



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 5, 2023 – 01:36 AM EDT

PDB ID : 7SGM  
Title : Crystal structure of a Fab variant containing a fluorescent noncanonical amino acid with blocked excited state proton transfer and in complex with its antigen, CD40L  
Authors : Henderson, J.N.; Mills, J.H.; Simmons, C.R.  
Deposited on : 2021-10-06  
Resolution : 2.00 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](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.

The types of validation reports are described at

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

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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 : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

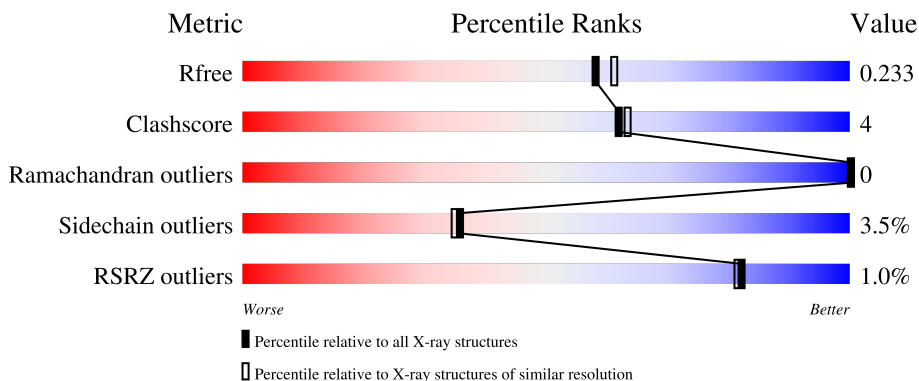
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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.



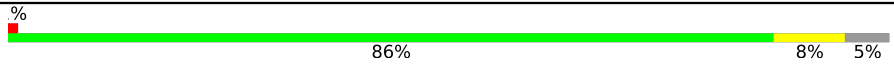
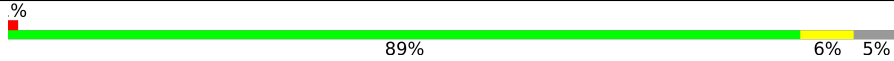

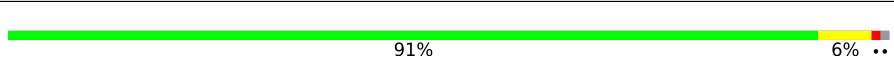
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	A	146	 77% 15% • 6%
1	B	146	 77% 16% • •
1	C	146	 79% 12% • 6%
2	H	226	 78% 15% 7%
2	K	226	 88% 7% 6%

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Mol	Chain	Length	Quality of chain
2	X	226	 <p>% 86% 8% 5%</p>
3	L	218	 <p>% 89% 6% 5%</p>
3	M	218	 <p>88% 11% .</p>
3	Y	218	 <p>91% 6% ..</p>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 14354 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 CD40 ligand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	137	1074	683	186	200	5	0	7	0
1	B	140	1083	689	185	204	5	0	5	0
1	C	137	1074	686	182	201	5	0	7	0

- Molecule 2 is a protein called 5c8\* Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	211	1566	990	251	317	8	0	5	0
2	K	213	1574	991	254	321	8	0	1	0
2	X	214	1590	1003	257	322	8	0	3	0

- Molecule 3 is a protein called 5c8\* Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	208	1606	1013	263	325	5	0	3	0
3	M	217	1679	1054	279	341	5	0	1	0
3	Y	216	1681	1055	280	340	6	0	3	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	8	4	1	3	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



