



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 12, 2022 – 01:17 PM EDT

PDB ID : 8DRW
Title : Product structure of SARS-CoV-2 Mpro C145A mutant in complex with nsp9-nsp10 (C9) cut site sequence
Authors : Lee, J.; Kenward, C.; Worrall, L.J.; Vuckovic, M.; Paetzel, M.; Strynadka, N.C.J.
Deposited on : 2022-07-21
Resolution : 2.67 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

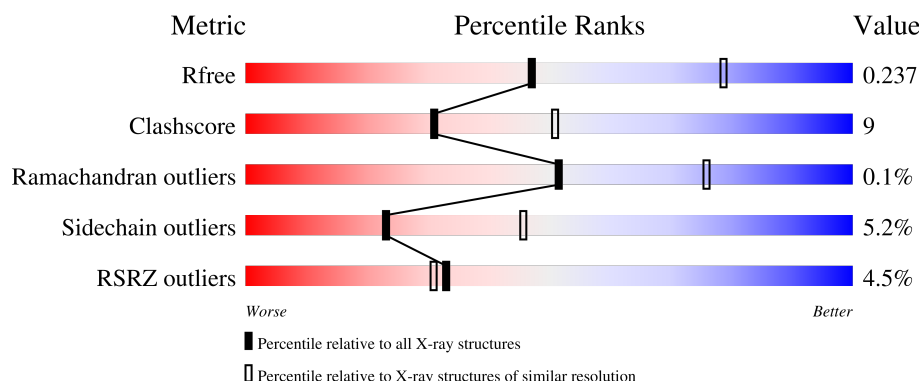
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	306	
1	B	306	
1	C	306	
1	D	306	
1	E	306	

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Mol	Chain	Length	Quality of chain
1	F	306	
1	G	306	
1	H	306	
1	I	306	
1	J	306	
1	K	306	
1	L	306	
1	M	306	
1	N	306	

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
4	PEG	A	404	-	-	X	-
5	PO4	G	403	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33657 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 Fusion protein of 3C-like proteinase nsp5 and nsp9-nsp10 (C9) cut site.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2351	1490	399	442	20			
1	B	306	Total	C	N	O	S	0	0	0
			2359	1491	404	443	21			
1	C	306	Total	C	N	O	S	0	0	0
			2363	1494	405	443	21			
1	D	306	Total	C	N	O	S	0	0	0
			2363	1494	405	443	21			
1	E	306	Total	C	N	O	S	0	0	0
			2359	1491	404	443	21			
1	F	306	Total	C	N	O	S	0	0	0
			2351	1488	399	443	21			
1	G	306	Total	C	N	O	S	0	1	0
			2333	1478	395	439	21			
1	H	306	Total	C	N	O	S	0	0	0
			2368	1499	405	443	21			
1	I	306	Total	C	N	O	S	0	0	0
			2347	1485	398	443	21			
1	J	306	Total	C	N	O	S	0	0	0
			2340	1482	398	440	20			
1	K	298	Total	C	N	O	S	0	0	0
			2208	1392	380	418	18			
1	L	306	Total	C	N	O	S	0	0	0
			2366	1497	404	444	21			
1	M	306	Total	C	N	O	S	0	0	0
			2370	1500	405	444	21			
1	N	306	Total	C	N	O	S	0	0	0
			2356	1489	405	441	21			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	145	ALA	CYS	conflict	UNP P0DTD1
B	145	ALA	CYS	conflict	UNP P0DTD1
C	145	ALA	CYS	conflict	UNP P0DTD1
D	145	ALA	CYS	conflict	UNP P0DTD1
E	145	ALA	CYS	conflict	UNP P0DTD1
F	145	ALA	CYS	conflict	UNP P0DTD1
G	145	ALA	CYS	conflict	UNP P0DTD1
H	145	ALA	CYS	conflict	UNP P0DTD1
I	145	ALA	CYS	conflict	UNP P0DTD1
J	145	ALA	CYS	conflict	UNP P0DTD1
K	145	ALA	CYS	conflict	UNP P0DTD1
L	145	ALA	CYS	conflict	UNP P0DTD1
M	145	ALA	CYS	conflict	UNP P0DTD1
N	145	ALA	CYS	conflict	UNP P0DTD1

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0
2	I	1	Total Na 1 1	0	0
2	J	1	Total Na 1 1	0	0
2	L	1	Total Na 1 1	0	0
2	M	1	Total Na 1 1	0	0
2	N	1	Total Na 1 1	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



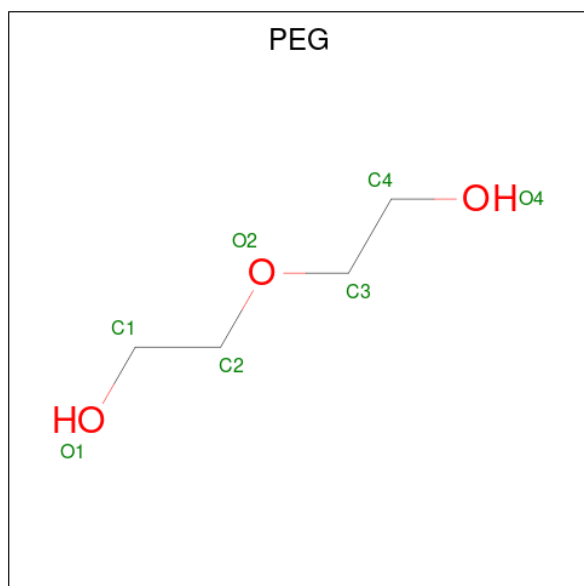
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			13	8	5		
3	E	1	Total	C	O	0	0
			10	6	4		
3	F	1	Total	C	O	0	0
			10	6	4		
3	F	1	Total	C	O	0	0
			10	6	4		
3	G	1	Total	C	O	0	0
			10	6	4		
3	H	1	Total	C	O	0	0
			10	6	4		
3	H	1	Total	C	O	0	0
			16	10	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			10	6	4		
3	I	1	Total	C	O	0	0
			10	6	4		
3	J	1	Total	C	O	0	0
			10	6	4		
3	J	1	Total	C	O	0	0
			16	10	6		
3	K	1	Total	C	O	0	0
			10	6	4		
3	L	1	Total	C	O	0	0
			10	6	4		
3	M	1	Total	C	O	0	0
			10	6	4		
3	N	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		

