



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 01:51 am BST

PDB ID : 6OL7
Title : Crystal structure of glVRC01 scFv in complex with anti-idiotypic iv8 scFv
Authors : Weidle, C.; Pancera, M.
Deposited on : 2019-04-15
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 : 2.11
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

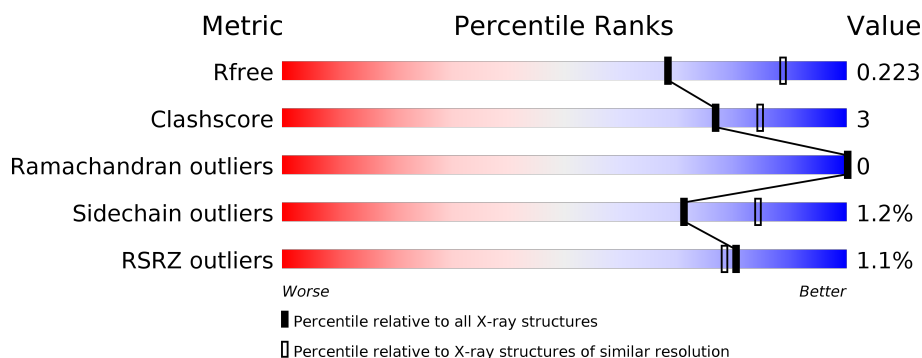
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	131	
1	E	131	
1	K	131	
1	P	131	
2	B	111	
2	F	111	

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Mol	Chain	Length	Quality of chain
2	L	111	
2	N	111	
3	C	141	
3	H	141	
3	I	141	
3	M	141	
4	D	125	
4	J	125	
4	O	125	
4	Q	125	

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
5	EDO	I	201	-	-	-	X
6	PEG	M	203	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 29736 atoms, of which 14050 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 iv8 Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	117	Total	C	H	N	O	S	0	0	0
			1814	584	889	156	181	4			
1	E	120	Total	C	H	N	O	S	0	0	0
			1841	591	902	159	185	4			
1	K	117	Total	C	H	N	O	S	0	0	0
			1814	584	889	156	181	4			
1	P	117	Total	C	H	N	O	S	0	0	0
			1814	584	889	156	181	4			

- Molecule 2 is a protein called glVRC01 Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	106	Total	C	H	N	O	S	0	0	0
			1569	504	769	133	161	2			
2	F	103	Total	C	H	N	O	S	0	0	0
			1548	498	760	130	158	2			
2	L	103	Total	C	H	N	O	S	0	0	0
			1548	498	760	130	158	2			
2	N	106	Total	C	H	N	O	S	0	0	0
			1569	504	769	133	161	2			

- Molecule 3 is a protein called glVRC01 Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	123	Total	C	H	N	O	S	0	0	0
			1873	604	911	170	182	6			
3	H	120	Total	C	H	N	O	S	0	0	0
			1836	593	892	167	178	6			
3	I	126	Total	C	H	N	O	S	0	0	0
			1888	607	916	173	186	6			
3	M	120	Total	C	H	N	O	S	0	0	0
			1836	593	892	167	178	6			

- Molecule 4 is a protein called iv8 Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	121	Total	C	H	N	O	S	0	1	0
			1836	593	905	152	182	4			
4	J	118	Total	C	H	N	O	S	0	0	0
			1791	581	883	145	178	4			
4	O	117	Total	C	H	N	O	S	0	0	0
			1780	578	878	144	176	4			
4	Q	117	Total	C	H	N	O	S	0	0	0
			1780	578	878	144	176	4			

