



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2024 – 10:41 am BST

PDB ID : 1HJS  
Title : Structure of two fungal beta-1,4-galactanases: searching for the basis for temperature and pH optimum.  
Authors : Le Nours, J.; Ryttersgaard, C.; Lo Leggio, L.; Ostergaard, P.R.; Borchert, T.V.; Christensen, L.L.H.; Larsen, S.  
Deposited on : 2003-02-27  
Resolution : 1.87 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

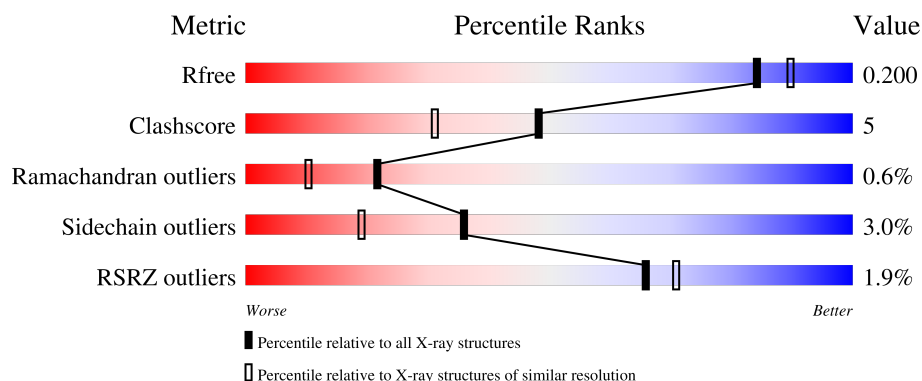
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.87 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	1090 (1.88-1.88)
Clashscore	180529	1144 (1.88-1.88)
Ramachandran outliers	177936	1135 (1.88-1.88)
Sidechain outliers	177891	1135 (1.88-1.88)
RSRZ outliers	164620	1090 (1.88-1.88)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	332	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>14%</div> <div>.</div> </div> </div>
1	B	332	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>
1	C	332	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>.</div> </div> </div>
1	D	332	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>

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	802	-	-	-	X
5	EPE	A	901	-	-	-	X

## 2 Entry composition [i](#)

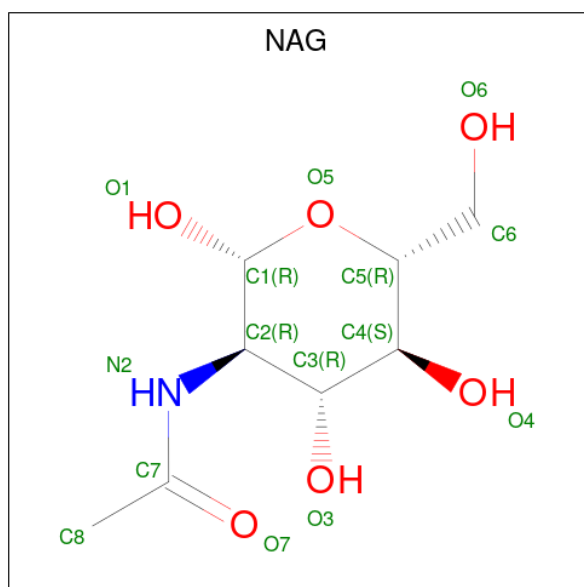
There are 6 unique types of molecules in this entry. The entry contains 11296 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-1,4-GALACTANASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	1	0
			2609	1661	446	494	8			
1	B	332	Total	C	N	O	S	0	1	0
			2609	1661	446	494	8			
1	C	332	Total	C	N	O	S	0	1	0
			2609	1661	446	494	8			
1	D	332	Total	C	N	O	S	0	1	0
			2609	1661	446	494	8			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



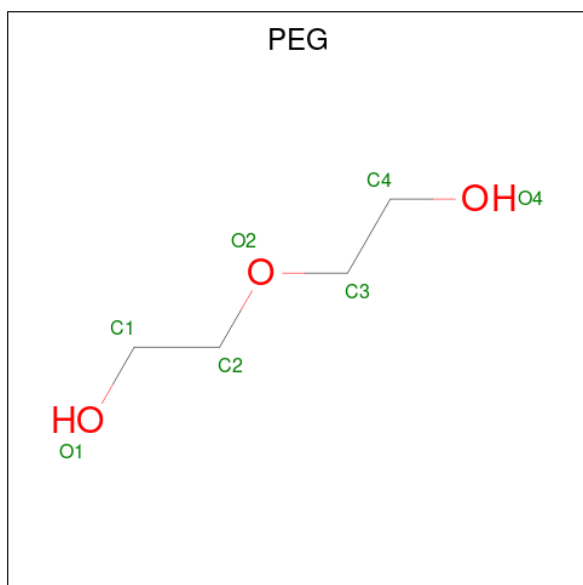
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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