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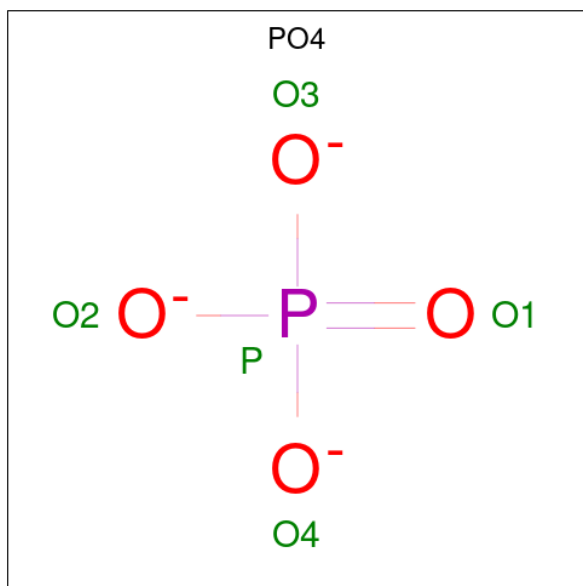
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		
4	G	1	Total	C	O	0	0
			7	4	3		
4	H	1	Total	C	O	0	0
			7	4	3		
4	H	1	Total	C	O	0	0
			7	4	3		
4	J	1	Total	C	O	0	0
			7	4	3		
4	J	1	Total	C	O	0	0
			7	4	3		
4	J	1	Total	C	O	0	0
			7	4	3		
4	J	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	I	1	Total	O	P	0	0
			5	4	1		
5	J	1	Total	O	P	0	0
			5	4	1		
5	J	1	Total	O	P	0	0
			5	4	1		
5	K	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		
5	M	1	Total	O	P	0	0
			5	4	1		

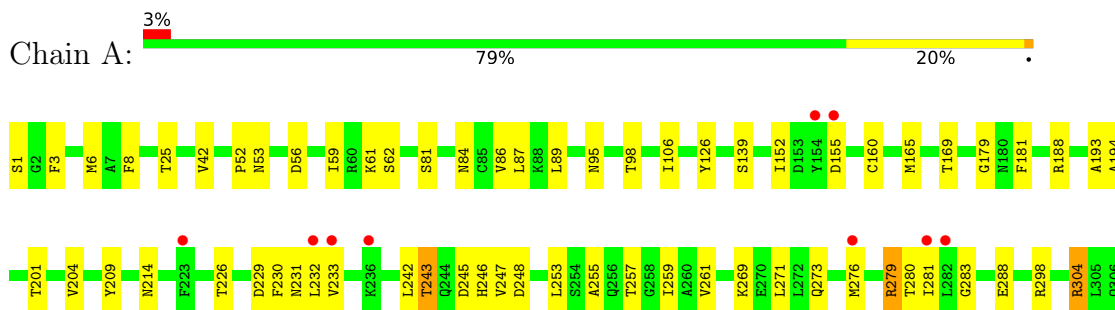
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total	O	0	0
			14	14		
6	B	16	Total	O	0	0
			16	16		
6	C	8	Total	O	0	0
			8	8		
6	D	33	Total	O	0	0
			33	33		
6	E	14	Total	O	0	0
			14	14		
6	F	16	Total	O	0	0
			16	16		
6	G	11	Total	O	0	0
			11	11		
6	H	19	Total	O	0	0
			19	19		
6	I	10	Total	O	0	0
			10	10		
6	J	15	Total	O	0	0
			15	15		
6	K	4	Total	O	0	0
			4	4		
6	L	24	Total	O	0	0
			24	24		
6	M	13	Total	O	0	0
			13	13		
6	N	13	Total	O	0	0
			13	13		

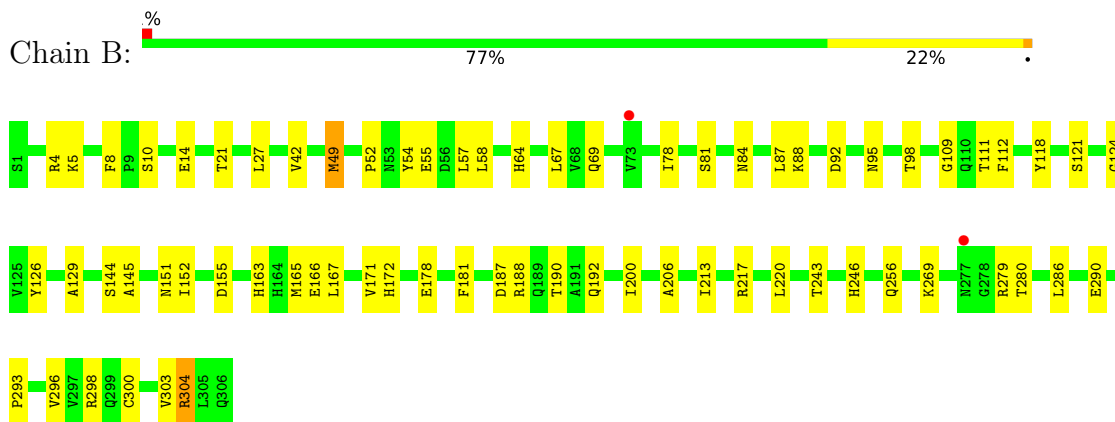
3 Residue-property plots [i](#)

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.

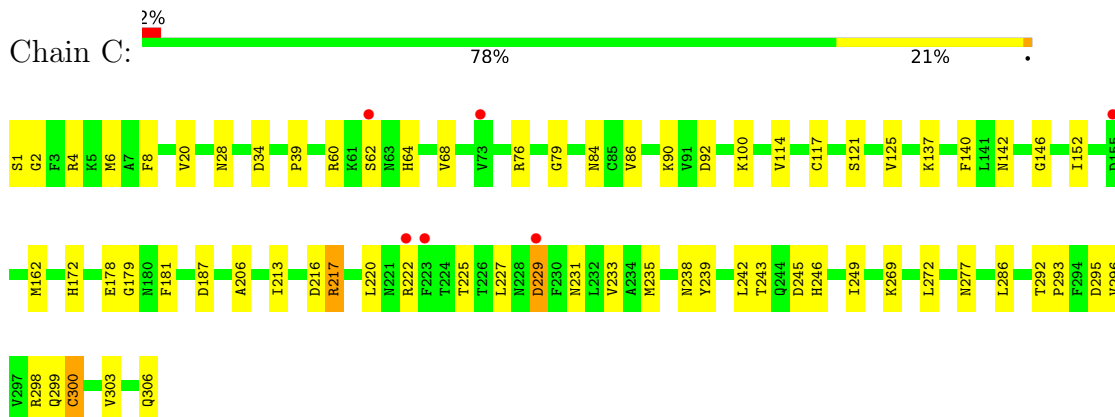
- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp9-nsp10 (C9) cut site



