



wwPDB X-ray Structure Validation Summary Report ⓘ

May 19, 2025 – 04:14 PM JST

PDB ID : 8ZNT / pdb_00008znt
Title : Catalytic antibody T99_C220A
Authors : Kobayashi, J.; Yoshida, H.; Tsuyuguchi, M.; Kato, R.
Deposited on : 2024-05-28
Resolution : 2.61 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 : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

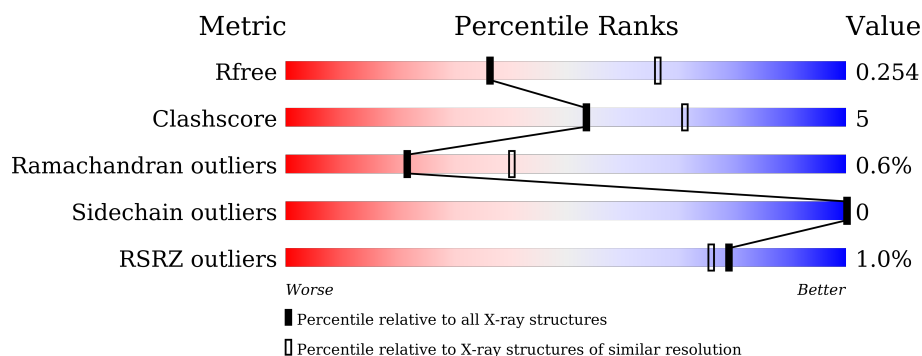
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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}	164625	4623 (2.64-2.60)
Clashscore	180529	5071 (2.64-2.60)
Ramachandran outliers	177936	5006 (2.64-2.60)
Sidechain outliers	177891	5006 (2.64-2.60)
RSRZ outliers	164620	4622 (2.64-2.60)

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	226	
1	B	226	
1	C	226	
1	D	226	
1	E	226	
1	F	226	

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Mol	Chain	Length	Quality of chain
1	G	226	<div><div>%</div><div><div></div><div>82%</div><div>14%</div><div></div></div><div></div></div>
1	H	226	<div><div>%</div><div><div></div><div>89%</div><div>9%</div><div></div></div><div></div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13868 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 Catalytic antibody T99_C220A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1672	1045	285	334	8			
1	B	217	Total	C	N	O	S	0	0	0
			1664	1040	284	333	7			
1	C	218	Total	C	N	O	S	0	0	0
			1672	1045	285	334	8			
1	D	217	Total	C	N	O	S	0	0	0
			1664	1040	284	333	7			
1	E	220	Total	C	N	O	S	0	0	0
			1686	1053	287	338	8			
1	F	218	Total	C	N	O	S	0	0	0
			1665	1040	284	334	7			
1	G	217	Total	C	N	O	S	0	0	0
			1660	1038	284	331	7			
1	H	223	Total	C	N	O	S	0	0	0
			1706	1068	290	341	7			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