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



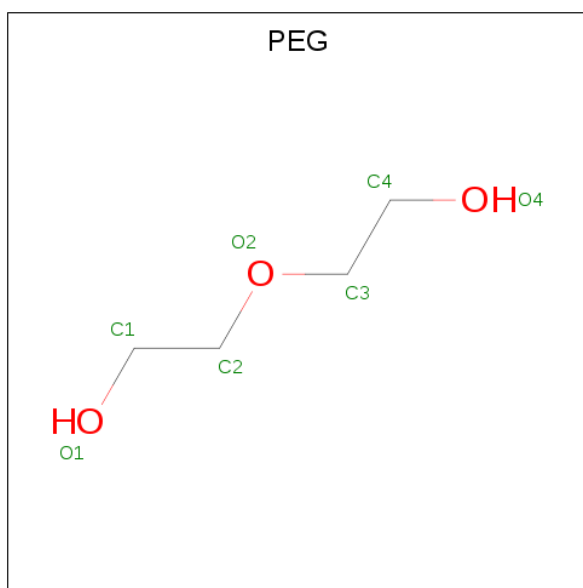
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	C	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total 10	C 2	H 6	O 2	0	0
5	D	1	Total 10	C 2	H 6	O 2	0	0
5	F	1	Total 10	C 2	H 6	O 2	0	0
5	F	1	Total 10	C 2	H 6	O 2	0	0
5	F	1	Total 10	C 2	H 6	O 2	0	0
5	H	1	Total 10	C 2	H 6	O 2	0	0
5	H	1	Total 10	C 2	H 6	O 2	0	0
5	I	1	Total 10	C 2	H 6	O 2	0	0
5	J	1	Total 10	C 2	H 6	O 2	0	0
5	K	1	Total 10	C 2	H 6	O 2	0	0
5	K	1	Total 10	C 2	H 6	O 2	0	0
5	K	1	Total 10	C 2	H 6	O 2	0	0
5	L	1	Total 10	C 2	H 6	O 2	0	0
5	M	1	Total 10	C 2	H 6	O 2	0	0
5	M	1	Total 10	C 2	H 6	O 2	0	0
5	N	1	Total 10	C 2	H 6	O 2	0	0
5	N	1	Total 10	C 2	H 6	O 2	0	0
5	N	1	Total 10	C 2	H 6	O 2	0	0
5	N	1	Total 10	C 2	H 6	O 2	0	0
5	O	1	Total 10	C 2	H 6	O 2	0	0
5	Q	1	Total 10	C 2	H 6	O 2	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			17	4	10	3		
6	F	1	Total	C	H	O	0	0
			17	4	10	3		
6	J	1	Total	C	H	O	0	0
			17	4	10	3		
6	J	1	Total	C	H	O	0	0
			17	4	10	3		
6	K	1	Total	C	H	O	0	0
			17	4	10	3		
6	K	1	Total	C	H	O	0	0
			17	4	10	3		
6	M	1	Total	C	H	O	0	0
			17	4	10	3		
6	N	1	Total	C	H	O	0	0
			17	4	10	3		
6	O	1	Total	C	H	O	0	0
			17	4	10	3		
6	Q	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	P	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	K	1	Total	Cl	0	0
			1	1		


- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	69	Total	O	0	0
			69	69		
8	B	55	Total	O	0	0
			55	55		
8	C	72	Total	O	0	0
			72	72		
8	D	96	Total	O	0	0
			96	96		
8	E	90	Total	O	0	0
			90	90		
8	F	71	Total	O	0	0
			71	71		
8	H	71	Total	O	0	0
			71	71		
8	I	97	Total	O	0	0
			97	97		
8	J	63	Total	O	0	0
			63	63		
8	K	62	Total	O	0	0
			62	62		
8	L	53	Total	O	0	0
			53	53		
8	M	76	Total	O	0	0
			76	76		
8	N	57	Total	O	0	0
			57	57		
8	O	62	Total	O	0	0
			62	62		
8	P	73	Total	O	0	0
			73	73		
8	Q	80	Total	O	0	0
			80	80		

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: iv8 Heavy Chain

Chain A: 




- Molecule 1: iv8 Heavy Chain

Chain E: 




- Molecule 1: iv8 Heavy Chain

Chain K: 



- Molecule 1: iv8 Heavy Chain

Chain P: 



- Molecule 2: glVRC01 Light Chain

Chain B: 

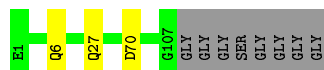
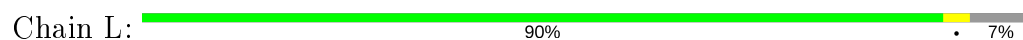


- Molecule 2: glVRC01 Light Chain

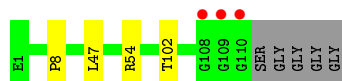
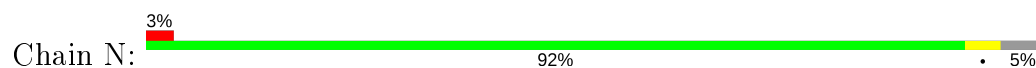
Chain F: 



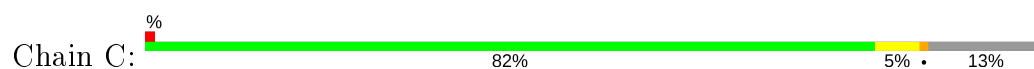
- Molecule 2: glVRC01 Light Chain



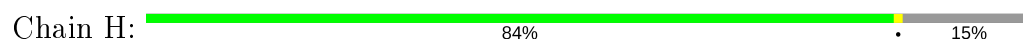
- Molecule 2: glVRC01 Light Chain



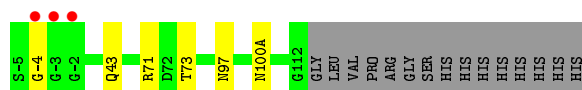
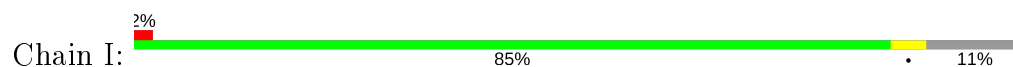
- Molecule 3: glVRC01 Heavy Chain