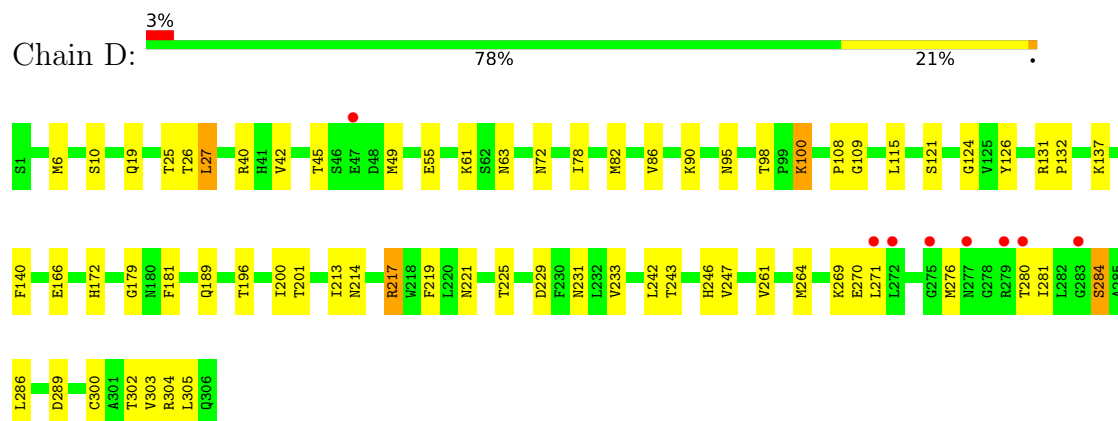
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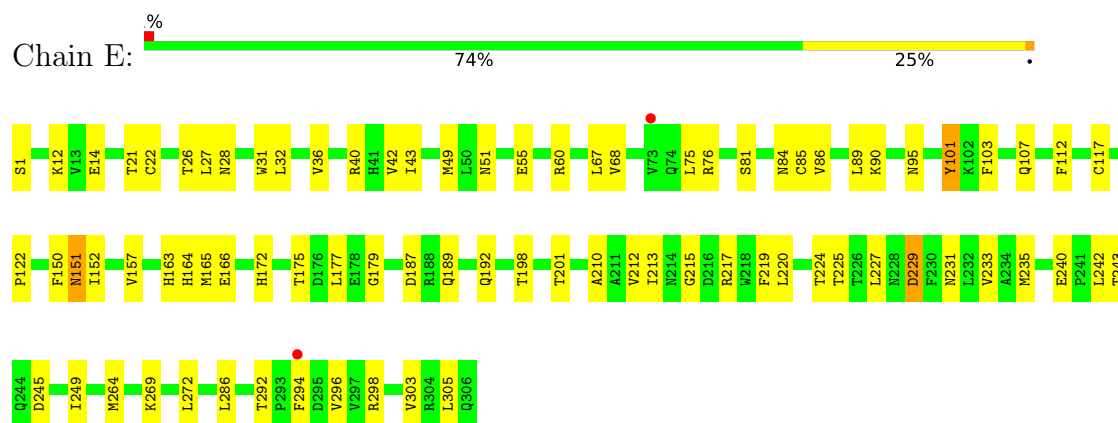
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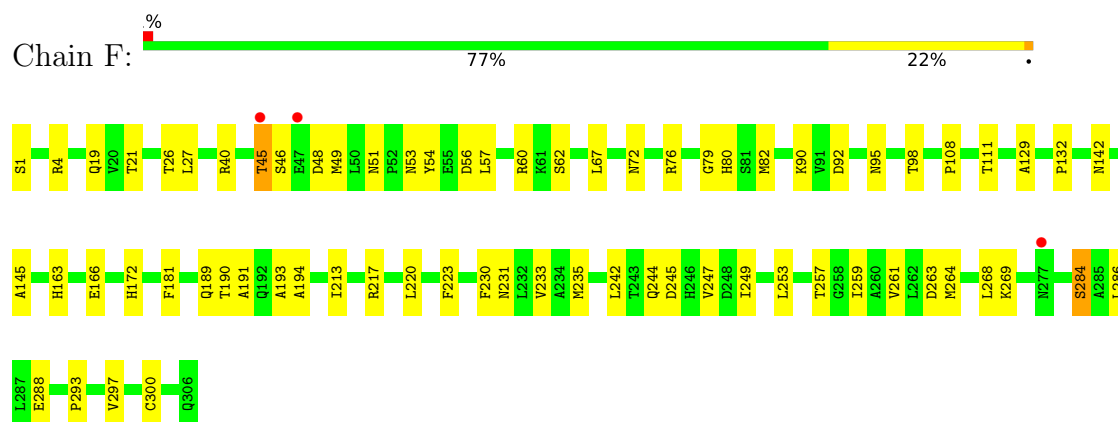
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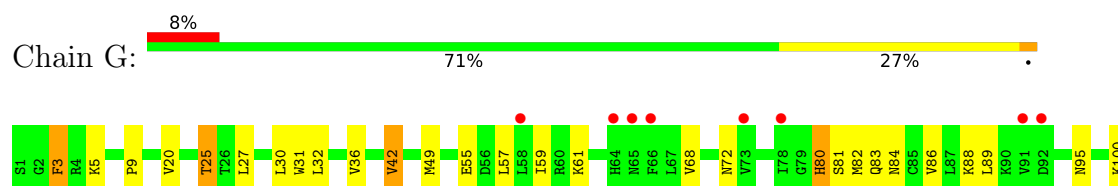
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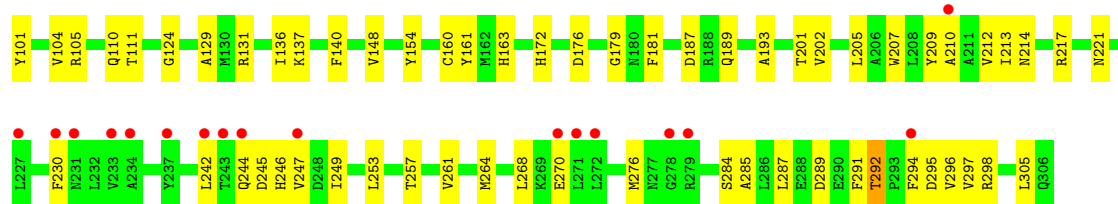


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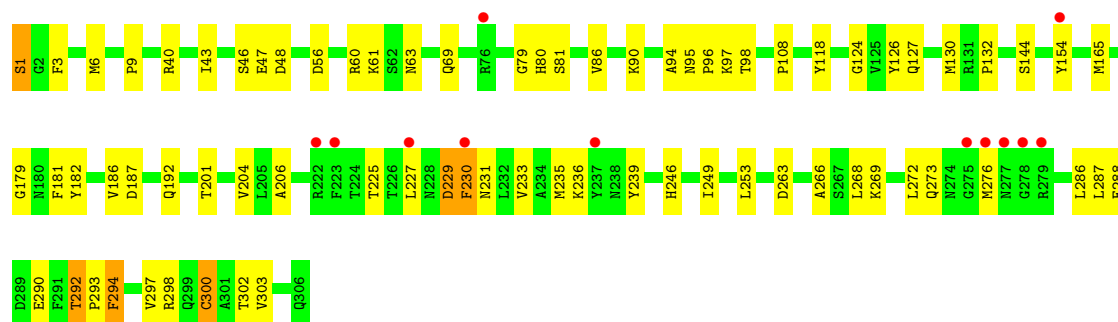
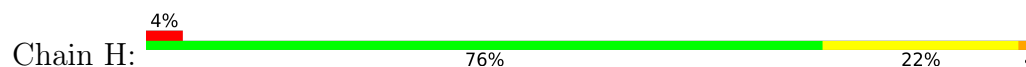