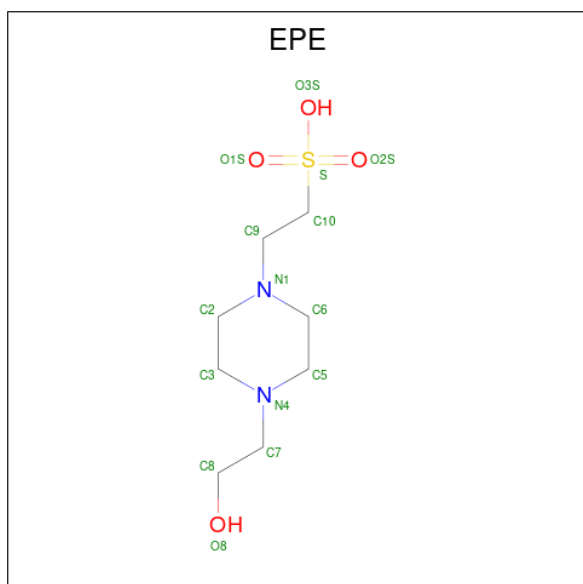
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total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

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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

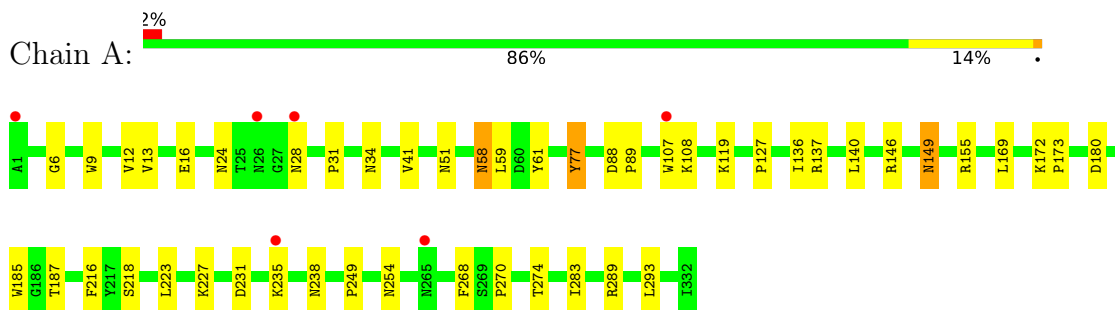
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	182	Total	O	0	0
			182	182		
6	B	163	Total	O	0	0
			163	163		
6	C	144	Total	O	0	0
			144	144		
6	D	154	Total	O	0	0
			154	154		

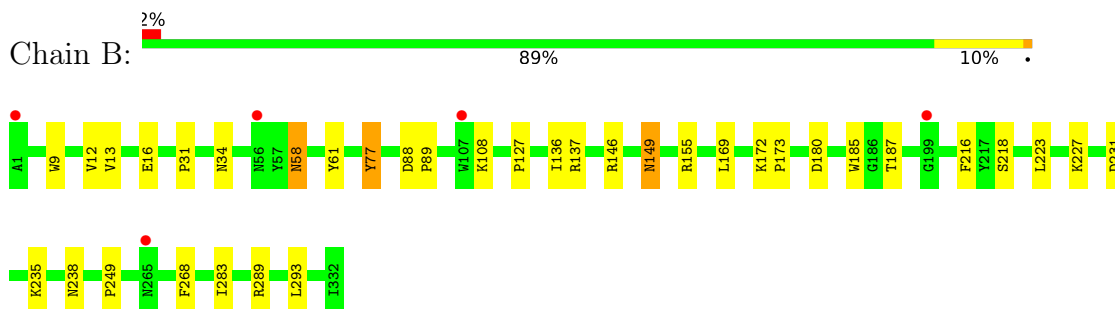
### 3 Residue-property plots [i](#)

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.

