



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:12 AM UTC

PDB ID : 8UKY / pdb_00008uky
Title : Crystal structure of BAK in complex with inhibiting antibody 14G6
Authors : Miller, M.S.; Czabotar, P.E.
Deposited on : 2023-10-15
Resolution : 2.40 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

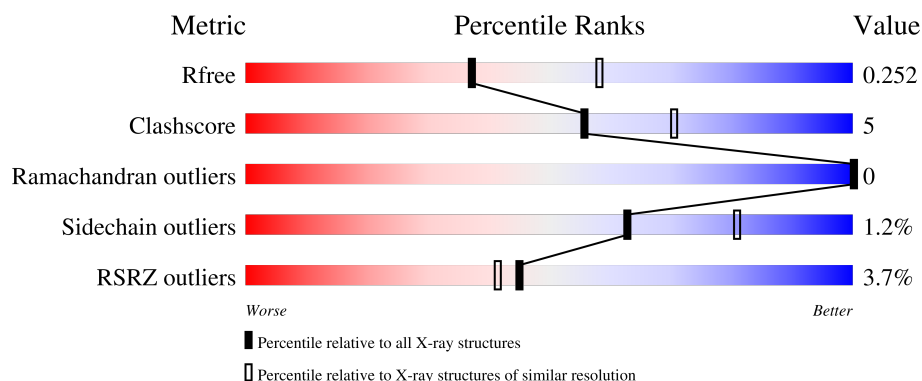
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 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	213	0% 90% 10%
1	L	213	2% 85% 14%
2	B	219	3% 90% 9%
2	H	219	3% 88% 9%
3	C	170	6% 76% 11% 13%

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Mol	Chain	Length	Quality of chain
3	D	170	7% 77% 13% 10%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 9336 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 14G6 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	0	0
			1640	1024	278	332	6			
1	A	213	Total	C	N	O	S	0	0	0
			1647	1027	279	334	7			

- Molecule 2 is a protein called 14G6 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	0	0
			1590	1007	259	319	5			
2	B	217	Total	C	N	O	S	0	0	0
			1612	1020	263	324	5			

- Molecule 3 is a protein called Bcl-2 homologous antagonist/killer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	148	Total	C	N	O	S	0	0	0
			1197	761	211	221	4			
3	D	153	Total	C	N	O	S	0	0	0
			1227	779	216	228	4			

There are 14 discrepancies between the modelled and reference sequences:

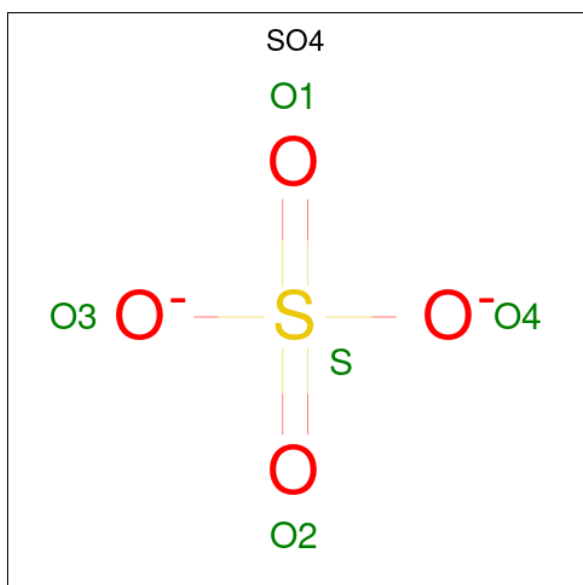
Chain	Residue	Modelled	Actual	Comment	Reference
C	17	GLY	-	expression tag	UNP Q16611
C	18	PRO	-	expression tag	UNP Q16611
C	19	LEU	-	expression tag	UNP Q16611
C	20	GLY	-	expression tag	UNP Q16611
C	21	SER	-	expression tag	UNP Q16611
C	22	MET	-	expression tag	UNP Q16611
C	166	SER	CYS	engineered mutation	UNP Q16611
D	17	GLY	-	expression tag	UNP Q16611

