



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 09:45 AM UTC

PDB ID : 6VL8 / pdb_00006vl8
Title : Anti-PEG antibody 6-3 Fab fragment in complex with PEG
Authors : Nicely, N.I.; Huckaby, J.T.; Lai, S.K.; Jacobs, T.M.
Deposited on : 2020-01-23
Resolution : 2.42 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

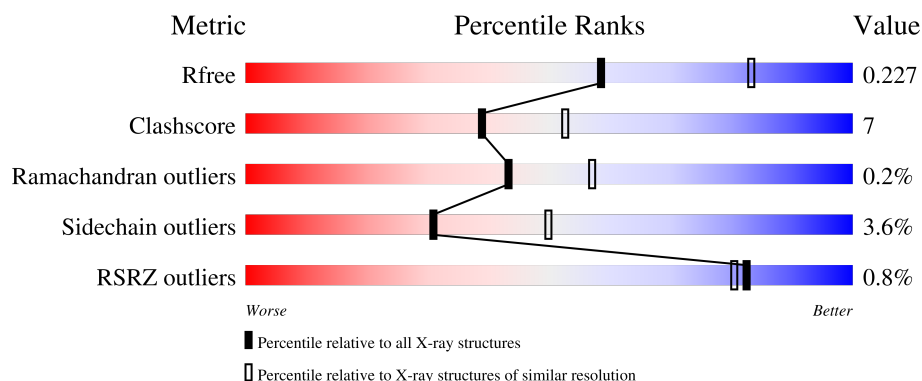
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	228	80% 11% 8%
1	C	228	75% 15% 8%
1	E	228	76% 16% 7%
1	H	228	83% 7% 8%
2	B	219	84% 15%

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Mol	Chain	Length	Quality of chain
2	D	219	
2	F	219	
2	L	219	

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
3	EDO	D	301	-	-	X	-
4	PEU	C	301	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13788 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 6-3 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1587	1019	261	301	6			
1	C	209	Total	C	N	O	S	0	0	0
			1589	1020	261	302	6			
1	E	211	Total	C	N	O	S	0	0	0
			1599	1025	263	305	6			
1	H	209	Total	C	N	O	S	0	0	0
			1587	1019	261	301	6			

- Molecule 2 is a protein called 6-3 Fab light chain.

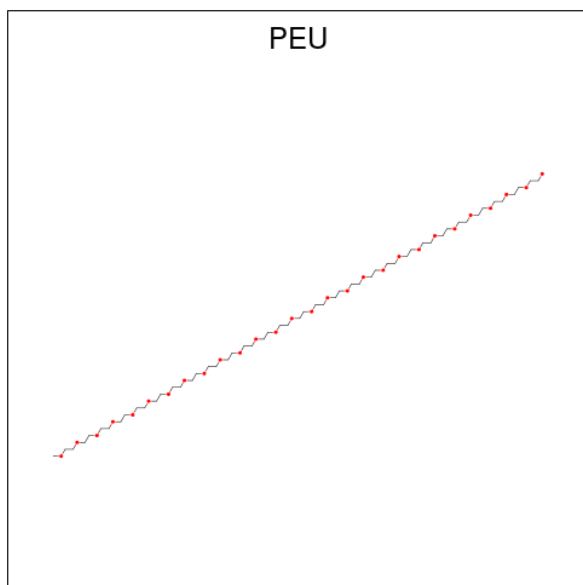
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1683	1056	278	342	7			
2	D	218	Total	C	N	O	S	0	0	0
			1683	1056	278	342	7			
2	F	218	Total	C	N	O	S	0	0	0
			1683	1056	278	342	7			
2	L	218	Total	C	N	O	S	0	1	0
			1688	1059	278	344	7			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 2,5,8,11,14,17,20,23,26,29,32,35,38,41,44,47,50,53,56,59,62,65,68,71,74,77,80-HEPTACOSAOXADOCTACONTAN-82-OL (CCD ID: PEU) (formula: C₅₅H₁₁₂O₂₈) (labeled as "Ligand of Interest" by depositor).