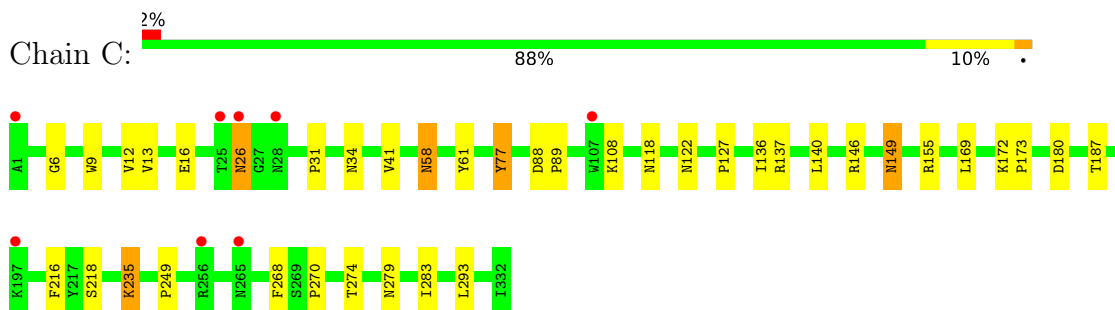
#### • Molecule 1: BETA-1,4-GALACTANASE



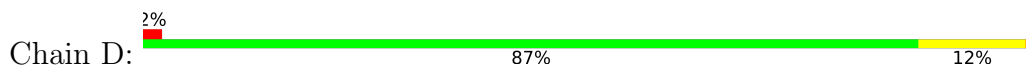
#### • Molecule 1: BETA-1,4-GALACTANASE



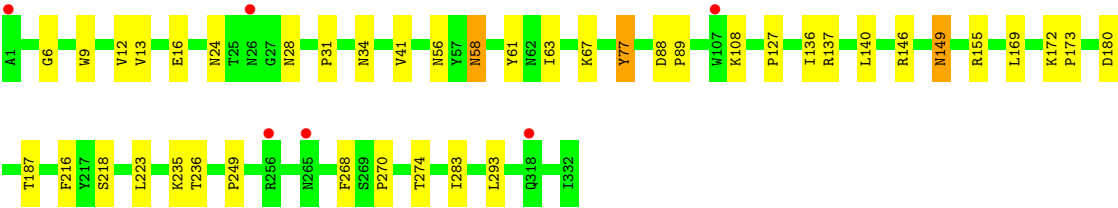
#### • Molecule 1: BETA-1,4-GALACTANASE



#### • Molecule 1: BETA-1,4-GALACTANASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.38Å 136.15Å 111.01Å 90.00° 119.02° 90.00°	Depositor
Resolution (Å)	19.84 – 1.87 19.84 – 1.87	Depositor EDS
% Data completeness (in resolution range)	95.4 (19.84-1.87) 95.4 (19.84-1.87)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 1.86Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.194 , 0.208 0.186 , 0.200	Depositor DCC
$R_{free}$ test set	10585 reflections (9.31%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.8	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 39.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EPE, PEG, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.32	0/2688	0.60	0/3677
1	B	0.32	0/2688	0.60	0/3677
1	C	0.31	0/2688	0.60	0/3677
1	D	0.31	0/2688	0.60	0/3677
All	All	0.32	0/10752	0.60	0/14708