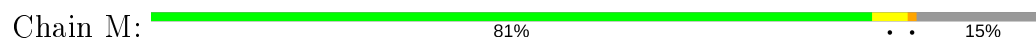
- Molecule 3: glVRC01 Heavy Chain



- Molecule 3: glVRC01 Heavy Chain



- Molecule 3: glVRC01 Heavy Chain

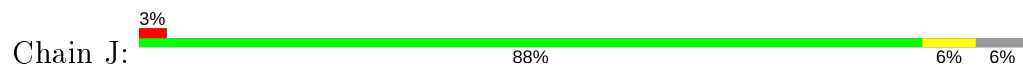


- Molecule 4: iv8 Light Chain

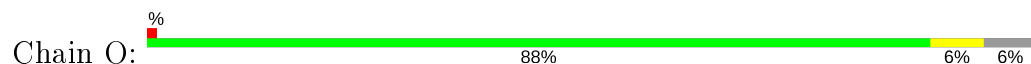




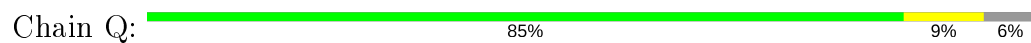
- Molecule 4: iv8 Light Chain



- Molecule 4: iv8 Light Chain



- Molecule 4: iv8 Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.58Å 107.94Å 116.96Å 85.49° 80.28° 84.17°	Depositor
Resolution (Å)	49.78 – 2.42 49.78 – 2.42	Depositor EDS
% Data completeness (in resolution range)	92.4 (49.78-2.42) 92.4 (49.78-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.174 , 0.224 0.174 , 0.223	Depositor DCC
R_{free} test set	4371 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.896	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	29736	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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, EDO, CL

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	0.26	0/947	0.48	0/1287
1	E	0.28	0/961	0.49	0/1305
1	K	0.26	0/947	0.49	0/1287
1	P	0.26	0/947	0.47	0/1287
2	B	0.27	0/818	0.46	0/1110
2	F	0.27	0/806	0.46	0/1095
2	L	0.26	0/806	0.46	0/1095
2	N	0.26	0/818	0.46	0/1110
3	C	0.26	0/987	0.47	0/1337
3	H	0.26	0/969	0.46	0/1313
3	I	0.25	0/997	0.46	0/1349
3	M	0.26	0/969	0.46	0/1313
4	D	0.26	0/954	0.44	0/1289
4	J	0.27	0/931	0.45	0/1260
4	O	0.26	0/925	0.45	0/1252
4	Q	0.26	0/925	0.45	0/1252
All	All	0.26	0/14707	0.46	0/19941

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	925	889	891	4	0
1	E	939	902	902	18	0
1	K	925	889	891	5	0
1	P	925	889	891	9	0
2	B	800	769	769	3	0
2	F	788	760	760	4	0
2	L	788	760	760	2	0
2	N	800	769	769	2	0
3	C	962	911	914	9	0
3	H	944	892	895	1	0
3	I	972	916	917	4	0
3	M	944	892	895	4	0
4	D	931	905	904	5	0
4	J	908	883	883	5	0
4	O	902	878	878	4	0
4	Q	902	878	878	7	0
5	A	8	12	12	0	0
5	B	16	24	24	1	0
5	C	4	6	6	0	0
5	D	8	12	12	0	0
5	F	12	18	18	1	0
5	H	8	12	12	0	0
5	I	4	6	6	0	0
5	J	4	6	6	0	0
5	K	12	18	18	0	0
5	L	4	6	6	0	0
5	M	8	12	12	0	0
5	N	16	24	24	0	0
5	O	4	6	6	0	0
5	Q	4	6	6	0	0
6	A	7	10	10	0	0
6	F	7	10	10	1	0
6	J	14	20	20	1	0
6	K	14	20	20	2	0
6	M	7	10	10	0	0
6	N	7	10	10	1	0
6	O	7	10	10	0	0
6	Q	7	10	10	0	0
7	K	1	0	0	0	0
7	P	1	0	0	0	0
8	A	69	0	0	0	0
8	B	55	0	0	1	0
8	C	72	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	96	0	0	3	0
8	E	90	0	0	3	0
8	F	71	0	0	2	1
8	H	71	0	0	1	0
8	I	97	0	0	3	0
8	J	63	0	0	0	0
8	K	62	0	0	0	1
8	L	53	0	0	2	0
8	M	76	0	0	1	0
8	N	57	0	0	2	0
8	O	62	0	0	1	0
8	P	73	0	0	3	0
8	Q	80	0	0	3	0
All	All	15686	14050	14065	87	1

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 3.