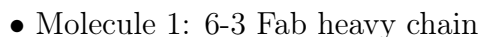
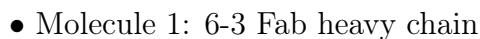
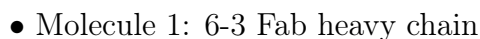


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			73	48	25		
4	E	1	Total	C	O	0	0
			73	48	25		

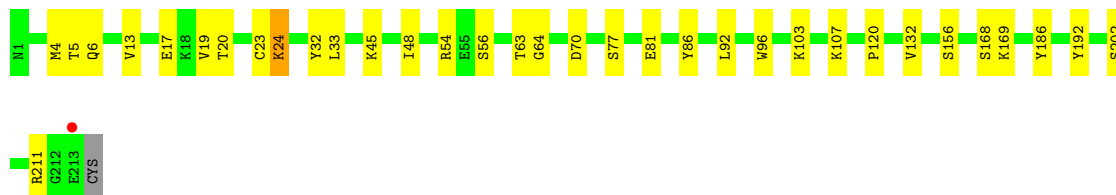
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	60	Total	O	0	0
			60	60		
5	B	85	Total	O	0	0
			85	85		
5	C	54	Total	O	0	0
			54	54		
5	D	64	Total	O	0	0
			64	64		
5	E	52	Total	O	0	0
			52	52		
5	F	55	Total	O	0	0
			55	55		
5	H	70	Total	O	0	0
			70	70		
5	L	91	Total	O	0	0
			91	91		

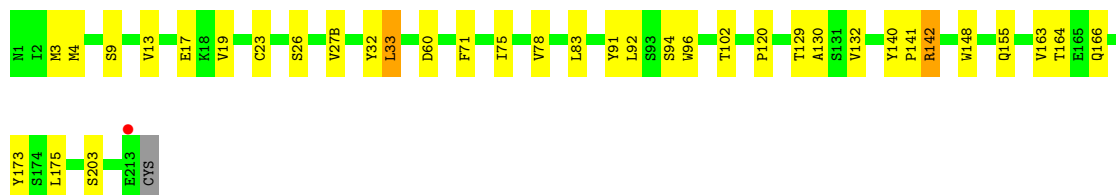
- Molecule 1: 6-3 Fab heavy chain



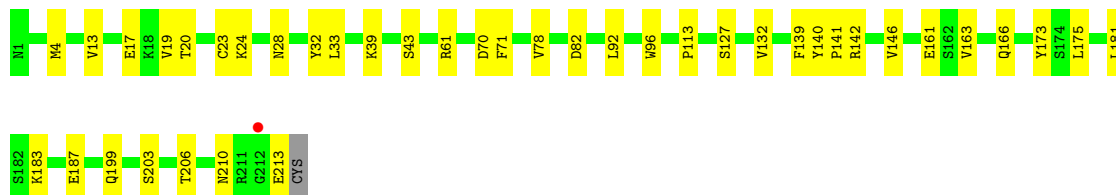
• Molecule 2: 6-3 Fab light chain

Chain B:  84% 15%

• Molecule 2: 6-3 Fab light chain

Chain D:  83% 16%

• Molecule 2: 6-3 Fab light chain

Chain F:  81% 18%

• Molecule 2: 6-3 Fab light chain

Chain L:  88% 11%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.11Å 87.79Å 116.07Å 90.00° 113.66° 90.00°	Depositor
Resolution (Å)	41.92 – 2.42 41.92 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.2 (41.92-2.42) 99.2 (41.92-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.184 , 0.240 (Not available) , 0.227	Depositor DCC
R_{free} test set	2006 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.813	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13788	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.9988e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PEU

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	0/1631	0.55	0/2223
1	C	0.33	0/1633	0.51	0/2226
1	E	0.32	0/1643	0.49	0/2239
1	H	0.37	0/1631	0.54	0/2223
2	B	0.36	0/1719	0.54	0/2334
2	D	0.35	0/1719	0.53	0/2334
2	F	0.32	0/1719	0.53	0/2334
2	L	0.39	0/1727	0.57	0/2345
All	All	0.35	0/13422	0.53	0/18258

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 [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	1587	0	1563	22	0
1	C	1589	0	1565	30	0
1	E	1599	0	1573	25	0
1	H	1587	0	1563	19	0
2	B	1683	0	1636	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1683	0	1636	32	0
2	F	1683	0	1636	23	0
2	L	1688	0	1640	16	0
3	A	4	0	6	0	0
3	D	4	0	6	5	0
3	H	4	0	6	0	0
4	C	73	0	96	30	0
4	E	73	0	96	14	0
5	A	60	0	0	2	0
5	B	85	0	0	2	0
5	C	54	0	0	2	0
5	D	64	0	0	2	0
5	E	52	0	0	2	0
5	F	55	0	0	2	0
5	H	70	0	0	1	0
5	L	91	0	0	2	0
All	All	13788	0	13022	179	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 7.