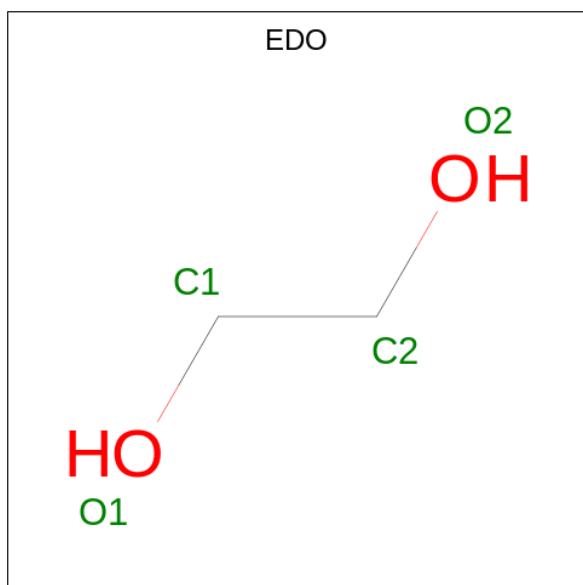
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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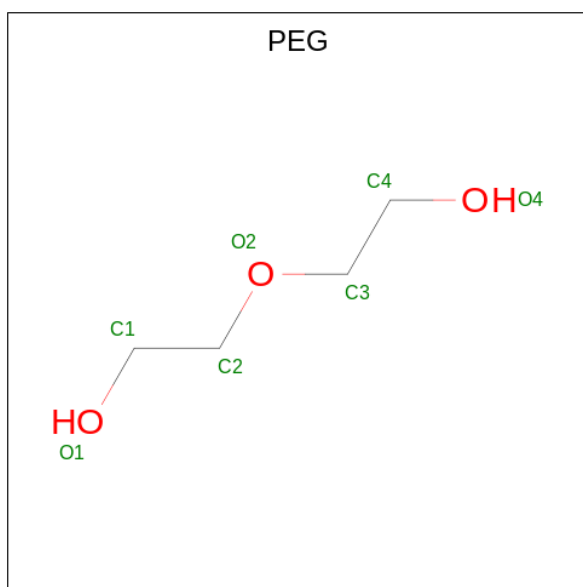
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		
5	B	2	Total	K	0	0
			2	2		
5	C	1	Total	K	0	0
			1	1		
5	D	1	Total	K	0	0
			1	1		
5	E	1	Total	K	0	0
			1	1		
5	F	1	Total	K	0	0
			1	1		
5	G	1	Total	K	0	0
			1	1		
5	H	1	Total	K	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	B	3	Total Cl 3 3	0	0
6	C	1	Total Cl 1 1	0	0
6	D	2	Total Cl 2 2	0	0
6	E	2	Total Cl 2 2	0	0
6	F	1	Total Cl 1 1	0	0
6	G	2	Total Cl 2 2	0	0
6	H	1	Total Cl 1 1	0	0


- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	24	Total O 24 24	0	0
7	B	16	Total O 16 16	0	0
7	C	12	Total O 12 12	0	0
7	D	18	Total O 18 18	0	0
7	E	18	Total O 18 18	0	0
7	F	22	Total O 22 22	0	0
7	G	31	Total O 31 31	0	0
7	H	18	Total O 18 18	0	0

3 Residue-property plots

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: Catalytic antibody T99_C220A

Chain A: 




• Molecule 1: Catalytic antibody T99_C220A

Chain B: 




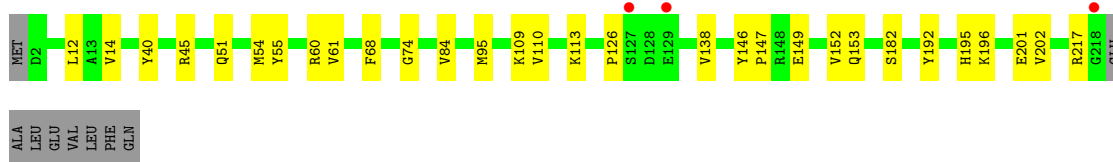
• Molecule 1: Catalytic antibody T99_C220A

Chain C: 




• Molecule 1: Catalytic antibody T99_C220A

Chain D: 