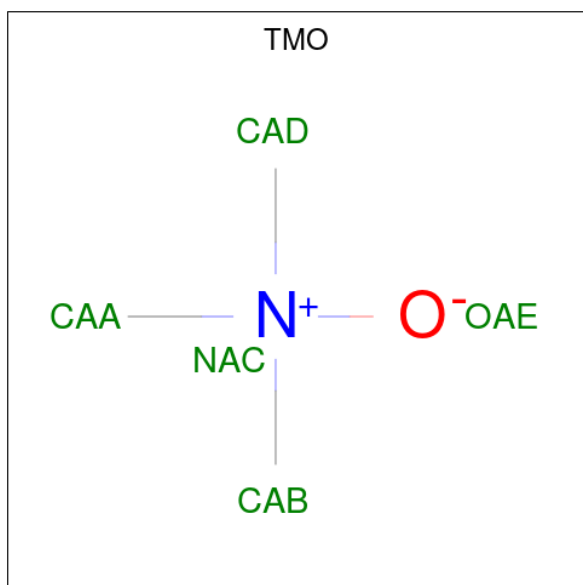
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	7	4	3	0	0
6	B	1	7	4	3	0	0
6	C	1	7	4	3	0	0
6	H	1	5	3	2	0	0
6	H	1	7	4	3	0	0
6	L	1	7	4	3	0	1
6	L	1	5	3	2	0	0
6	L	1	7	4	3	0	0
6	K	1	7	4	3	0	0
6	M	1	7	4	3	0	1
6	X	1	7	4	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	Y	1	Total	C	O	0	0
			6	4	2		
6	Y	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is trimethylamine oxide (three-letter code: TMO) (formula: C<sub>3</sub>H<sub>9</sub>NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	1
			5	3	1	1		
7	M	1	Total	C	N	O	0	1
			5	3	1	1		
7	Y	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	107	Total	O	0	9
			107	107		
8	B	99	Total	O	0	7
			99	99		
8	C	98	Total	O	0	6
			98	98		
8	H	97	Total	O	0	0
			97	97		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
8	L	178	Total 178	O 178	0	1
8	K	160	Total 160	O 160	0	1
8	M	200	Total 200	O 200	0	0
8	X	150	Total 150	O 150	0	0
8	Y	187	Total 187	O 187	0	2



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


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.

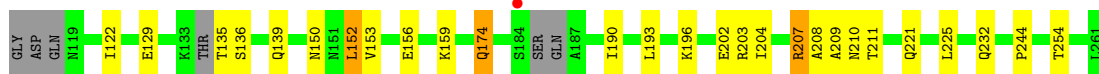
- Molecule 1: CD40 ligand

Chain A: 




- Molecule 1: CD40 ligand

Chain B: 




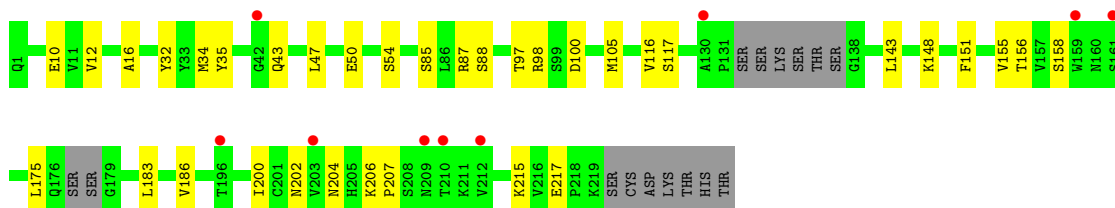
- Molecule 1: CD40 ligand

Chain C: 




- Molecule 2: 5c8\* Fab heavy chain

Chain H: 



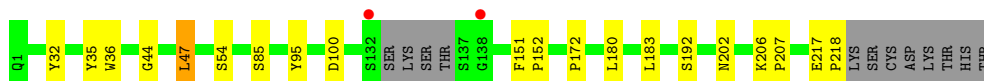
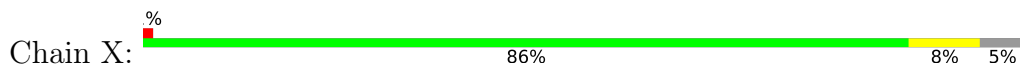
- Molecule 2: 5c8\* Fab heavy chain