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	2609	0	2501	34	0
1	B	2609	0	2501	22	0
1	C	2609	0	2501	26	0
1	D	2609	0	2501	27	0
2	A	14	0	13	2	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
3	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	15	0	0	0	0
4	A	28	0	40	4	0
4	B	28	0	40	3	0
4	C	14	0	20	3	0
4	D	21	0	30	1	0
5	A	15	0	17	2	0
6	A	182	0	0	3	0
6	B	163	0	0	1	0
6	C	144	0	0	0	0
6	D	154	0	0	1	0
All	All	11296	0	10203	112	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 (112) 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)
5:A:901:EPE:H101	6:A:2180:HOH:O	1.79	0.81
1:B:185:TRP:HB3	4:B:806:PEG:H11	1.63	0.78
1:A:24:ASN:HD21	1:A:28:ASN:HB2	1.48	0.78
1:B:137:ARG:HD3	1:B:180:ASP:OD1	1.85	0.76
1:C:137:ARG:HD3	1:C:180:ASP:OD1	1.86	0.76
1:D:137:ARG:HD3	1:D:180:ASP:OD1	1.86	0.75
1:A:137:ARG:HD3	1:A:180:ASP:OD1	1.86	0.74
1:C:58:ASN:ND2	1:C:61:TYR:H	1.92	0.67
1:A:119:LYS:HD3	4:A:801:PEG:H22	1.77	0.67
1:A:59:LEU:HB3	4:A:801:PEG:H32	1.76	0.66
1:B:238[A]:ASN:OD1	1:B:289:ARG:HD2	1.96	0.66
1:A:58:ASN:ND2	1:A:61:TYR:H	1.93	0.66
1:D:24:ASN:HD21	1:D:28:ASN:HB2	1.59	0.66
1:D:58:ASN:ND2	1:D:61:TYR:H	1.92	0.66
1:B:58:ASN:ND2	1:B:61:TYR:H	1.92	0.66
1:C:58:ASN:C	1:C:58:ASN:HD22	1.99	0.66
1:D:58:ASN:HD22	1:D:58:ASN:C	1.98	0.65
1:A:58:ASN:HD22	1:A:58:ASN:C	2.00	0.64
1:B:58:ASN:C	1:B:58:ASN:HD22	2.00	0.63
1:A:107:TRP:CH2	2:A:601:NAG:H3	2.35	0.61
1:D:236:THR:OG1	4:D:802:PEG:H42	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:LYS:HD2	4:C:802:PEG:C4	2.32	0.59
1:D:24:ASN:ND2	1:D:28:ASN:HB2	2.18	0.58
1:C:235:LYS:HD2	4:C:802:PEG:O4	2.04	0.57
1:A:24:ASN:ND2	1:A:28:ASN:HB2	2.18	0.57
1:A:107:TRP:CZ3	2:A:601:NAG:H3	2.40	0.56
1:C:249:PRO:HG2	1:C:268:PHE:CD1	2.40	0.56
1:B:249:PRO:HG2	1:B:268:PHE:CD1	2.41	0.55
1:D:169:LEU:O	1:D:172:LYS:HD2	2.06	0.55
1:B:169:LEU:O	1:B:172:LYS:HD2	2.07	0.55
1:A:249:PRO:HG2	1:A:268:PHE:CD1	2.42	0.54
1:C:146:ARG:O	1:C:149:ASN:HB2	2.08	0.54
1:A:146:ARG:O	1:A:149:ASN:HB2	2.08	0.54
1:A:169:LEU:O	1:A:172:LYS:HD2	2.08	0.53
1:C:169:LEU:O	1:C:172:LYS:HD2	2.09	0.53
1:D:146:ARG:O	1:D:149:ASN:HB2	2.08	0.53
1:D:249:PRO:HG2	1:D:268:PHE:CD1	2.43	0.53
1:B:293:LEU:C	1:B:293:LEU:HD23	2.29	0.53
1:C:293:LEU:C	1:C:293:LEU:HD23	2.29	0.53
1:B:146:ARG:O	1:B:149:ASN:HB2	2.08	0.52
1:D:293:LEU:C	1:D:293:LEU:HD23	2.30	0.52
1:A:293:LEU:C	1:A:293:LEU:HD23	2.31	0.52
1:D:88:ASP:HB2	1:D:89:PRO:CD	2.41	0.51
1:A:88:ASP:HB2	1:A:89:PRO:CD	2.42	0.50
1:A:137:ARG:HD2	1:A:187:THR:HG21	1.93	0.50
1:B:88:ASP:HB2	1:B:89:PRO:CD	2.41	0.50
1:D:12:VAL:O	1:D:16:GLU:HG3	2.12	0.49
1:C:12:VAL:O	1:C:16:GLU:HG3	2.13	0.49
1:C:88:ASP:HB2	1:C:89:PRO:CD	2.42	0.49