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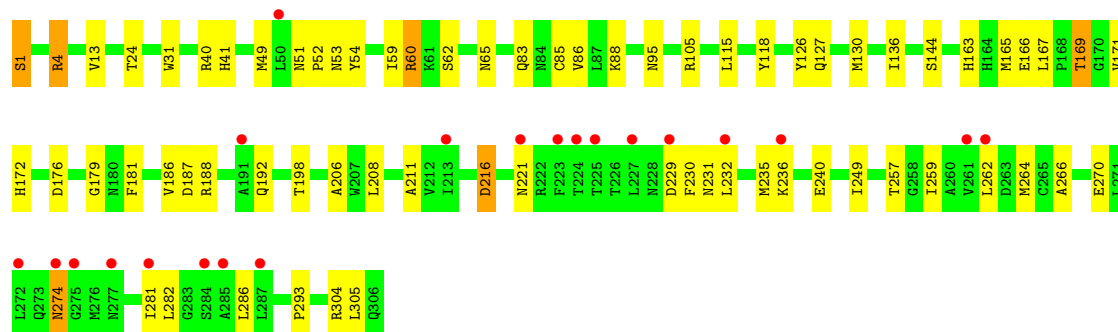




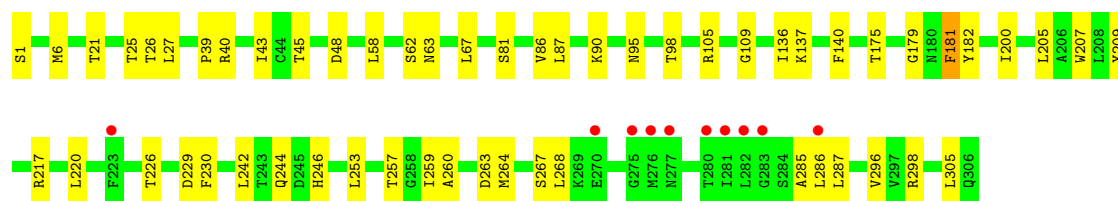
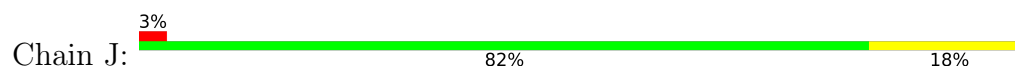
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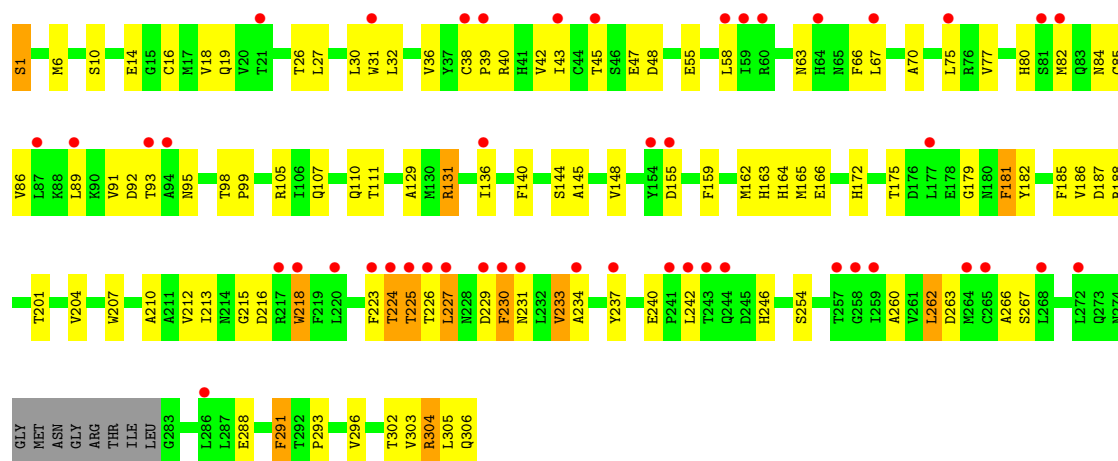


- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp9-nsp10 (C9) cut site

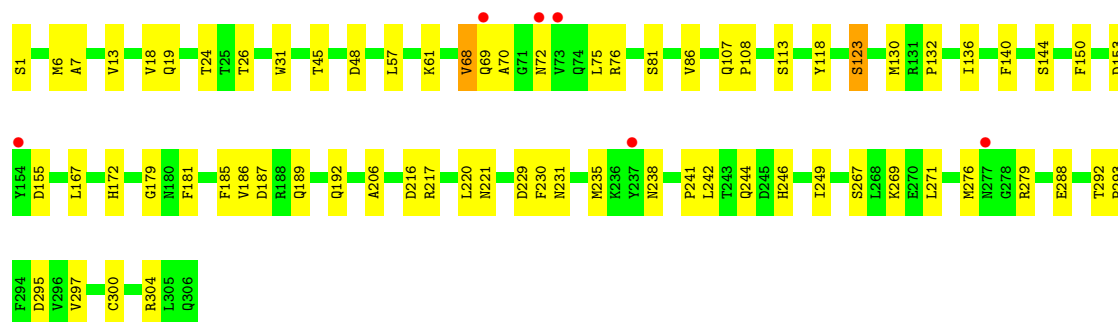


- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp9-nsp10 (C9) cut site

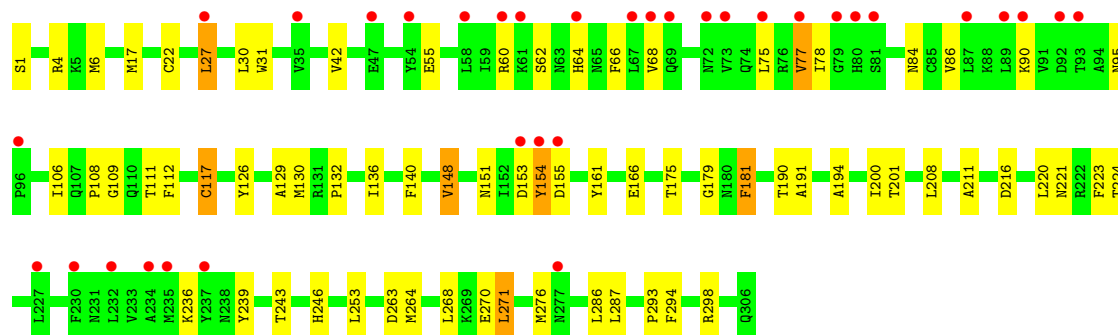
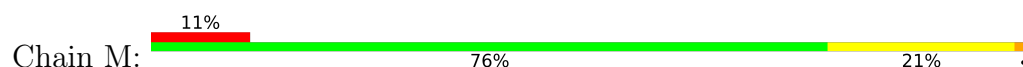




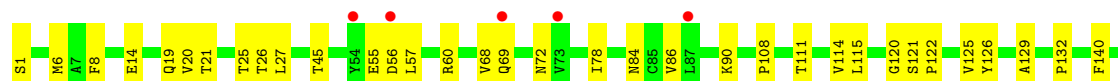
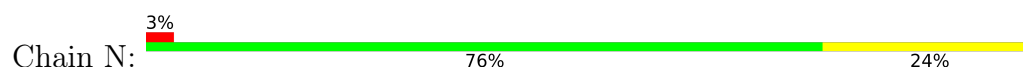
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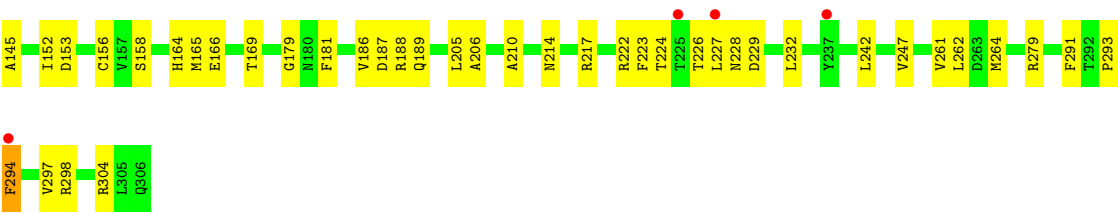