The worst 5 of 179 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:B:96:TRP:HE1	4:E:301:PEU:HCQ2	1.12	1.11
1:A:96:TRP:H	4:E:301:PEU:HCN1	1.16	1.06
4:C:301:PEU:HCQ1	2:D:96:TRP:HE1	1.19	1.04
2:L:70[A]:ASP:OD1	5:L:301:HOH:O	1.85	0.93
4:C:301:PEU:HAJ2	1:H:96:TRP:H	1.35	0.91

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	205/228 (90%)	194 (95%)	11 (5%)	0	100	100
1	C	205/228 (90%)	193 (94%)	12 (6%)	0	100	100
1	E	207/228 (91%)	196 (95%)	10 (5%)	1 (0%)	24	35
1	H	205/228 (90%)	195 (95%)	8 (4%)	2 (1%)	12	18
2	B	216/219 (99%)	209 (97%)	6 (3%)	1 (0%)	24	35
2	D	216/219 (99%)	210 (97%)	6 (3%)	0	100	100
2	F	216/219 (99%)	205 (95%)	11 (5%)	0	100	100
2	L	217/219 (99%)	207 (95%)	10 (5%)	0	100	100
All	All	1687/1788 (94%)	1609 (95%)	74 (4%)	4 (0%)	43	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	211	ARG
1	H	65	GLY
1	H	96	TRP
1	E	101	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	174/193 (90%)	166 (95%)	8 (5%)	24	39
1	C	175/193 (91%)	167 (95%)	8 (5%)	24	39
1	E	176/193 (91%)	171 (97%)	5 (3%)	38	58
1	H	174/193 (90%)	172 (99%)	2 (1%)	65	81
2	B	193/194 (100%)	182 (94%)	11 (6%)	18	31
2	D	193/194 (100%)	188 (97%)	5 (3%)	40	61
2	F	193/194 (100%)	184 (95%)	9 (5%)	23	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	194/194 (100%)	189 (97%)	5 (3%)	40 61
All	All	1472/1548 (95%)	1419 (96%)	53 (4%)	31 50

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	129	THR
1	E	180	SER
2	L	20	THR
2	D	132	VAL
1	E	58	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	204	GLN
2	F	147	GLN
2	L	160	GLN
2	F	199	GLN
2	D	22	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
4	PEU	E	301	-	72,72,82	1.44	11 (15%)	71,71,81	0.51	0
3	EDO	A	301	-	3,3,3	0.44	0	2,2,2	0.88	0
3	EDO	H	301	-	3,3,3	0.52	0	2,2,2	0.11	0
4	PEU	C	301	-	72,72,82	1.26	7 (9%)	71,71,81	0.52	0
3	EDO	D	301	-	3,3,3	0.55	0	2,2,2	0.20	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	PEU	E	301	-	-	35/70/70/80	-
3	EDO	A	301	-	-	1/1/1/1	-
3	EDO	H	301	-	-	0/1/1/1	-
4	PEU	C	301	-	-	35/70/70/80	-
3	EDO	D	301	-	-	0/1/1/1	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	301	PEU	CAG-CAF	4.00	1.69	1.49
4	E	301	PEU	CAD-CAC	3.78	1.69	1.49
4	C	301	PEU	CCR-CCQ	3.35	1.65	1.49
4	E	301	PEU	CCR-CCQ	3.26	1.65	1.49
4	C	301	PEU	CAG-CAF	3.16	1.64	1.49

There are no bond angle outliers.

There are no chirality outliers.

5 of 71 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	301	PEU	CCO-CCN-OCM-CCL
4	E	301	PEU	CBQ-CBR-OBS-CBT
4	C	301	PEU	CCG-CCF-OCE-CCD

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Mol	Chain	Res	Type	Atoms
4	C	301	PEU	OAH-CAI-CAJ-OAK
4	E	301	PEU	OAK-CAL-CAM-OAN

There are no ring outliers.

