



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:55 pm BST

PDB ID : 4K1P  
Title : Structure of the NheA component of the Nhe toxin from *Bacillus cereus*  
Authors : Ganash, M.; Phung, D.; Artymiuk, P.J.  
Deposited on : 2013-04-05  
Resolution : 2.05 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.

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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 : 1.8.5 (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

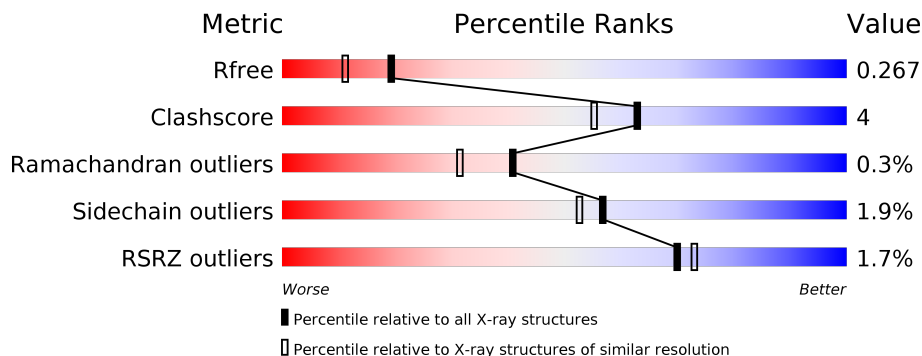
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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  $\geq 3$ , 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	360	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">85% 9% 6%</p>
1	B	360	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">86% 10% •</p>
1	C	360	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">82% 9% • 8%</p>
1	D	360	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">85% 11% •</p>
1	E	360	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">80% 9% 10%</p>
1	F	360	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">81% 9% 10%</p>

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Mol	Chain	Length	Quality of chain
1	G	360	 <p>% 80% 10% 10%</p>
1	H	360	 <p>% 82% 11% 7%</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22614 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 NheA.

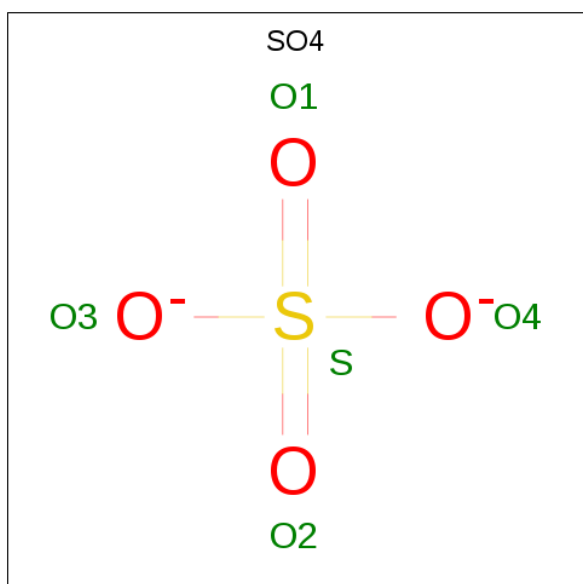
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	339	Total 2689	C 1685	N 458	O 539	S 7	0	0	0
1	B	346	Total 2740	C 1721	N 466	O 546	S 7	0	0	0
1	C	330	Total 2570	C 1614	N 438	O 511	S 7	0	0	3
1	D	346	Total 2743	C 1723	N 466	O 547	S 7	0	0	0
1	E	325	Total 2562	C 1607	N 442	O 506	S 7	0	0	0
1	F	325	Total 2581	C 1622	N 435	O 517	S 7	0	0	0
1	G	325	Total 2552	C 1598	N 439	O 508	S 7	0	0	1
1	H	336	Total 2646	C 1662	N 455	O 522	S 7	0	0	0

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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