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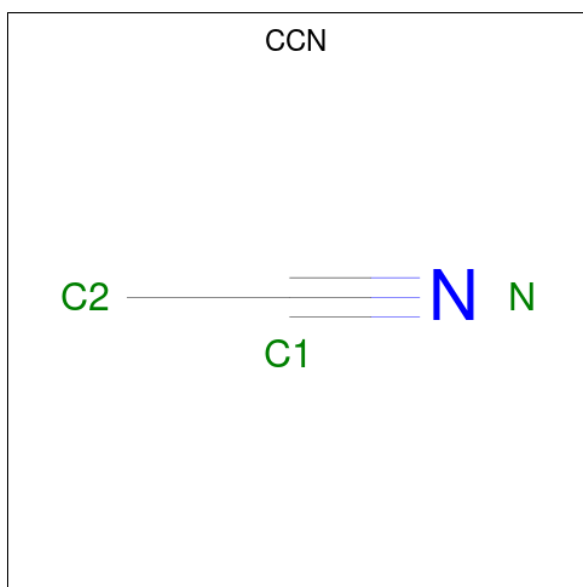
Chain	Residue	Modelled	Actual	Comment	Reference
D	18	PRO	-	expression tag	UNP Q16611
D	19	LEU	-	expression tag	UNP Q16611
D	20	GLY	-	expression tag	UNP Q16611
D	21	SER	-	expression tag	UNP Q16611
D	22	MET	-	expression tag	UNP Q16611
D	166	SER	CYS	engineered mutation	UNP Q16611

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



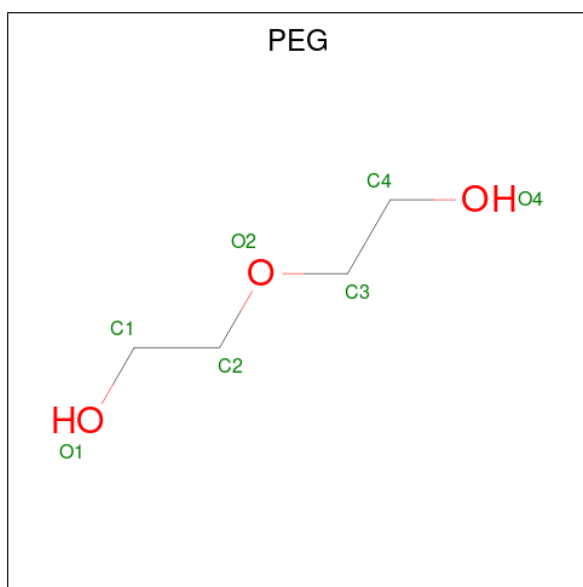
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is ACETONITRILE (CCD ID: CCN) (formula: C₂H₃N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	N	0	0
			3	2	1		
5	L	1	Total	C	N	0	0
			3	2	1		
5	L	1	Total	C	N	0	0
			3	2	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



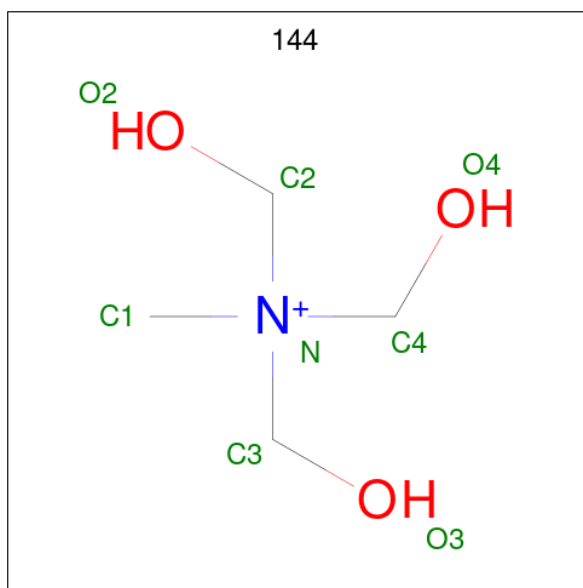
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			7	4	3		

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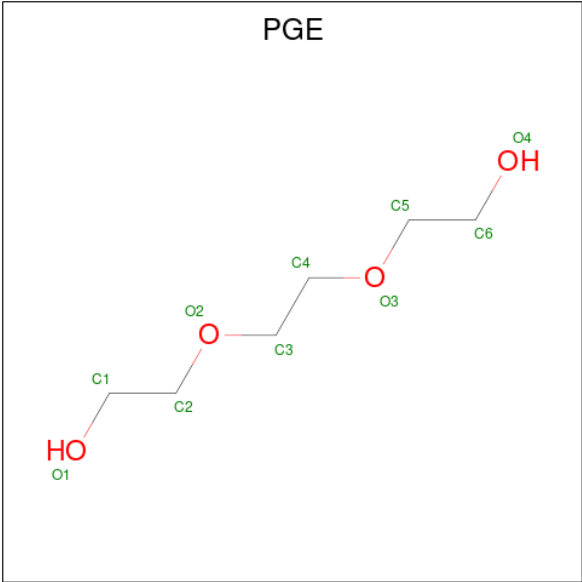
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			7	4	3		
6	H	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is TRIS-HYDROXYMETHYL-METHYL-AMMONIUM (CCD ID: 144) (formula: $C_4H_{12}NO_3$).



