-	11/60/60/60	-
5	NAG	E	402	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	401	FO4	C16-C-C1-C2
4	E	401	FO4	O-C-C1-C2
4	E	401	FO4	C41-O2-P-O5
5	A	403	NAG	C8-C7-N2-C2
5	A	403	NAG	O7-C7-N2-C2
5	E	403	NAG	C8-C7-N2-C2
5	E	403	NAG	O7-C7-N2-C2
4	E	401	FO4	C41-O2-P-O4
4	A	401	FO4	C27-C28-C29-C30
4	E	401	FO4	C36-C37-C38-C39
5	E	402	NAG	C4-C5-C6-O6
5	E	402	NAG	O5-C5-C6-O6
4	E	401	FO4	C41-O2-P-O3
4	A	401	FO4	O4-C42-C43-N1
4	A	401	FO4	C30-C31-C32-C33
4	A	401	FO4	C33-C34-C35-C36
4	A	401	FO4	C3-C4-C5-C6
4	E	401	FO4	C29-C30-C31-C32
5	A	402	NAG	C3-C2-N2-C7
4	A	401	FO4	C29-C30-C31-C32
4	A	401	FO4	C37-C38-C39-C40
4	A	401	FO4	C10-C11-C12-C13
4	A	401	FO4	C-C16-N-C17
4	A	401	FO4	O1-C17-C18-C19
4	A	401	FO4	C6-C7-C8-C9

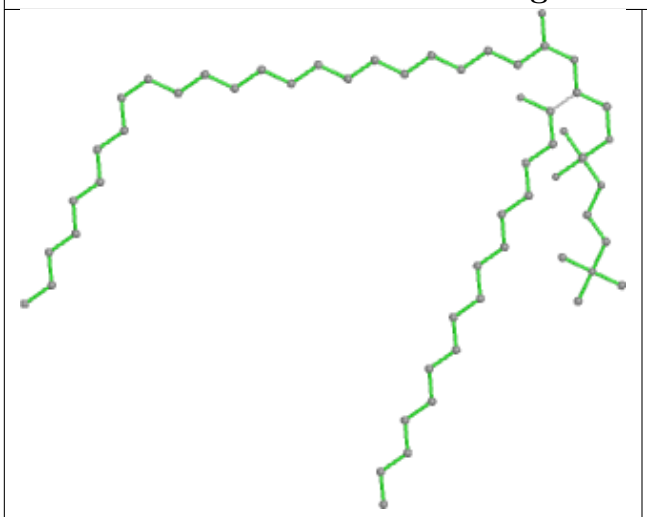
There are no ring outliers.

No monomer is involved in short contacts.

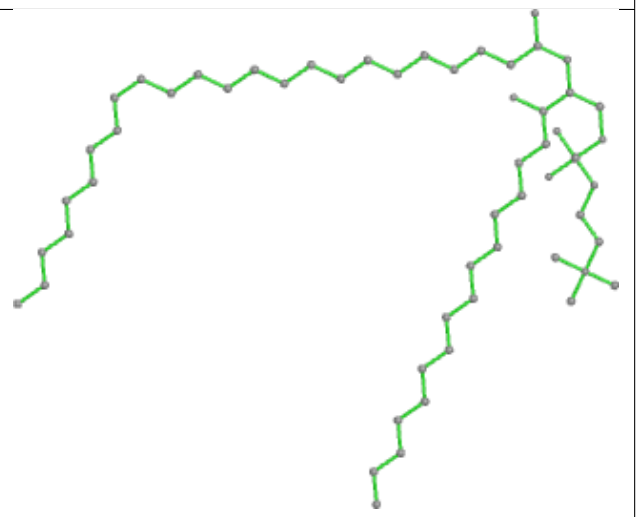
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