Chain K: 

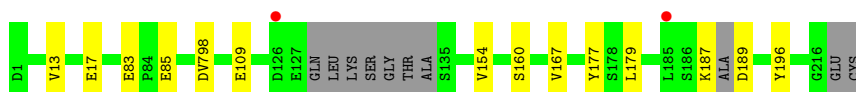
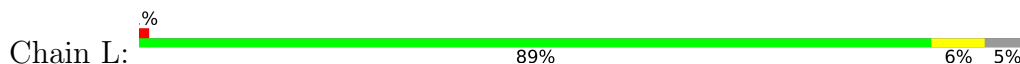




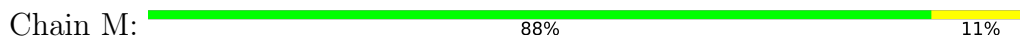
- Molecule 2: 5c8\* Fab heavy chain



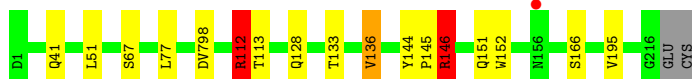
- Molecule 3: 5c8\* Fab light chain



- Molecule 3: 5c8\* Fab light chain



- Molecule 3: 5c8\* Fab light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	226.85Å 131.25Å 97.30Å 90.00° 109.10° 90.00°	Depositor
Resolution (Å)	48.42 – 2.00 48.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (48.42-2.00) 97.6 (48.37-2.00)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.193 , 0.228 0.199 , 0.233	Depositor DCC
$R_{free}$ test set	8919 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtrriage
Anisotropy	0.299	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14354	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: PEG, DV7, TRS, TMO, NAG

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	0.82	0/1113	1.08	1/1507 (0.1%)
1	B	0.89	2/1116 (0.2%)	1.01	0/1511
1	C	0.82	0/1116	1.08	3/1511 (0.2%)
2	H	0.76	0/1608	0.95	1/2189 (0.0%)
2	K	0.81	0/1611	0.96	0/2198
2	X	0.79	0/1633	0.96	0/2224
3	L	0.83	1/1635 (0.1%)	0.94	0/2227
3	M	0.88	1/1704 (0.1%)	0.97	1/2317 (0.0%)
3	Y	0.84	0/1709	1.03	6/2323 (0.3%)
All	All	0.82	4/13245 (0.0%)	0.99	12/18007 (0.1%)

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
2	H	0	1
2	X	0	1
3	L	0	1
3	M	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	156	GLU	CD-OE2	6.13	1.32	1.25
3	L	83	GLU	CD-OE1	5.86	1.32	1.25
3	M	83	GLU	CD-OE1	5.83	1.32	1.25
1	B	202	GLU	CD-OE1	5.37	1.31	1.25

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	146	ARG	CG-CD-NE	-9.13	92.62	111.80
3	Y	112[A]	ARG	NE-CZ-NH2	-7.11	116.75	120.30
3	Y	112[B]	ARG	NE-CZ-NH2	-7.11	116.75	120.30
3	Y	146	ARG	NE-CZ-NH2	-7.08	116.76	120.30
3	Y	112[A]	ARG	NE-CZ-NH1	7.06	123.83	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	43[B]	GLN	Peptide
3	L	160	SER	Peptide
3	M	161	GLY	Peptide
2	X	217	GLU	Peptide

