



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 02:47 PM BST

PDB ID : 6VL8
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 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 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 : 2.14.2
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) : 2.14.2

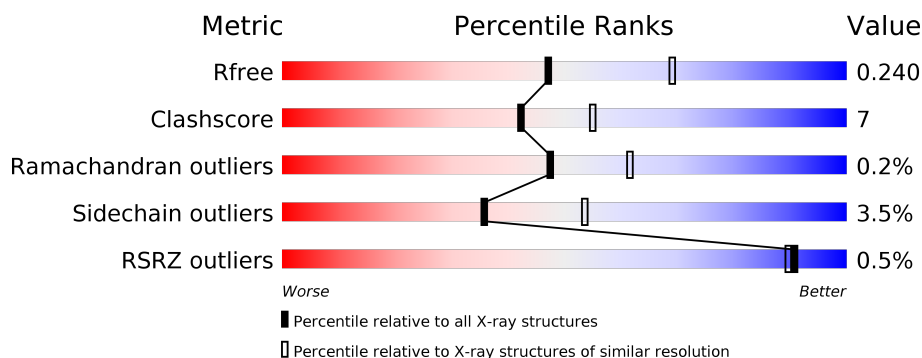
1 Overall quality at a glance

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.



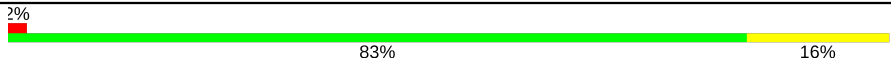

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 on 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	<div> <div>79%</div> <div>13%</div> <div>8%</div> </div>
1	C	228	<div> <div>75%</div> <div>16%</div> <div>8%</div> </div>
1	E	228	<div> <div>%</div> <div>77%</div> <div>16%</div> <div>7%</div> </div>
1	H	228	<div> <div>83%</div> <div>8%</div> <div>8%</div> </div>
2	B	219	<div> <div>85%</div> <div>14%</div> </div>
2	D	219	<div> <div>83%</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
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.

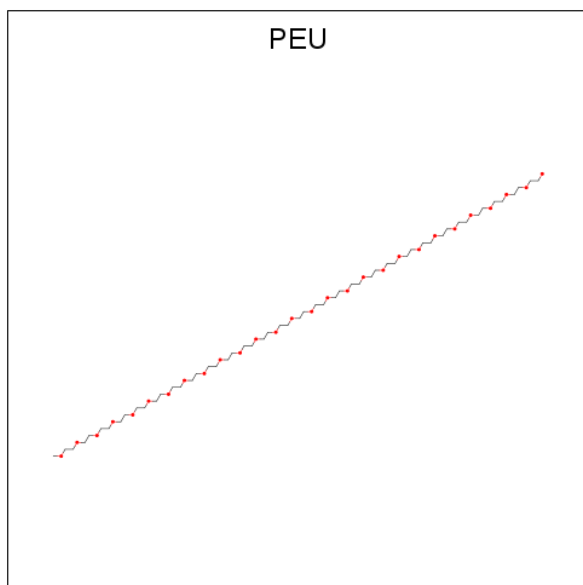
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1683	1056	278	342	7			
2	D	218	Total	C	N	O	S	0	0	0
			1683	1056	278	342	7			
2	F	218	Total	C	N	O	S	0	0	0
			1683	1056	278	342	7			
2	L	218	Total	C	N	O	S	0	1	0
			1688	1059	278	344	7			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: 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 (three-letter code: PEU) (formula: $C_{55}H_{112}O_{28}$) (labeled as "Ligand of Interest" by author).



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		

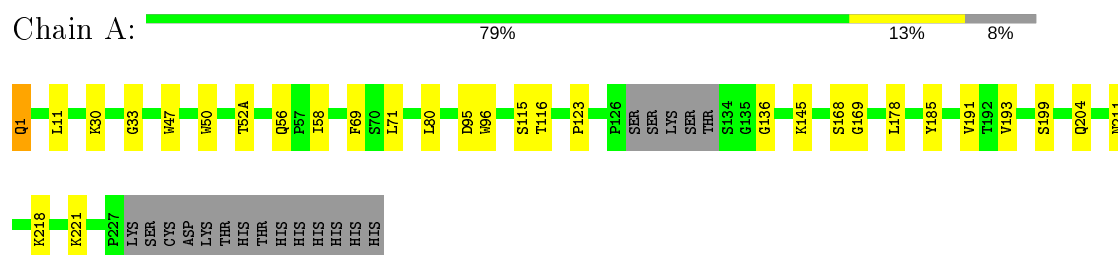
- Molecule 5 is water.

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		

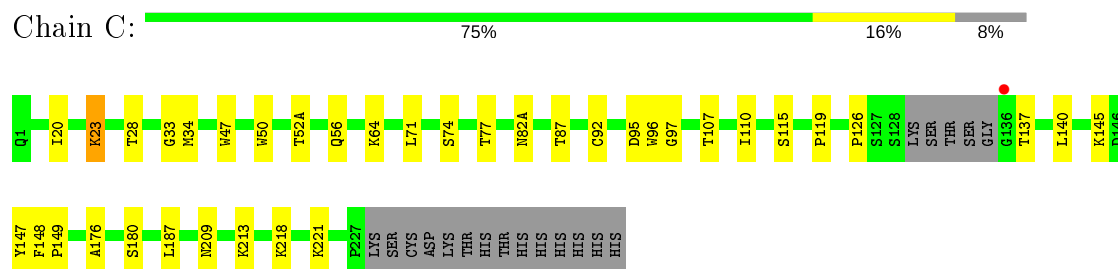
3 Residue-property plots

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.

