



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:22 pm BST

PDB ID : 4M5Y  
Title : Crystal structure of broadly neutralizing Fab 5J8  
Authors : Lee, P.S.; Wilson, I.A.  
Deposited on : 2013-08-08  
Resolution : 1.55 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](mailto: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.

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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 : 2.11  
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) : 2.11

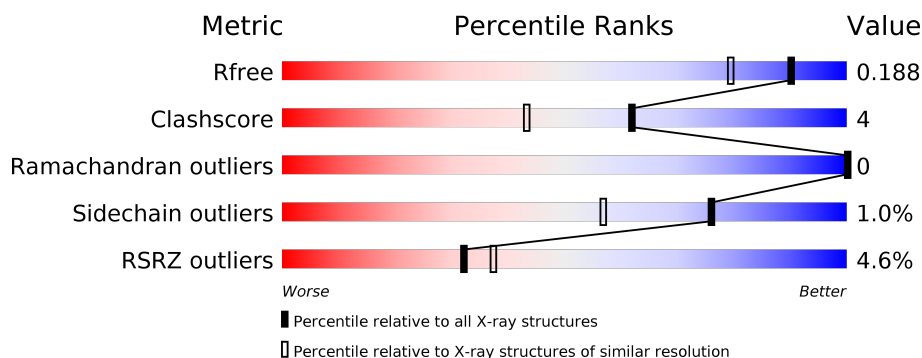
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.55 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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  $\geq 3$ , 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	H	233	<div> <div>10%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>7%</div> </div> </div>
1	I	233	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>•</div> </div> </div>
2	L	214	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>6%</div> <div>•</div> </div> </div>
2	M	214	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>•</div> <div>•</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	I	302	-	-	X	-
3	PEG	I	303	-	-	X	-
4	PG4	H	305	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7570 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.

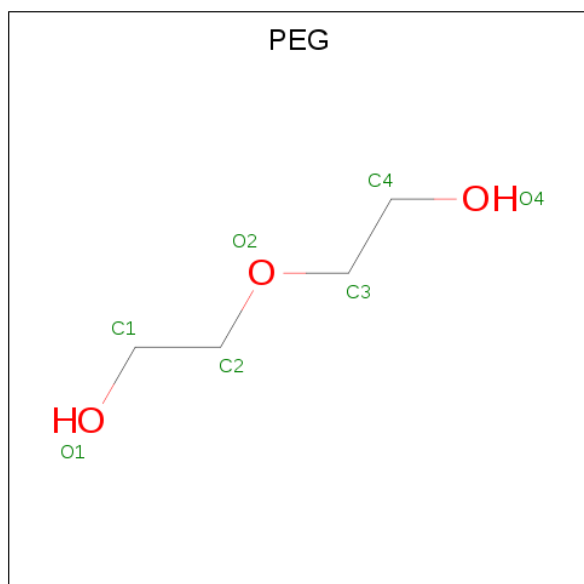
- Molecule 1 is a protein called Fab 5J8 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	217	Total	C	N	O	S	0	9	0
			1683	1079	270	330	4			
1	I	224	Total	C	N	O	S	0	10	0
			1727	1110	276	337	4			

- Molecule 2 is a protein called Fab 5J8 light chain.

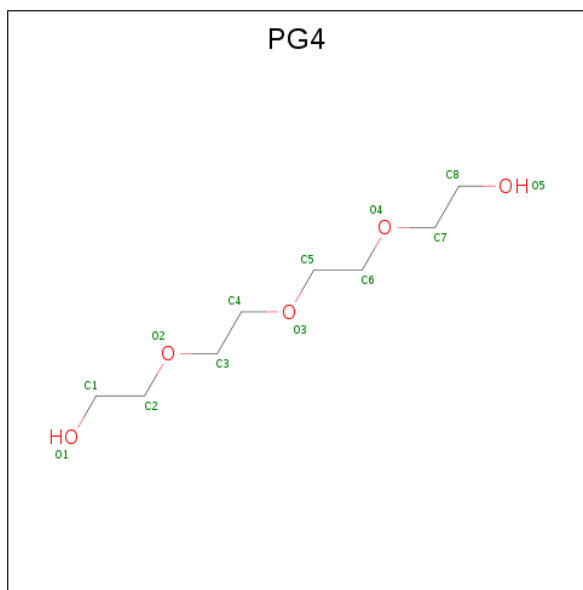
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	4	0
			1599	1004	267	324	4			
2	M	211	Total	C	N	O	S	0	5	0
			1598	1004	264	326	4			