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

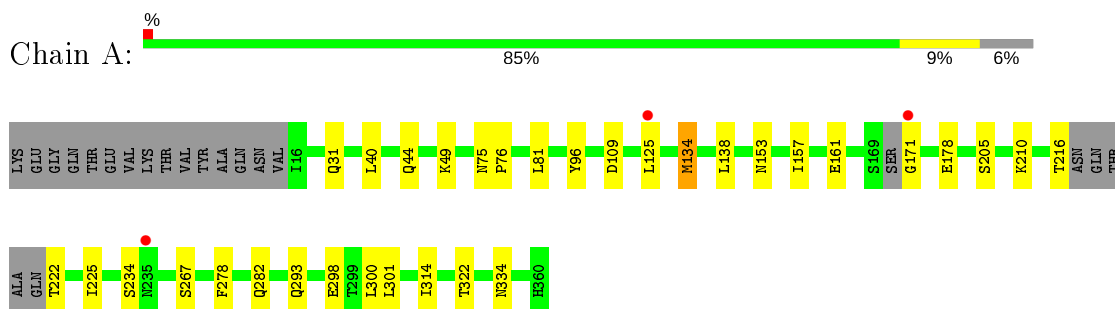
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	217	Total	O	0	0
			217	217		
4	B	184	Total	O	0	0
			184	184		
4	C	226	Total	O	0	0
			226	226		
4	D	213	Total	O	0	0
			213	213		
4	E	166	Total	O	0	0
			166	166		
4	F	205	Total	O	0	0
			205	205		
4	G	155	Total	O	0	0
			155	155		
4	H	141	Total	O	0	0
			141	141		

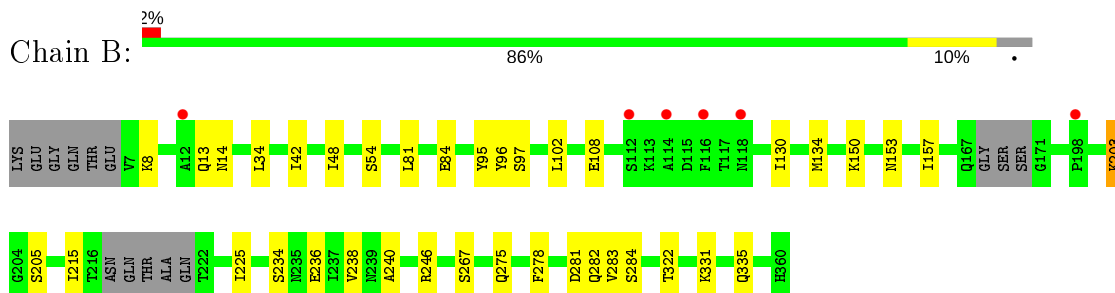
### 3 Residue-property plots [i](#)

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.

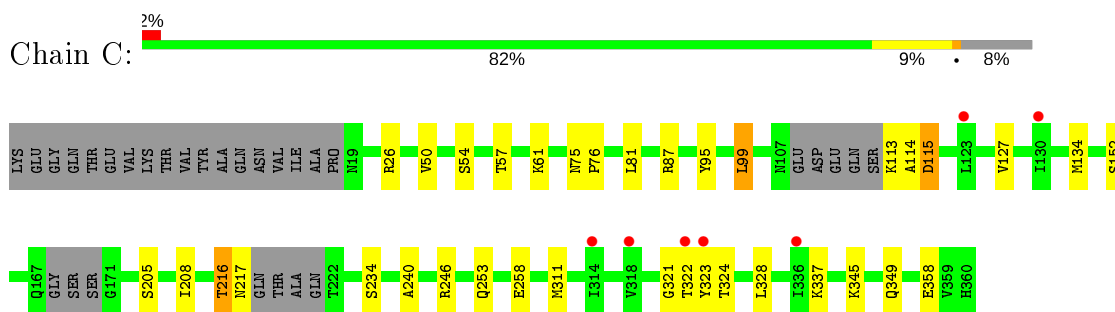
- Molecule 1: NheA



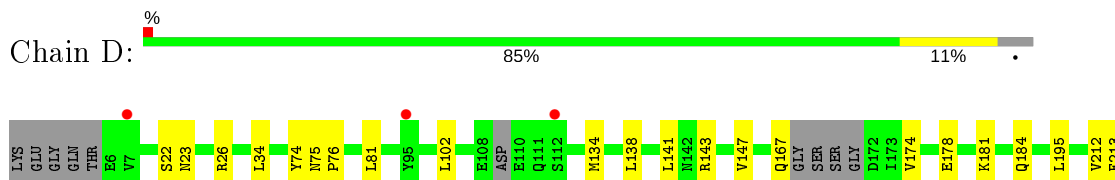
- Molecule 1: NheA



- Molecule 1: NheA

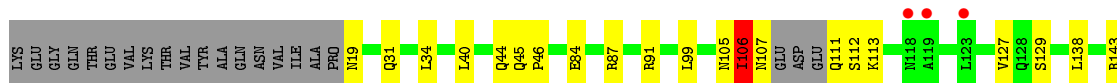
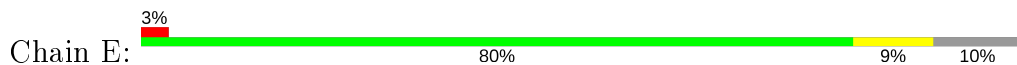