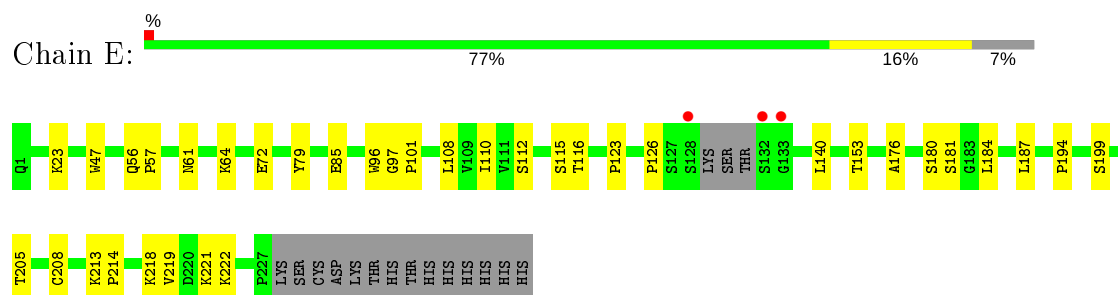
- Molecule 1: 6-3 Fab heavy chain



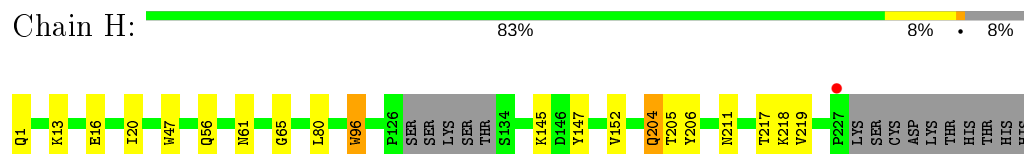
- Molecule 1: 6-3 Fab heavy chain



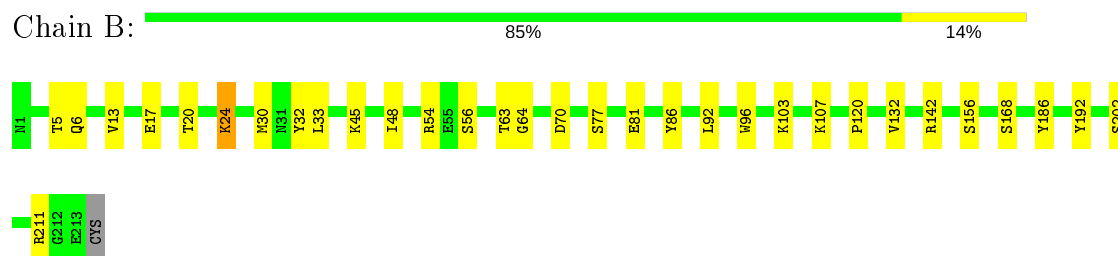
- Molecule 1: 6-3 Fab heavy chain



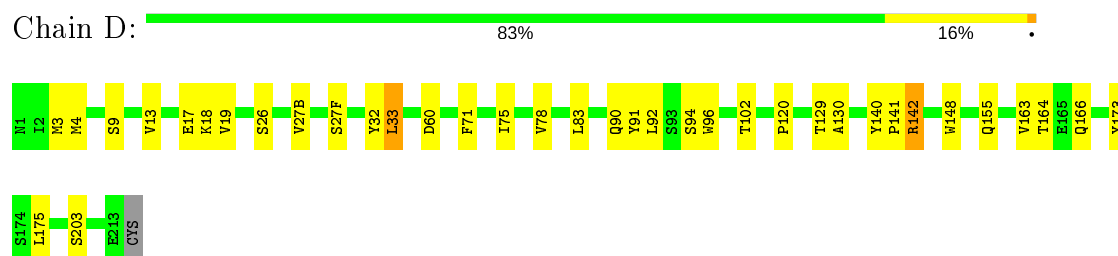
- Molecule 1: 6-3 Fab heavy chain



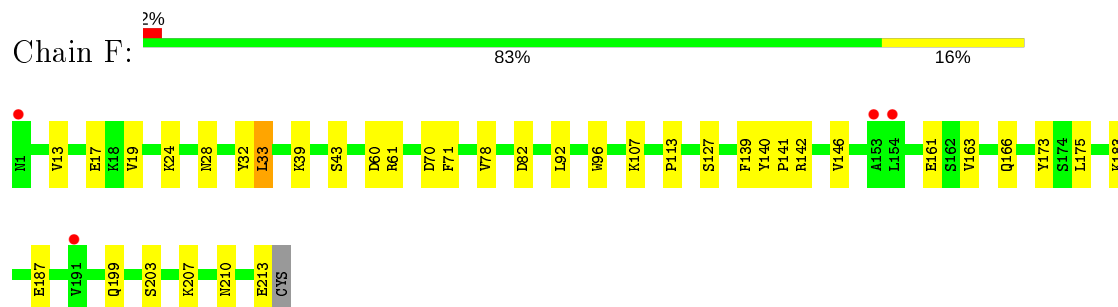
- Molecule 2: 6-3 Fab light chain



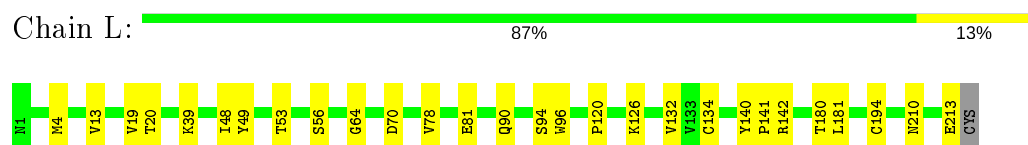
- Molecule 2: 6-3 Fab light chain



- Molecule 2: 6-3 Fab light chain



- Molecule 2: 6-3 Fab light chain



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 0.184 , 0.240	Depositor DCC
R_{free} test set	2000 reflections (2.57%)	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)	0.32 , 35.0	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: PEU, EDO