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C O 7 4 3	0	0
3	H	1	Total C O 7 4 3	0	0
3	H	1	Total C O 7 4 3	0	0
3	H	1	Total C O 7 4 3	0	0
3	L	1	Total C O 7 4 3	0	0
3	I	1	Total C O 7 4 3	0	0
3	I	1	Total C O 7 4 3	0	0
3	I	1	Total C O 7 4 3	0	0
3	I	1	Total C O 7 4 3	0	0
3	I	1	Total C O 7 4 3	0	0
3	M	1	Total C O 7 4 3	0	0
3	M	1	Total C O 7 4 3	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			13	8	5		

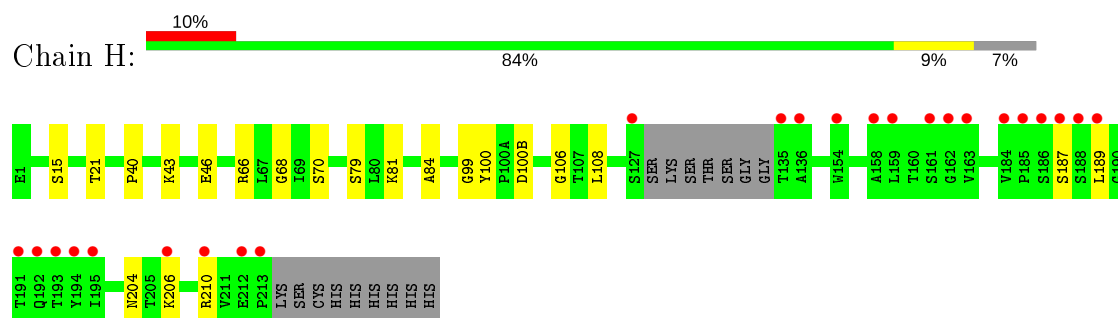
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	209	Total	O	0	0
			209	209		
5	L	194	Total	O	0	0
			194	194		
5	I	240	Total	O	0	0
			240	240		
5	M	223	Total	O	0	0
			223	223		

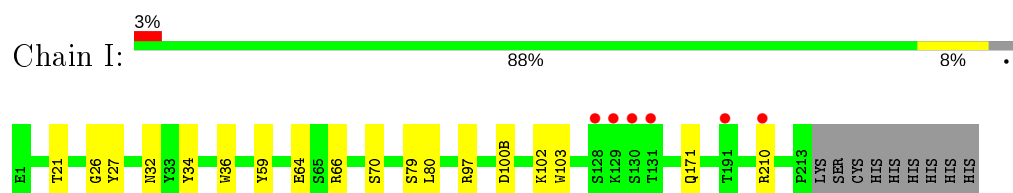
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

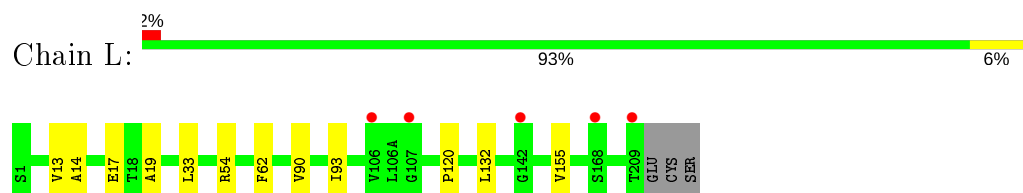
- Molecule 1: Fab 5J8 heavy chain



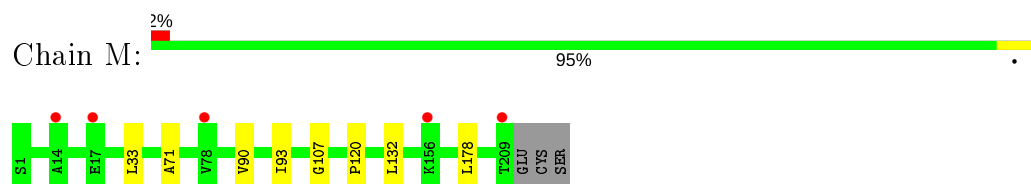
- Molecule 1: Fab 5J8 heavy chain



- Molecule 2: Fab 5J8 light chain



- Molecule 2: Fab 5J8 light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.57Å 99.98Å 144.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 1.55 49.15 – 1.55	Depositor EDS
% Data completeness (in resolution range)	96.8 (49.15-1.55) 96.7 (49.15-1.55)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 1.55Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.172 , 0.186 0.173 , 0.188	Depositor DCC
$R_{free}$ test set	9216 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7570	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	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 41.33 % 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 2.3987e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: PG4, PEG