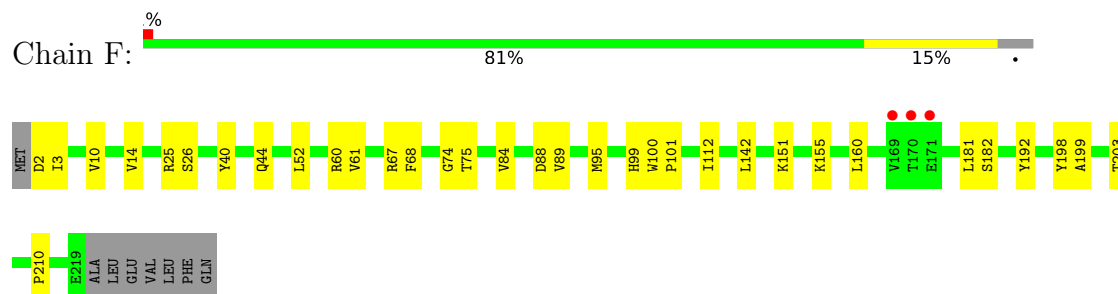


• Molecule 1: Catalytic antibody T99_C220A

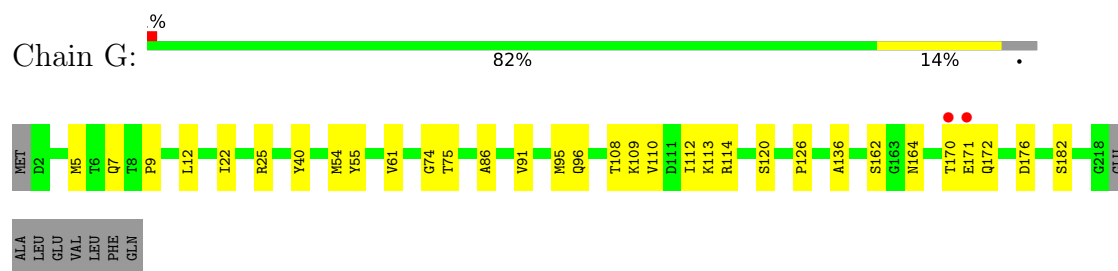
Chain E: 



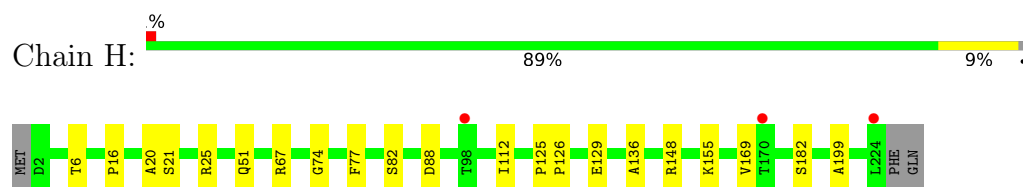
● Molecule 1: Catalytic antibody T99_C220A



● Molecule 1: Catalytic antibody T99_C220A



● Molecule 1: Catalytic antibody T99_C220A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.08Å 85.33Å 104.58Å 106.77° 91.44° 116.91°	Depositor
Resolution (Å)	28.11 – 2.61 28.11 – 2.61	Depositor EDS
% Data completeness (in resolution range)	97.9 (28.11-2.61) 97.9 (28.11-2.61)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.195 , 0.254 0.197 , 0.254	Depositor DCC
R_{free} test set	3290 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13868	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: EDO, CL, PEG, GOL, K

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	0.12	0/1710	0.32	0/2323
1	B	0.12	0/1702	0.32	0/2313
1	C	0.12	0/1710	0.35	0/2323
1	D	0.12	0/1702	0.36	0/2313
1	E	0.12	0/1724	0.36	0/2342
1	F	0.13	0/1703	0.34	0/2316
1	G	0.13	0/1698	0.33	0/2308
1	H	0.13	0/1744	0.35	0/2371
All	All	0.13	0/13693	0.34	0/18609

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	1672	0	1623	12	0
1	B	1664	0	1611	10	0
1	C	1672	0	1622	14	0
1	D	1664	0	1611	19	0
1	E	1686	0	1634	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1665	0	1602	22	0
1	G	1660	0	1607	23	0
1	H	1706	0	1655	15	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	1	0
2	E	24	0	32	1	0
2	F	18	0	24	0	0
2	G	30	0	40	1	0
2	H	6	0	8	0	0
3	A	28	0	42	2	0
3	B	16	0	24	1	0
3	C	28	0	42	2	0
3	D	32	0	48	2	0
3	E	20	0	30	2	0
3	F	20	0	30	2	0
3	G	20	0	30	5	0
3	H	24	0	36	4	0
4	A	7	0	10	1	0
4	G	7	0	10	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	1	0	0	0	0
6	B	3	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
6	G	2	0	0	0	0
6	H	1	0	0	0	0
7	A	24	0	0	0	0
7	B	16	0	0	0	0
7	C	12	0	0	0	0
7	D	18	0	0	0	0
7	E	18	0	0	0	0
7	F	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	31	0	0	0	0
7	H	18	0	0	1	0
All	All	13868	0	13395	130	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.