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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	275.64Å 217.22Å 104.64Å 90.00° 110.98° 90.00°	Depositor
Resolution (Å)	67.10 – 2.67 67.10 – 2.67	Depositor EDS
% Data completeness (in resolution range)	74.7 (67.10-2.67) 74.7 (67.10-2.67)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.205 , 0.239 0.203 , 0.237	Depositor DCC
R_{free} test set	1997 reflections (1.65%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h-2*k,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	33657	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, NA, 1PE, PO4

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	0.25	0/2403	0.48	0/3269
1	B	0.25	0/2410	0.49	0/3276
1	C	0.25	0/2414	0.49	0/3280
1	D	0.26	0/2414	0.50	0/3280
1	E	0.25	0/2410	0.49	0/3276
1	F	0.25	0/2402	0.49	0/3266
1	G	0.25	0/2387	0.49	0/3249
1	H	0.27	0/2420	0.50	0/3288
1	I	0.27	0/2398	0.50	0/3262
1	J	0.26	0/2392	0.48	0/3254
1	K	0.32	0/2257	0.57	0/3077
1	L	0.25	0/2418	0.48	0/3287
1	M	0.25	0/2422	0.48	0/3291
1	N	0.26	0/2407	0.50	0/3271
All	All	0.26	0/33554	0.50	0/45626

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2351	0	2292	41	0
1	B	2359	0	2308	53	0
1	C	2363	0	2319	40	0
1	D	2363	0	2319	41	0
1	E	2359	0	2308	46	0
1	F	2351	0	2297	44	0
1	G	2333	0	2261	54	0
1	H	2368	0	2321	48	0
1	I	2347	0	2285	45	0
1	J	2340	0	2266	32	0
1	K	2208	0	2051	84	0
1	L	2366	0	2315	39	0
1	M	2370	0	2326	47	0
1	N	2356	0	2306	34	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	H	1	0	0	1	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
3	A	10	0	13	1	0
3	B	20	0	26	5	0
3	C	20	0	26	1	0
3	D	33	0	43	2	0
3	E	10	0	13	0	0
3	F	20	0	26	3	0
3	G	10	0	13	1	0
3	H	36	0	48	5	0
3	I	10	0	13	0	0
3	J	26	0	35	3	0
3	K	10	0	13	1	0
3	L	10	0	13	1	0
3	M	10	0	13	3	0
3	N	10	0	13	1	0
4	A	21	0	30	6	0
4	B	42	0	60	2	0
4	C	14	0	20	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	14	0	20	1	0
4	E	14	0	20	0	0
4	F	14	0	20	2	0
4	G	7	0	10	3	0
4	H	14	0	20	2	0
4	J	42	0	60	1	0
4	L	21	0	30	1	0
4	M	7	0	10	0	0
4	N	21	0	30	2	0
5	A	10	0	0	0	0
5	B	15	0	0	2	0
5	C	15	0	0	1	0
5	D	5	0	0	0	0
5	E	10	0	0	0	0
5	F	15	0	0	1	0
5	G	10	0	0	0	0
5	H	15	0	0	0	0
5	I	5	0	0	0	0
5	J	10	0	0	0	0
5	K	5	0	0	0	0
5	L	15	0	0	0	0
5	M	5	0	0	0	0
6	A	14	0	0	3	0
6	B	16	0	0	1	0
6	C	8	0	0	2	0
6	D	33	0	0	3	0
6	E	14	0	0	2	0
6	F	16	0	0	0	0
6	G	11	0	0	1	0
6	H	19	0	0	1	0
6	I	10	0	0	0	0
6	J	15	0	0	0	0
6	K	4	0	0	0	0
6	L	24	0	0	0	0
6	M	13	0	0	0	0
6	N	13	0	0	0	0
All	All	33657	0	32612	599	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 9.

The worst 5 of 599 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:I:62:SER:H	1:I:65:ASN:HD22	1.25	0.82
1:K:226:THR:HG22	1:K:229:ASP:HB2	1.62	0.82
1:J:86:VAL:HG13	1:J:179:GLY:HA2	1.62	0.81
1:K:86:VAL:HG13	1:K:179:GLY:HA2	1.62	0.80
1:A:231:ASN:HD21	1:A:242:LEU:H	1.29	0.80

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	304/306 (99%)	294 (97%)	10 (3%)	0	100	100
1	B	304/306 (99%)	297 (98%)	7 (2%)	0	100	100
1	C	304/306 (99%)	296 (97%)	8 (3%)	0	100	100
1	D	304/306 (99%)	297 (98%)	7 (2%)	0	100	100
1	E	304/306 (99%)	296 (97%)	8 (3%)	0	100	100
1	F	304/306 (99%)	294 (97%)	10 (3%)	0	100	100
1	G	305/306 (100%)	297 (97%)	7 (2%)	1 (0%)	41	64
1	H	304/306 (99%)	298 (98%)	5 (2%)	1 (0%)	41	64
1	I	304/306 (99%)	298 (98%)	6 (2%)	0	100	100
1	J	304/306 (99%)	298 (98%)	6 (2%)	0	100	100
1	K	294/306 (96%)	276 (94%)	18 (6%)	0	100	100
1	L	304/306 (99%)	299 (98%)	5 (2%)	0	100	100
1	M	304/306 (99%)	296 (97%)	7 (2%)	1 (0%)	41	64
1	N	304/306 (99%)	296 (97%)	8 (3%)	0	100	100
All	All	4247/4284 (99%)	4132 (97%)	112 (3%)	3 (0%)	51	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	154	TYR
1	G	154	TYR
1	H	154	TYR

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	258/262 (98%)	247 (96%)	11 (4%)	29	54
1	B	260/262 (99%)	254 (98%)	6 (2%)	50	76
1	C	261/262 (100%)	249 (95%)	12 (5%)	27	51
1	D	261/262 (100%)	248 (95%)	13 (5%)	24	47
1	E	260/262 (99%)	245 (94%)	15 (6%)	20	41
1	F	259/262 (99%)	249 (96%)	10 (4%)	32	58
1	G	253/262 (97%)	238 (94%)	15 (6%)	19	40
1	H	261/262 (100%)	249 (95%)	12 (5%)	27	51
1	I	258/262 (98%)	246 (95%)	12 (5%)	26	50
1	J	254/262 (97%)	245 (96%)	9 (4%)	36	62
1	K	226/262 (86%)	203 (90%)	23 (10%)	7	15
1	L	261/262 (100%)	245 (94%)	16 (6%)	18	38
1	M	262/262 (100%)	251 (96%)	11 (4%)	30	55
1	N	259/262 (99%)	238 (92%)	21 (8%)	11	25
All	All	3593/3668 (98%)	3407 (95%)	186 (5%)	23	46

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	1	SER
1	L	107	GLN
1	K	67	LEU
1	K	230	PHE
1	L	279	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	142	ASN
1	N	228	ASN
1	K	203	ASN
1	M	151	ASN
1	F	84	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 94 ligands modelled in this entry, 12 are monoatomic - leaving 82 for Mogul analysis.