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	0.41	0/1631	0.60	0/2223
1	C	0.42	0/1633	0.56	0/2226
1	E	0.41	0/1643	0.55	0/2239
1	H	0.45	0/1631	0.59	0/2223
2	B	0.46	0/1719	0.59	0/2334
2	D	0.45	0/1719	0.60	0/2334
2	F	0.41	0/1719	0.59	0/2334
2	L	0.50	2/1727 (0.1%)	0.61	0/2345
All	All	0.44	2/13422 (0.0%)	0.59	0/18258

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	194	CYS	CB-SG	-5.94	1.72	1.81
2	L	134	CYS	CB-SG	-5.88	1.72	1.81

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	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1589	0	1565	28	0
1	E	1599	0	1573	25	0
1	H	1587	0	1563	21	0
2	B	1683	0	1636	17	0
2	D	1683	0	1636	32	0
2	F	1683	0	1636	22	0
2	L	1688	0	1640	17	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	180	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.

All (180) 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
2:D:94:SER:H	3:D:301:EDO:H11	1.36	0.89
2:D:142:ARG:HH11	2:D:163:VAL:HG21	1.40	0.85
2:B:96:TRP:NE1	4:E:301:PEU:HCQ2	1.92	0.84
1:A:96:TRP:HE1	4:E:301:PEU:HCG2	1.43	0.82
4:C:301:PEU:HCC1	3:D:301:EDO:H22	1.63	0.78
1:E:97:GLY:H	4:E:301:PEU:HAM2	1.49	0.78
4:C:301:PEU:HCQ1	2:D:96:TRP:NE1	1.99	0.75
1:C:96:TRP:CZ2	4:C:301:PEU:HCD1	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:VAL:HG11	2:D:19:VAL:HG12	1.73	0.70
4:C:301:PEU:HBQ1	1:H:96:TRP:HE1	1.58	0.69
2:B:13:VAL:HG13	2:B:17:GLU:HB2	1.75	0.69
1:C:64:LYS:O	5:C:401:HOH:O	2.10	0.69
1:E:96:TRP:HE1	4:E:301:PEU:HBN1	1.56	0.69
4:C:301:PEU:CAJ	1:H:96:TRP:H	2.05	0.69
1:C:97:GLY:H	4:C:301:PEU:HCK1	1.59	0.68
1:C:96:TRP:HE1	4:C:301:PEU:HBA2	1.60	0.66
1:E:213:LYS:H	1:E:213:LYS:HE2	1.61	0.66
4:C:301:PEU:HCT2	3:D:301:EDO:O1	1.96	0.66
1:H:211:ASN:OD1	1:H:218:LYS:HE2	1.96	0.65
1:C:96:TRP:HE1	4:C:301:PEU:HCG1	1.62	0.65
1:A:96:TRP:N	4:E:301:PEU:HCN1	2.02	0.65
2:B:24:LYS:HD3	2:B:70:ASP:OD2	1.97	0.64
2:F:24:LYS:HE2	2:F:70:ASP:OD1	1.99	0.63
1:H:1:GLN:OE1	1:H:1:GLN:N	2.21	0.62
4:C:301:PEU:HAJ2	1:H:96:TRP:N	2.13	0.62
1:E:96:TRP:NE1	4:E:301:PEU:HBN1	2.15	0.62
1:E:96:TRP:HE1	4:E:301:PEU:HBQ2	1.64	0.62
4:C:301:PEU:HCN2	2:D:96:TRP:CZ2	2.36	0.61
4:C:301:PEU:HCT1	2:D:96:TRP:CD1	2.35	0.61
2:D:142:ARG:HH21	2:D:142:ARG:HB3	1.66	0.61
1:C:96:TRP:H	4:C:301:PEU:HCN1	1.66	0.60
1:E:97:GLY:N	4:E:301:PEU:HAM2	2.16	0.60
2:D:60:ASP:N	2:D:60:ASP:OD1	2.32	0.60
2:D:3:MET:HB2	2:D:26:SER:HB3	1.82	0.60
2:F:199:GLN:NE2	5:F:301:HOH:O	2.34	0.60
1:C:96:TRP:HZ2	4:C:301:PEU:HCD1	1.67	0.58
1:C:47:TRP:CD1	2:D:96:TRP:HB2	2.38	0.58
1:C:126:PRO:HG3	1:C:140:LEU:HB3	1.86	0.57
4:C:301:PEU:HCQ2	2:D:91:TYR:HB2	1.86	0.57
1:E:194:PRO:HG2	1:E:199:SER:HB3	1.87	0.57
1:A:47:TRP:CD1	2:B:96:TRP:HB2	2.40	0.56
2:D:94:SER:N	3:D:301:EDO:H11	2.14	0.56
1:E:218:LYS:NZ	5:E:405:HOH:O	2.38	0.56
2:F:166:GLN:HG3	2:F:173:TYR:CZ	2.40	0.56
1:H:204:GLN:HG3	1:H:205:THR:N	2.19	0.56
1:A:52(A):THR:HA	1:A:71:LEU:HD11	1.88	0.55