The worst 5 of 130 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:G:40:TYR:OH	1:G:95:MET:HE3	1.69	0.93
1:G:40:TYR:OH	1:G:95:MET:CE	2.37	0.72
1:G:5:MET:HE3	1:G:96:GLN:HG2	1.73	0.71
1:B:67:ARG:NH1	1:B:83:ARG:O	2.24	0.68
1:C:19:SER:HB2	1:C:83:ARG:H	1.57	0.68

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	216/226 (96%)	210 (97%)	5 (2%)	1 (0%)	25	45
1	B	215/226 (95%)	209 (97%)	5 (2%)	1 (0%)	25	45
1	C	216/226 (96%)	208 (96%)	6 (3%)	2 (1%)	14	29
1	D	215/226 (95%)	209 (97%)	5 (2%)	1 (0%)	25	45
1	E	218/226 (96%)	210 (96%)	6 (3%)	2 (1%)	14	29
1	F	216/226 (96%)	211 (98%)	4 (2%)	1 (0%)	25	45
1	G	215/226 (95%)	208 (97%)	5 (2%)	2 (1%)	14	29
1	H	221/226 (98%)	215 (97%)	5 (2%)	1 (0%)	25	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1732/1808 (96%)	1680 (97%)	41 (2%)	11 (1%)	22	40

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	170	THR
1	G	171	GLU
1	C	34	ASP
1	E	74	GLY
1	B	73	SER

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	190/197 (96%)	190 (100%)	0	100	100
1	B	189/197 (96%)	189 (100%)	0	100	100
1	C	190/197 (96%)	190 (100%)	0	100	100
1	D	189/197 (96%)	189 (100%)	0	100	100
1	E	191/197 (97%)	191 (100%)	0	100	100
1	F	188/197 (95%)	188 (100%)	0	100	100
1	G	188/197 (95%)	188 (100%)	0	100	100
1	H	193/197 (98%)	193 (100%)	0	100	100
All	All	1518/1576 (96%)	1518 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	18	GLN
1	C	195	HIS

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Mol	Chain	Res	Type
1	G	205	GLN
1	F	195	HIS
1	B	195	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](#)

