



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2025 – 04:50 PM JST

PDB ID : 8Z95
Title : Humanized anti-PEG h6.3 Fab in complex with PEG
Authors : Lin, Y.C.; Chang, C.Y.; Su, Y.C.
Deposited on : 2024-04-22
Resolution : 2.26 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) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

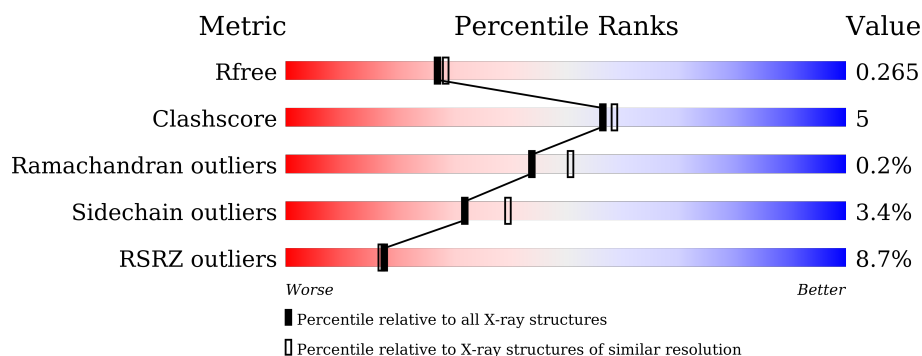
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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}	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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	219	<div> <div>16%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>5%</div> </div> </div>
1	H	219	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>.</div> </div> </div>
2	B	219	<div> <div>10%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
2	L	219	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6790 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.

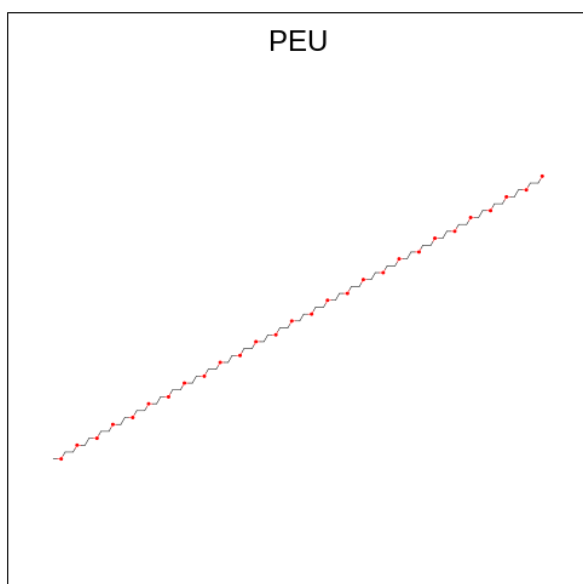
- Molecule 1 is a protein called Heavy chain of Anti-PEG antibody h6-3 Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1580	1008	260	306	6			
1	H	212	Total	C	N	O	S	0	0	0
			1604	1023	265	310	6			

- Molecule 2 is a protein called Light chain of Anti-PEG antibody h6-3 Fab fragment.

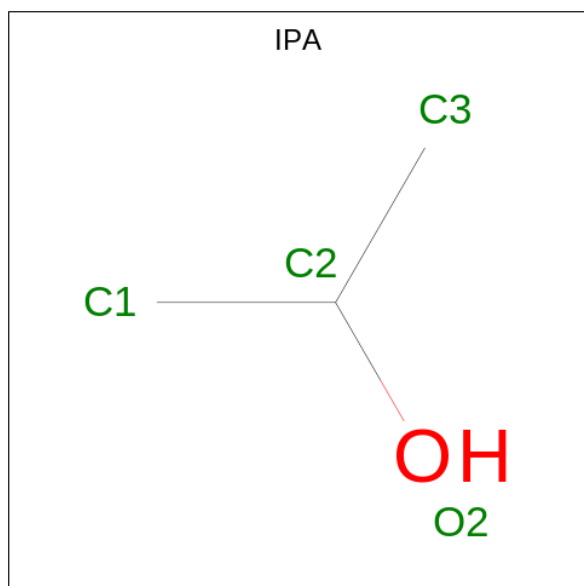
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1678	1055	278	339	6			
2	L	216	Total	C	N	O	S	0	0	0
			1674	1053	277	338	6			