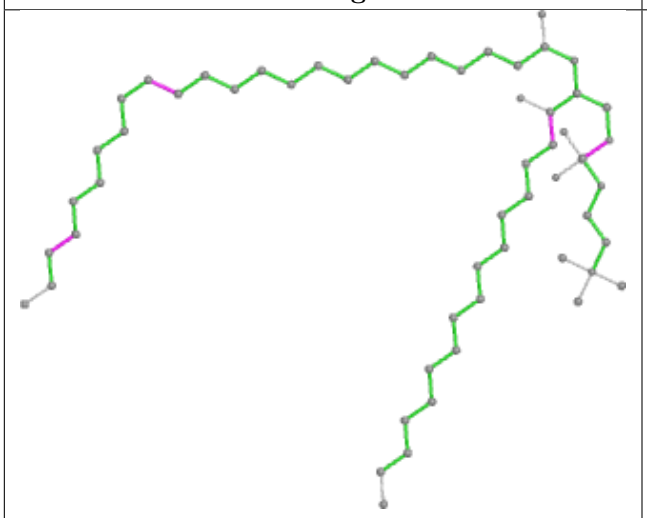
Ligand FO4 E 401



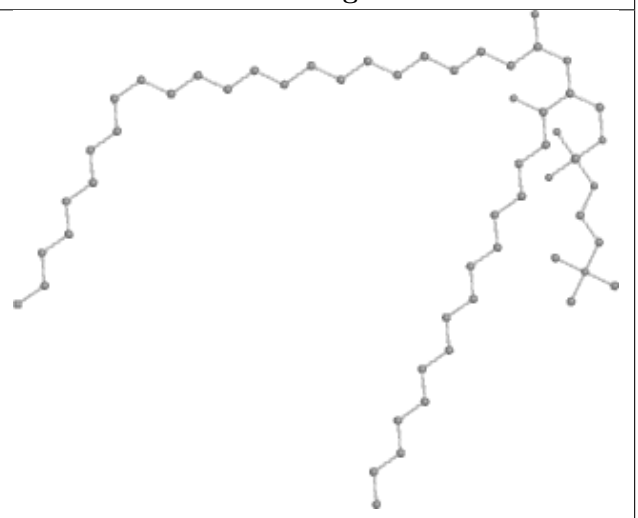
Bond lengths



Bond angles

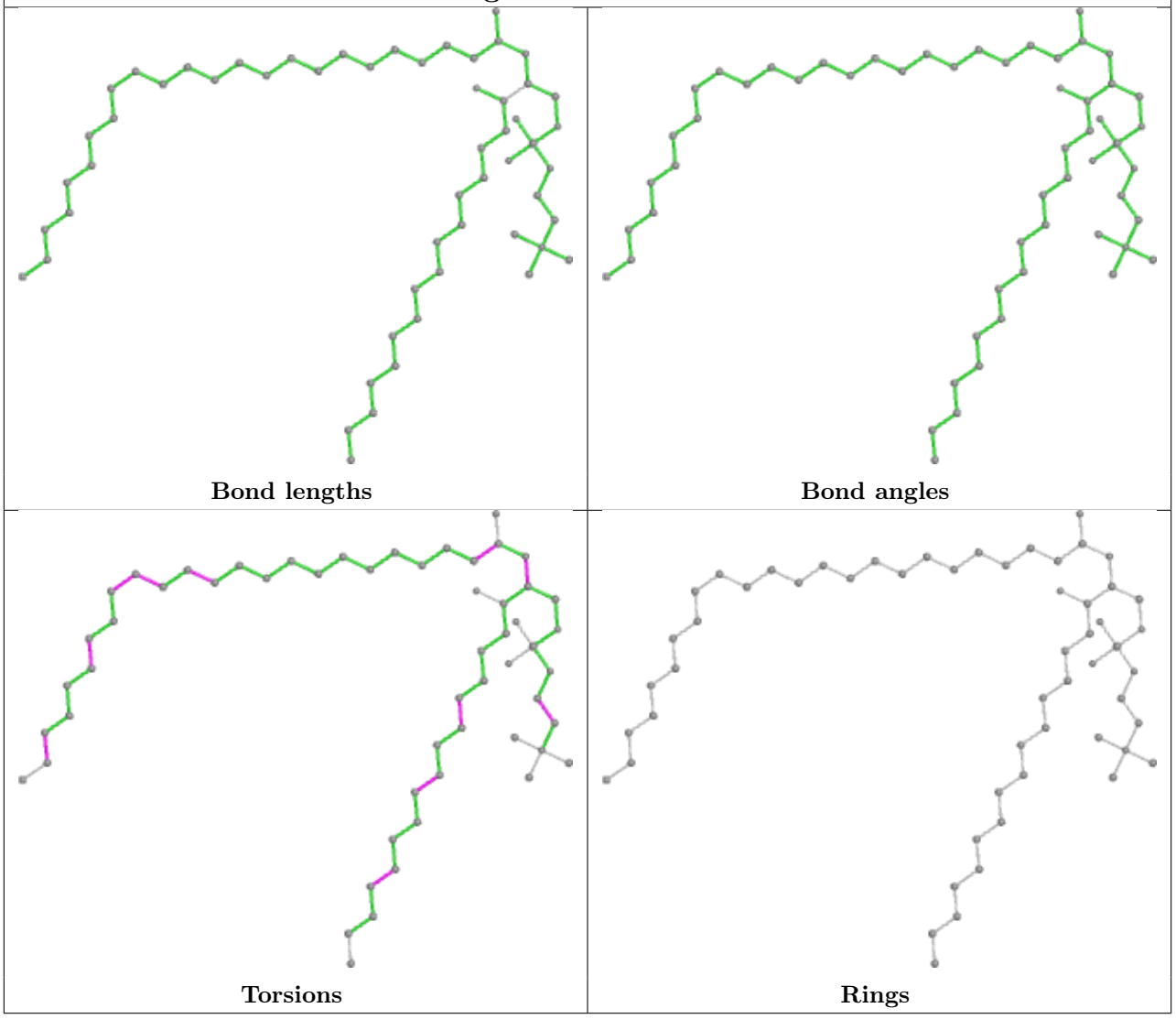


Torsions



Rings

Ligand FO4 A 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	271/347 (78%)	0.86	38 (14%) 2 4	30, 46, 121, 162	0
1	E	268/347 (77%)	1.01	44 (16%) 1 2	26, 45, 122, 161	0
2	B	98/100 (98%)	0.62	6 (6%) 21 30	28, 42, 85, 112	0
2	F	98/100 (98%)	0.80	12 (12%) 4 7	32, 68, 114, 130	0
3	D	127/127 (100%)	0.19	2 (1%) 72 80	38, 57, 80, 105	0
3	G	127/127 (100%)	0.03	2 (1%) 72 80	31, 43, 62, 110	0
All	All	989/1148 (86%)	0.68	104 (10%) 6 10	26, 49, 114, 162	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	197	PRO	8.7
1	A	109	ALA	8.5
1	E	277	TRP	8.2
1	E	258	GLY	8.1
1	E	256	ALA	8.0
1	E	190	TRP	7.5
1	A	198	GLY	7.4
1	E	275	LEU	7.3
1	E	254	GLY	6.5
1	A	195	PRO	6.4
1	E	257	ALA	6.4
1	E	203	LEU	6.2
1	A	258	GLY	6.2
1	A	256	ALA	6.2
1	A	254	GLY	6.0
1	E	276	TYR	6.0
1	A	199	PRO	5.9
1	A	106	PRO	5.8
1	E	252	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
1	E	260	SER	5.4
2	F	98	ASP	5.4
1	A	200	GLY	5.4
1	E	261	CYS	5.3
1	A	252	VAL	5.1
1	A	204	LEU	4.9
1	E	4	MET	4.8
1	A	202	LEU	4.8
1	A	251	VAL	4.6
1	A	203	LEU	4.6
1	A	196	SER	4.6
1	A	257	ALA	4.6
1	E	223	GLY	4.5