1:A:221:LYS:NZ	5:A:404:HOH:O	2.31	0.55
1:C:96:TRP:NE1	4:C:301:PEU:HBA2	2.21	0.55
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ASN:HB3	1:C:218:LYS:NZ	2.22	0.55
1:E:47:TRP:CD1	2:F:96:TRP:HB2	2.42	0.55
4:C:301:PEU:HCN2	2:D:96:TRP:HZ2	1.72	0.54
1:H:1:GLN:H3	1:H:1:GLN:CD	2.04	0.54
1:C:47:TRP:CG	2:D:96:TRP:HB2	2.42	0.54
2:L:210:ASN:O	2:L:213:GLU:HG2	2.08	0.54
1:E:205:THR:HG23	1:E:222:LYS:HE3	1.91	0.53
1:C:97:GLY:N	4:C:301:PEU:HCK1	2.24	0.53
1:A:193:VAL:HB	1:H:1:GLN:H1	1.75	0.52
2:L:13:VAL:HG11	2:L:19:VAL:HG22	1.92	0.51
4:C:301:PEU:HAP2	2:L:49:TYR:CD2	2.45	0.51
1:C:119:PRO:HB3	1:C:147:TYR:HB3	1.91	0.51
4:C:301:PEU:OCV	3:D:301:EDO:O2	2.25	0.51
1:C:145:LYS:HE3	5:D:429:HOH:O	2.10	0.51
2:B:54:ARG:HH21	2:B:63:THR:HG22	1.75	0.51
4:C:301:PEU:HCD2	5:L:305:HOH:O	2.11	0.51
2:F:146:VAL:HG22	2:F:161:GLU:OE2	2.09	0.51
1:E:126:PRO:HG3	1:E:140:LEU:HB3	1.92	0.50
1:A:1:GLN:NE2	1:H:204:GLN:HG2	2.27	0.50
4:C:301:PEU:HBO2	1:H:96:TRP:NE1	2.27	0.50
2:F:210:ASN:O	2:F:213:GLU:HG2	2.12	0.50
2:D:142:ARG:HG3	2:D:173:TYR:CZ	2.46	0.49
1:H:47:TRP:CD1	2:L:96:TRP:HB2	2.48	0.49
2:B:202:SER:OG	5:B:301:HOH:O	2.20	0.49
1:C:23:LYS:HE3	1:C:77:THR:OG1	2.13	0.49
1:E:47:TRP:CG	2:F:96:TRP:HB2	2.48	0.49
4:C:301:PEU:HBO2	1:H:96:TRP:HE1	1.78	0.49
1:C:34:MET:HE2	1:C:92:CYS:HB2	1.95	0.48
5:E:408:HOH:O	2:F:28:ASN:HB3	2.13	0.48
1:E:23:LYS:HB2	1:E:23:LYS:HE2	1.69	0.48
2:F:183:LYS:NZ	2:F:187:GLU:OE2	2.39	0.47
2:D:142:ARG:NH2	2:D:142:ARG:HB3	2.29	0.47
2:F:166:GLN:HG3	2:F:173:TYR:CE1	2.50	0.47
1:A:123:PRO:HD3	1:A:221:LYS:HE3	1.95	0.47
1:C:52(A):THR:HA	1:C:71:LEU:HD11	1.96	0.47
2:F:163:VAL:HG22	2:F:175:LEU:HD12	1.97	0.47
4:C:301:PEU:HBE1	5:H:445:HOH:O	2.14	0.47
2:L:126:LYS:HE2	2:L:126:LYS:HB3	1.70	0.47
1:C:209:ASN:HB3	1:C:218:LYS:HZ3	1.80	0.47
2:B:186:TYR:O	2:B:192:TYR:OH	2.32	0.47
1:C:96:TRP:H	4:C:301:PEU:CCN	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:301:PEU:HBT1	4:E:301:PEU:HBQ1	1.45	0.47
2:B:103:LYS:HE3	5:B:379:HOH:O	2.14	0.47
2:D:32:TYR:HB2	2:D:92:LEU:HB2	1.96	0.46
1:E:85:GLU:CD	1:E:85:GLU:H	2.19	0.46
1:A:95:ASP:OD1	4:E:301:PEU:HCO1	2.16	0.46
1:E:153:THR:HG23	1:E:213:LYS:NZ	2.30	0.46
2:D:163:VAL:HG22	2:D:175:LEU:HD12	1.97	0.46
2:D:166:GLN:HG3	2:D:173:TYR:CZ	2.51	0.45
2:D:19:VAL:HG22	2:D:75:ILE:HB	1.97	0.45
2:D:83:LEU:HB2	5:D:424:HOH:O	2.15	0.45
2:F:33:LEU:HD13	2:F:71:PHE:CD2	2.51	0.45
2:F:32:TYR:HB2	2:F:92:LEU:HB2	1.99	0.45
1:E:61:ASN:HA	1:E:64:LYS:HD2	1.97	0.45
1:A:69:PHE:HE1	1:A:80:LEU:HD13	1.81	0.45
2:L:140:TYR:CG	2:L:141:PRO:HA	2.51	0.45
1:A:47:TRP:CG	2:B:96:TRP:HB2	2.52	0.45
1:A:1:GLN:H3	1:A:1:GLN:CD	2.16	0.45
2:L:180:THR:O	2:L:181:LEU:HD23	2.17	0.45
2:D:13:VAL:CG1	2:D:19:VAL:HG12	2.44	0.45
2:D:4:MET:HE2	2:D:90:GLN:HB3	1.98	0.45
1:C:87:THR:HG23	1:C:110:ILE:HA	1.98	0.44
1:C:95:ASP:HA	4:C:301:PEU:HCO1	1.99	0.44
2:F:113:PRO:HB3	2:F:139:PHE:HB3	1.98	0.44
1:A:178:LEU:HD13	1:A:185:TYR:CZ	2.53	0.44