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	$\# Z > 2$
5	PO4	E	406	-	4,4,4	0.90	0	6,6,6	0.45	0
4	PEG	D	405	-	6,6,6	0.11	0	5,5,5	0.08	0
3	1PE	E	402	-	9,9,15	0.09	0	8,8,14	0.16	0
5	PO4	H	407	-	4,4,4	0.91	0	6,6,6	0.43	0
5	PO4	I	403	-	4,4,4	0.93	0	6,6,6	0.42	0
4	PEG	A	404	-	6,6,6	0.08	0	5,5,5	0.07	0
5	PO4	G	404	-	4,4,4	0.91	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	1PE	H	405	-	9,9,15	0.12	0	8,8,14	0.13	0
3	1PE	J	404	-	9,9,15	0.12	0	8,8,14	0.13	0
3	1PE	K	401	-	9,9,15	0.11	0	8,8,14	0.11	0
3	1PE	F	403	-	9,9,15	0.11	0	8,8,14	0.13	0
4	PEG	L	403	-	6,6,6	0.10	0	5,5,5	0.10	0
4	PEG	C	403	-	6,6,6	0.12	0	5,5,5	0.05	0
3	1PE	C	402	-	9,9,15	0.10	0	8,8,14	0.13	0
4	PEG	B	407	-	6,6,6	0.11	0	5,5,5	0.09	0
4	PEG	N	403	-	6,6,6	0.11	0	5,5,5	0.07	0
3	1PE	I	402	-	9,9,15	0.12	0	8,8,14	0.12	0
3	1PE	D	404	-	12,12,15	0.11	0	11,11,14	0.13	0
4	PEG	E	403	-	6,6,6	0.11	0	5,5,5	0.09	0
4	PEG	B	409	-	6,6,6	0.12	0	5,5,5	0.09	0
4	PEG	B	403	-	6,6,6	0.12	0	5,5,5	0.07	0
3	1PE	C	405	-	9,9,15	0.11	0	8,8,14	0.13	0
4	PEG	L	402	-	6,6,6	0.11	0	5,5,5	0.09	0
5	PO4	B	410	-	4,4,4	0.92	0	6,6,6	0.41	0
3	1PE	J	405	-	15,15,15	0.54	0	14,14,14	0.25	0
4	PEG	E	404	-	6,6,6	0.11	0	5,5,5	0.10	0
4	PEG	A	403	-	6,6,6	0.11	0	5,5,5	0.09	0
4	PEG	B	404	-	6,6,6	0.11	0	5,5,5	0.09	0
3	1PE	L	404	-	9,9,15	0.11	0	8,8,14	0.14	0
5	PO4	L	407	-	4,4,4	0.91	0	6,6,6	0.42	0
4	PEG	D	406	-	6,6,6	0.10	0	5,5,5	0.10	0
4	PEG	J	409	-	6,6,6	0.50	0	5,5,5	0.48	0
5	PO4	J	411	-	4,4,4	0.92	0	6,6,6	0.44	0
4	PEG	J	406	-	6,6,6	0.11	0	5,5,5	0.10	0
4	PEG	H	404	-	6,6,6	0.11	0	5,5,5	0.08	0
5	PO4	C	407	-	4,4,4	0.91	0	6,6,6	0.44	0
3	1PE	B	402	-	9,9,15	0.11	0	8,8,14	0.14	0
5	PO4	B	411	-	4,4,4	0.92	0	6,6,6	0.42	0
4	PEG	A	405	-	6,6,6	0.11	0	5,5,5	0.08	0
3	1PE	D	403	-	9,9,15	0.10	0	8,8,14	0.14	0
4	PEG	B	406	-	6,6,6	0.12	0	5,5,5	0.09	0
3	1PE	M	402	-	9,9,15	0.11	0	8,8,14	0.14	0
5	PO4	G	403	-	4,4,4	0.92	0	6,6,6	0.44	0
4	PEG	C	404	-	6,6,6	0.11	0	5,5,5	0.09	0
5	PO4	M	404	-	4,4,4	0.91	0	6,6,6	0.43	0
4	PEG	H	406	-	6,6,6	0.10	0	5,5,5	0.10	0
5	PO4	E	405	-	4,4,4	0.91	0	6,6,6	0.43	0
5	PO4	H	408	-	4,4,4	0.90	0	6,6,6	0.44	0
5	PO4	J	410	-	4,4,4	0.90	0	6,6,6	0.44	0
4	PEG	J	408	-	6,6,6	0.25	0	5,5,5	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	M	403	-	6,6,6	0.11	0	5,5,5	0.09	0
3	1PE	H	403	-	15,15,15	0.12	0	14,14,14	0.21	0
5	PO4	L	406	-	4,4,4	0.91	0	6,6,6	0.42	0
4	PEG	F	405	-	6,6,6	0.11	0	5,5,5	0.09	0
5	PO4	B	412	-	4,4,4	0.92	0	6,6,6	0.42	0
3	1PE	B	408	-	9,9,15	0.11	0	8,8,14	0.13	0
3	1PE	D	402	-	9,9,15	0.11	0	8,8,14	0.14	0
4	PEG	N	402	-	6,6,6	0.11	0	5,5,5	0.07	0
4	PEG	F	402	-	6,6,6	0.11	0	5,5,5	0.10	0
3	1PE	G	401	-	9,9,15	0.12	0	8,8,14	0.20	0
5	PO4	A	406	-	4,4,4	0.91	0	6,6,6	0.41	0
3	1PE	H	402	-	9,9,15	0.13	0	8,8,14	0.18	0
5	PO4	C	406	-	4,4,4	0.93	0	6,6,6	0.42	0
5	PO4	F	407	-	4,4,4	0.91	0	6,6,6	0.43	0
4	PEG	B	405	-	6,6,6	0.11	0	5,5,5	0.09	0
5	PO4	K	402	-	4,4,4	0.91	0	6,6,6	0.44	0
4	PEG	N	405	-	6,6,6	0.12	0	5,5,5	0.06	0
5	PO4	A	407	-	4,4,4	0.91	0	6,6,6	0.43	0
4	PEG	J	403	-	6,6,6	0.11	0	5,5,5	0.10	0
5	PO4	H	409	-	4,4,4	0.91	0	6,6,6	0.44	0
4	PEG	J	407	-	6,6,6	0.11	0	5,5,5	0.09	0
5	PO4	L	408	-	4,4,4	0.93	0	6,6,6	0.42	0
3	1PE	N	404	-	9,9,15	0.12	0	8,8,14	0.12	0
3	1PE	F	404	-	9,9,15	0.11	0	8,8,14	0.12	0
4	PEG	G	402	-	6,6,6	0.11	0	5,5,5	0.05	0
4	PEG	J	402	-	6,6,6	0.11	0	5,5,5	0.09	0
5	PO4	F	408	-	4,4,4	0.91	0	6,6,6	0.42	0
3	1PE	A	402	-	9,9,15	0.10	0	8,8,14	0.13	0
5	PO4	C	408	-	4,4,4	0.91	0	6,6,6	0.44	0
5	PO4	F	406	-	4,4,4	0.92	0	6,6,6	0.42	0
4	PEG	L	405	-	6,6,6	0.11	0	5,5,5	0.08	0
5	PO4	D	407	-	4,4,4	0.90	0	6,6,6	0.43	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	1PE	H	402	-	-	3/7/7/13	-
4	PEG	E	403	-	-	1/4/4/4	-
4	PEG	B	409	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	B	403	-	-	1/4/4/4	-
4	PEG	B	405	-	-	3/4/4/4	-
4	PEG	C	404	-	-	1/4/4/4	-
4	PEG	D	405	-	-	3/4/4/4	-
3	1PE	E	402	-	-	4/7/7/13	-
4	PEG	H	406	-	-	1/4/4/4	-
3	1PE	C	405	-	-	3/7/7/13	-
4	PEG	L	402	-	-	2/4/4/4	-
3	1PE	J	405	-	-	9/13/13/13	-
4	PEG	N	405	-	-	2/4/4/4	-
4	PEG	E	404	-	-	0/4/4/4	-
4	PEG	A	403	-	-	2/4/4/4	-
4	PEG	B	404	-	-	2/4/4/4	-
3	1PE	L	404	-	-	3/7/7/13	-
4	PEG	A	404	-	-	2/4/4/4	-
4	PEG	J	403	-	-	1/4/4/4	-
4	PEG	J	408	-	-	3/4/4/4	-
4	PEG	M	403	-	-	2/4/4/4	-
4	PEG	D	406	-	-	2/4/4/4	-
3	1PE	H	405	-	-	5/7/7/13	-
4	PEG	J	407	-	-	2/4/4/4	-
3	1PE	J	404	-	-	5/7/7/13	-
3	1PE	K	401	-	-	5/7/7/13	-
4	PEG	J	409	-	-	1/4/4/4	-
3	1PE	F	403	-	-	6/7/7/13	-
4	PEG	L	403	-	-	3/4/4/4	-
4	PEG	C	403	-	-	2/4/4/4	-
3	1PE	H	403	-	-	6/13/13/13	-
4	PEG	J	406	-	-	2/4/4/4	-
3	1PE	N	404	-	-	4/7/7/13	-
3	1PE	C	402	-	-	4/7/7/13	-
3	1PE	F	404	-	-	4/7/7/13	-
4	PEG	H	404	-	-	1/4/4/4	-
4	PEG	B	407	-	-	1/4/4/4	-
4	PEG	G	402	-	-	2/4/4/4	-
4	PEG	J	402	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	A	402	-	-	3/7/7/13	-
4	PEG	F	405	-	-	1/4/4/4	-
3	1PE	B	402	-	-	4/7/7/13	-
3	1PE	M	402	-	-	2/7/7/13	-
3	1PE	B	408	-	-	4/7/7/13	-
3	1PE	D	402	-	-	4/7/7/13	-
4	PEG	A	405	-	-	2/4/4/4	-
4	PEG	N	402	-	-	1/4/4/4	-
4	PEG	F	402	-	-	2/4/4/4	-
4	PEG	N	403	-	-	2/4/4/4	-
3	1PE	D	403	-	-	4/7/7/13	-
3	1PE	G	401	-	-	4/7/7/13	-
3	1PE	I	402	-	-	3/7/7/13	-
4	PEG	L	405	-	-	2/4/4/4	-
4	PEG	B	406	-	-	2/4/4/4	-
3	1PE	D	404	-	-	4/10/10/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 153 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	405	1PE	C16-C26-OH6-C15
3	D	403	1PE	OH5-C14-C24-OH4
4	A	404	PEG	O2-C3-C4-O4
3	A	402	1PE	OH6-C15-C25-OH5
3	H	403	1PE	OH6-C15-C25-OH5