- Molecule 3 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 (three-letter code: PEU) (formula: $C_{55}H_{112}O_{28}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			70	46	24		

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	3	1		

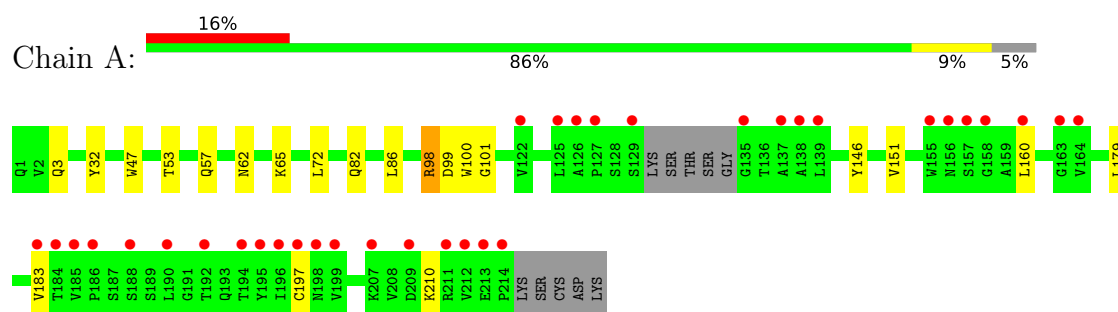
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	B	35	Total	O	0	0
			35	35		
5	H	68	Total	O	0	0
			68	68		
5	L	51	Total	O	0	0
			51	51		

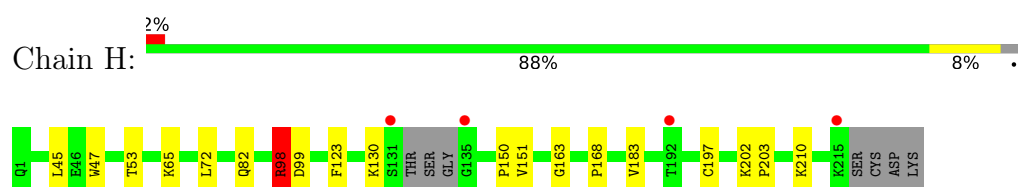
3 Residue-property plots

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.

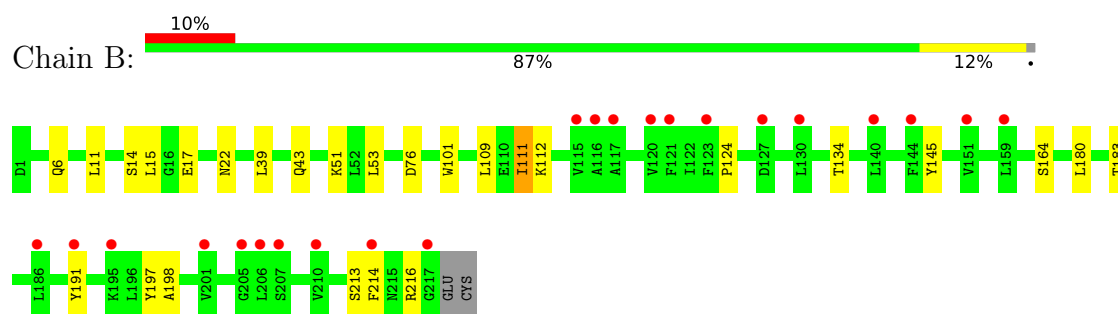
- Molecule 1: Heavy chain of Anti-PEG antibody h6-3 Fab fragment