Of 87 ligands modelled in this entry, 22 are monoatomic - leaving 65 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	$\# Z > 2$
3	EDO	G	309	-	3,3,3	0.45	0	2,2,2	0.34	0
2	GOL	F	303	-	5,5,5	0.92	0	5,5,5	0.97	0
2	GOL	F	302	-	5,5,5	0.96	0	5,5,5	0.94	0
3	EDO	A	307	-	3,3,3	0.43	0	2,2,2	0.42	0
3	EDO	B	302	-	3,3,3	0.46	0	2,2,2	0.35	0
3	EDO	B	305	-	3,3,3	0.49	0	2,2,2	0.21	0
3	EDO	C	304	-	3,3,3	0.46	0	2,2,2	0.38	0
3	EDO	D	307	-	3,3,3	0.46	0	2,2,2	0.36	0
2	GOL	B	301	-	5,5,5	0.96	0	5,5,5	0.93	0
3	EDO	G	308	-	3,3,3	0.46	0	2,2,2	0.37	0
3	EDO	D	306	-	3,3,3	0.47	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	H	304	-	3,3,3	0.46	0	2,2,2	0.33	0
2	GOL	C	301	-	5,5,5	0.89	0	5,5,5	1.00	0
3	EDO	B	303	-	3,3,3	0.44	0	2,2,2	0.32	0
2	GOL	H	301	-	5,5,5	0.87	0	5,5,5	1.03	0
3	EDO	G	310	-	3,3,3	0.45	0	2,2,2	0.36	0
3	EDO	C	306	-	3,3,3	0.48	0	2,2,2	0.26	0
3	EDO	H	303	-	3,3,3	0.46	0	2,2,2	0.29	0
3	EDO	H	302	-	3,3,3	0.46	0	2,2,2	0.37	0
3	EDO	H	305	-	3,3,3	0.46	0	2,2,2	0.34	0
3	EDO	C	308	-	3,3,3	0.49	0	2,2,2	0.22	0
3	EDO	G	307	-	3,3,3	0.44	0	2,2,2	0.41	0
2	GOL	G	305	-	5,5,5	0.94	0	5,5,5	0.95	0
3	EDO	E	305	-	3,3,3	0.49	0	2,2,2	0.28	0
3	EDO	E	308	-	3,3,3	0.46	0	2,2,2	0.37	0
3	EDO	F	305	-	3,3,3	0.45	0	2,2,2	0.36	0
3	EDO	F	307	-	3,3,3	0.44	0	2,2,2	0.39	0
3	EDO	H	307	-	3,3,3	0.46	0	2,2,2	0.37	0
2	GOL	F	301	-	5,5,5	0.88	0	5,5,5	1.07	0
3	EDO	E	307	-	3,3,3	0.47	0	2,2,2	0.27	0
2	GOL	E	301	-	5,5,5	0.89	0	5,5,5	1.03	0
2	GOL	E	302	-	5,5,5	0.93	0	5,5,5	0.94	0
3	EDO	D	302	-	3,3,3	0.48	0	2,2,2	0.29	0
3	EDO	D	308	-	3,3,3	0.47	0	2,2,2	0.30	0
3	EDO	C	305	-	3,3,3	0.49	0	2,2,2	0.16	0
3	EDO	H	306	-	3,3,3	0.45	0	2,2,2	0.38	0
3	EDO	F	306	-	3,3,3	0.44	0	2,2,2	0.44	0
2	GOL	E	303	-	5,5,5	0.90	0	5,5,5	1.00	0
2	GOL	G	302	-	5,5,5	0.94	0	5,5,5	0.96	0
3	EDO	C	307	-	3,3,3	0.48	0	2,2,2	0.22	0
3	EDO	E	306	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	A	305	-	3,3,3	0.47	0	2,2,2	0.22	0
3	EDO	G	306	-	3,3,3	0.46	0	2,2,2	0.34	0
2	GOL	E	304	-	5,5,5	0.94	0	5,5,5	0.95	0
2	GOL	G	304	-	5,5,5	0.97	0	5,5,5	0.95	0
2	GOL	A	301	-	5,5,5	0.91	0	5,5,5	0.98	0
3	EDO	C	303	-	3,3,3	0.46	0	2,2,2	0.38	0
3	EDO	A	306	-	3,3,3	0.44	0	2,2,2	0.42	0
3	EDO	A	308	-	3,3,3	0.46	0	2,2,2	0.37	0
3	EDO	C	302	-	3,3,3	0.46	0	2,2,2	0.36	0
4	PEG	G	311	-	6,6,6	0.13	0	5,5,5	0.07	0
3	EDO	A	303	-	3,3,3	0.45	0	2,2,2	0.38	0
3	EDO	D	304	-	3,3,3	0.42	0	2,2,2	0.35	0
3	EDO	F	304	-	3,3,3	0.49	0	2,2,2	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	A	309	-	6,6,6	0.13	0	5,5,5	0.07	0