## 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	1074	0	1056	19	0
1	B	1083	0	1060	16	0
1	C	1074	0	1064	16	0
2	H	1566	0	1503	18	0
2	K	1574	0	1513	8	0
2	X	1590	0	1546	9	0
3	L	1606	0	1488	8	0
3	M	1679	0	1582	16	0
3	Y	1681	0	1591	11	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
5	A	8	0	12	1	0
6	A	7	0	10	0	0
6	B	7	0	10	0	0
6	C	7	0	10	0	0
6	H	12	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	7	0	10	0	0
6	L	19	0	25	0	0
6	M	7	0	10	0	0
6	X	7	0	10	0	0
6	Y	13	0	17	0	0
7	L	5	0	9	0	0
7	M	5	0	9	0	0
7	Y	5	0	9	0	0
8	A	107	0	0	3	0
8	B	99	0	0	1	0
8	C	98	0	0	2	0
8	H	97	0	0	1	0
8	K	160	0	0	1	0
8	L	178	0	0	2	0
8	M	200	0	0	0	0
8	X	150	0	0	0	0
8	Y	187	0	0	2	0
All	All	14354	0	12598	113	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.

The worst 5 of 113 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:M:146[B]:ARG:HH11	3:M:146[B]:ARG:HG2	1.34	0.91
3:L:13[A]:VAL:HG13	3:L:17:GLU:HB3	1.63	0.80
1:C:232[B]:GLN:NE2	8:C:401:HOH:O	2.18	0.75
1:A:208:ALA:HB2	1:A:225:LEU:HD21	1.72	0.72
1:B:135:THR:O	1:B:244:PRO:HG2	1.89	0.71

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	138/146 (94%)	134 (97%)	4 (3%)	0	100	100
1	B	139/146 (95%)	135 (97%)	4 (3%)	0	100	100
1	C	138/146 (94%)	132 (96%)	6 (4%)	0	100	100
2	H	210/226 (93%)	200 (95%)	10 (5%)	0	100	100
2	K	210/226 (93%)	205 (98%)	5 (2%)	0	100	100
2	X	213/226 (94%)	207 (97%)	6 (3%)	0	100	100
3	L	204/218 (94%)	195 (96%)	9 (4%)	0	100	100
3	M	215/218 (99%)	207 (96%)	8 (4%)	0	100	100
3	Y	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
All	All	1683/1770 (95%)	1626 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	116/122 (95%)	112 (97%)	4 (3%)	37	36
1	B	116/122 (95%)	104 (90%)	12 (10%)	7	4
1	C	117/122 (96%)	111 (95%)	6 (5%)	24	19
2	H	172/194 (89%)	161 (94%)	11 (6%)	17	13
2	K	176/194 (91%)	172 (98%)	4 (2%)	50	53
2	X	179/194 (92%)	173 (97%)	6 (3%)	37	36
3	L	176/191 (92%)	176 (100%)	0	100	100
3	M	186/191 (97%)	180 (97%)	6 (3%)	39	38
3	Y	188/191 (98%)	182 (97%)	6 (3%)	39	38
All	All	1426/1521 (94%)	1371 (96%)	55 (4%)	36	30

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	148	LYS
2	K	186	VAL
3	Y	195	VAL
3	Y	112[A]	ARG
2	H	155	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	X	43	GLN
3	Y	214	ASN
3	L	164	GLN
2	K	197	GLN
2	K	209	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](#)

3 non-standard protein/DNA/RNA residues 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	DV7	L	98	3	18,19,20	1.08	1 (5%)	21,26,28	1.39	4 (19%)
3	DV7	Y	98	3	18,19,20	1.30	3 (16%)	21,26,28	1.66	4 (19%)
3	DV7	M	98	3	18,19,20	1.11	1 (5%)	21,26,28	1.44	4 (19%)

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	DV7	L	98	3	-	2/6/7/9	0/2/2/2
3	DV7	Y	98	3	-	1/6/7/9	0/2/2/2
3	DV7	M	98	3	-	1/6/7/9	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	98	DV7	CH1-CT	2.65	1.43	1.39
3	M	98	DV7	CH1-CT	2.50	1.42	1.39
3	Y	98	DV7	CG-CD	2.41	1.54	1.50
3	Y	98	DV7	CB-CA	-2.40	1.50	1.53
3	L	98	DV7	CH1-CT	2.28	1.42	1.39