3 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	301	PEU	14	0
4	C	301	PEU	30	0
3	D	301	EDO	5	0

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

Ligand PEU E 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEU C 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers ⓘ

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	209/228 (91%)	-0.26	3 (1%) 73 70	29, 41, 57, 87	0
1	C	209/228 (91%)	-0.23	1 (0%) 87 86	32, 42, 64, 90	2 (0%)
1	E	211/228 (92%)	-0.05	2 (0%) 81 79	33, 48, 77, 124	1 (0%)
1	H	209/228 (91%)	-0.29	4 (1%) 66 63	29, 39, 58, 76	0
2	B	218/219 (99%)	-0.27	1 (0%) 87 86	28, 40, 62, 80	0
2	D	218/219 (99%)	-0.13	1 (0%) 87 86	31, 46, 63, 93	0
2	F	218/219 (99%)	0.08	1 (0%) 87 86	31, 49, 83, 107	0
2	L	218/219 (99%)	-0.39	0 100 100	27, 36, 48, 67	1 (0%)
All	All	1710/1788 (95%)	-0.19	13 (0%) 82 80	27, 42, 69, 124	4 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	SER	4.1
1	C	128	SER	3.6
1	H	126	PRO	3.6
1	A	126	PRO	3.2
2	F	212	GLY	3.0

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

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

6.3 Carbohydrates [i](#)

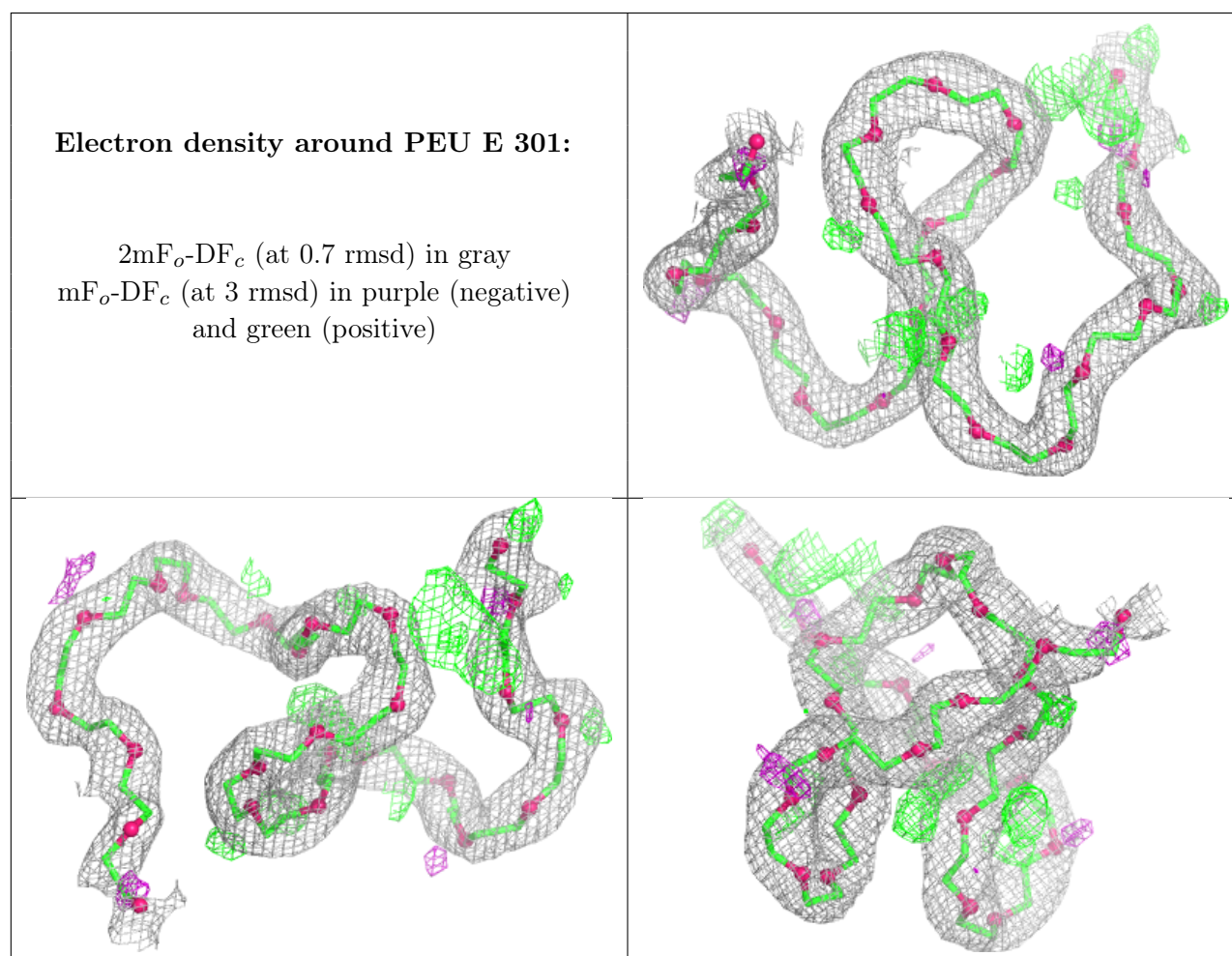
There are no oligosaccharides in this entry.