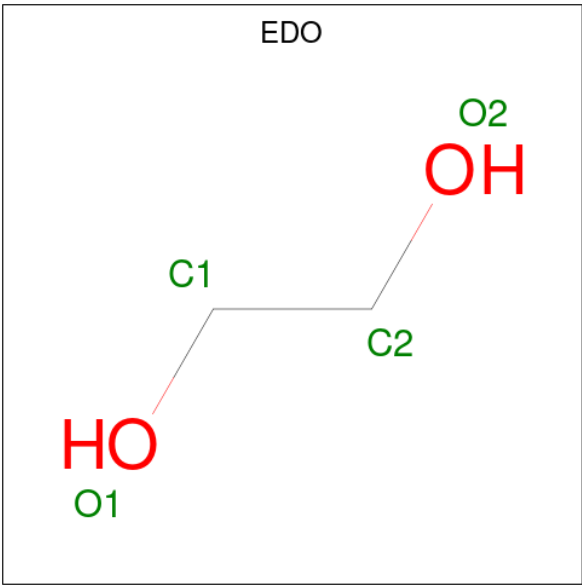
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	H	1	Total	C	N	O	0	0
			8	4	1	3		
7	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	H	1	Total	C	O	0	0
			10	6	4		
8	H	1	Total	C	O	0	0
			10	6	4		
8	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



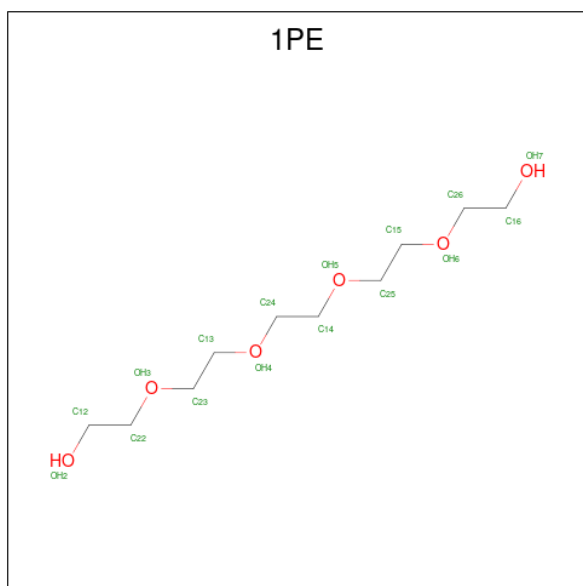
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			16	10	6		

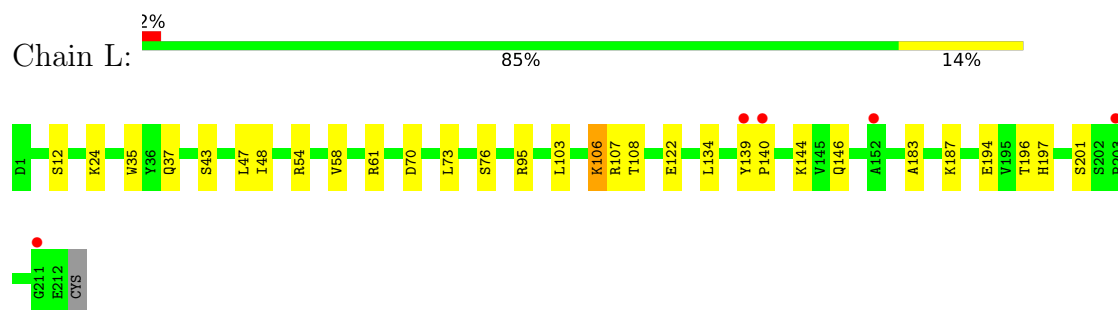
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	54	Total	O	0	0
			54	54		
11	H	62	Total	O	0	0
			62	62		
11	C	19	Total	O	0	0
			19	19		
11	A	48	Total	O	0	0
			48	48		
11	B	71	Total	O	0	0
			71	71		
11	D	19	Total	O	0	0
			19	19		

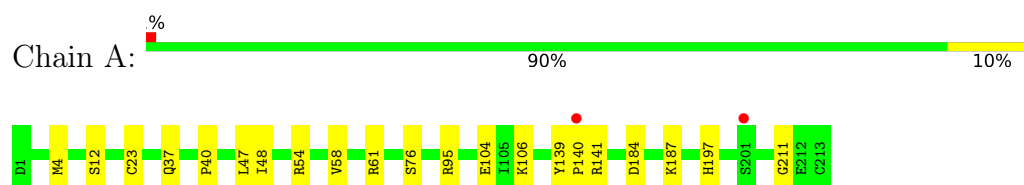
3 Residue-property plots [i](#)

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.