- Molecule 1: NheA

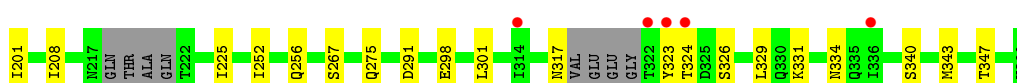
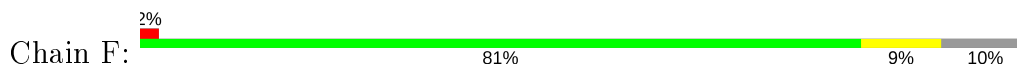




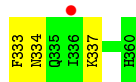
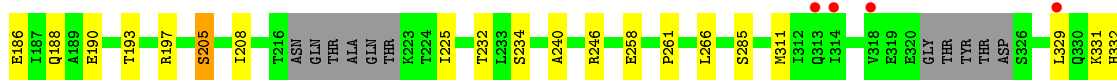
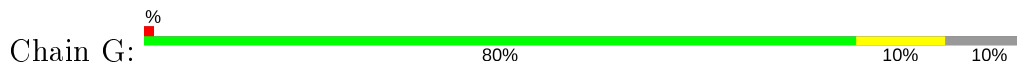
• Molecule 1: NheA



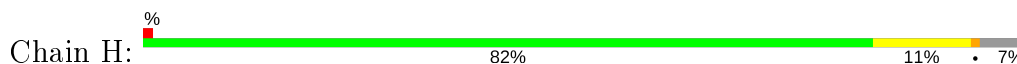
• Molecule 1: NheA



• Molecule 1: NheA



• Molecule 1: NheA





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	309.01Å 58.24Å 173.00Å 90.00° 110.61° 90.00°	Depositor
Resolution (Å)	49.90 – 2.05 49.85 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.90-2.05) 98.5 (49.85-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.05Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.212 , 0.262 0.214 , 0.267	Depositor DCC
$R_{free}$ test set	8966 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.6	Xtrriage
Anisotropy	0.752	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 55.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22614	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8571e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, EDO

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	0.35	0/2717	0.48	0/3669
1	B	0.32	0/2770	0.45	0/3745
1	C	0.34	0/2590	0.48	0/3491
1	D	0.34	0/2768	0.50	0/3739
1	E	0.32	0/2583	0.46	0/3482
1	F	0.35	0/2603	0.47	0/3510
1	G	0.33	0/2576	0.46	0/3476
1	H	0.29	0/2674	0.43	0/3612
All	All	0.33	0/21281	0.47	0/28724

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	2689	0	2684	31	1
1	B	2740	0	2734	22	0
1	C	2570	0	2529	18	0
1	D	2743	0	2721	31	1
1	E	2562	0	2543	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2581	0	2562	22	0
1	G	2552	0	2522	23	0
1	H	2646	0	2637	22	0
2	A	4	0	6	0	0
2	B	4	0	6	1	0
2	D	4	0	6	0	0
2	E	3	0	3	1	0
2	G	4	0	6	0	0
3	B	5	0	0	0	0
4	A	217	0	0	4	0
4	B	184	0	0	2	1
4	C	226	0	0	3	1
4	D	213	0	0	1	0
4	E	166	0	0	2	0
4	F	205	0	0	4	0
4	G	155	0	0	2	0
4	H	141	0	0	2	0
All	All	22614	0	20959	180	2

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 4.