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	98	DV7	CG-CD-CE2	3.77	123.00	118.62
3	Y	98	DV7	OH1-CZ2-CE2	-3.35	118.37	121.56
3	M	98	DV7	CH2-CT-CH1	-3.14	116.74	120.17
3	L	98	DV7	OH1-CZ2-CE2	-2.95	118.75	121.56
3	Y	98	DV7	OH1-CZ1-CE1	2.84	120.83	117.17

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	98	DV7	O-C-CA-CB
3	L	98	DV7	CE2-CD-CG-CB
3	M	98	DV7	CE2-CD-CG-CB
3	Y	98	DV7	CE2-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

20 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
6	PEG	Y	303	-	6,6,6	0.16	0	5,5,5	0.08	0
6	PEG	B	302	-	6,6,6	0.21	0	5,5,5	0.14	0
4	NAG	C	301	1	14,14,15	0.82	0	17,19,21	2.10	3 (17%)
6	PEG	C	302	-	6,6,6	0.24	0	5,5,5	0.19	0
6	PEG	L	304	-	6,6,6	0.14	0	5,5,5	0.12	0
5	TRS	A	302	-	7,7,7	0.11	0	9,9,9	0.35	0
6	PEG	A	303	-	6,6,6	0.16	0	5,5,5	0.11	0
6	PEG	Y	302	-	5,5,6	0.28	0	4,4,5	0.19	0
4	NAG	B	301	1	14,14,15	0.93	0	17,19,21	2.71	4 (23%)
7	TMO	M	301[A]	-	4,4,4	0.94	0	6,6,6	0.05	0
7	TMO	L	301[B]	-	4,4,4	1.08	1 (25%)	6,6,6	0.08	0
6	PEG	H	301	-	4,4,6	0.24	0	3,3,5	0.17	0
6	PEG	L	303	-	4,4,6	0.26	0	3,3,5	0.21	0
6	PEG	X	301	-	6,6,6	0.19	0	5,5,5	0.14	0
4	NAG	A	301	1	14,14,15	0.98	1 (7%)	17,19,21	2.05	5 (29%)
7	TMO	Y	301	-	4,4,4	0.97	0	6,6,6	0.07	0
6	PEG	M	302[B]	-	6,6,6	0.11	0	5,5,5	0.10	0
6	PEG	H	302	-	6,6,6	0.22	0	5,5,5	0.13	0
6	PEG	K	301	-	6,6,6	0.15	0	5,5,5	0.06	0
6	PEG	L	302[A]	-	6,6,6	0.21	0	5,5,5	0.14	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	NAG	A	301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	301	1	-	0/6/23/26	0/1/1/1
6	PEG	C	302	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	L	304	-	-	0/4/4/4	-
6	PEG	Y	302	-	-	2/3/3/4	-
5	TRS	A	302	-	-	3/9/9/9	-
6	PEG	M	302[B]	-	-	2/4/4/4	-
4	NAG	B	301	1	-	2/6/23/26	0/1/1/1
6	PEG	H	302	-	-	3/4/4/4	-
6	PEG	L	302[A]	-	-	3/4/4/4	-
6	PEG	H	301	-	-	2/2/2/4	-
6	PEG	Y	303	-	-	2/4/4/4	-
6	PEG	B	302	-	-	2/4/4/4	-
6	PEG	K	301	-	-	2/4/4/4	-
6	PEG	A	303	-	-	2/4/4/4	-
6	PEG	L	303	-	-	1/2/2/4	-
6	PEG	X	301	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	NAG	O5-C1	2.18	1.47	1.43
7	L	301[B]	TMO	OAE-NAC	-2.11	1.39	1.42

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	NAG	C1-O5-C5	9.89	125.60	112.19
4	C	301	NAG	C1-O5-C5	7.02	121.71	112.19
4	A	301	NAG	C1-O5-C5	5.99	120.31	112.19
4	A	301	NAG	C1-C2-N2	3.13	115.84	110.49
4	A	301	NAG	C6-C5-C4	-2.55	107.04	113.00