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	H	0.44	0/1751	0.65	0/2394
1	I	0.45	0/1805	0.66	0/2468
2	L	0.39	0/1650	0.57	0/2261
2	M	0.40	0/1652	0.59	0/2264
All	All	0.42	0/6858	0.62	0/9387

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	H	1683	0	1661	22	0
1	I	1727	0	1726	18	0
2	L	1599	0	1564	8	0
2	M	1598	0	1563	9	0
3	H	28	0	40	9	0
3	I	35	0	50	15	0
3	L	7	0	10	0	0
3	M	14	0	20	2	0
4	H	13	0	18	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	209	0	0	6	0
5	I	240	0	0	4	0
5	L	194	0	0	0	0
5	M	223	0	0	0	0
All	All	7570	0	6652	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 4.

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)
1:H:81:LYS:HB3	4:H:305:PG4:H11	1.59	0.84
1:H:84:ALA:HB1	3:H:303:PEG:H32	1.63	0.80
1:I:97:ARG:HB2	3:I:302:PEG:H22	1.73	0.70
1:H:108:LEU:HB2	3:H:304:PEG:H32	1.78	0.66
1:H:46:GLU:OE1	5:H:536:HOH:O	2.14	0.66
3:I:302:PEG:O4	5:I:575:HOH:O	2.14	0.65
1:H:99:GLY:HA3	3:I:303:PEG:H31	1.80	0.63
2:M:132[A]:LEU:HD12	2:M:178:LEU:HD23	1.79	0.62
1:H:21[B]:THR:HG22	1:H:79[B]:SER:OG	2.00	0.62
1:I:70[B]:SER:OG	3:I:304:PEG:H32	2.00	0.62
1:I:97:ARG:HH11	3:I:302:PEG:H32	1.66	0.61
1:H:70[B]:SER:OG	4:H:305:PG4:O4	2.12	0.61
1:I:21[B]:THR:HG22	1:I:79[B]:SER:OG	2.01	0.61
2:L:14:ALA:HB3	2:L:17:GLU:HG3	1.87	0.57
1:I:21[B]:THR:HG23	5:I:596:HOH:O	2.06	0.56
4:H:305:PG4:O5	5:H:472:HOH:O	2.18	0.56
2:M:120:PRO:HD3	2:M:132[A]:LEU:CD2	2.38	0.54
1:H:70[A]:SER:OG	4:H:305:PG4:H82	2.07	0.54
1:H:81:LYS:CB	4:H:305:PG4:H11	2.35	0.53
1:I:97:ARG:NH1	3:I:302:PEG:H32	2.24	0.52
1:H:21[B]:THR:HG23	5:H:575:HOH:O	2.09	0.52
1:H:100(B):ASP:HB3	2:L:93[A]:ILE:HD11	1.93	0.51
1:H:43:LYS:NZ	3:H:302:PEG:H12	2.26	0.51
1:I:102:LYS:HB3	3:I:301:PEG:H11	1.92	0.50
1:I:171:GLN:NE2	5:I:592:HOH:O	2.40	0.50
1:I:27:TYR:HA	3:I:303:PEG:H32	1.94	0.49
3:H:303:PEG:H42	5:H:481:HOH:O	2.13	0.49
1:H:15:SER:OG	3:H:301:PEG:H22	2.14	0.48
3:I:302:PEG:H41	5:I:582:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:120:PRO:HD3	2:L:132:LEU:CD2	2.43	0.48
1:I:26:GLY:O	3:I:303:PEG:H32	2.13	0.47
1:H:100(B):ASP:HB3	2:L:93[A]:ILE:CD1	2.44	0.47
1:I:102:LYS:HD2	3:I:301:PEG:H11	1.97	0.46
2:L:54[B]:ARG:HD3	2:L:62:PHE:O	2.16	0.45
2:M:33:LEU:HD12	2:M:90[A]:VAL:HG13	1.98	0.45
3:H:301:PEG:H42	5:H:573:HOH:O	2.17	0.45
1:I:100(B):ASP:HB3	2:M:93:ILE:HD11	1.98	0.45
2:M:33:LEU:HD22	2:M:71:ALA:CB	2.46	0.45
2:L:54[A]:ARG:HD3	2:L:62:PHE:O	2.17	0.45
1:H:40:PRO:HB3	3:H:302:PEG:H21	1.99	0.45
2:M:107:GLY:H	3:M:302:PEG:H12	1.82	0.45
1:H:99:GLY:C	3:I:303:PEG:H22	2.37	0.44
1:I:36:TRP:CG	1:I:80[A]:LEU:HD12	2.53	0.44
1:H:100:TYR:CD2	3:I:303:PEG:H21	2.52	0.44
1:H:68:GLY:HA3	4:H:305:PG4:H62	2.00	0.43
1:I:59:TYR:HD2	1:I:64:GLU:HG3	1.81	0.43
3:H:302:PEG:H41	5:H:579:HOH:O	2.17	0.43
1:I:100(B):ASP:HB3	2:M:93:ILE:CD1	2.48	0.43
1:I:34:TYR:HE2	3:I:302:PEG:H31	1.84	0.43
1:I:103:TRP:HB2	3:I:301:PEG:H42	2.00	0.42
2:M:107:GLY:N	3:M:302:PEG:H12	2.35	0.42
1:H:106:GLY:O	3:H:304:PEG:H11	2.19	0.41
2:L:33:LEU:HD12	2:L:90[A]:VAL:HG13	2.01	0.41
1:H:81:LYS:HB3	4:H:305:PG4:C1	2.41	0.41
2:M:120:PRO:HD3	2:M:132[A]:LEU:HD23	2.03	0.40
1:H:189:LEU:HA	1:H:189:LEU:HD23	1.91	0.40
2:L:13:VAL:HG11	2:L:19:ALA:HB2	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	H	222/233 (95%)	217 (98%)	5 (2%)	0	100	100
1	I	232/233 (100%)	228 (98%)	4 (2%)	0	100	100
2	L	213/214 (100%)	207 (97%)	6 (3%)	0	100	100
2	M	214/214 (100%)	210 (98%)	4 (2%)	0	100	100
All	All	881/894 (98%)	862 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	H	196/201 (98%)	192 (98%)	4 (2%)	55	26
1	I	202/201 (100%)	200 (99%)	2 (1%)	76	57
2	L	182/181 (101%)	181 (100%)	1 (0%)	88	78
2	M	183/181 (101%)	183 (100%)	0	100	100
All	All	763/764 (100%)	756 (99%)	7 (1%)	76	61