All (87) 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:K:32:SER:O	1:K:71:ARG:NH2	2.08	0.86
4:O:17:GLU:OE2	8:O:301:HOH:O	1.98	0.81
2:F:50:ASP:OD1	5:F:202:EDO:O1	1.99	0.80
3:C:84:SER:H	3:C:114:LEU:HD12	1.47	0.79
1:E:64:LYS:O	8:E:201:HOH:O	2.01	0.77
3:H:54:SER:O	8:H:301:HOH:O	2.03	0.76
3:M:1:GLN:OE1	8:M:301:HOH:O	2.04	0.76
4:Q:27:GLN:OE1	8:Q:301:HOH:O	2.03	0.75
4:D:112:SER:OG	8:D:301:HOH:O	2.10	0.70
4:J:61:ARG:NH2	4:J:82:ASP:OD1	2.25	0.69
3:C:84:SER:HB2	3:C:114:LEU:HB3	1.72	0.69
6:N:205:PEG:O1	8:N:301:HOH:O	2.10	0.68
1:E:3:LYS:NZ	8:E:203:HOH:O	2.25	0.68
4:J:96:TRP:O	6:K:205:PEG:H21	1.94	0.68
3:I:43:GLN:OE1	8:I:301:HOH:O	2.13	0.67
2:L:6:GLN:O	8:L:301:HOH:O	2.11	0.67
1:E:32:SER:O	1:E:71:ARG:NH2	2.29	0.66
3:C:82(B):ARG:O	8:C:301:HOH:O	2.12	0.66
4:Q:27:GLN:NE2	8:Q:303:HOH:O	2.26	0.65
4:O:61:ARG:NH2	4:O:82:ASP:OD1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:204:PEG:O4	8:F:301:HOH:O	2.05	0.63
3:M:23:LYS:NZ	3:M:75:ILE:O	2.31	0.63
4:Q:54:ARG:NE	4:Q:62:PHE:O	2.30	0.62
1:P:83:ARG:NH1	8:P:304:HOH:O	2.33	0.62
1:P:31:ASN:OD1	8:P:301:HOH:O	2.16	0.61
4:Q:55:GLU:OE1	8:Q:302:HOH:O	2.17	0.60
4:D:40:PRO:O	8:D:302:HOH:O	2.17	0.59
2:L:70:ASP:OD1	8:L:302:HOH:O	2.17	0.59
1:E:12:VAL:HG21	1:E:82(C):LEU:HD13	1.85	0.59
1:P:1:GLU:N	8:P:303:HOH:O	2.31	0.59
1:A:10:ASP:OD1	1:A:11:PHE:N	2.37	0.58
4:D:54[B]:ARG:NH2	4:D:60:ASP:OD1	2.38	0.55
4:Q:61:ARG:NH2	4:Q:82:ASP:OD1	2.41	0.54
2:F:27:GLN:OE1	6:J:203:PEG:O1	2.22	0.54
1:P:32:SER:O	1:P:71:ARG:NH2	2.38	0.54
3:C:96:LYS:NZ	8:C:304:HOH:O	2.33	0.53
1:E:0:SER:HA	1:E:26:GLY:HA2	1.90	0.53
1:K:35:SER:OG	1:K:95:GLN:OE1	2.23	0.51
3:I:100(A):ASN:OD1	8:I:302:HOH:O	2.19	0.51
1:E:86:ASP:OD1	8:E:202:HOH:O	2.19	0.50
1:K:47:TRP:O	6:K:205:PEG:H11	2.10	0.50
2:B:70:ASP:OD1	8:B:301:HOH:O	2.19	0.50
1:E:2:VAL:H	1:E:26:GLY:HA3	1.77	0.50
1:E:2:VAL:N	1:E:25:SER:O	2.43	0.49