1:B:137:ARG:HD2	1:B:187:THR:HG21	1.94	0.49
1:D:137:ARG:HD2	1:D:187:THR:HG21	1.93	0.49
1:C:137:ARG:HD2	1:C:187:THR:HG21	1.94	0.49
1:B:12:VAL:O	1:B:16:GLU:HG3	2.14	0.48
1:D:58:ASN:ND2	1:D:58:ASN:C	2.66	0.48
1:C:127:PRO:O	1:C:173:PRO:HB3	2.13	0.48
1:D:127:PRO:O	1:D:173:PRO:HB3	2.13	0.48
1:B:58:ASN:ND2	1:B:58:ASN:C	2.67	0.48
1:C:58:ASN:ND2	1:C:58:ASN:C	2.67	0.48
1:D:56:ASN:HB2	6:D:2037:HOH:O	2.14	0.48
1:A:58:ASN:ND2	1:A:58:ASN:C	2.68	0.47
1:B:127:PRO:O	1:B:173:PRO:HB3	2.14	0.47
1:C:58:ASN:HD21	1:C:61:TYR:H	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:PRO:HD2	1:C:34:ASN:HD22	1.80	0.47
1:D:63:ILE:O	1:D:67:LYS:HG3	2.13	0.47
1:B:31:PRO:HD2	1:B:34:ASN:HD22	1.80	0.47
1:D:58:ASN:HD21	1:D:61:TYR:H	1.62	0.47
1:D:223:LEU:HB3	1:D:283:ILE:HD11	1.96	0.47
1:B:231:ASP:HB3	4:B:805:PEG:H32	1.96	0.46
1:A:127:PRO:O	1:A:173:PRO:HB3	2.14	0.46
1:C:31:PRO:HB2	1:C:34:ASN:ND2	2.31	0.46
1:A:31:PRO:HB2	1:A:34:ASN:ND2	2.31	0.46
1:A:31:PRO:HD2	1:A:34:ASN:HD22	1.81	0.46
1:D:12:VAL:HG13	1:D:13:VAL:N	2.31	0.45
1:C:279:ASN:O	1:C:283:ILE:HG12	2.16	0.45
1:A:12:VAL:O	1:A:16:GLU:HG3	2.15	0.45
1:B:58:ASN:HD21	1:B:61:TYR:H	1.63	0.45
1:B:31:PRO:HB2	1:B:34:ASN:ND2	2.31	0.45
1:C:12:VAL:HG13	1:C:13:VAL:N	2.32	0.45
1:B:223:LEU:HB3	1:B:283:ILE:HD11	1.98	0.45
1:A:12:VAL:HG13	1:A:13:VAL:N	2.31	0.45
1:A:146:ARG:HE	5:A:901:EPE:C7	2.29	0.45
4:A:801:PEG:H31	6:A:2040:HOH:O	2.15	0.45
1:D:31:PRO:HD2	1:D:34:ASN:HD22	1.82	0.44
1:A:185:TRP:HB3	4:A:806:PEG:H11	1.99	0.44
1:C:26:ASN:HD22	1:C:26:ASN:HA	1.56	0.44
1:D:77:TYR:C	1:D:77:TYR:CD1	2.91	0.44
4:B:801:PEG:H41	6:B:2085:HOH:O	2.18	0.44
1:B:12:VAL:HG13	1:B:13:VAL:N	2.33	0.44
1:B:77:TYR:CD1	1:B:77:TYR:C	2.91	0.43
1:C:118:ASN:O	1:C:122:ASN:ND2	2.52	0.43
1:C:77:TYR:C	1:C:77:TYR:CD1	2.92	0.43
1:D:31:PRO:HB2	1:D:34:ASN:ND2	2.32	0.43
1:D:63:ILE:CG2	1:D:67:LYS:HE3	2.48	0.43
1:A:77:TYR:C	1:A:77:TYR:CD1	2.92	0.42
1:A:270:PRO:O	1:A:274:THR:HG23	2.19	0.42
1:A:58:ASN:HD21	1:A:61:TYR:H	1.64	0.42
1:A:223:LEU:HD22	1:A:283:ILE:CD1	2.49	0.42
1:A:223:LEU:HB3	1:A:283:ILE:HD11	2.02	0.42
1:A:238[A]:ASN:ND2	1:A:289:ARG:HD2	2.34	0.42
1:C:235:LYS:HD2	4:C:802:PEG:H41	1.98	0.42
1:B:227:LYS:HE3	1:B:231:ASP:OD2	2.20	0.41
1:C:6:GLY:HA2	1:C:41:VAL:HG13	2.02	0.41
1:D:140:LEU:HD23	1:D:140:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLY:HA2	1:A:41:VAL:HG13	2.01	0.41
1:A:140:LEU:HD23	1:A:140:LEU:N	2.35	0.41
1:A:227:LYS:HE3	1:A:231:ASP:OD2	2.21	0.41
1:C:140:LEU:N	1:C:140:LEU:HD23	2.35	0.41
1:A:51:ASN:HB2	6:A:2032:HOH:O	2.21	0.41
1:A:149:ASN:HD22	1:A:149:ASN:HA	1.69	0.41
1:C:270:PRO:O	1:C:274:THR:HG23	2.20	0.41
1:D:6:GLY:HA2	1:D:41:VAL:HG13	2.03	0.40
1:D:270:PRO:O	1:D:274:THR:HG23	2.21	0.40