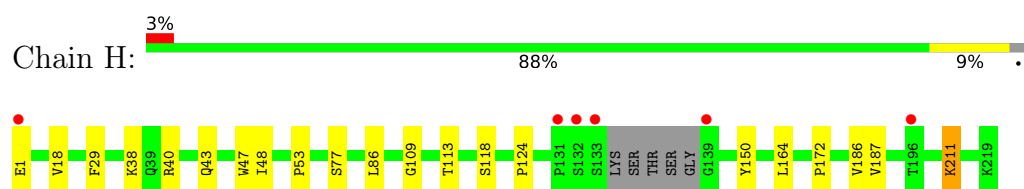
- Molecule 1: 14G6 Fab light chain



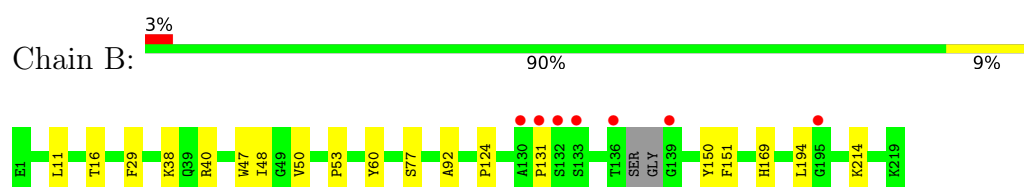
- Molecule 1: 14G6 Fab light chain



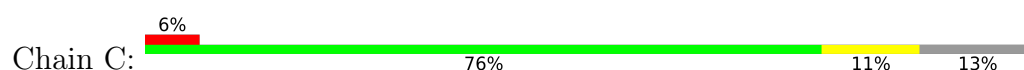
- Molecule 2: 14G6 Fab heavy chain

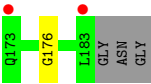
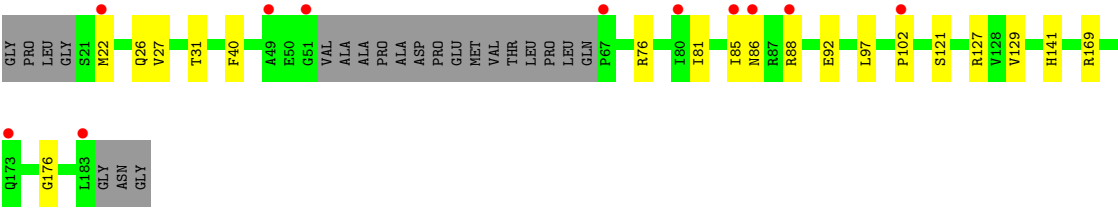


- Molecule 2: 14G6 Fab heavy chain

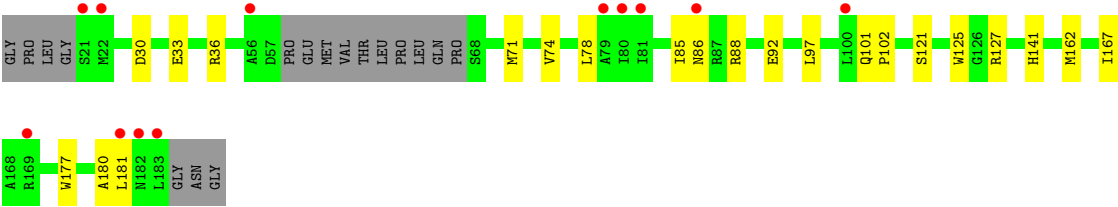
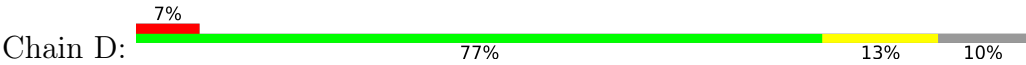


- Molecule 3: Bcl-2 homologous antagonist/killer





● Molecule 3: Bcl-2 homologous antagonist/killer



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.55Å 72.62Å 75.28Å 103.01° 103.98° 112.15°	Depositor
Resolution (Å)	45.38 – 2.40 45.38 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.4 (45.38-2.40) 96.5 (45.38-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.215 , 0.252 0.216 , 0.252	Depositor DCC
R_{free} test set	2415 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9336	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, 1PE, 144, CCN, SO4, EDO, PGE