3:C:83:ARG:NH2	8:C:309:HOH:O	2.46	0.49
2:B:31:SER:O	5:B:202:EDO:O1	2.19	0.48
3:C:14:PRO:HG3	3:C:114:LEU:HB2	1.94	0.48
2:F:24:ARG:NH1	8:F:303:HOH:O	2.44	0.48
1:K:12:VAL:HG21	1:K:82(C):LEU:HD13	1.96	0.48
1:P:35:SER:OG	1:P:95:GLN:OE1	2.28	0.48
2:F:45:ARG:HH12	3:I:-4:GLY:HA2	1.79	0.47
4:Q:50:TRP:O	4:Q:51:ALA:HB3	2.15	0.47
4:J:50:TRP:O	4:J:51:ALA:HB3	2.15	0.47
1:A:12:VAL:HG21	1:A:82(C):LEU:HD13	1.97	0.46
3:M:20:VAL:HG13	3:M:107:THR:HG21	1.97	0.46
1:E:0:SER:HA	1:E:26:GLY:CA	2.45	0.45
1:P:12:VAL:HG21	1:P:82(C):LEU:HD13	1.98	0.45
1:P:38:ARG:HG3	1:P:48:VAL:HG21	1.97	0.45
2:N:54:ARG:NH2	8:N:305:HOH:O	2.50	0.44
4:O:50:TRP:O	4:O:51:ALA:HB3	2.17	0.44
4:D:25:SER:O	8:D:304:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:MET:HB3	1:A:82(C):LEU:HD21	1.99	0.44
1:P:82:MET:HB3	1:P:82(C):LEU:HD21	2.00	0.44
2:N:8:PRO:O	2:N:102:THR:HG23	2.18	0.44
1:E:64:LYS:O	1:E:65:ASP:HB2	2.18	0.43
1:A:12:VAL:HG21	1:A:82(C):LEU:CD1	2.48	0.43
3:C:14:PRO:HG3	3:C:114:LEU:H	1.83	0.43
1:E:1:GLU:H	1:E:26:GLY:HA3	1.82	0.43
4:O:15:LEU:HD13	4:O:16:GLY:N	2.33	0.43
3:C:82(B):ARG:NH1	8:C:303:HOH:O	2.44	0.43
4:Q:32:TYR:HB2	4:Q:92:TYR:HB2	2.01	0.42
2:B:8:PRO:O	2:B:102:THR:HG23	2.18	0.42
1:E:1:GLU:H	1:E:26:GLY:CA	2.32	0.42
3:C:83:ARG:NH1	8:C:301:HOH:O	2.53	0.42
1:E:2:VAL:N	1:E:26:GLY:HA3	2.34	0.42
4:D:50:TRP:O	4:D:51:ALA:HB3	2.20	0.41
4:J:94:TYR:HH	4:J:96:TRP:HZ2	1.66	0.41
1:P:2:VAL:HG11	1:P:102:VAL:HG21	2.02	0.41
1:E:12:VAL:HG21	1:E:82(C):LEU:CD1	2.49	0.41
1:K:82:MET:HB3	1:K:82(C):LEU:HD21	2.03	0.41
1:E:35:SER:OG	1:E:95:GLN:OE1	2.25	0.41
3:I:73:THR:O	8:I:303:HOH:O	2.22	0.41
1:E:10:ASP:OD1	1:E:11:PHE:N	2.54	0.40
3:M:20:VAL:CG1	3:M:107:THR:HG21	2.51	0.40
1:E:0:SER:HA	1:E:26:GLY:N	2.37	0.40
4:J:27(C):LEU:HD11	4:J:29:GLN:HA	2.03	0.40
1:E:-2:GLY:HA2	1:E:76:ASN:HB2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:307:HOH:O	8:K:357:HOH:O[1_455]	2.16	0.04