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	331/332 (100%)	318 (96%)	11 (3%)	2 (1%)	22	10
1	B	331/332 (100%)	318 (96%)	11 (3%)	2 (1%)	22	10
1	C	331/332 (100%)	317 (96%)	12 (4%)	2 (1%)	22	10
1	D	331/332 (100%)	318 (96%)	11 (3%)	2 (1%)	22	10
All	All	1324/1328 (100%)	1271 (96%)	45 (3%)	8 (1%)	22	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	SER
1	B	218	SER
1	C	218	SER
1	D	218	SER
1	B	136	ILE
1	D	136	ILE

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Mol	Chain	Res	Type
1	A	136	ILE
1	C	136	ILE

### 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	280/279 (100%)	271 (97%)	9 (3%)	34	17
1	B	280/279 (100%)	272 (97%)	8 (3%)	37	20
1	C	280/279 (100%)	271 (97%)	9 (3%)	34	17
1	D	280/279 (100%)	272 (97%)	8 (3%)	37	20
All	All	1120/1116 (100%)	1086 (97%)	34 (3%)	36	19

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TRP
1	A	58	ASN
1	A	77	TYR
1	A	108	LYS
1	A	149	ASN
1	A	155	ARG
1	A	216	PHE
1	A	235	LYS
1	A	254	ASN
1	B	9	TRP
1	B	58	ASN
1	B	77	TYR
1	B	108	LYS
1	B	149	ASN
1	B	155	ARG
1	B	216	PHE
1	B	235	LYS
1	C	9	TRP
1	C	26	ASN

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Mol	Chain	Res	Type
1	C	58	ASN
1	C	77	TYR
1	C	108	LYS
1	C	149	ASN
1	C	155	ARG
1	C	216	PHE
1	C	235	LYS
1	D	9	TRP
1	D	58	ASN
1	D	77	TYR
1	D	108	LYS
1	D	149	ASN
1	D	155	ARG
1	D	216	PHE
1	D	235	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	39	ASN
1	A	58	ASN
1	A	149	ASN
1	A	254	ASN
1	A	330	GLN
1	B	34	ASN
1	B	39	ASN
1	B	58	ASN
1	B	122	ASN
1	B	149	ASN
1	B	330	GLN
1	C	26	ASN
1	C	34	ASN
1	C	39	ASN
1	C	58	ASN
1	C	122	ASN
1	C	149	ASN
1	C	330	GLN
1	D	34	ASN
1	D	39	ASN
1	D	58	ASN
1	D	122	ASN

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Mol	Chain	Res	Type
1	D	149	ASN
1	D	330	GLN