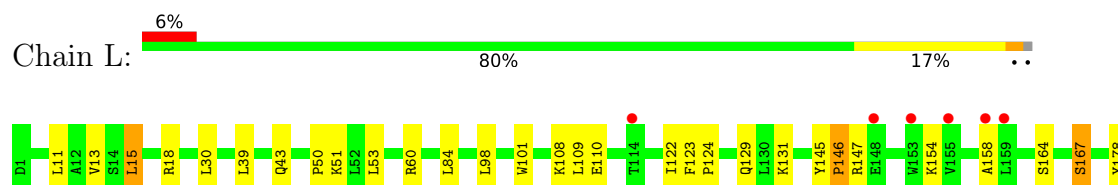
- Molecule 1: Heavy chain of Anti-PEG antibody h6-3 Fab fragment

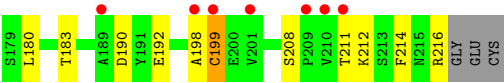


- Molecule 2: Light chain of Anti-PEG antibody h6-3 Fab fragment



- Molecule 2: Light chain of Anti-PEG antibody h6-3 Fab fragment





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	245.37Å 43.57Å 110.15Å 90.00° 111.70° 90.00°	Depositor
Resolution (Å)	29.81 – 2.26 29.81 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.81-2.26) 98.9 (29.81-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.209 , 0.261 0.217 , 0.265	Depositor DCC
R_{free} test set	2640 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6790	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, 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	0.37	0/1623	0.69	0/2217
1	H	0.44	0/1647	0.76	1/2247 (0.0%)
2	B	0.38	0/1715	0.71	0/2330
2	L	0.41	0/1711	0.76	0/2325
All	All	0.40	0/6696	0.73	1/9119 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	H	0	1
2	L	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	98	ARG	NE-CZ-NH2	-6.52	117.04	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	ARG	Sidechain
1	H	98	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	L	18	ARG	Sidechain
2	L	60	ARG	Sidechain

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	1580	0	1539	12	0
1	H	1604	0	1570	12	0
2	B	1678	0	1631	16	0
2	L	1674	0	1628	25	0
3	A	70	0	92	4	0
4	B	4	0	8	0	0
5	A	26	0	0	0	0
5	B	35	0	0	1	0
5	H	68	0	0	0	0
5	L	51	0	0	0	0
All	All	6790	0	6468	59	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 5.