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	115/131 (88%)	112 (97%)	3 (3%)	0	100	100
1	E	118/131 (90%)	111 (94%)	7 (6%)	0	100	100
1	K	115/131 (88%)	113 (98%)	2 (2%)	0	100	100
1	P	115/131 (88%)	113 (98%)	2 (2%)	0	100	100
2	B	104/111 (94%)	98 (94%)	6 (6%)	0	100	100
2	F	101/111 (91%)	97 (96%)	4 (4%)	0	100	100
2	L	101/111 (91%)	97 (96%)	4 (4%)	0	100	100
2	N	104/111 (94%)	97 (93%)	7 (7%)	0	100	100
3	C	121/141 (86%)	119 (98%)	2 (2%)	0	100	100
3	H	118/141 (84%)	116 (98%)	2 (2%)	0	100	100
3	I	124/141 (88%)	120 (97%)	4 (3%)	0	100	100
3	M	118/141 (84%)	118 (100%)	0	0	100	100
4	D	120/125 (96%)	117 (98%)	3 (2%)	0	100	100
4	J	116/125 (93%)	113 (97%)	3 (3%)	0	100	100
4	O	115/125 (92%)	112 (97%)	3 (3%)	0	100	100
4	Q	115/125 (92%)	112 (97%)	3 (3%)	0	100	100
All	All	1820/2032 (90%)	1765 (97%)	55 (3%)	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	A	102/111 (92%)	101 (99%)	1 (1%)	76	87
1	E	103/111 (93%)	101 (98%)	2 (2%)	57	74
1	K	102/111 (92%)	101 (99%)	1 (1%)	76	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	102/111 (92%)	101 (99%)	1 (1%)	76	87
2	B	85/86 (99%)	85 (100%)	0	100	100
2	F	85/86 (99%)	83 (98%)	2 (2%)	49	67
2	L	85/86 (99%)	84 (99%)	1 (1%)	71	84
2	N	85/86 (99%)	84 (99%)	1 (1%)	71	84
3	C	100/113 (88%)	97 (97%)	3 (3%)	41	59
3	H	98/113 (87%)	97 (99%)	1 (1%)	76	87
3	I	100/113 (88%)	98 (98%)	2 (2%)	55	72
3	M	98/113 (87%)	96 (98%)	2 (2%)	55	72
4	D	101/101 (100%)	101 (100%)	0	100	100
4	J	100/101 (99%)	100 (100%)	0	100	100
4	O	99/101 (98%)	99 (100%)	0	100	100
4	Q	99/101 (98%)	98 (99%)	1 (1%)	76	87
All	All	1544/1644 (94%)	1526 (99%)	18 (1%)	71	84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
3	C	71	ARG
3	C	101	GLN
3	C	114	LEU
1	E	1	GLU
1	E	58	HIS
2	F	27	GLN
2	F	47	LEU
3	H	71	ARG
3	I	71	ARG
3	I	97	ASN
1	K	58	HIS
2	L	27	GLN
3	M	71	ARG
3	M	107	THR
2	N	47	LEU
1	P	58	HIS
4	Q	103	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 40 ligands modelled in this entry, 2 are monoatomic - leaving 38 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	EDO	F	203	-	3,3,3	0.46	0	2,2,2	0.30	0
5	EDO	H	202	-	3,3,3	0.46	0	2,2,2	0.26	0
5	EDO	N	201	-	3,3,3	0.44	0	2,2,2	0.32	0
5	EDO	L	201	-	3,3,3	0.43	0	2,2,2	0.28	0
5	EDO	D	202	-	3,3,3	0.45	0	2,2,2	0.28	0
6	PEG	A	203	-	6,6,6	0.47	0	5,5,5	0.33	0
6	PEG	J	203	-	6,6,6	0.50	0	5,5,5	0.30	0
5	EDO	N	203	-	3,3,3	0.46	0	2,2,2	0.30	0
5	EDO	O	201	-	3,3,3	0.47	0	2,2,2	0.28	0
6	PEG	O	202	-	6,6,6	0.48	0	5,5,5	0.26	0
5	EDO	K	202	-	3,3,3	0.48	0	2,2,2	0.29	0
6	PEG	J	202	-	6,6,6	0.49	0	5,5,5	0.22	0
5	EDO	K	203	-	3,3,3	0.47	0	2,2,2	0.22	0
5	EDO	A	202	-	3,3,3	0.47	0	2,2,2	0.23	0
5	EDO	H	201	-	3,3,3	0.46	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	D	201	-	3,3,3	0.47	0	2,2,2	0.30	0