There are no ring outliers.

35 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	405	PEG	1	0
4	A	404	PEG	4	0
3	H	405	1PE	1	0
3	J	404	1PE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	401	1PE	1	0
4	L	403	PEG	1	0
4	C	403	PEG	1	0
3	C	402	1PE	1	0
4	B	407	PEG	1	0
4	N	403	PEG	1	0
3	D	404	1PE	1	0
4	B	403	PEG	1	0
5	B	410	PO4	1	0
3	J	405	1PE	2	0
3	L	404	1PE	1	0
4	H	404	PEG	1	0
3	B	402	1PE	2	0
5	B	411	PO4	1	0
4	A	405	PEG	2	0
3	D	403	1PE	1	0
3	M	402	1PE	3	0
4	C	404	PEG	1	0
4	H	406	PEG	1	0
3	H	403	1PE	4	0
3	B	408	1PE	3	0
4	F	402	PEG	2	0
3	G	401	1PE	1	0
5	C	406	PO4	1	0
4	N	405	PEG	1	0
4	J	403	PEG	1	0
3	N	404	1PE	1	0
3	F	404	1PE	3	0
4	G	402	PEG	3	0
5	F	408	PO4	1	0
3	A	402	1PE	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

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	306/306 (100%)	0.16	9 (2%) 51 51	42, 56, 96, 119	0
1	B	306/306 (100%)	0.06	2 (0%) 87 88	42, 53, 78, 133	0
1	C	306/306 (100%)	0.17	6 (1%) 65 65	44, 64, 98, 128	0
1	D	306/306 (100%)	0.20	8 (2%) 56 55	41, 56, 86, 131	0
1	E	306/306 (100%)	0.10	2 (0%) 87 88	48, 61, 99, 124	0
1	F	306/306 (100%)	0.14	3 (0%) 82 82	43, 58, 88, 129	0
1	G	306/306 (100%)	0.56	25 (8%) 11 9	48, 73, 112, 142	0
1	H	306/306 (100%)	0.28	12 (3%) 39 37	44, 57, 100, 151	0
1	I	306/306 (100%)	0.39	21 (6%) 16 14	45, 64, 103, 126	0
1	J	306/306 (100%)	0.19	10 (3%) 46 45	41, 55, 107, 139	0
1	K	298/306 (97%)	0.92	47 (15%) 2 1	52, 87, 140, 176	0
1	L	306/306 (100%)	0.18	6 (1%) 65 65	47, 62, 91, 117	0
1	M	306/306 (100%)	0.56	34 (11%) 5 4	48, 73, 108, 143	0
1	N	306/306 (100%)	0.29	9 (2%) 51 51	49, 67, 103, 141	0
All	All	4276/4284 (99%)	0.30	194 (4%) 33 31	41, 63, 106, 176	0

The worst 5 of 194 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	268	LEU	6.0
1	K	225	THR	5.8
1	K	234	ALA	5.8
1	K	259	ILE	5.6
1	G	278	GLY	5.0