All (59) 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:A:301:PEU:HCl2	2:B:101:TRP:CZ2	2.24	0.72
2:L:84:LEU:HD11	2:L:109:LEU:HD21	1.72	0.71
3:A:301:PEU:HCl2	2:B:101:TRP:HZ2	1.63	0.63
1:A:151:VAL:CG2	1:A:179:LEU:HD21	2.30	0.61
1:A:100:TRP:H	3:A:301:PEU:HCl1	1.67	0.58
2:L:84:LEU:CD1	2:L:109:LEU:HD21	2.34	0.57
2:L:124:PRO:HB3	2:L:214:PHE:CE2	2.41	0.56
1:H:98:ARG:CD	1:H:99:ASP:O	2.53	0.56
2:B:11:LEU:HD23	2:B:109:LEU:HD13	1.86	0.55
1:A:98:ARG:HD2	1:A:99:ASP:O	2.06	0.55
1:H:47:TRP:CD1	2:L:101:TRP:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:LYS:NZ	5:B:401:HOH:O	2.40	0.54
1:A:32:TYR:HB3	1:A:98:ARG:HD3	1.90	0.53
2:L:154:LYS:HA	2:L:158:ALA:O	2.10	0.52
1:H:98:ARG:HD3	1:H:99:ASP:O	2.10	0.52
2:L:43:GLN:HB2	2:L:53:LEU:HD11	1.93	0.51
1:H:98:ARG:HD2	1:H:99:ASP:O	2.11	0.50
2:L:147:ARG:HH11	2:L:147:ARG:HG2	1.76	0.50
1:A:146:TYR:OH	1:A:179:LEU:HD23	2.12	0.49
2:L:154:LYS:CG	2:L:198:ALA:HB3	2.43	0.49
2:B:43:GLN:HB2	2:B:53:LEU:HD11	1.95	0.49
2:B:14:SER:HB2	2:B:17:GLU:HG3	1.95	0.48
2:L:30:LEU:C	2:L:30:LEU:HD13	2.36	0.47
1:A:160:LEU:HD21	1:A:183:VAL:HG21	1.98	0.46
2:B:191:TYR:HA	2:B:197:TYR:OH	2.15	0.45
1:H:202:LYS:N	1:H:203:PRO:CD	2.79	0.45
1:A:101:GLY:H	3:A:301:PEU:HBE1	1.80	0.45
1:A:179:LEU:HD12	1:A:179:LEU:C	2.37	0.45
2:L:154:LYS:HG2	2:L:198:ALA:HB3	1.99	0.45
1:A:32:TYR:CB	1:A:98:ARG:HD3	2.47	0.45
2:L:216:ARG:HG2	2:L:216:ARG:HH11	1.82	0.44
1:A:47:TRP:CD1	2:B:101:TRP:HB2	2.53	0.44
1:H:45:LEU:HD11	2:L:50:PRO:HG3	2.00	0.43
1:H:53:THR:HA	1:H:72:LEU:HD11	2.00	0.43
2:L:122:ILE:HG13	2:L:212:LYS:HB3	2.00	0.43
2:L:110:GLU:OE1	2:L:178:TYR:OH	2.28	0.43
2:L:192:GLU:O	2:L:216:ARG:NH2	2.52	0.42
2:L:164:SER:HA	2:L:183:THR:O	2.20	0.42
2:L:145:TYR:HA	2:L:146:PRO:HA	1.88	0.42
1:H:47:TRP:CG	2:L:101:TRP:HB2	2.54	0.42
2:B:6:GLN:HA	2:B:22:ASN:O	2.20	0.42
2:B:112:LYS:HA	2:B:145:TYR:OH	2.20	0.42
1:H:163:GLY:O	1:H:183:VAL:HA	2.20	0.42
2:B:180:LEU:C	2:B:180:LEU:HD23	2.41	0.41
1:H:168:PRO:O	2:L:167:SER:OG	2.35	0.41
2:B:164:SER:HA	2:B:183:THR:O	2.20	0.41
2:B:198:ALA:HB2	2:B:213:SER:HB3	2.02	0.41
2:L:15:LEU:HD12	2:L:15:LEU:HA	1.91	0.41
1:A:62:ASN:HA	1:A:65:LYS:HE2	2.01	0.41
2:B:15:LEU:HD12	2:B:111:ILE:HG12	2.01	0.41
1:H:123:PHE:CE2	2:L:129:GLN:HG3	2.55	0.41
1:A:53:THR:HA	1:A:72:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:PRO:HB3	2:B:214:PHE:CE2	2.56	0.41
2:L:11:LEU:HG	2:L:13:VAL:HG23	2.02	0.41
2:L:199:CYS:O	2:L:211:THR:HA	2.21	0.41
2:B:15:LEU:CD1	2:B:111:ILE:HG12	2.51	0.40
2:L:180:LEU:C	2:L:180:LEU:HD23	2.41	0.40
2:L:123:PHE:HA	2:L:124:PRO:HD2	1.93	0.40
1:H:197:CYS:SG	1:H:210:LYS:HB3	2.62	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	205/219 (94%)	196 (96%)	9 (4%)	0	100	100
1	H	208/219 (95%)	201 (97%)	6 (3%)	1 (0%)	25	25
2	B	215/219 (98%)	205 (95%)	9 (4%)	1 (0%)	25	25
2	L	214/219 (98%)	203 (95%)	11 (5%)	0	100	100
All	All	842/876 (96%)	805 (96%)	35 (4%)	2 (0%)	44	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	216	ARG
1	H	130	LYS