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	0.09	0/1682	0.33	0/2279
1	L	0.09	0/1675	0.32	0/2271
2	B	0.10	0/1650	0.31	0/2247
2	H	0.11	0/1628	0.31	0/2218
3	C	0.15	0/1225	0.31	0/1655
3	D	0.09	0/1255	0.27	0/1698
All	All	0.11	0/9115	0.31	0/12368

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

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	1647	0	1589	13	0
1	L	1640	0	1584	18	0
2	B	1612	0	1586	14	0
2	H	1590	0	1561	15	0
3	C	1197	0	1141	12	0
3	D	1227	0	1168	14	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	0	0	0
4	L	5	0	0	0	0
5	L	9	0	9	1	0
6	A	14	0	20	1	0
6	B	14	0	20	2	0
6	D	7	0	10	1	0
6	H	14	0	20	1	0
6	L	7	0	10	0	0
7	B	8	0	12	0	0
7	H	8	0	12	1	0
8	A	10	0	14	2	0
8	H	20	0	28	3	0
9	A	8	0	12	0	0
10	A	16	0	22	1	0
11	A	48	0	0	1	0
11	B	71	0	0	1	0
11	C	19	0	0	0	0
11	D	19	0	0	0	0
11	H	62	0	0	0	0
11	L	54	0	0	0	0
All	All	9336	0	8818	84	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 5.