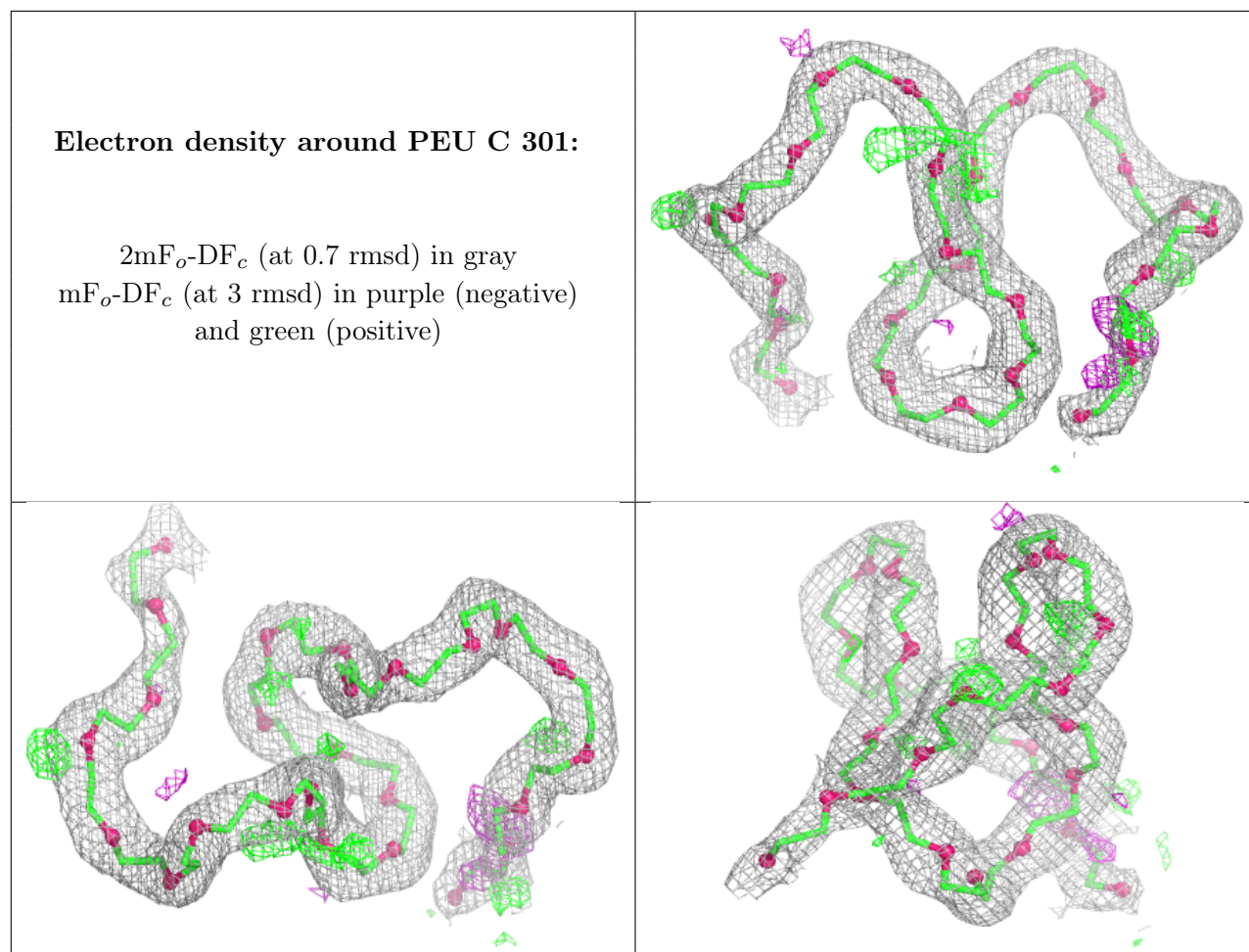
6.4 Ligands [i](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	301	4/4	0.85	0.17	41,42,43,47	0
3	EDO	D	301	4/4	0.92	0.19	40,42,42,49	0
4	PEU	E	301	73/83	0.92	0.11	28,37,45,49	0
4	PEU	C	301	73/83	0.93	0.11	26,36,44,46	0
3	EDO	H	301	4/4	0.97	0.07	35,36,38,42	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.