2:D:140:TYR:CG	2:D:141:PRO:HA	2.53	0.44
2:B:13:VAL:CG1	2:B:17:GLU:HB2	2.47	0.44
2:B:48:ILE:HD13	2:B:64:GLY:N	2.33	0.44
2:L:39:LYS:NZ	2:L:81:GLU:O	2.49	0.44
1:A:1:GLN:HE22	1:H:204:GLN:HG2	1.83	0.44
1:A:136:GLY:HA3	1:C:28:THR:OG1	2.17	0.44
1:E:123:PRO:HD3	1:E:221:LYS:HE2	2.00	0.44
4:E:301:PEU:HAL1	4:E:301:PEU:HAI2	1.68	0.43
2:L:48:ILE:HD13	2:L:64:GLY:N	2.33	0.43
2:B:81:GLU:HA	2:B:168:SER:HB2	2.00	0.43
1:E:176:ALA:HA	1:E:187:LEU:HB3	2.00	0.43
2:L:48:ILE:HA	2:L:53:THR:O	2.19	0.43
1:E:116:THR:HG21	1:E:214:PRO:O	2.19	0.43
4:C:301:PEU:HCO2	4:C:301:PEU:HCL2	1.55	0.43
1:C:20:ILE:HD12	1:C:107:THR:HG21	1.99	0.43
2:D:120:PRO:HG3	2:D:130:ALA:HB1	2.01	0.43
1:E:108:LEU:HD21	1:E:110:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLY:HA3	1:A:50:TRP:NE1	2.34	0.43
2:L:13:VAL:HG22	2:L:78:VAL:HG11	2.01	0.43
1:E:56:GLN:HA	1:E:57:PRO:HD3	1.89	0.43
2:F:146:VAL:O	2:F:146:VAL:HG23	2.19	0.43
2:F:142:ARG:HB2	2:F:173:TYR:CE2	2.54	0.43
2:B:30:MET:HB2	2:B:30:MET:HE3	1.78	0.42
1:E:97:GLY:H	4:E:301:PEU:HAO2	1.85	0.42
2:L:120:PRO:HD3	2:L:132:VAL:HG22	2.01	0.42
1:C:176:ALA:HA	1:C:187:LEU:HB3	2.01	0.42
2:B:32:TYR:HB2	2:B:92:LEU:HB2	2.01	0.42
2:F:39:LYS:HD2	5:F:327:HOH:O	2.18	0.42
2:D:9:SER:O	2:D:102:THR:HA	2.19	0.42
1:A:1:GLN:N	1:A:1:GLN:OE1	2.35	0.42
2:F:140:TYR:CG	2:F:141:PRO:HA	2.54	0.42
1:A:169:GLY:O	1:A:191:VAL:HA	2.19	0.42
1:A:58:ILE:HD13	2:F:28:ASN:HA	2.02	0.42
2:D:148:TRP:HB2	2:D:155:GLN:HB2	2.00	0.42
2:D:17:GLU:O	2:D:78:VAL:HG23	2.20	0.42
2:D:163:VAL:HG12	2:D:164:THR:O	2.19	0.42
1:H:13:LYS:O	1:H:16:GLU:HG3	2.20	0.42
1:A:204:GLN:OE1	5:A:401:HOH:O	2.21	0.41
1:H:20:ILE:HD12	1:H:80:LEU:HD23	2.01	0.41
4:C:301:PEU:HAC2	2:L:94:SER:N	2.35	0.41
1:E:208:CYS:SG	1:E:221:LYS:HB3	2.60	0.41
1:H:217:THR:HG22	1:H:219:VAL:HG13	2.02	0.41
1:A:1:GLN:NE2	1:H:206:TYR:CE1	2.89	0.41
2:D:33:LEU:HD13	2:D:71:PHE:CD2	2.55	0.41
1:H:147:TYR:CE2	1:H:152:VAL:HG13	2.56	0.41
2:D:27(B):VAL:HA	2:D:92:LEU:HD22	2.02	0.41
2:F:17:GLU:O	2:F:78:VAL:HG23	2.21	0.41
1:H:47:TRP:CG	2:L:96:TRP:HB2	2.55	0.41
1:E:72:GLU:HB2	1:E:79:TYR:HE2	1.85	0.41
2:L:13:VAL:CG2	2:L:78:VAL:HG11	2.51	0.41
1:A:33:GLY:HA3	1:A:50:TRP:HE1	1.85	0.41
1:E:181:SER:HB2	1:E:184:LEU:HD12	2.01	0.41
2:L:4:MET:HE2	2:L:90:GLN:HB3	2.02	0.41
2:B:6:GLN:NE2	2:B:86:TYR:O	2.45	0.41
1:C:82(A):ASN:ND2	5:C:411:HOH:O	2.54	0.41
2:F:61:ARG:HH21	2:F:82:ASP:CG	2.25	0.41
2:F:61:ARG:NH2	2:F:82:ASP:OD1	2.54	0.40
1:C:33:GLY:HA3	1:C:50:TRP:HE1	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:LYS:HB2	1:H:145:LYS:HE2	1.94	0.40
1:C:148:PHE:HA	1:C:149:PRO:HA	1.82	0.40
1:A:11:LEU:HD23	1:A:116:THR:HG22	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	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%)	29	40
1	H	205/228 (90%)	195 (95%)	8 (4%)	2 (1%)	15	22
2	B	216/219 (99%)	209 (97%)	6 (3%)	1 (0%)	29	40
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%)	47	61