All (84) 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:D:30:ASP:HB3	3:D:71:MET:HE2	1.56	0.85
1:L:134:LEU:HD22	2:H:186:VAL:HG11	1.70	0.72
3:D:71:MET:HE1	3:D:177:TRP:HB2	1.76	0.67
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.75	0.67
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.75	0.65
3:D:125:TRP:H	6:D:201:PEG:H22	1.61	0.64
1:A:40:PRO:HA	10:A:303:1PE:H221	1.80	0.64
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.81	0.62
3:D:121:SER:HB2	3:D:127:ARG:HH22	1.65	0.60
6:H:302:PEG:H21	3:C:40:PHE:HA	1.81	0.60
2:B:214:LYS:NZ	11:B:401:HOH:O	2.35	0.60
1:L:12:SER:HB2	1:L:106:LYS:HG3	1.82	0.59
3:D:97:LEU:HD22	3:D:102:PRO:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:PRO:HB3	2:B:150:TYR:HB3	1.84	0.58
1:A:140:PRO:HD2	1:A:197:HIS:CE1	2.39	0.58
3:C:22:MET:CE	3:C:176:GLY:HA3	2.35	0.57
2:H:113:THR:H	8:H:304:PGE:H12	1.71	0.56
3:D:88:ARG:O	3:D:92:GLU:HG2	2.07	0.55
3:D:74:VAL:HG22	3:D:181:LEU:HG	1.87	0.55
3:C:22:MET:HE3	3:C:176:GLY:HA3	1.89	0.55
1:A:211:GLY:H	6:A:301:PEG:H31	1.70	0.54
2:B:47:TRP:HZ2	2:B:50:VAL:HG13	1.73	0.54
5:L:304:CCN:H21	2:H:47:TRP:H	1.71	0.54
6:B:301:PEG:H21	6:B:302:PEG:H22	1.90	0.54
1:L:140:PRO:HD2	1:L:197:HIS:CE1	2.43	0.53
3:C:22:MET:HG3	3:C:27:VAL:HG23	1.89	0.53
2:B:38:LYS:HB2	2:B:48:ILE:HD11	1.90	0.53
3:C:102:PRO:HD2	3:C:141:HIS:CD2	2.43	0.53
3:D:78:LEU:HD21	3:D:180:ALA:HB1	1.91	0.52
1:L:61:ARG:HB2	1:L:76:SER:O	2.10	0.52
3:D:102:PRO:HD2	3:D:141:HIS:CD2	2.45	0.51
1:L:48:ILE:HD13	1:L:54:ARG:HA	1.91	0.51
2:B:131:PRO:HG3	2:B:194:LEU:HD11	1.92	0.51
3:C:97:LEU:HD22	3:C:102:PRO:HG3	1.92	0.50
1:L:144:LYS:HB3	1:L:196:THR:HB	1.93	0.49
1:L:139:TYR:HB3	1:L:140:PRO:HD3	1.94	0.48
1:L:95:ARG:HD3	2:H:47:TRP:CE2	2.47	0.48
3:C:85:ILE:HG13	3:C:86:ASN:N	2.29	0.48
2:H:29:PHE:CD2	2:H:77:SER:HA	2.48	0.48
1:A:61:ARG:HB2	1:A:76:SER:O	2.13	0.47
2:B:47:TRP:CZ2	2:B:50:VAL:HG13	2.49	0.47
3:C:88:ARG:O	3:C:92:GLU:HG2	2.14	0.47
2:B:60:TYR:HD2	6:B:301:PEG:H32	1.79	0.47
3:D:85:ILE:HG13	3:D:86:ASN:N	2.29	0.47
1:A:106:LYS:NZ	11:A:404:HOH:O	2.48	0.47
8:A:307:PGE:H52	2:B:169:HIS:CE1	2.50	0.47
2:H:172:PRO:HA	7:H:303:144:H22	1.98	0.46
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.98	0.46
1:L:183:ALA:O	1:L:187:LYS:HG3	2.16	0.45
1:A:139:TYR:HB3	1:A:140:PRO:HD3	1.98	0.45
2:H:18:VAL:HG22	2:H:86:LEU:HD11	1.98	0.45
3:C:121:SER:HB2	3:C:127:ARG:HH22	1.81	0.45
8:A:307:PGE:H52	2:B:169:HIS:ND1	2.32	0.44
2:H:211:LYS:HB3	2:H:211:LYS:HE3	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:146:GLN:NE2	1:L:194:GLU:OE1	2.50	0.44
1:A:95:ARG:HD3	2:B:47:TRP:CE2	2.52	0.44
2:H:113:THR:N	8:H:304:PGE:H12	2.33	0.44
1:L:54:ARG:HG2	1:L:58:VAL:HB	2.00	0.44
2:H:40:ARG:NH1	2:H:43:GLN:HG3	2.33	0.44
3:D:121:SER:HB2	3:D:127:ARG:NH2	2.33	0.43
2:B:40:ARG:HG2	2:B:92:ALA:HB2	1.99	0.43
2:B:29:PHE:CD2	2:B:77:SER:HA	2.54	0.43
2:H:29:PHE:CE2	2:H:53:PRO:HB3	2.54	0.43
2:H:164:LEU:HD21	2:H:187:VAL:HG21	2.00	0.42
2:B:29:PHE:CE2	2:B:53:PRO:HB3	2.55	0.42
1:L:107:ARG:HG2	1:L:108:THR:N	2.35	0.42
1:L:43:SER:OG	2:H:109:GLY:O	2.29	0.42
3:D:162:MET:HA	3:D:167:ILE:HB	2.02	0.42
1:A:4:MET:HE3	1:A:23:CYS:SG	2.60	0.42
1:L:35:TRP:CD2	1:L:73:LEU:HB2	2.56	0.41
1:L:35:TRP:CE2	1:L:73:LEU:HB2	2.55	0.41
1:L:103:LEU:HD23	1:L:103:LEU:HA	1.95	0.41
1:A:12:SER:HB3	1:A:106:LYS:HB2	2.03	0.41
3:D:33:GLU:OE2	3:D:36:ARG:NH1	2.52	0.41
3:C:81:ILE:HD11	3:C:129:VAL:HG11	2.03	0.41
1:L:24:LYS:NZ	1:L:70:ASP:OD1	2.44	0.41
2:B:11:LEU:HD11	2:B:151:PHE:CZ	2.56	0.41
3:D:101:GLN:H	3:D:101:GLN:HG2	1.67	0.41
1:A:48:ILE:HD13	1:A:54:ARG:HA	2.03	0.40
1:A:184:ASP:HA	1:A:187:LYS:HE2	2.03	0.40
3:C:27:VAL:O	3:C:31:THR:OG1	2.38	0.40
1:A:54:ARG:HG2	1:A:58:VAL:HB	2.02	0.40
3:C:121:SER:HB2	3:C:127:ARG:NH2	2.37	0.40
8:H:304:PGE:H1	8:H:304:PGE:H32	1.91	0.40

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	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
1	L	210/213 (99%)	200 (95%)	10 (5%)	0	100	100
2	B	213/219 (97%)	210 (99%)	3 (1%)	0	100	100
2	H	210/219 (96%)	207 (99%)	3 (1%)	0	100	100
3	C	144/170 (85%)	142 (99%)	2 (1%)	0	100	100
3	D	149/170 (88%)	147 (99%)	2 (1%)	0	100	100
All	All	1137/1204 (94%)	1108 (97%)	29 (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	187/187 (100%)	185 (99%)	2 (1%)	65	82
1	L	186/187 (100%)	183 (98%)	3 (2%)	55	76
2	B	183/184 (100%)	182 (100%)	1 (0%)	81	91
2	H	180/184 (98%)	177 (98%)	3 (2%)	53	74
3	C	123/138 (89%)	120 (98%)	3 (2%)	43	65
3	D	125/138 (91%)	125 (100%)	0	100	100
All	All	984/1018 (97%)	972 (99%)	12 (1%)	63	81