1	E	230	THR	4.5
1	E	255	GLU	4.4
2	F	15	ALA	4.4
1	E	248	THR	4.4
1	A	197	PRO	4.3
1	E	220	TRP	4.3
1	A	194	GLY	4.3
2	F	17	ASN	4.3
2	F	97	ARG	4.3
1	E	228	GLN	4.2
1	E	253	ALA	4.1
1	E	259	LEU	4.1
1	E	205	VAL	4.0
1	A	253	ALA	3.9
1	E	204	LEU	3.9
3	G	127	SER	3.9
1	A	201	ARG	3.9
2	B	73	THR	3.9
1	A	255	GLU	3.9
2	F	77	GLU	3.9
2	F	14	PRO	3.8
1	A	277	TRP	3.8
1	E	191	LEU	3.8
1	A	205	VAL	3.7
1	E	227	GLN	3.7
1	A	221	MET	3.6
1	E	206	CYS	3.6
1	E	278	GLY	3.5
1	A	276	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	225	GLN	3.5
1	E	229	GLY	3.4
1	A	193	ARG	3.4
1	E	247	ALA	3.4
1	E	251	VAL	3.3
1	E	196	SER	3.2
1	A	249	LEU	3.2
1	A	259	LEU	3.2
1	A	250	ASP	3.2
1	A	108	ASN	3.1
2	B	98	ASP	3.1
3	D	1	GLN	3.0
2	B	15	ALA	3.0
1	E	195	PRO	3.0
1	A	222	ARG	2.9
1	E	192	SER	2.9
2	F	76	ASP	2.9
2	F	75	LYS	2.9
2	F	96	ASP	2.8
1	E	222	ARG	2.8
1	A	220	TRP	2.7
1	A	226	GLU	2.7
1	A	275	LEU	2.7
2	B	97	ARG	2.6
2	B	1	ILE	2.6
1	E	226	GLU	2.6
1	E	5	GLN	2.6
1	E	249	LEU	2.6
2	F	92	ILE	2.5
1	E	207	HIS	2.5
1	A	261	CYS	2.5
3	D	2	VAL	2.4
1	E	218	VAL	2.4
1	E	231	GLN	2.4
1	E	244	TYR	2.3
1	E	194	GLY	2.3
1	A	278	GLY	2.3
2	B	16	GLU	2.2
2	F	18	GLY	2.2
3	G	1	GLN	2.1
1	E	274	VAL	2.1
1	A	11	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	42	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