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%)	165 (95%)	9 (5%)	23	37
1	C	175/193 (91%)	167 (95%)	8 (5%)	27	42
1	E	176/193 (91%)	172 (98%)	4 (2%)	50	68
1	H	174/193 (90%)	171 (98%)	3 (2%)	60	77
2	B	193/194 (100%)	183 (95%)	10 (5%)	23	37
2	D	193/194 (100%)	187 (97%)	6 (3%)	40	58
2	F	193/194 (100%)	184 (95%)	9 (5%)	26	41
2	L	194/194 (100%)	191 (98%)	3 (2%)	65	79
All	All	1472/1548 (95%)	1420 (96%)	52 (4%)	36	53

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	30	LYS
1	A	56	GLN
1	A	115	SER
1	A	145	LYS
1	A	168	SER
1	A	199	SER
1	A	211	ASN
1	A	218	LYS
2	B	5	THR
2	B	20	THR
2	B	24	LYS
2	B	33	LEU
2	B	45	LYS
2	B	56	SER
2	B	77	SER
2	B	107	LYS
2	B	142	ARG
2	B	156	SER

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Mol	Chain	Res	Type
1	C	23	LYS
1	C	56	GLN
1	C	74	SER
1	C	115	SER
1	C	137	THR
1	C	180	SER
1	C	213	LYS
1	C	221	LYS
2	D	18	LYS
2	D	27(F)	SER
2	D	33	LEU
2	D	129	THR
2	D	142	ARG
2	D	203	SER
1	E	112	SER
1	E	115	SER
1	E	180	SER
1	E	219	VAL
2	F	13	VAL
2	F	19	VAL
2	F	33	LEU
2	F	43	SER
2	F	60	ASP
2	F	107	LYS
2	F	127	SER
2	F	203	SER
2	F	207	LYS
1	H	56	GLN
1	H	61	ASN
1	H	204	GLN
2	L	20	THR
2	L	56	SER
2	L	142	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
2	D	1	ASN
2	F	199	GLN
1	H	216	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
3	EDO	H	301	-	3,3,3	0.54	0	2,2,2	0.05	0
4	PEU	E	301	-	72,72,82	1.42	11 (15%)	71,71,81	0.51	0
4	PEU	C	301	-	72,72,82	1.24	6 (8%)	71,71,81	0.53	0
3	EDO	D	301	-	3,3,3	0.58	0	2,2,2	0.26	0
3	EDO	A	301	-	3,3,3	0.48	0	2,2,2	0.88	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	EDO	H	301	-	-	0/1/1/1	-
4	PEU	E	301	-	-	33/70/70/80	-
4	PEU	C	301	-	-	34/70/70/80	-
3	EDO	D	301	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	301	-	-	1/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	301	PEU	CAG-CAF	3.90	1.69	1.49
4	E	301	PEU	CAD-CAC	3.75	1.69	1.49
4	C	301	PEU	CCR-CCQ	3.27	1.65	1.49
4	E	301	PEU	CCR-CCQ	3.19	1.65	1.49
4	C	301	PEU	CAG-CAF	3.08	1.64	1.49
4	E	301	PEU	CCT-CCU	2.77	1.64	1.49
4	C	301	PEU	CCT-CCU	2.60	1.63	1.49
4	E	301	PEU	OAE-CAD	2.55	1.53	1.42
4	E	301	PEU	OAE-CAF	2.40	1.52	1.42
4	E	301	PEU	CBT-CBU	2.40	1.61	1.49
4	C	301	PEU	CBZ-CCA	2.28	1.60	1.49
4	C	301	PEU	CCO-CCN	2.27	1.60	1.49
4	E	301	PEU	CCF-CCG	2.26	1.60	1.49
4	E	301	PEU	CAJ-CAI	2.24	1.60	1.49
4	E	301	PEU	CBQ-CBR	2.10	1.59	1.49
4	C	301	PEU	OCS-CCR	2.05	1.50	1.42
4	E	301	PEU	CCC-CCD	2.05	1.59	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	301	PEU	CBQ-CBR-OBS-CBT
4	C	301	PEU	CCO-CCN-OCM-CCL
4	C	301	PEU	CCG-CCF-OCE-CCD
4	E	301	PEU	OBJ-CBK-CBL-OBM
4	E	301	PEU	OAK-CAL-CAM-OAN
4	E	301	PEU	OBV-CBW-CBX-OBY
4	C	301	PEU	OAH-CAI-CAJ-OAK
4	E	301	PEU	OAT-CAU-CAV-OAW
4	C	301	PEU	OCP-CCQ-CCR-OCS
4	C	301	PEU	OAK-CAL-CAM-OAN
4	C	301	PEU	OAE-CAF-CAG-OAH
4	E	301	PEU	OBD-CCH-CCI-OCJ
4	C	301	PEU	OAW-CAX-CAY-OAZ