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	106	LYS
1	L	122	GLU
1	L	201	SER
2	H	1	GLU

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Mol	Chain	Res	Type
2	H	118	SER
2	H	211	LYS
3	C	26	GLN
3	C	76	ARG
3	C	169	ARG
1	A	104	GLU
1	A	141	ARG
2	B	16	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	79	GLN
1	L	146	GLN
2	H	176	GLN
2	H	209	ASN
3	C	29	GLN
3	C	43	HIS
3	C	73	GLN
1	A	159	GLN
1	A	198	GLN
2	B	176	GLN
3	D	43	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

22 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	D	201	-	6,6,6	0.50	0	5,5,5	0.29	0
6	PEG	H	302	-	6,6,6	0.12	0	5,5,5	0.08	0
9	EDO	A	302	-	3,3,3	0.42	0	2,2,2	0.42	0
6	PEG	B	301	-	6,6,6	0.14	0	5,5,5	0.13	0
6	PEG	H	301	-	6,6,6	0.50	0	5,5,5	0.27	0
4	SO4	A	305	-	4,4,4	0.24	0	6,6,6	0.07	0
6	PEG	L	303	-	6,6,6	0.50	0	5,5,5	0.25	0
6	PEG	B	302	-	6,6,6	0.52	0	5,5,5	0.27	0
9	EDO	A	304	-	3,3,3	0.42	0	2,2,2	0.42	0
5	CCN	L	302	-	2,2,2	0.90	0	1,1,1	0.63	0
8	PGE	H	304	-	9,9,9	0.30	0	8,8,8	0.31	0
5	CCN	L	304	-	2,2,2	0.90	0	1,1,1	0.62	0
4	SO4	L	301	-	4,4,4	0.24	0	6,6,6	0.07	0
7	144	B	303	-	1,7,7	1.24	0	3,9,9	0.13	0
10	1PE	A	303	-	15,15,15	0.12	0	14,14,14	0.24	0
6	PEG	A	306	-	6,6,6	0.23	0	5,5,5	0.22	0
7	144	H	303	-	1,7,7	1.23	0	3,9,9	0.08	0
5	CCN	L	305	-	2,2,2	0.90	0	1,1,1	0.62	0
6	PEG	A	301	-	6,6,6	0.52	0	5,5,5	0.29	0
8	PGE	H	305	-	9,9,9	0.31	0	8,8,8	0.40	0
4	SO4	B	304	-	4,4,4	0.24	0	6,6,6	0.07	0
8	PGE	A	307	-	9,9,9	0.11	0	8,8,8	0.21	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
6	PEG	L	303	-	-	1/4/4/4	-
6	PEG	B	302	-	-	0/4/4/4	-
6	PEG	D	201	-	-	1/4/4/4	-
6	PEG	H	302	-	-	0/4/4/4	-
7	144	B	303	-	-	0/0/9/9	-
8	PGE	H	305	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	302	-	-	0/1/1/1	-
6	PEG	B	301	-	-	3/4/4/4	-
10	1PE	A	303	-	-	7/13/13/13	-
6	PEG	A	306	-	-	3/4/4/4	-
7	144	H	303	-	-	0/0/9/9	-
9	EDO	A	304	-	-	0/1/1/1	-
8	PGE	A	307	-	-	4/7/7/7	-
6	PEG	H	301	-	-	0/4/4/4	-
8	PGE	H	304	-	-	1/7/7/7	-
6	PEG	A	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	303	1PE	OH5-C14-C24-OH4
10	A	303	1PE	OH6-C15-C25-OH5
6	L	303	PEG	O1-C1-C2-O2
8	H	305	PGE	O3-C5-C6-O4
8	A	307	PGE	O1-C1-C2-O2
6	A	306	PEG	O1-C1-C2-O2
6	B	301	PEG	O2-C3-C4-O4
8	A	307	PGE	O2-C3-C4-O3
10	A	303	1PE	OH4-C13-C23-OH3
8	H	305	PGE	C1-C2-O2-C3
6	A	306	PEG	C4-C3-O2-C2
6	B	301	PEG	C4-C3-O2-C2
8	H	305	PGE	O2-C3-C4-O3
6	A	306	PEG	C1-C2-O2-C3
8	A	307	PGE	C4-C3-O2-C2
10	A	303	1PE	C13-C23-OH3-C22
6	D	201	PEG	O1-C1-C2-O2
6	B	301	PEG	C1-C2-O2-C3
8	H	304	PGE	C1-C2-O2-C3
10	A	303	1PE	C25-C15-OH6-C26
10	A	303	1PE	OH7-C16-C26-OH6
10	A	303	1PE	C12-C22-OH3-C23
8	A	307	PGE	C6-C5-O3-C4