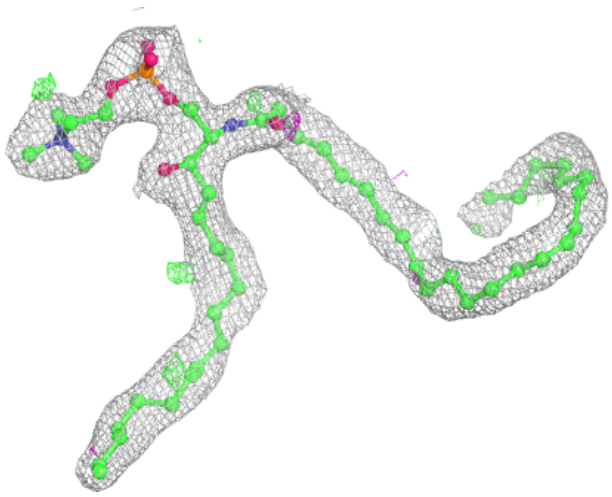
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

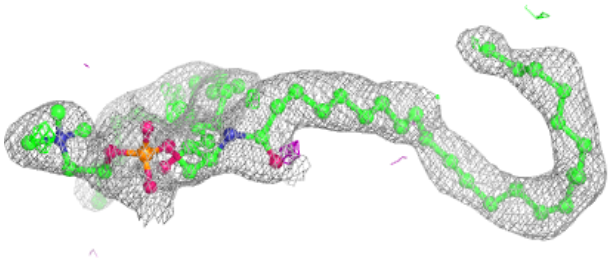
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	A	402	14/15	0.81	0.15	60,67,78,87	0
4	FO4	E	401	56/56	0.90	0.20	29,46,63,71	0
4	FO4	A	401	56/56	0.91	0.18	28,45,70,77	0
5	NAG	E	403	14/15	0.91	0.16	34,43,52,55	0
5	NAG	E	402	14/15	0.93	0.12	41,46,55,58	0
5	NAG	A	403	14/15	0.96	0.13	36,44,57,60	0

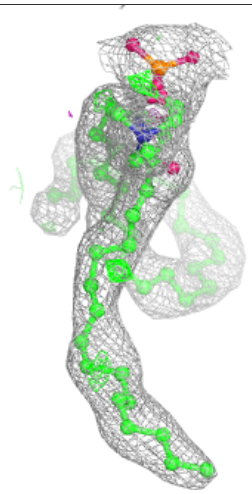
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FO4 E 401:

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

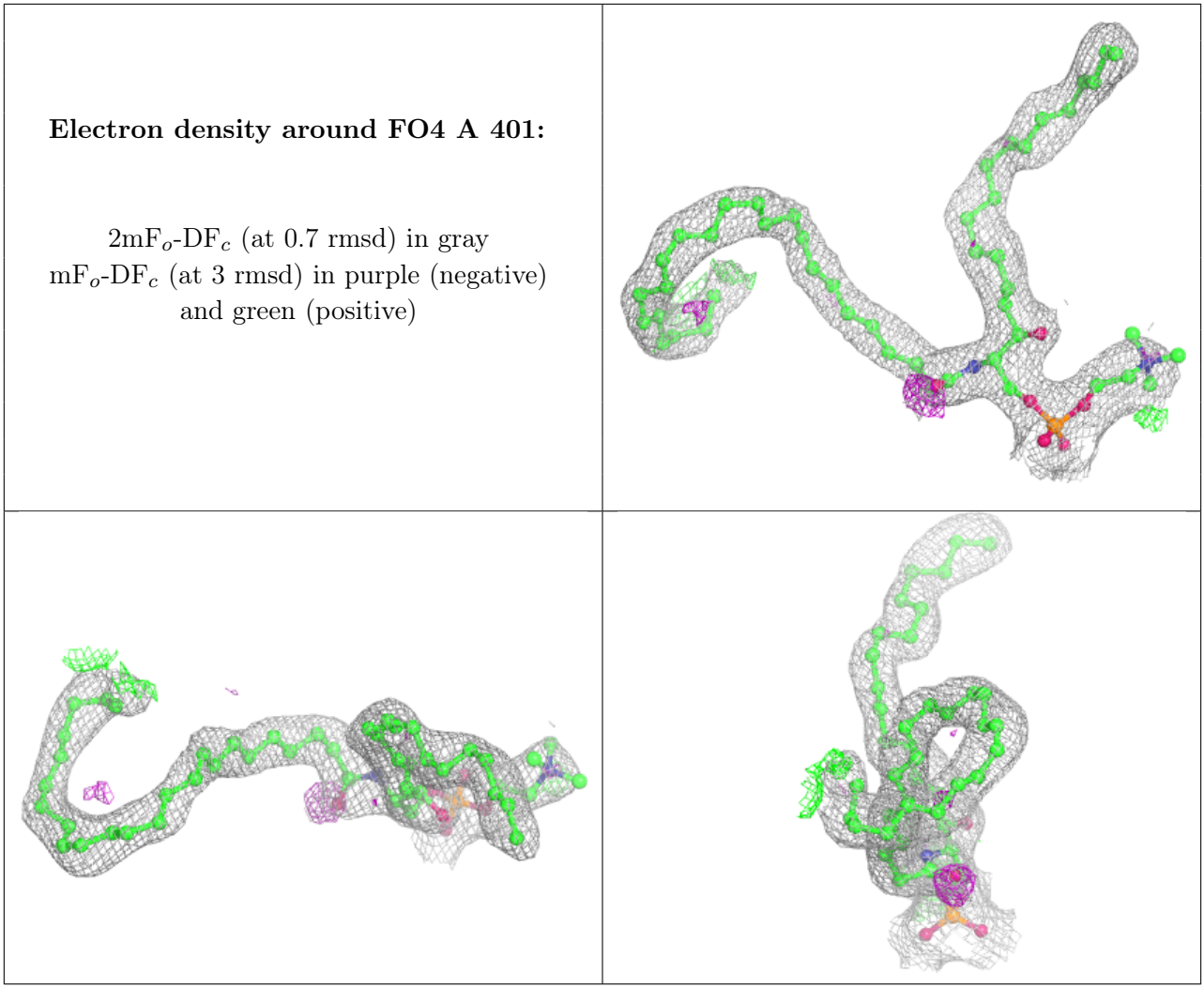






Electron density around FO4 A 401:

$2mF_o$-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.