3	EDO	D	305	-	3,3,3	0.45	0	2,2,2	0.39	0
3	EDO	A	302	-	3,3,3	0.48	0	2,2,2	0.32	0
3	EDO	D	301	-	3,3,3	0.47	0	2,2,2	0.31	0
3	EDO	F	308	-	3,3,3	0.48	0	2,2,2	0.23	0
3	EDO	A	304	-	3,3,3	0.47	0	2,2,2	0.34	0
3	EDO	D	303	-	3,3,3	0.46	0	2,2,2	0.30	0
3	EDO	E	309	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	B	304	5	3,3,3	0.47	0	2,2,2	0.28	0
2	GOL	G	303	-	5,5,5	0.89	0	5,5,5	0.99	0
2	GOL	G	301	-	5,5,5	0.92	0	5,5,5	0.93	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	EDO	G	309	-	-	0/1/1/1	-
2	GOL	F	303	-	-	0/4/4/4	-
2	GOL	F	302	-	-	1/4/4/4	-
3	EDO	A	307	-	-	0/1/1/1	-
3	EDO	B	302	-	-	0/1/1/1	-
3	EDO	B	305	-	-	0/1/1/1	-
3	EDO	C	304	-	-	0/1/1/1	-
3	EDO	D	307	-	-	0/1/1/1	-
2	GOL	B	301	-	-	2/4/4/4	-
3	EDO	G	308	-	-	0/1/1/1	-
3	EDO	D	306	-	-	0/1/1/1	-
3	EDO	H	304	-	-	0/1/1/1	-
2	GOL	C	301	-	-	0/4/4/4	-
3	EDO	B	303	-	-	0/1/1/1	-
2	GOL	H	301	-	-	1/4/4/4	-
3	EDO	G	310	-	-	0/1/1/1	-
3	EDO	C	306	-	-	1/1/1/1	-
3	EDO	H	303	-	-	0/1/1/1	-
3	EDO	H	302	-	-	0/1/1/1	-
3	EDO	H	305	-	-	1/1/1/1	-
3	EDO	C	308	-	-	0/1/1/1	-
3	EDO	G	307	-	-	0/1/1/1	-
2	GOL	G	305	-	-	2/4/4/4	-
3	EDO	E	305	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	E	308	-	-	1/1/1/1	-
3	EDO	F	305	-	-	0/1/1/1	-
3	EDO	F	307	-	-	0/1/1/1	-
3	EDO	H	307	-	-	0/1/1/1	-
2	GOL	F	301	-	-	2/4/4/4	-
3	EDO	E	307	-	-	0/1/1/1	-
2	GOL	E	301	-	-	2/4/4/4	-
2	GOL	E	302	-	-	2/4/4/4	-
3	EDO	D	302	-	-	0/1/1/1	-
3	EDO	D	308	-	-	0/1/1/1	-
3	EDO	C	305	-	-	0/1/1/1	-
3	EDO	H	306	-	-	0/1/1/1	-
3	EDO	F	306	-	-	0/1/1/1	-
2	GOL	E	303	-	-	2/4/4/4	-
2	GOL	G	302	-	-	0/4/4/4	-
3	EDO	C	307	-	-	0/1/1/1	-
3	EDO	E	306	-	-	0/1/1/1	-
3	EDO	A	305	-	-	0/1/1/1	-
3	EDO	G	306	-	-	0/1/1/1	-
2	GOL	E	304	-	-	2/4/4/4	-
2	GOL	G	304	-	-	1/4/4/4	-
2	GOL	A	301	-	-	2/4/4/4	-
3	EDO	C	303	-	-	0/1/1/1	-
3	EDO	A	306	-	-	0/1/1/1	-
3	EDO	A	308	-	-	0/1/1/1	-
3	EDO	C	302	-	-	0/1/1/1	-
4	PEG	G	311	-	-	1/4/4/4	-
3	EDO	A	303	-	-	0/1/1/1	-
3	EDO	D	304	-	-	0/1/1/1	-
3	EDO	F	304	-	-	0/1/1/1	-
4	PEG	A	309	-	-	0/4/4/4	-
3	EDO	D	305	-	-	0/1/1/1	-
3	EDO	A	302	-	-	0/1/1/1	-
3	EDO	D	301	-	-	0/1/1/1	-
3	EDO	F	308	-	-	0/1/1/1	-
3	EDO	A	304	-	-	0/1/1/1	-
3	EDO	D	303	-	-	0/1/1/1	-
3	EDO	E	309	-	-	0/1/1/1	-
3	EDO	B	304	5	-	0/1/1/1	-
2	GOL	G	303	-	-	0/4/4/4	-
2	GOL	G	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	GOL	O1-C1-C2-C3
2	B	301	GOL	O1-C1-C2-C3
2	E	301	GOL	C1-C2-C3-O3
2	E	302	GOL	C1-C2-C3-O3
2	E	303	GOL	O1-C1-C2-C3