### 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](#)

29 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	$\# Z  > 2$
4	PEG	A	805	-	6,6,6	0.75	0	5,5,5	1.45	1 (20%)
3	SO4	A	704	-	4,4,4	1.81	1 (25%)	6,6,6	0.91	0
3	SO4	D	703	-	4,4,4	1.88	2 (50%)	6,6,6	0.90	0
3	SO4	A	703	-	4,4,4	1.88	2 (50%)	6,6,6	0.89	0
3	SO4	C	705	-	4,4,4	1.88	2 (50%)	6,6,6	0.90	0
3	SO4	C	703	-	4,4,4	1.88	2 (50%)	6,6,6	0.89	0
3	SO4	B	705	-	4,4,4	1.88	2 (50%)	6,6,6	0.90	0
2	NAG	A	601	1	14,14,15	0.48	0	17,19,21	0.62	0
5	EPE	A	901	-	15,15,15	1.35	3 (20%)	18,20,20	1.05	2 (11%)
4	PEG	D	802	-	6,6,6	0.62	0	5,5,5	1.42	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PEG	B	802	-	6,6,6	0.74	0	5,5,5	1.43	1 (20%)
2	NAG	B	601	1	14,14,15	0.50	0	17,19,21	0.61	0
4	PEG	D	806	-	6,6,6	0.70	0	5,5,5	1.43	1 (20%)
3	SO4	A	702	-	4,4,4	1.82	2 (50%)	6,6,6	0.88	0
4	PEG	D	805	-	6,6,6	0.67	0	5,5,5	1.48	1 (20%)
4	PEG	C	802	-	6,6,6	0.64	0	5,5,5	1.44	1 (20%)
4	PEG	A	801	-	6,6,6	0.70	0	5,5,5	1.45	1 (20%)
4	PEG	B	801	-	6,6,6	0.71	0	5,5,5	1.45	1 (20%)
4	PEG	B	805	-	6,6,6	0.73	0	5,5,5	1.45	1 (20%)
2	NAG	D	601	1	14,14,15	0.49	0	17,19,21	0.62	0
3	SO4	B	703	-	4,4,4	1.87	2 (50%)	6,6,6	0.89	0
2	NAG	C	601	1	14,14,15	0.49	0	17,19,21	0.61	0
3	SO4	D	701	-	4,4,4	1.85	2 (50%)	6,6,6	0.89	0
3	SO4	A	701	-	4,4,4	1.85	2 (50%)	6,6,6	0.90	0
4	PEG	A	802	-	6,6,6	0.64	0	5,5,5	1.40	1 (20%)
4	PEG	A	806	-	6,6,6	0.75	0	5,5,5	1.46	1 (20%)
4	PEG	C	805	-	6,6,6	0.72	0	5,5,5	1.44	1 (20%)
3	SO4	D	705	-	4,4,4	1.89	2 (50%)	6,6,6	0.86	0
4	PEG	B	806	-	6,6,6	0.74	0	5,5,5	1.42	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	805	-	-	2/4/4/4	-
4	PEG	D	805	-	-	2/4/4/4	-
5	EPE	A	901	-	-	1/9/19/19	0/1/1/1
4	PEG	D	802	-	-	2/4/4/4	-
2	NAG	C	601	1	-	0/6/23/26	0/1/1/1
4	PEG	C	802	-	-	1/4/4/4	-
4	PEG	A	801	-	-	2/4/4/4	-
4	PEG	D	806	-	-	1/4/4/4	-
4	PEG	B	801	-	-	3/4/4/4	-
4	PEG	B	805	-	-	1/4/4/4	-
4	PEG	A	802	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	601	1	-	0/6/23/26	0/1/1/1
2	NAG	B	601	1	-	0/6/23/26	0/1/1/1
4	PEG	A	806	-	-	2/4/4/4	-
4	PEG	C	805	-	-	2/4/4/4	-
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1
4	PEG	B	802	-	-	1/4/4/4	-
4	PEG	B	806	-	-	1/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	703	SO4	O1-S	3.12	1.62	1.46
3	B	705	SO4	O1-S	3.11	1.62	1.46
3	B	703	SO4	O1-S	3.10	1.62	1.46
3	D	703	SO4	O1-S	3.09	1.62	1.46
3	C	705	SO4	O1-S	3.08	1.62	1.46
3	A	703	SO4	O1-S	3.07	1.62	1.46
3	A	701	SO4	O1-S	3.06	1.62	1.46
3	D	701	SO4	O1-S	3.05	1.62	1.46
3	D	705	SO4	O1-S	3.00	1.62	1.46
3	A	704	SO4	O1-S	2.98	1.62	1.46
3	A	702	SO4	O1-S	2.98	1.62	1.46
5	A	901	EPE	C6-N1	2.35	1.53	1.46
5	A	901	EPE	C10-S	2.31	1.80	1.77
3	D	705	SO4	O3-S	-2.24	1.29	1.47
5	A	901	EPE	C2-N1	2.20	1.53	1.46
3	A	703	SO4	O3-S	-2.11	1.30	1.47
3	C	705	SO4	O3-S	-2.11	1.30	1.47
3	B	705	SO4	O3-S	-2.07	1.30	1.47
3	D	703	SO4	O3-S	-2.07	1.30	1.47
3	A	702	SO4	O3-S	-2.06	1.31	1.47
3	B	703	SO4	O3-S	-2.05	1.31	1.47
3	D	701	SO4	O3-S	-2.05	1.31	1.47
3	C	703	SO4	O3-S	-2.05	1.31	1.47
3	A	701	SO4	O3-S	-2.04	1.31	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	PEG	O2-C2-C1	2.54	121.22	110.07
4	D	805	PEG	O2-C2-C1	2.53	121.18	110.07
4	C	802	PEG	O2-C2-C1	2.50	121.06	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	PEG	O2-C2-C1	2.49	121.00	110.07
4	B	805	PEG	O2-C2-C1	2.49	121.00	110.07
4	A	806	PEG	O2-C2-C1	2.48	120.98	110.07
4	D	806	PEG	O2-C2-C1	2.46	120.89	110.07
4	A	805	PEG	O2-C2-C1	2.45	120.85	110.07
4	D	802	PEG	O2-C2-C1	2.45	120.82	110.07
4	B	802	PEG	O2-C2-C1	2.43	120.73	110.07
4	A	802	PEG	O2-C2-C1	2.42	120.72	110.07
4	C	805	PEG	O2-C2-C1	2.40	120.62	110.07
4	B	806	PEG	O2-C2-C1	2.38	120.52	110.07
5	A	901	EPE	C9-N1-C6	-2.21	105.59	111.23
5	A	901	EPE	C7-N4-C5	-2.11	105.84	111.23

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	801	PEG	O2-C3-C4-O4
4	B	801	PEG	O1-C1-C2-O2
4	B	805	PEG	O2-C3-C4-O4
4	C	805	PEG	O2-C3-C4-O4
4	D	805	PEG	O2-C3-C4-O4
4	D	806	PEG	O1-C1-C2-O2
4	A	801	PEG	O2-C3-C4-O4
4	B	806	PEG	O2-C3-C4-O4
4	C	805	PEG	O1-C1-C2-O2
4	D	802	PEG	O1-C1-C2-O2
4	D	802	PEG	O2-C3-C4-O4
4	D	805	PEG	O1-C1-C2-O2
4	B	802	PEG	O2-C3-C4-O4
4	A	802	PEG	O2-C3-C4-O4
4	A	806	PEG	O2-C3-C4-O4
4	A	801	PEG	C4-C3-O2-C2
4	A	805	PEG	O1-C1-C2-O2
4	C	802	PEG	C4-C3-O2-C2
4	A	802	PEG	O1-C1-C2-O2
4	B	801	PEG	C4-C3-O2-C2
5	A	901	EPE	N4-C7-C8-O8
4	A	806	PEG	O1-C1-C2-O2
4	A	805	PEG	O2-C3-C4-O4