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
5	PO4	C	407	5/5	0.69	0.23	104,105,121,128	0
5	PO4	E	405	5/5	0.69	0.23	105,111,127,131	0
5	PO4	G	403	5/5	0.69	0.45	113,113,125,129	0
5	PO4	A	407	5/5	0.72	0.32	92,93,107,124	0
2	NA	C	401	1/1	0.75	0.13	99,99,99,99	0
4	PEG	H	406	7/7	0.76	0.33	69,73,76,77	0
4	PEG	M	403	7/7	0.76	0.34	77,88,91,92	0
5	PO4	C	406	5/5	0.77	0.22	98,101,119,120	0
3	1PE	C	405	10/16	0.77	0.26	68,71,73,75	0
5	PO4	B	412	5/5	0.78	0.25	92,102,107,117	0
4	PEG	B	406	7/7	0.79	0.26	59,64,74,77	0
4	PEG	J	406	7/7	0.80	0.22	60,65,80,84	0
4	PEG	N	402	7/7	0.80	0.34	61,63,67,69	0
5	PO4	A	406	5/5	0.80	0.28	74,89,102,105	0
5	PO4	M	404	5/5	0.80	0.34	114,115,130,131	0
4	PEG	J	402	7/7	0.81	0.30	65,67,71,75	0
4	PEG	E	404	7/7	0.81	0.24	57,59,64,66	0
5	PO4	J	410	5/5	0.81	0.24	81,83,98,110	0
5	PO4	B	411	5/5	0.81	0.26	90,90,113,121	0
3	1PE	D	404	13/16	0.82	0.23	65,74,80,80	0
2	NA	A	401	1/1	0.82	0.05	81,81,81,81	0
4	PEG	L	403	7/7	0.82	0.41	69,74,81,87	0
4	PEG	B	403	7/7	0.83	0.18	74,75,79,83	0
4	PEG	J	409	7/7	0.83	0.20	62,65,70,71	0
2	NA	H	401	1/1	0.83	0.28	103,103,103,103	0
2	NA	I	401	1/1	0.83	0.51	116,116,116,116	0
4	PEG	H	404	7/7	0.83	0.34	65,68,71,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	1PE	H	403	16/16	0.83	0.27	49,62,71,76	0
3	1PE	K	401	10/16	0.83	0.27	80,87,91,91	0
5	PO4	B	410	5/5	0.83	0.23	87,88,98,104	0
4	PEG	A	403	7/7	0.84	0.29	62,67,69,77	0
3	1PE	D	403	10/16	0.84	0.20	62,68,78,81	0
5	PO4	F	406	5/5	0.84	0.24	88,91,106,111	0
4	PEG	D	406	7/7	0.85	0.22	60,64,67,74	0
5	PO4	F	407	5/5	0.85	0.25	73,75,86,106	0
4	PEG	B	405	7/7	0.85	0.19	45,60,67,69	0
5	PO4	H	409	5/5	0.85	0.21	66,68,79,94	0
5	PO4	C	408	5/5	0.85	0.26	84,93,106,120	0
5	PO4	L	408	5/5	0.85	0.35	93,97,103,117	0
2	NA	B	401	1/1	0.85	0.06	52,52,52,52	0
3	1PE	B	408	10/16	0.86	0.26	49,55,61,70	0
5	PO4	L	407	5/5	0.86	0.37	105,107,123,133	0
5	PO4	E	406	5/5	0.86	0.32	78,86,92,102	0
4	PEG	N	405	7/7	0.86	0.23	57,67,69,71	0
5	PO4	K	402	5/5	0.87	0.17	108,117,122,136	0
3	1PE	F	404	10/16	0.87	0.21	53,63,72,74	0
3	1PE	G	401	10/16	0.87	0.28	60,63,69,73	0
3	1PE	M	402	10/16	0.87	0.23	56,62,71,75	0
2	NA	E	401	1/1	0.88	0.06	58,58,58,58	0
5	PO4	I	403	5/5	0.88	0.29	87,87,104,107	0
4	PEG	L	402	7/7	0.88	0.31	70,72,78,80	0
5	PO4	D	407	5/5	0.88	0.22	85,86,101,119	0
3	1PE	J	404	10/16	0.88	0.24	53,59,62,69	0
5	PO4	G	404	5/5	0.88	0.26	83,92,96,120	0
5	PO4	H	407	5/5	0.88	0.15	80,83,98,101	0
3	1PE	H	402	10/16	0.89	0.26	56,62,70,71	0
4	PEG	B	404	7/7	0.89	0.28	63,66,75,79	0
4	PEG	F	405	7/7	0.89	0.24	69,71,72,73	0
3	1PE	N	404	10/16	0.89	0.23	59,62,65,65	0
3	1PE	F	403	10/16	0.89	0.26	58,65,68,72	0
4	PEG	C	404	7/7	0.89	0.25	49,52,61,63	0
3	1PE	B	402	10/16	0.90	0.20	52,57,64,65	0
4	PEG	D	405	7/7	0.90	0.20	57,62,70,73	0
4	PEG	G	402	7/7	0.90	0.28	51,52,59,61	0
3	1PE	D	402	10/16	0.90	0.21	53,57,66,67	0
5	PO4	L	406	5/5	0.91	0.18	58,66,89,91	0
2	NA	M	401	1/1	0.92	0.12	76,76,76,76	0
3	1PE	J	405	16/16	0.92	0.21	42,53,66,70	0
2	NA	N	401	1/1	0.92	0.23	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	1PE	L	404	10/16	0.92	0.21	50,57,60,63	0
4	PEG	N	403	7/7	0.92	0.22	54,54,60,64	0
4	PEG	B	407	7/7	0.92	0.23	47,54,58,62	0
3	1PE	E	402	10/16	0.92	0.21	55,63,66,71	0
4	PEG	J	403	7/7	0.92	0.20	43,47,51,52	0
2	NA	F	401	1/1	0.92	0.33	88,88,88,88	0
3	1PE	I	402	10/16	0.92	0.17	49,52,57,57	0
4	PEG	A	404	7/7	0.93	0.24	44,48,55,57	0
4	PEG	B	409	7/7	0.93	0.23	58,64,69,79	0
4	PEG	F	402	7/7	0.93	0.19	54,61,63,72	0
4	PEG	A	405	7/7	0.93	0.15	52,53,55,58	0
3	1PE	H	405	10/16	0.93	0.15	66,68,69,71	10
5	PO4	H	408	5/5	0.93	0.18	75,83,99,110	0
4	PEG	J	408	7/7	0.93	0.19	62,63,67,70	0
3	1PE	C	402	10/16	0.94	0.18	56,62,65,65	0
4	PEG	E	403	7/7	0.94	0.21	49,54,59,62	0
2	NA	D	401	1/1	0.94	0.26	76,76,76,76	0
4	PEG	J	407	7/7	0.94	0.21	61,64,70,71	0
2	NA	J	401	1/1	0.94	0.15	104,104,104,104	0
5	PO4	F	408	5/5	0.94	0.17	65,69,79,83	0
4	PEG	C	403	7/7	0.95	0.20	49,52,55,56	0
4	PEG	L	405	7/7	0.95	0.18	52,54,59,60	0
2	NA	L	401	1/1	0.95	0.09	62,62,62,62	0
3	1PE	A	402	10/16	0.95	0.24	48,53,60,66	0
5	PO4	J	411	5/5	0.97	0.13	63,70,78,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.