There are no ring outliers.

22 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	309	EDO	2	0
3	D	306	EDO	1	0
2	C	301	GOL	1	0
3	G	310	EDO	2	0
3	H	305	EDO	2	0
3	C	308	EDO	1	0
3	F	307	EDO	1	0
3	H	307	EDO	1	0
3	E	307	EDO	1	0
3	H	306	EDO	1	0
2	E	303	GOL	1	0
3	E	306	EDO	1	0
3	A	305	EDO	1	0
3	G	306	EDO	1	0
3	C	303	EDO	1	0
3	A	308	EDO	1	0
4	A	309	PEG	1	0
3	D	305	EDO	1	0
3	F	308	EDO	1	0
3	E	309	EDO	1	0
3	B	304	EDO	1	0
2	G	301	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	218/226 (96%)	-0.08	1 (0%) 87 85	31, 49, 75, 98	0
1	B	217/226 (96%)	-0.15	0 100 100	32, 48, 67, 79	0
1	C	218/226 (96%)	0.06	3 (1%) 73 69	34, 56, 73, 97	0
1	D	217/226 (96%)	-0.23	3 (1%) 73 69	33, 46, 65, 73	0
1	E	220/226 (97%)	-0.13	3 (1%) 73 69	31, 46, 69, 89	0
1	F	218/226 (96%)	-0.17	3 (1%) 73 69	33, 46, 69, 83	0
1	G	217/226 (96%)	-0.31	2 (0%) 81 77	31, 43, 59, 90	0
1	H	223/226 (98%)	-0.09	3 (1%) 74 71	33, 50, 71, 87	0
All	All	1748/1808 (96%)	-0.14	18 (1%) 79 76	31, 48, 69, 98	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	169	VAL	3.2
1	A	218	GLY	3.0
1	E	170	THR	2.9
1	F	171	GLU	2.7
1	D	127	SER	2.6