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	187	SER
1	H	204	ASN
1	H	206	LYS
1	H	210	ARG
2	L	155	VAL
1	I	32	ASN
1	I	210	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	53	HIS

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Mol	Chain	Res	Type
1	I	53	HIS
1	I	171	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

13 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	PEG	I	302	-	6,6,6	0.43	0	5,5,5	0.32	0
3	PEG	M	302	-	6,6,6	0.35	0	5,5,5	0.40	0
3	PEG	H	301	-	6,6,6	0.41	0	5,5,5	0.76	0
3	PEG	I	303	-	6,6,6	0.39	0	5,5,5	0.59	0
3	PEG	H	304	-	6,6,6	0.43	0	5,5,5	0.36	0
3	PEG	L	301	-	6,6,6	0.43	0	5,5,5	0.45	0
4	PG4	H	305	-	12,12,12	0.38	0	11,11,11	0.87	0
3	PEG	M	301	-	6,6,6	0.45	0	5,5,5	0.29	0
3	PEG	I	304	-	6,6,6	0.43	0	5,5,5	0.42	0
3	PEG	I	305	-	6,6,6	0.49	0	5,5,5	0.18	0
3	PEG	H	303	-	6,6,6	0.40	0	5,5,5	0.74	0
3	PEG	I	301	-	6,6,6	0.48	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEG	H	302	-	6,6,6	0.55	0	5,5,5	0.54	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	PEG	I	302	-	-	2/4/4/4	-
3	PEG	M	302	-	-	2/4/4/4	-
3	PEG	H	301	-	-	1/4/4/4	-
3	PEG	I	303	-	-	2/4/4/4	-
3	PEG	H	304	-	-	1/4/4/4	-
3	PEG	L	301	-	-	3/4/4/4	-
4	PG4	H	305	-	-	6/10/10/10	-
3	PEG	M	301	-	-	0/4/4/4	-
3	PEG	I	304	-	-	2/4/4/4	-
3	PEG	I	305	-	-	1/4/4/4	-
3	PEG	H	303	-	-	4/4/4/4	-
3	PEG	I	301	-	-	2/4/4/4	-
3	PEG	H	302	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	305	PG4	O2-C3-C4-O3
4	H	305	PG4	O1-C1-C2-O2
3	I	304	PEG	O1-C1-C2-O2
3	I	301	PEG	O1-C1-C2-O2
3	M	302	PEG	O1-C1-C2-O2
3	I	305	PEG	O2-C3-C4-O4
3	H	303	PEG	O2-C3-C4-O4
3	M	302	PEG	C4-C3-O2-C2
3	I	303	PEG	O1-C1-C2-O2
3	I	301	PEG	O2-C3-C4-O4
3	I	303	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	L	301	PEG	O2-C3-C4-O4
3	H	303	PEG	O1-C1-C2-O2
4	H	305	PG4	C3-C4-O3-C5
3	H	304	PEG	C4-C3-O2-C2
3	L	301	PEG	C1-C2-O2-C3
3	L	301	PEG	C4-C3-O2-C2
3	I	304	PEG	C4-C3-O2-C2
3	H	302	PEG	O1-C1-C2-O2
3	H	303	PEG	C1-C2-O2-C3
3	I	302	PEG	O2-C3-C4-O4
3	I	302	PEG	C1-C2-O2-C3
3	H	301	PEG	O1-C1-C2-O2
4	H	305	PG4	C8-C7-O4-C6
4	H	305	PG4	C5-C6-O4-C7
3	H	303	PEG	C4-C3-O2-C2
4	H	305	PG4	O3-C5-C6-O4