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	201	PEG	1	0
6	H	302	PEG	1	0
6	B	301	PEG	2	0
6	B	302	PEG	1	0
8	H	304	PGE	3	0
5	L	304	CCN	1	0
10	A	303	1PE	1	0
7	H	303	144	1	0
6	A	301	PEG	1	0
8	A	307	PGE	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	213/213 (100%)	0.29	2 (0%) 81 78	34, 50, 72, 100	0
1	L	212/213 (99%)	0.41	5 (2%) 59 55	36, 53, 76, 89	0
2	B	217/219 (99%)	0.26	7 (3%) 50 46	33, 43, 75, 107	0
2	H	214/219 (97%)	0.31	6 (2%) 55 51	32, 48, 73, 125	0
3	C	148/170 (87%)	0.66	11 (7%) 20 17	41, 59, 99, 124	0
3	D	153/170 (90%)	0.73	12 (7%) 19 15	37, 65, 101, 114	0
All	All	1157/1204 (96%)	0.41	43 (3%) 45 41	32, 51, 86, 125	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	183	LEU	4.3
1	L	140	PRO	3.9
1	A	140	PRO	3.7
2	B	131	PRO	3.6
2	B	136	THR	3.5
2	B	139	GLY	3.4
3	C	22	MET	3.4
3	D	56	ALA	3.3
3	D	21	SER	3.1
1	L	203	PRO	3.0
3	C	49	ALA	2.9
3	C	85	ILE	2.9
3	D	86	ASN	2.9
3	D	182	ASN	2.9
3	C	67	PRO	2.8
2	B	132	SER	2.7
3	D	22	MET	2.6
1	L	139	TYR	2.6
2	H	133	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	132	SER	2.6
3	C	173	GLN	2.5
3	D	80	ILE	2.5
3	D	79	ALA	2.5
3	D	169	ARG	2.4
2	H	196	THR	2.4
2	B	133	SER	2.4
2	H	139	GLY	2.3
3	C	80	ILE	2.3
2	B	195	GLY	2.3
2	B	130	ALA	2.3
1	A	201	SER	2.3
3	C	102	PRO	2.2
1	L	152	ALA	2.2
3	D	81	ILE	2.2
3	C	86	ASN	2.2
3	C	183	LEU	2.2
3	C	88	ARG	2.2
3	C	51	GLY	2.2
1	L	211	GLY	2.2
3	D	100	LEU	2.1
2	H	131	PRO	2.1
2	H	1	GLU	2.0
3	D	181	LEU	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	CCN	L	302	3/3	0.62	0.20	53,53,56,56	0
9	EDO	A	302	4/4	0.63	0.21	72,73,74,74	0
4	SO4	B	304	5/5	0.66	0.14	143,143,143,144	0
8	PGE	A	307	10/10	0.74	0.22	64,73,75,75	0
7	144	B	303	8/8	0.74	0.19	52,56,59,59	0
6	PEG	B	301	7/7	0.75	0.20	78,81,88,90	0
6	PEG	D	201	7/7	0.79	0.17	61,64,70,71	0
10	1PE	A	303	16/16	0.79	0.17	56,68,70,71	0
4	SO4	L	301	5/5	0.80	0.11	118,119,120,120	0
6	PEG	H	301	7/7	0.80	0.16	60,61,63,64	0
9	EDO	A	304	4/4	0.81	0.14	56,58,58,59	0
5	CCN	L	304	3/3	0.81	0.17	42,42,43,43	0
6	PEG	H	302	7/7	0.82	0.14	61,62,64,65	0
4	SO4	A	305	5/5	0.82	0.10	116,117,117,117	0
6	PEG	B	302	7/7	0.82	0.17	74,75,78,80	0
6	PEG	L	303	7/7	0.83	0.11	55,60,61,61	0
5	CCN	L	305	3/3	0.84	0.14	51,51,53,54	0
6	PEG	A	301	7/7	0.85	0.19	47,52,63,67	0
8	PGE	H	305	10/10	0.85	0.13	57,60,64,64	0
8	PGE	H	304	10/10	0.86	0.14	51,65,69,70	0
7	144	H	303	8/8	0.88	0.10	49,52,53,54	0
6	PEG	A	306	7/7	0.88	0.17	33,40,43,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.