All (180) 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:A:171:GLY:HA2	1:D:212:VAL:CG2	1.81	1.08
1:C:323:TYR:CD1	1:C:323:TYR:CD2	2.44	0.99
1:A:134:MET:HE1	1:A:300:LEU:HG	1.54	0.90
1:A:171:GLY:HA2	1:D:212:VAL:HG21	1.60	0.82
1:A:314:ILE:CD1	1:A:314:ILE:CB	2.60	0.79
1:A:134:MET:CE	1:A:300:LEU:HG	2.13	0.77
1:A:81:LEU:HD21	1:A:134:MET:HG3	1.66	0.76
1:A:171:GLY:CA	1:D:212:VAL:CG2	2.65	0.73
1:G:147:VAL:HG22	1:H:147:VAL:HG22	1.72	0.72
1:C:321:GLY:C	1:C:323:TYR:N	2.44	0.70
1:F:145:LYS:HE2	1:F:291:ASP:HA	1.73	0.69
1:G:147:VAL:HG22	1:H:147:VAL:CG2	2.23	0.69
1:B:215:ILE:HD12	1:B:215:ILE:O	1.94	0.67
1:C:57:THR:HG22	1:C:61:LYS:HE3	1.77	0.66
1:F:95:TYR:OH	1:F:95:TYR:CD1	2.48	0.66
1:F:27:MET:HG3	4:F:523:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:ILE:HD12	1:E:267:SER:HB3	1.81	0.63
1:G:331:LYS:C	1:G:333:PHE:H	2.00	0.63
1:A:153:ASN:ND2	4:A:661:HOH:O	2.19	0.62
1:E:127:VAL:HG21	1:E:311:MET:SD	2.39	0.62
1:A:157:ILE:O	1:A:161:GLU:HG3	2.00	0.60
1:B:205:SER:HB3	1:B:234:SER:HB3	1.83	0.60
1:D:278:PHE:O	1:D:282:GLN:HG3	2.02	0.60
1:A:205:SER:HB3	1:A:234:SER:HB3	1.84	0.59
1:E:105:ASN:C	1:E:107:ASN:H	2.05	0.59
1:H:193:THR:O	1:H:197:ARG:HG2	2.03	0.59
1:A:171:GLY:HA2	1:D:212:VAL:HG23	1.82	0.59
1:G:143:ARG:O	1:G:147:VAL:HG23	2.03	0.58
1:F:166:LEU:O	1:F:167:GLN:C	2.42	0.58
1:B:215:ILE:C	1:B:215:ILE:HD12	2.25	0.58
1:D:231:GLY:HA3	4:D:502:HOH:O	2.03	0.57
1:A:278:PHE:O	1:A:282:GLN:HG3	2.05	0.57
1:B:150:LYS:NZ	4:B:515:HOH:O	2.27	0.56
1:G:205:SER:HB3	1:G:234:SER:HB3	1.86	0.56
1:A:225:ILE:HD12	1:A:267:SER:HB3	1.88	0.55
1:D:181:LYS:HE3	1:D:280:GLU:OE1	2.06	0.55
1:H:48:ILE:HG13	1:H:49:LYS:N	2.22	0.55
1:A:178:GLU:OE1	4:A:640:HOH:O	2.18	0.54
1:B:48:ILE:HD13	1:B:275:GLN:HG2	1.90	0.54
1:H:309:ASN:O	1:H:313:GLN:HG2	2.07	0.54
1:A:134:MET:HE1	1:A:300:LEU:C	2.28	0.54
1:E:173:ILE:HD11	1:E:270:GLU:CB	2.37	0.54
1:E:40:LEU:O	1:E:44:GLN:HG3	2.08	0.54
1:H:173:ILE:HD11	1:H:269:THR:HB	1.89	0.54
1:D:81:LEU:HD21	1:D:134:MET:HG3	1.90	0.54
1:E:19:ASN:CA	4:E:664:HOH:O	2.56	0.54
1:C:127:VAL:HG21	1:C:311:MET:SD	2.47	0.54
1:F:81:LEU:HD21	1:F:134:MET:HG3	1.89	0.53
1:B:54:SER:OG	4:B:627:HOH:O	2.19	0.53
1:A:225:ILE:CD1	1:A:267:SER:HB3	2.38	0.53
1:F:225:ILE:CD1	1:F:267:SER:HB3	2.38	0.53
1:G:331:LYS:C	1:G:333:PHE:N	2.63	0.53
1:B:203:LYS:HG2	1:B:236:GLU:HG2	1.90	0.52