There are no ring outliers.

10 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	302	PEG	6	0
3	M	302	PEG	2	0
3	H	301	PEG	2	0
3	I	303	PEG	5	0
3	H	304	PEG	2	0
4	H	305	PG4	7	0
3	I	304	PEG	1	0
3	H	303	PEG	2	0
3	I	301	PEG	3	0
3	H	302	PEG	3	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	H	217/233 (93%)	0.37	24 (11%) 5 5	12, 20, 63, 78	0
1	I	224/233 (96%)	0.06	6 (2%) 54 62	11, 19, 48, 61	0
2	L	211/214 (98%)	0.01	5 (2%) 59 65	14, 27, 47, 61	0
2	M	211/214 (98%)	-0.11	5 (2%) 59 65	15, 26, 42, 57	0
All	All	863/894 (96%)	0.08	40 (4%) 32 37	11, 24, 51, 78	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	185	PRO	5.4
1	I	130	SER	5.2
1	H	162	GLY	5.1
2	L	209	THR	5.1
1	H	184	VAL	5.1
1	H	189	LEU	4.5
2	L	168	SER	4.5
2	M	209	THR	4.3
1	H	135	THR	4.2
1	H	187	SER	4.2
1	I	131	THR	4.1
1	H	136	ALA	3.7
1	H	186	SER	3.7
1	H	158	ALA	3.5
1	H	195	ILE	3.4
1	I	128	SER	3.4
1	H	188	SER	3.3
1	H	191	THR	3.3
1	H	159	LEU	3.2
1	H	194	TYR	3.1
1	H	161	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	M	156	LYS	3.1
1	H	213	PRO	3.0
1	H	210	ARG	3.0
1	I	129	LYS	3.0
1	H	206	LYS	3.0
1	H	127	SER	2.9
2	L	107	GLY	2.9
2	M	14	ALA	2.8
1	H	163	VAL	2.6
1	H	212	GLU	2.5
1	I	191	THR	2.5
1	I	210	ARG	2.4
2	L	106	VAL	2.3
1	H	193	THR	2.2
1	H	192	GLN	2.2
1	H	154	TRP	2.2
2	M	78	VAL	2.1
2	L	142	GLY	2.1
2	M	17	GLU	2.1

## 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 carbohydrates 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<sup>th</sup> 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	PEG	H	302	7/7	0.71	0.24	37,46,52,58	0
3	PEG	M	301	7/7	0.72	0.26	46,50,55,55	0
3	PEG	I	302	7/7	0.73	0.21	40,50,59,65	0
3	PEG	I	305	7/7	0.76	0.29	44,53,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEG	H	301	7/7	0.78	0.28	42,46,53,60	0
3	PEG	H	304	7/7	0.79	0.22	49,53,56,60	0
3	PEG	I	301	7/7	0.81	0.18	31,37,43,43	0
3	PEG	L	301	7/7	0.83	0.22	35,49,58,59	0
4	PG4	H	305	13/13	0.84	0.32	25,49,61,61	0
3	PEG	I	304	7/7	0.87	0.24	30,40,52,55	0
3	PEG	H	303	7/7	0.87	0.33	25,48,58,59	0
3	PEG	M	302	7/7	0.88	0.35	29,49,58,63	0
3	PEG	I	303	7/7	0.93	0.16	21,30,39,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.