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAG	2	0
5	A	901	EPE	2	0
4	D	802	PEG	1	0
4	C	802	PEG	3	0
4	A	801	PEG	3	0
4	B	801	PEG	1	0
4	B	805	PEG	1	0
4	A	806	PEG	1	0
4	B	806	PEG	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	332/332 (100%)	-0.18	6 (1%) 67 72	9, 14, 23, 33	1 (0%)
1	B	332/332 (100%)	-0.15	5 (1%) 71 77	10, 15, 23, 30	1 (0%)
1	C	332/332 (100%)	-0.10	8 (2%) 59 64	10, 15, 24, 37	1 (0%)
1	D	332/332 (100%)	-0.11	6 (1%) 67 72	10, 15, 24, 33	1 (0%)
All	All	1328/1328 (100%)	-0.14	25 (1%) 66 71	9, 15, 24, 37	4 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	107	TRP	4.6
1	D	107	TRP	4.1
1	C	1	ALA	3.8
1	A	107	TRP	3.7
1	A	265	ASN	3.2
1	A	1	ALA	3.2
1	B	107	TRP	3.1
1	B	1	ALA	3.1
1	C	26	ASN	2.9
1	B	265	ASN	2.7
1	D	265	ASN	2.6
1	D	1	ALA	2.5
1	C	28	ASN	2.5
1	C	265	ASN	2.5
1	A	26	ASN	2.4
1	B	56	ASN	2.4
1	C	25	THR	2.4
1	D	318	GLN	2.4
1	D	256	ARG	2.4
1	B	199	GLY	2.4
1	C	197	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	26	ASN	2.3
1	C	256	ARG	2.1
1	A	28	ASN	2.0
1	A	235	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	EPE	A	901	15/15	0.49	0.48	92,93,95,95	0
4	PEG	A	801	7/7	0.55	0.27	47,47,48,48	0
4	PEG	A	802	7/7	0.56	0.42	81,81,82,82	0
4	PEG	D	806	7/7	0.64	0.32	68,68,68,68	0
4	PEG	B	806	7/7	0.66	0.26	53,54,54,55	0
4	PEG	D	805	7/7	0.67	0.32	70,70,70,70	0
3	SO4	B	705	5/5	0.68	0.26	97,97,97,97	0
4	PEG	D	802	7/7	0.70	0.31	64,64,64,64	0
4	PEG	A	806	7/7	0.70	0.23	45,46,46,46	0
3	SO4	D	705	5/5	0.72	0.26	83,83,83,83	0
4	PEG	C	805	7/7	0.72	0.30	64,64,64,64	0
4	PEG	C	802	7/7	0.73	0.34	72,73,73,73	0
2	NAG	C	601	14/15	0.75	0.12	27,29,31,31	0
4	PEG	B	802	7/7	0.76	0.20	51,51,51,51	0
2	NAG	D	601	14/15	0.77	0.13	27,29,31,32	0
4	PEG	B	801	7/7	0.77	0.20	48,48,48,48	0
3	SO4	D	703	5/5	0.78	0.18	82,82,82,83	0
2	NAG	B	601	14/15	0.79	0.12	27,28,31,32	0
4	PEG	B	805	7/7	0.79	0.25	67,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PEG	A	805	7/7	0.79	0.24	61,61,61,62	0
3	SO4	C	705	5/5	0.80	0.20	89,89,89,89	0
2	NAG	A	601	14/15	0.81	0.11	27,28,30,31	0
3	SO4	A	703	5/5	0.82	0.16	57,57,57,57	0
3	SO4	B	703	5/5	0.82	0.15	58,58,58,58	0
3	SO4	C	703	5/5	0.85	0.14	55,55,56,56	0
3	SO4	A	704	5/5	0.90	0.12	32,33,33,33	0
3	SO4	A	701	5/5	0.93	0.10	44,44,44,44	0
3	SO4	A	702	5/5	0.93	0.11	34,34,35,35	0
3	SO4	D	701	5/5	0.94	0.10	36,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.