5	EDO	B	201	-	3,3,3	0.50	0	2,2,2	0.22	0
5	EDO	N	204	-	3,3,3	0.46	0	2,2,2	0.28	0
6	PEG	F	204	-	6,6,6	0.50	0	5,5,5	0.42	0
5	EDO	K	201	-	3,3,3	0.45	0	2,2,2	0.31	0
6	PEG	N	205	-	6,6,6	0.48	0	5,5,5	0.29	0
5	EDO	M	201	-	3,3,3	0.44	0	2,2,2	0.35	0
5	EDO	I	201	-	3,3,3	0.47	0	2,2,2	0.24	0
5	EDO	N	202	-	3,3,3	0.46	0	2,2,2	0.24	0
5	EDO	M	202	-	3,3,3	0.45	0	2,2,2	0.29	0
5	EDO	F	202	-	3,3,3	0.41	0	2,2,2	0.25	0
5	EDO	B	203	-	3,3,3	0.47	0	2,2,2	0.26	0
5	EDO	C	201	-	3,3,3	0.47	0	2,2,2	0.25	0
5	EDO	B	202	-	3,3,3	0.44	0	2,2,2	0.25	0
5	EDO	J	201	-	3,3,3	0.46	0	2,2,2	0.28	0
6	PEG	M	203	-	6,6,6	0.48	0	5,5,5	0.38	0
5	EDO	F	201	-	3,3,3	0.49	0	2,2,2	0.27	0
5	EDO	Q	201	-	3,3,3	0.48	0	2,2,2	0.28	0
6	PEG	K	204	-	6,6,6	0.49	0	5,5,5	0.37	0
6	PEG	Q	202	-	6,6,6	0.48	0	5,5,5	0.58	0
5	EDO	B	204	-	3,3,3	0.47	0	2,2,2	0.29	0
6	PEG	K	205	-	6,6,6	0.50	0	5,5,5	0.41	0
5	EDO	A	201	-	3,3,3	0.49	0	2,2,2	0.23	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
5	EDO	F	203	-	-	1/1/1/1	-
5	EDO	H	202	-	-	0/1/1/1	-
5	EDO	N	201	-	-	0/1/1/1	-
5	EDO	L	201	-	-	1/1/1/1	-
5	EDO	D	202	-	-	0/1/1/1	-
6	PEG	A	203	-	-	0/4/4/4	-
6	PEG	J	203	-	-	2/4/4/4	-
5	EDO	N	203	-	-	0/1/1/1	-
5	EDO	O	201	-	-	0/1/1/1	-
6	PEG	O	202	-	-	1/4/4/4	-
5	EDO	K	202	-	-	0/1/1/1	-
6	PEG	J	202	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	K	203	-	-	1/1/1/1	-
5	EDO	A	202	-	-	0/1/1/1	-
5	EDO	H	201	-	-	0/1/1/1	-
5	EDO	D	201	-	-	0/1/1/1	-
5	EDO	B	201	-	-	0/1/1/1	-
5	EDO	N	204	-	-	0/1/1/1	-
6	PEG	F	204	-	-	1/4/4/4	-
5	EDO	K	201	-	-	0/1/1/1	-
6	PEG	N	205	-	-	1/4/4/4	-
5	EDO	M	201	-	-	0/1/1/1	-
5	EDO	I	201	-	-	0/1/1/1	-
5	EDO	N	202	-	-	0/1/1/1	-
5	EDO	M	202	-	-	0/1/1/1	-
5	EDO	F	202	-	-	1/1/1/1	-
5	EDO	B	203	-	-	0/1/1/1	-
5	EDO	C	201	-	-	1/1/1/1	-
5	EDO	B	202	-	-	0/1/1/1	-
5	EDO	J	201	-	-	0/1/1/1	-
6	PEG	M	203	-	-	1/4/4/4	-
5	EDO	F	201	-	-	0/1/1/1	-
5	EDO	Q	201	-	-	0/1/1/1	-
6	PEG	K	204	-	-	1/4/4/4	-
6	PEG	Q	202	-	-	4/4/4/4	-
5	EDO	B	204	-	-	0/1/1/1	-
6	PEG	K	205	-	-	4/4/4/4	-
5	EDO	A	201	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	Q	202	PEG	C4-C3-O2-C2
6	J	202	PEG	O1-C1-C2-O2
6	J	203	PEG	O2-C3-C4-O4
6	J	203	PEG	O1-C1-C2-O2
6	F	204	PEG	O2-C3-C4-O4
6	M	203	PEG	O1-C1-C2-O2
5	K	203	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	C	201	EDO	O1-C1-C2-O2
6	N	205	PEG	O1-C1-C2-O2
6	Q	202	PEG	O2-C3-C4-O4
6	Q	202	PEG	C1-C2-O2-C3
6	J	202	PEG	C4-C3-O2-C2
6	K	205	PEG	C4-C3-O2-C2
6	K	205	PEG	O1-C1-C2-O2
6	K	204	PEG	C1-C2-O2-C3
5	F	203	EDO	O1-C1-C2-O2
6	O	202	PEG	O2-C3-C4-O4
6	K	205	PEG	O2-C3-C4-O4
5	L	201	EDO	O1-C1-C2-O2
5	F	202	EDO	O1-C1-C2-O2
6	Q	202	PEG	O1-C1-C2-O2
6	K	205	PEG	C1-C2-O2-C3