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	302	TRS	C1-C-C3-O3
5	A	302	TRS	C2-C-C3-O3
6	K	301	PEG	O1-C1-C2-O2
4	A	301	NAG	C4-C5-C6-O6
4	B	301	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	302	TRS	1	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 [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, 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	A	137/146 (93%)	-0.33	0 <a href="#">100</a> <a href="#">100</a>	11, 18, 38, 50	0
1	B	140/146 (95%)	-0.32	1 (0%) <a href="#">87</a> <a href="#">87</a>	10, 19, 38, 53	0
1	C	137/146 (93%)	-0.38	0 <a href="#">100</a> <a href="#">100</a>	11, 18, 35, 47	0
2	H	211/226 (93%)	0.00	9 (4%) <a href="#">35</a> <a href="#">34</a>	15, 36, 65, 79	0
2	K	213/226 (94%)	-0.51	1 (0%) <a href="#">91</a> <a href="#">90</a>	17, 28, 41, 52	0
2	X	214/226 (94%)	-0.56	2 (0%) <a href="#">84</a> <a href="#">83</a>	14, 26, 40, 51	0
3	L	207/218 (94%)	-0.44	2 (0%) <a href="#">82</a> <a href="#">81</a>	12, 21, 55, 72	0
3	M	216/218 (99%)	-0.53	1 (0%) <a href="#">91</a> <a href="#">90</a>	11, 20, 43, 60	0
3	Y	215/218 (98%)	-0.57	1 (0%) <a href="#">91</a> <a href="#">90</a>	11, 20, 44, 55	0
All	All	1690/1770 (95%)	-0.41	17 (1%) <a href="#">82</a> <a href="#">81</a>	10, 23, 48, 79	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	42[A]	GLY	3.0
2	H	210	THR	2.9
3	L	185	LEU	2.8
2	X	132	SER	2.8
2	H	209	ASN	2.7

### 6.2 Non-standard residues in protein, DNA, RNA chains [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	DV7	L	98	18/19	0.95	0.08	18,21,23,23	0
3	DV7	M	98	18/19	0.95	0.09	18,20,21,22	0
3	DV7	Y	98	18/19	0.96	0.09	16,20,21,21	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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
6	PEG	C	302	7/7	0.62	0.19	48,48,56,57	0
4	NAG	A	301	14/15	0.65	0.30	43,52,56,56	0
6	PEG	H	302	7/7	0.73	0.30	66,66,67,68	0
6	PEG	X	301	7/7	0.75	0.23	56,59,61,61	0
6	PEG	A	303	7/7	0.77	0.18	58,60,66,67	0
6	PEG	L	303	5/7	0.79	0.20	58,58,59,60	0
6	PEG	Y	303	7/7	0.80	0.18	54,55,59,59	0
6	PEG	L	304	7/7	0.81	0.14	55,60,61,62	0
6	PEG	B	302	7/7	0.82	0.23	53,55,57,57	0
6	PEG	K	301	7/7	0.83	0.18	49,51,54,56	0
6	PEG	M	302[B]	7/7	0.83	0.38	21,23,25,27	7
4	NAG	B	301	14/15	0.84	0.22	39,49,51,55	0
4	NAG	C	301	14/15	0.84	0.21	32,43,46,50	0
5	TRS	A	302	8/8	0.85	0.16	50,53,56,58	0
6	PEG	H	301	5/7	0.87	0.17	44,45,49,49	0
7	TMO	M	301[A]	5/5	0.88	0.42	27,28,29,31	5
7	TMO	L	301[B]	5/5	0.91	0.38	24,24,25,25	5
6	PEG	L	302[A]	7/7	0.91	0.24	24,24,26,26	7
6	PEG	Y	302	6/7	0.92	0.12	48,48,49,52	0
7	TMO	Y	301	5/5	0.92	0.13	60,61,61,64	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.