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	176/185 (95%)	170 (97%)	6 (3%)	32	40
1	H	179/185 (97%)	175 (98%)	4 (2%)	47	56
2	B	191/193 (99%)	187 (98%)	4 (2%)	48	57
2	L	191/193 (99%)	180 (94%)	11 (6%)	17	16
All	All	737/756 (98%)	712 (97%)	25 (3%)	32	40

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	57	GLN
1	A	82	GLN
1	A	86	LEU
1	A	197	CYS
1	A	210	LYS
2	B	39	LEU
2	B	76	ASP
2	B	111	ILE
2	B	134	THR
1	H	65	LYS
1	H	82	GLN
1	H	150	PRO
1	H	151	VAL
2	L	15	LEU
2	L	39	LEU
2	L	51	LYS
2	L	98	LEU
2	L	108	LYS
2	L	131	LYS
2	L	146	PRO
2	L	167	SER
2	L	190	ASP
2	L	199	CYS
2	L	208	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	48	GLN
2	L	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](#)

2 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	$\# Z > 2$
3	PEU	A	301	-	69,69,82	1.23	8 (11%)	68,68,81	1.25	8 (11%)
4	IPA	B	301	-	3,3,3	0.35	0	3,3,3	0.15	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
3	PEU	A	301	-	-	33/67/67/80	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	PEU	OBV-CBX	2.46	1.52	1.42
3	A	301	PEU	OBV-CBU	2.41	1.52	1.42
3	A	301	PEU	OBP-CBQ	2.32	1.52	1.42
3	A	301	PEU	OAN-CAO	2.29	1.52	1.42
3	A	301	PEU	OBM-CBN	2.15	1.51	1.42
3	A	301	PEU	OAB-CAC	2.12	1.53	1.42
3	A	301	PEU	OAT-CAS	2.12	1.51	1.42
3	A	301	PEU	OAQ-CAP	2.11	1.51	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	PEU	OAK-CAJ-CAI	2.97	123.79	110.39
3	A	301	PEU	OAN-CAM-CAL	2.70	122.58	110.39
3	A	301	PEU	CBF-OBG-CBH	2.59	124.50	113.29
3	A	301	PEU	CAI-OAH-CAG	2.48	124.03	113.29
3	A	301	PEU	CBI-OBJ-CBK	2.44	123.87	113.29
3	A	301	PEU	CCG-OBC-CBB	2.44	123.84	113.29
3	A	301	PEU	OBV-CBW-CBX	2.44	121.38	110.39
3	A	301	PEU	OBS-CBR-CBQ	2.02	119.50	110.39

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	PEU	OBV-CBW-CBX-OBV
3	A	301	PEU	OAH-CAI-CAJ-OAK
3	A	301	PEU	OAE-CAF-CAG-OAH
3	A	301	PEU	OBM-CBN-CBO-OBP
3	A	301	PEU	OAZ-CBA-CBB-OBC
3	A	301	PEU	CAJ-CAI-OAH-CAG
3	A	301	PEU	OAN-CAO-CAP-OAQ
3	A	301	PEU	CAI-CAJ-OAK-CAL
3	A	301	PEU	OBS-CBT-CBU-OBV
3	A	301	PEU	OAK-CAL-CAM-OAN
3	A	301	PEU	OBD-CBE-CBF-OBG
3	A	301	PEU	OBD-CCH-CCI-OCJ
3	A	301	PEU	OBJ-CBK-CBL-OBM
3	A	301	PEU	OBV-CBZ-CCA-OCB
3	A	301	PEU	OBP-CBQ-CBR-OBS
3	A	301	PEU	OAW-CAX-CAY-OAZ
3	A	301	PEU	OAQ-CAR-CAS-OAT