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	203	PEG	1	0
6	F	204	PEG	1	0
6	N	205	PEG	1	0
5	F	202	EDO	1	0
5	B	202	EDO	1	0
6	K	205	PEG	2	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	117/131 (89%)	-0.18	0 100 100	19, 29, 52, 70	0
1	E	120/131 (91%)	0.06	3 (2%) 57 54	21, 30, 58, 193	0
1	K	117/131 (89%)	-0.13	0 100 100	19, 27, 48, 77	0
1	P	117/131 (89%)	-0.15	0 100 100	22, 31, 52, 73	0
2	B	106/111 (95%)	-0.35	0 100 100	21, 28, 44, 62	0
2	F	103/111 (92%)	-0.26	0 100 100	20, 27, 46, 62	0
2	L	103/111 (92%)	-0.30	0 100 100	24, 32, 46, 66	0
2	N	106/111 (95%)	-0.13	3 (2%) 53 50	24, 33, 55, 78	0
3	C	123/141 (87%)	-0.07	2 (1%) 72 69	24, 32, 52, 122	1 (0%)
3	H	120/141 (85%)	-0.33	0 100 100	19, 31, 53, 58	0
3	I	126/141 (89%)	-0.04	3 (2%) 59 56	19, 27, 45, 173	0
3	M	120/141 (85%)	-0.24	0 100 100	23, 37, 51, 63	0
4	D	121/125 (96%)	-0.13	4 (3%) 46 44	18, 28, 50, 182	0
4	J	118/125 (94%)	-0.06	4 (3%) 45 43	18, 27, 51, 111	0
4	O	117/125 (93%)	-0.18	1 (0%) 84 82	22, 32, 53, 71	0
4	Q	117/125 (93%)	-0.25	0 100 100	22, 30, 46, 65	0
All	All	1851/2032 (91%)	-0.17	20 (1%) 80 78	18, 30, 52, 193	1 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	-1	GLY	7.8
1	E	-2	GLY	7.4
1	E	0	SER	7.3
3	C	113	GLY	6.5
4	D	115	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
3	C	114	LEU	6.2
3	I	-2	GLY	4.9
4	D	114	GLY	3.6
4	J	112	SER	3.5
4	J	110	GLY	3.5
4	J	109	GLY	3.4
4	D	112	SER	3.3
4	J	111	GLY	3.2
2	N	109	GLY	2.8
3	I	-4	GLY	2.6
2	N	110	GLY	2.5
4	D	113	GLY	2.3
4	O	111	GLY	2.1
3	I	-3	GLY	2.1
2	N	108	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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, 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(Å ²)	Q<0.9
5	EDO	N	204	4/4	0.52	0.30	63,80,96,96	0
6	PEG	O	202	7/7	0.60	0.29	64,79,100,113	0
5	EDO	C	201	4/4	0.65	0.28	43,54,58,65	0
5	EDO	I	201	4/4	0.70	0.46	54,67,89,89	0
5	EDO	H	201	4/4	0.71	0.38	46,56,64,68	0
6	PEG	J	202	7/7	0.73	0.24	42,54,83,83	0
6	PEG	N	205	7/7	0.73	0.34	74,100,134,134	0
6	PEG	M	203	7/7	0.74	0.45	50,64,77,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	PEG	A	203	7/7	0.78	0.40	34,56,84,84	0
6	PEG	F	204	7/7	0.78	0.31	43,55,77,77	0
6	PEG	K	204	7/7	0.78	0.36	32,46,60,60	0
5	EDO	K	203	4/4	0.79	0.30	58,69,81,81	0
5	EDO	A	202	4/4	0.79	0.31	43,52,56,62	0
6	PEG	Q	202	7/7	0.79	0.32	41,66,83,86	0
5	EDO	B	204	4/4	0.80	0.24	40,55,58,70	0
5	EDO	M	202	4/4	0.82	0.29	56,67,73,75	0
5	EDO	F	203	4/4	0.85	0.14	50,60,64,70	0
5	EDO	D	202	4/4	0.86	0.25	42,73,108,108	0
6	PEG	K	205	7/7	0.86	0.26	26,39,48,50	0
5	EDO	M	201	4/4	0.87	0.13	40,48,60,60	0
5	EDO	O	201	4/4	0.87	0.21	54,65,72,72	0
5	EDO	N	203	4/4	0.87	0.28	47,56,67,67	0
5	EDO	B	201	4/4	0.87	0.24	37,47,65,65	0
5	EDO	J	201	4/4	0.87	0.22	45,54,62,62	0
5	EDO	A	201	4/4	0.87	0.29	23,28,45,45	0
5	EDO	Q	201	4/4	0.88	0.21	28,55,73,73	0
5	EDO	K	201	4/4	0.88	0.26	44,53,65,65	0
6	PEG	J	203	7/7	0.88	0.27	39,49,71,71	0
5	EDO	N	202	4/4	0.90	0.27	42,55,66,67	0
5	EDO	K	202	4/4	0.90	0.14	41,50,62,62	0
5	EDO	B	203	4/4	0.90	0.20	37,50,59,64	0
5	EDO	F	201	4/4	0.91	0.17	28,47,57,57	0
5	EDO	D	201	4/4	0.92	0.16	46,56,73,73	0
5	EDO	F	202	4/4	0.93	0.20	30,37,43,48	0
5	EDO	H	202	4/4	0.93	0.13	43,52,57,61	0
5	EDO	L	201	4/4	0.93	0.15	22,27,34,41	0
7	CL	K	206	1/1	0.93	0.18	41,41,41,41	0
7	CL	P	201	1/1	0.95	0.14	51,51,51,51	0
5	EDO	B	202	4/4	0.97	0.17	26,31,40,48	0
5	EDO	N	201	4/4	0.98	0.13	24,29,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.