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

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
3	EDO	G	309	4/4	0.72	0.16	51,56,62,76	0
3	EDO	H	306	4/4	0.72	0.20	61,62,69,72	0
2	GOL	E	301	6/6	0.76	0.16	44,51,54,60	0
3	EDO	E	306	4/4	0.77	0.19	51,65,65,70	0
3	EDO	F	308	4/4	0.78	0.20	38,41,55,62	0
3	EDO	G	308	4/4	0.78	0.17	45,52,53,57	0
2	GOL	G	303	6/6	0.79	0.14	54,58,64,70	0
3	EDO	D	305	4/4	0.80	0.20	46,54,57,68	0
3	EDO	A	307	4/4	0.80	0.19	58,59,62,71	0
3	EDO	E	308	4/4	0.80	0.21	48,52,61,65	0
3	EDO	F	304	4/4	0.80	0.19	40,42,51,64	0
3	EDO	G	306	4/4	0.82	0.17	46,51,56,61	0
3	EDO	B	302	4/4	0.82	0.14	42,50,58,59	0
3	EDO	F	307	4/4	0.83	0.13	58,61,61,65	0
3	EDO	D	308	4/4	0.83	0.19	59,59,61,68	0
3	EDO	E	307	4/4	0.83	0.16	50,58,60,66	0
3	EDO	B	305	4/4	0.84	0.15	47,55,59,61	0
3	EDO	C	308	4/4	0.84	0.17	53,55,59,60	0
3	EDO	C	302	4/4	0.85	0.17	49,50,53,60	0
4	PEG	G	311	7/7	0.85	0.15	53,58,67,74	0
3	EDO	C	304	4/4	0.86	0.15	60,62,65,65	0
2	GOL	G	304	6/6	0.86	0.12	36,39,53,61	0
3	EDO	D	301	4/4	0.86	0.13	47,55,58,62	0
3	EDO	C	303	4/4	0.86	0.19	42,52,60,74	0
3	EDO	D	307	4/4	0.86	0.11	50,59,61,70	0
3	EDO	F	305	4/4	0.86	0.13	43,55,57,58	0
3	EDO	F	306	4/4	0.86	0.15	47,66,68,70	0
2	GOL	F	302	6/6	0.87	0.15	43,51,56,58	0
3	EDO	A	304	4/4	0.87	0.11	40,44,46,49	0
3	EDO	H	304	4/4	0.87	0.19	50,62,69,72	0
3	EDO	E	305	4/4	0.87	0.15	41,44,59,60	0
3	EDO	C	307	4/4	0.87	0.14	45,49,51,53	0
5	K	B	306	1/1	0.87	0.11	65,65,65,65	0
3	EDO	D	302	4/4	0.88	0.21	46,58,61,64	0
2	GOL	A	301	6/6	0.88	0.13	50,56,61,66	0
3	EDO	H	303	4/4	0.88	0.18	47,61,62,67	0
3	EDO	D	306	4/4	0.88	0.12	42,50,53,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	E	304	6/6	0.88	0.14	53,57,59,59	0
4	PEG	A	309	7/7	0.88	0.18	36,54,65,68	0
2	GOL	B	301	6/6	0.88	0.16	52,60,65,72	0
3	EDO	G	307	4/4	0.88	0.13	40,43,56,57	0
5	K	H	308	1/1	0.88	0.08	65,65,65,65	0
3	EDO	A	308	4/4	0.89	0.11	50,51,59,64	0
5	K	F	309	1/1	0.89	0.09	63,63,63,63	0
3	EDO	E	309	4/4	0.89	0.11	48,57,58,62	0
3	EDO	H	307	4/4	0.90	0.15	58,58,60,66	0
5	K	B	307	1/1	0.90	0.22	99,99,99,99	0
3	EDO	A	302	4/4	0.90	0.13	43,58,64,65	0
2	GOL	F	303	6/6	0.90	0.18	39,47,56,61	0
3	EDO	D	303	4/4	0.91	0.10	35,40,41,53	0
3	EDO	A	303	4/4	0.91	0.09	47,52,55,64	0
3	EDO	C	305	4/4	0.91	0.13	39,43,49,57	0
2	GOL	G	305	6/6	0.91	0.11	46,53,59,59	0
3	EDO	A	305	4/4	0.91	0.14	38,46,47,59	0
3	EDO	G	310	4/4	0.91	0.11	48,58,64,70	0
3	EDO	A	306	4/4	0.91	0.11	40,48,49,53	0
2	GOL	C	301	6/6	0.91	0.09	49,55,71,71	0
2	GOL	H	301	6/6	0.92	0.09	45,50,58,74	0
3	EDO	B	304	4/4	0.92	0.13	51,54,56,61	0
3	EDO	C	306	4/4	0.92	0.11	41,44,55,55	0
2	GOL	E	303	6/6	0.92	0.12	47,50,63,64	0
2	GOL	F	301	6/6	0.92	0.12	45,48,51,59	0
3	EDO	H	305	4/4	0.92	0.13	40,51,56,58	0
2	GOL	G	302	6/6	0.92	0.11	41,54,60,63	0
3	EDO	H	302	4/4	0.93	0.12	34,46,47,52	0
5	K	C	309	1/1	0.93	0.07	55,55,55,55	0
3	EDO	D	304	4/4	0.93	0.16	37,43,52,57	0
3	EDO	B	303	4/4	0.93	0.12	32,44,47,49	0
5	K	D	309	1/1	0.94	0.06	54,54,54,54	0
2	GOL	G	301	6/6	0.94	0.15	44,51,58,71	0
2	GOL	E	302	6/6	0.94	0.10	48,52,59,65	0
6	CL	A	311	1/1	0.94	0.08	60,60,60,60	0
6	CL	D	311	1/1	0.94	0.09	52,52,52,52	0
6	CL	B	308	1/1	0.96	0.10	50,50,50,50	0
6	CL	C	310	1/1	0.96	0.06	59,59,59,59	0
6	CL	D	310	1/1	0.96	0.06	50,50,50,50	0
5	K	A	310	1/1	0.96	0.08	53,53,53,53	0
6	CL	B	309	1/1	0.97	0.05	50,50,50,50	0
5	K	G	312	1/1	0.97	0.04	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CL	E	312	1/1	0.97	0.07	52,52,52,52	0
6	CL	E	311	1/1	0.98	0.05	48,48,48,48	0
6	CL	B	310	1/1	0.98	0.05	45,45,45,45	0
6	CL	F	310	1/1	0.98	0.05	48,48,48,48	0
6	CL	G	313	1/1	0.98	0.08	43,43,43,43	0
6	CL	H	309	1/1	0.98	0.06	60,60,60,60	0
6	CL	G	314	1/1	0.99	0.09	52,52,52,52	0
5	K	E	310	1/1	0.99	0.02	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.