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Mol	Chain	Res	Type	Atoms
4	E	301	PEU	OAW-CAX-CAY-OAZ
4	E	301	PEU	OCP-CCQ-CCR-OCS
4	C	301	PEU	OBD-CBE-CBF-OBG
4	E	301	PEU	CBA-CBB-OBC-CCG
4	C	301	PEU	OBG-CBH-CBI-OBJ
4	C	301	PEU	OBJ-CBK-CBL-OBM
4	C	301	PEU	OCJ-CCK-CCL-OCM
4	C	301	PEU	OBS-CBT-CBU-OBV
4	C	301	PEU	OBP-CBQ-CBR-OBS
4	C	301	PEU	OCE-CCF-CCG-OBC
4	C	301	PEU	OCM-CCN-CCO-OCP
4	E	301	PEU	CAI-CAJ-OAK-CAL
4	E	301	PEU	OAN-CAO-CAP-OAQ
4	C	301	PEU	OAB-CAC-CAD-OAE
3	A	301	EDO	O1-C1-C2-O2
4	E	301	PEU	OCJ-CCK-CCL-OCM
4	E	301	PEU	OBS-CBT-CBU-OBV
4	C	301	PEU	OCB-CCC-CCD-OCE
4	E	301	PEU	OAE-CAF-CAG-OAH
4	E	301	PEU	OBP-CBQ-CBR-OBS
4	E	301	PEU	CAJ-CAI-OAH-CAG
4	E	301	PEU	OBZ-CBZ-CCA-OCB
4	E	301	PEU	OBG-CBH-CBI-OBJ
4	E	301	PEU	CCN-CCO-OCP-CCQ
4	C	301	PEU	CCD-CCC-OCB-CCA
4	C	301	PEU	CCH-CCI-OCJ-CCK
4	E	301	PEU	CCA-CBZ-OBZ-CBX
4	C	301	PEU	CAI-CAJ-OAK-CAL
4	C	301	PEU	CAC-CAD-OAE-CAF
4	C	301	PEU	CBF-CBE-OBG-CCH
4	E	301	PEU	CAV-CAU-OAT-CAS
4	C	301	PEU	CBO-CBN-OBM-CBL
4	E	301	PEU	CBZ-CCA-OCB-CCC
4	C	301	PEU	CBI-CBH-OBG-CBF
4	C	301	PEU	CAL-CAM-OAN-CAO
4	C	301	PEU	CBR-CBQ-OBP-CBO
4	E	301	PEU	CBU-CBT-OBS-CBR
4	E	301	PEU	CBI-CBH-OBG-CBF
4	C	301	PEU	CCA-CBZ-OBZ-CBX
4	E	301	PEU	CBX-CBW-OBV-CBU
4	E	301	PEU	OCM-CCN-CCO-OCP
4	C	301	PEU	CBA-CBB-OBC-CCG

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Mol	Chain	Res	Type	Atoms
4	C	301	PEU	CBK-CBL-OBM-CBN
4	C	301	PEU	CCI-CCH-OB-DBE
4	E	301	PEU	CBT-CBU-OBV-CBW
4	C	301	PEU	CBU-CBT-OBS-CBR
4	E	301	PEU	OAH-CAI-CAJ-OAK
4	E	301	PEU	OBM-CBN-CBO-OBP
4	E	301	PEU	CAP-CAO-OAN-CAM
4	E	301	PEU	OAQ-CAR-CAS-OAT
4	E	301	PEU	OAZ-CBA-CBB-OBC
4	E	301	PEU	CCL-CCK-OCJ-CCI
4	C	301	PEU	OAZ-CBA-CBB-OBC
4	C	301	PEU	CAF-CAG-OAH-CAI
4	C	301	PEU	OB-DBE-CCI-OCJ





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 [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	209/228 (91%)	-0.33	0 100 100	29, 41, 57, 87	0
1	C	209/228 (91%)	-0.25	1 (0%) 91 89	32, 42, 64, 90	2 (0%)
1	E	211/228 (92%)	-0.29	3 (1%) 75 73	33, 48, 77, 124	1 (0%)
1	H	209/228 (91%)	-0.30	1 (0%) 91 89	29, 39, 58, 76	0
2	B	218/219 (99%)	-0.30	0 100 100	28, 40, 62, 80	0
2	D	218/219 (99%)	-0.23	0 100 100	31, 46, 63, 93	0
2	F	218/219 (99%)	-0.10	4 (1%) 68 65	31, 49, 83, 107	0
2	L	218/219 (99%)	-0.30	0 100 100	27, 36, 48, 67	0
All	All	1710/1788 (95%)	-0.26	9 (0%) 91 89	27, 42, 69, 124	3 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	132	SER	5.7
1	E	133	GLY	4.6
2	F	154	LEU	3.5
2	F	153	ALA	2.8
1	C	136	GLY	2.7
2	F	191	VAL	2.7
1	H	227	PRO	2.4
1	E	128	SER	2.4
2	F	1	ASN	2.3

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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