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Mol	Chain	Res	Type	Atoms
3	A	301	PEU	CAS-CAR-OAQ-CAP
3	A	301	PEU	CBU-CBT-OBS-CBR
3	A	301	PEU	CCL-CCK-OCJ-CCI
3	A	301	PEU	CAU-CAV-OAW-CAX
3	A	301	PEU	CBT-CBU-OBV-CBW
3	A	301	PEU	CCO-CCN-OCM-CCL
3	A	301	PEU	CBB-CBA-OAZ-CAY
3	A	301	PEU	CBW-CBX-OBY-CBZ
3	A	301	PEU	CCC-CCD-OCE-CCF
3	A	301	PEU	CAV-CAU-OAT-CAS
3	A	301	PEU	CBF-CBE-OB-DBD-CCH
3	A	301	PEU	OCJ-CCK-CCL-OCM
3	A	301	PEU	CCI-CCH-OB-DBD-CBE
3	A	301	PEU	CAM-CAL-OAK-CAJ
3	A	301	PEU	OBG-CBH-CBI-OB-DBJ
3	A	301	PEU	OCE-CCF-CCG-OCB

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	PEU	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 A 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 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	209/219 (95%)	0.79	35 (16%) 5 5	20, 47, 80, 104	0
1	H	212/219 (96%)	-0.06	4 (1%) 66 66	13, 28, 57, 95	0
2	B	217/219 (99%)	0.64	22 (10%) 14 13	16, 44, 73, 88	0
2	L	216/219 (98%)	0.30	13 (6%) 29 28	13, 31, 66, 77	0
All	All	854/876 (97%)	0.42	74 (8%) 17 17	13, 35, 73, 104	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	153	TRP	4.6
1	A	212	VAL	4.4
2	B	217	GLY	4.2
1	A	126	ALA	3.8
1	A	185	VAL	3.6
1	A	196	ILE	3.5
2	B	205	GLY	3.4
1	A	190	LEU	3.4
2	B	130	LEU	3.4
1	A	194	THR	3.3
2	L	199	CYS	3.3
2	L	209	PRO	3.2
1	A	135	GLY	3.2
1	A	197	CYS	3.1
1	A	192	THR	3.0
2	L	159	LEU	3.0
2	B	206	LEU	2.9
1	A	155	TRP	2.8
1	A	183	VAL	2.8
2	B	116	ALA	2.8
2	B	140	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	210	VAL	2.8
2	L	211	THR	2.8
1	A	127	PRO	2.8
1	A	163	GLY	2.8
2	B	121	PHE	2.7
1	A	138	ALA	2.7
1	A	186	PRO	2.7
2	L	189	ALA	2.6
1	A	139	LEU	2.6
1	A	156	ASN	2.6
1	A	209	ASP	2.6
2	B	207	SER	2.5
1	A	137	ALA	2.5
1	A	214	PRO	2.5
1	A	122	VAL	2.5
1	H	215	LYS	2.5
2	B	117	ALA	2.5
2	B	120	VAL	2.5
2	B	123	PHE	2.4
2	L	158	ALA	2.4
2	B	127	ASP	2.4
1	A	158	GLY	2.4
1	H	135	GLY	2.4
1	A	125	LEU	2.4
2	B	186	LEU	2.4
2	L	155	VAL	2.3
1	A	199	VAL	2.3
1	A	164	VAL	2.3
2	B	115	VAL	2.3
2	L	210	VAL	2.3
1	A	195	TYR	2.2
2	L	198	ALA	2.2
2	B	159	LEU	2.2
2	L	114	THR	2.2
1	A	160	LEU	2.2
2	B	144	PHE	2.2
1	A	207	LYS	2.2
2	B	201	VAL	2.2
2	B	195	LYS	2.1
2	B	214	PHE	2.1
1	A	188	SER	2.1
1	H	192	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	191	TYR	2.1
2	B	151	VAL	2.1
1	A	157	SER	2.1
1	H	131	SER	2.1
1	A	184	THR	2.1
1	A	213	GLU	2.1
2	L	148	GLU	2.0
1	A	211	ARG	2.0
1	A	198	ASN	2.0
2	L	201	VAL	2.0
1	A	129	SER	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](#)