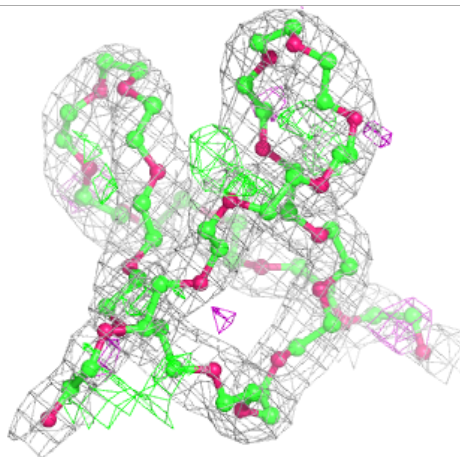
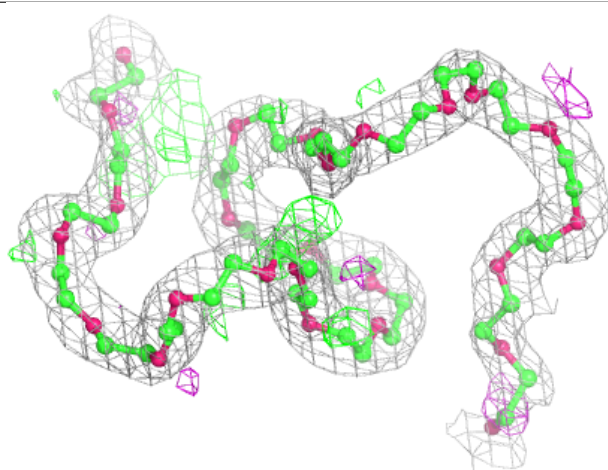
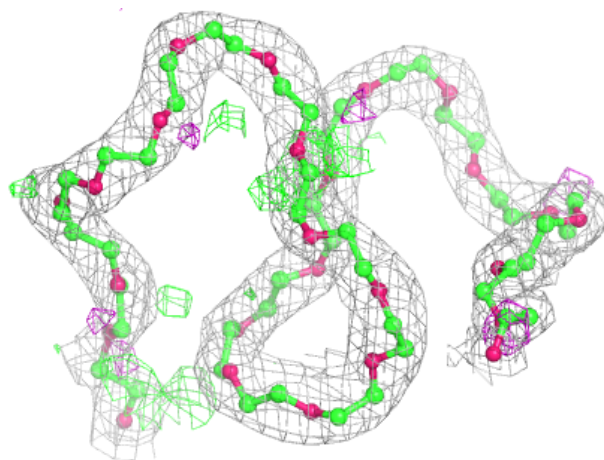
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

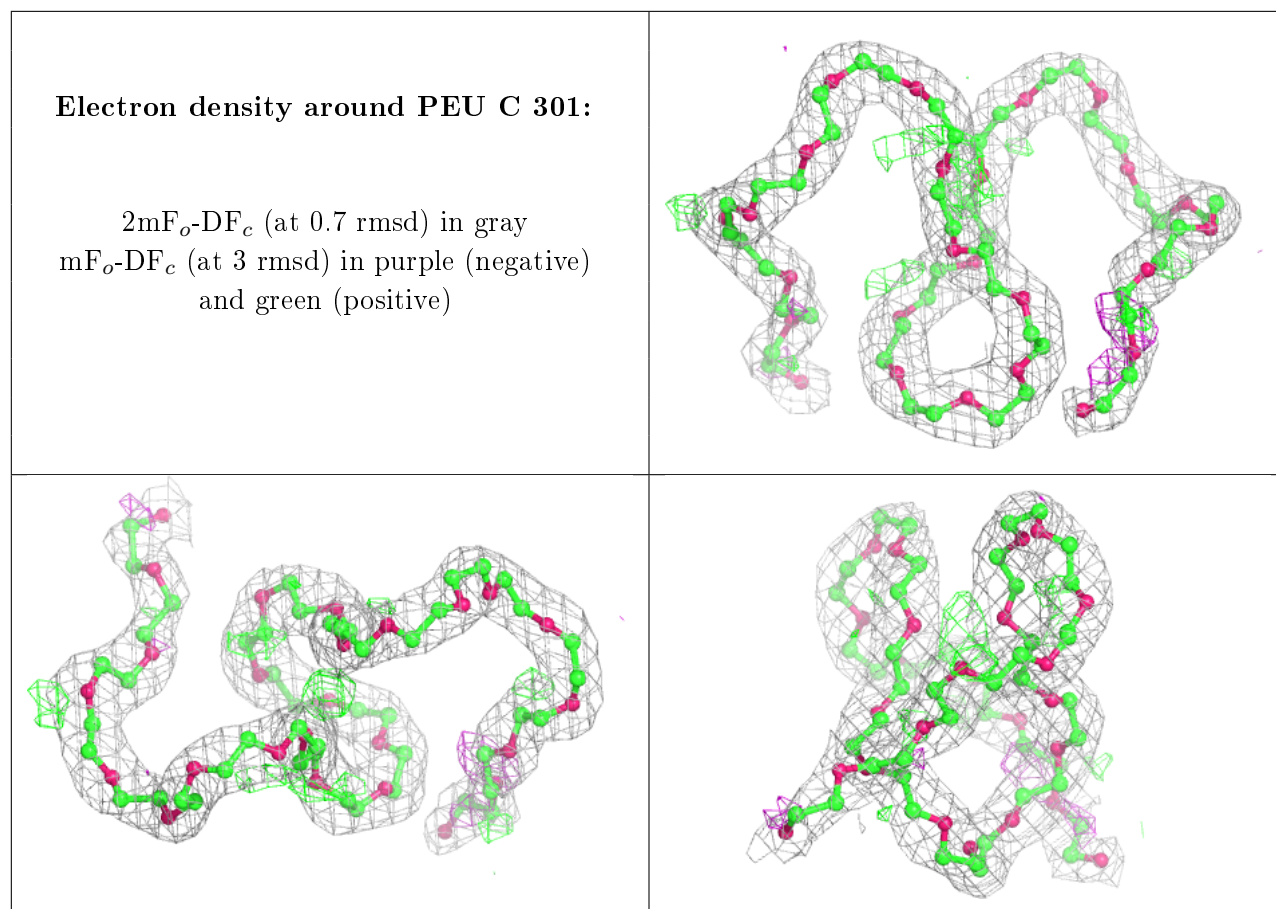
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	A	301	4/4	0.88	0.17	41,42,43,47	0
3	EDO	D	301	4/4	0.92	0.22	40,42,42,49	0
4	PEU	E	301	73/83	0.94	0.21	28,37,45,49	0
4	PEU	C	301	73/83	0.94	0.24	26,36,44,46	0
3	EDO	H	301	4/4	0.98	0.14	35,36,38,42	0

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.

Electron density around PEU E 301:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.