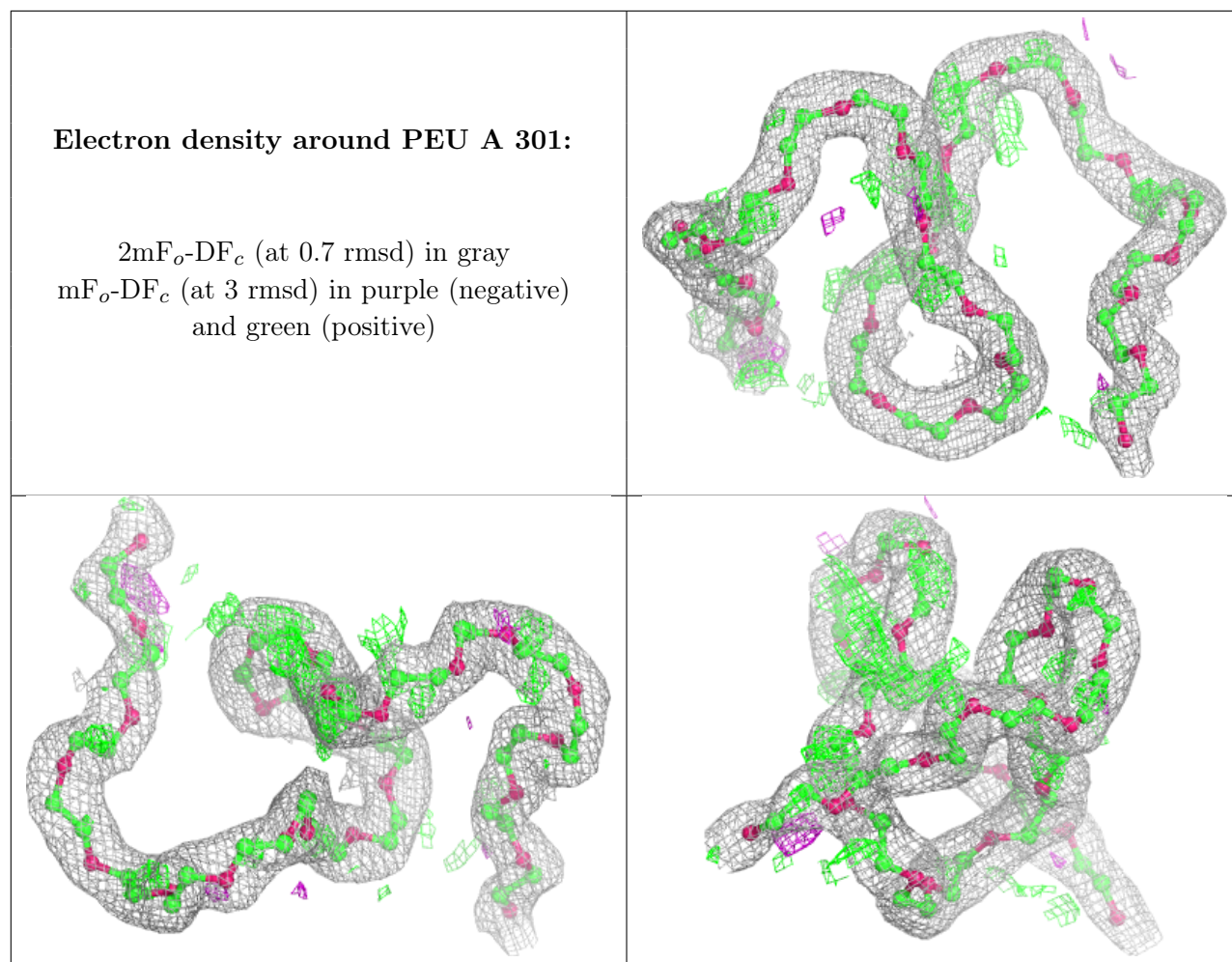
There are no monosaccharides in this entry.

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, 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(\AA^2)	Q<0.9
4	IPA	B	301	4/4	0.88	0.14	30,30,32,32	0
3	PEU	A	301	70/83	0.90	0.12	19,29,37,42	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.