1:F:275:GLN:HG2	4:F:600:HOH:O	2.09	0.52
1:H:75:ASN:N	1:H:76:PRO:CD	2.72	0.52
1:A:216:THR:HG22	1:A:222:THR:CA	2.39	0.52
1:C:152:SER:HB2	4:C:548:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:ASN:C	1:E:107:ASN:N	2.62	0.52
1:A:171:GLY:HA2	1:D:212:VAL:HG22	1.83	0.52
1:E:138:LEU:HD22	1:E:298:GLU:HG3	1.92	0.51
1:F:326:SER:O	1:F:329:LEU:HB3	2.10	0.51
1:G:186:GLU:O	1:G:190:GLU:HG2	2.11	0.51
1:B:84:GLU:HG2	1:B:130:ILE:CG1	2.40	0.51
1:C:216:THR:HG22	1:C:217:ASN:N	2.24	0.51
1:D:222:THR:N	1:D:222:THR:O	2.44	0.51
1:H:131:GLN:O	1:H:135:GLU:HG2	2.10	0.51
1:E:143:ARG:O	1:E:147:VAL:HG23	2.10	0.51
1:C:240:ALA:O	1:C:246:ARG:HD3	2.11	0.50
1:B:278:PHE:O	1:B:282:GLN:HG3	2.11	0.50
1:F:317:ASN:HB2	1:F:323:TYR:CE2	2.46	0.50
1:G:329:LEU:O	1:G:333:PHE:HB2	2.12	0.50
1:A:134:MET:CE	1:A:300:LEU:CG	2.89	0.50
1:D:26:ARG:HD2	1:D:349:GLN:OE1	2.11	0.50
1:E:34:LEU:HD21	1:E:191:LEU:HB3	1.94	0.50
1:G:127:VAL:HG21	1:G:311:MET:SD	2.52	0.50
1:D:143:ARG:O	1:D:147:VAL:HG23	2.10	0.50
1:G:188:GLN:OE1	1:G:285:SER:HB3	2.12	0.50
1:H:172:ASP:N	1:H:172:ASP:OD1	2.44	0.49
1:H:40:LEU:O	1:H:44:GLN:HG3	2.13	0.49
1:D:34:LEU:HD13	1:D:195:LEU:HD12	1.93	0.49
1:G:240:ALA:O	1:G:246:ARG:NH1	2.42	0.49
1:H:300:LEU:HA	4:H:455:HOH:O	2.12	0.49
1:D:358:GLU:HB3	1:D:360:HIS:NE2	2.28	0.48
1:A:134:MET:HE1	1:A:301:LEU:N	2.29	0.48
1:C:258:GLU:HG3	4:C:505:HOH:O	2.12	0.48
1:C:253:GLN:NE2	4:C:546:HOH:O	2.30	0.48
1:C:75:ASN:HB3	1:C:76:PRO:HD3	1.96	0.48
1:C:87:ARG:HB2	1:C:87:ARG:CZ	2.44	0.48
1:E:173:ILE:HD11	1:E:270:GLU:HB3	1.95	0.48
1:H:83:GLN:NE2	4:H:472:HOH:O	2.46	0.48
1:E:272:GLU:HA	1:E:275:GLN:OE1	2.13	0.48
1:H:350:PHE:CD2	1:H:350:PHE:C	2.87	0.48
1:B:153:ASN:O	1:B:157:ILE:HG12	2.14	0.48
1:G:173:ILE:HD13	1:G:266:LEU:HD12	1.95	0.48
1:B:81:LEU:HD21	1:B:134:MET:HG3	1.96	0.47
1:E:31:GLN:OE1	1:E:293:GLN:HG3	2.14	0.47
1:F:138:LEU:HD12	1:F:301:LEU:HD22	1.96	0.47
1:H:342:GLU:OE1	1:H:345:LYS:HE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:TYR:HB3	1:D:141:LEU:CD2	2.46	0.46
1:D:174:VAL:O	1:D:178:GLU:HG3	2.14	0.46
1:H:314:ILE:O	1:H:318:VAL:HG23	2.14	0.46
1:E:173:ILE:HD11	1:E:270:GLU:HB2	1.97	0.46
1:A:134:MET:HE1	1:A:300:LEU:CG	2.37	0.46
1:B:95:TYR:O	1:B:96:TYR:C	2.50	0.46
1:A:171:GLY:CA	1:D:212:VAL:HG23	2.43	0.46
1:B:238:VAL:O	1:B:246:ARG:HG3	2.16	0.46
1:F:83:GLN:HG2	4:F:454:HOH:O	2.16	0.46
1:F:343:MET:O	1:F:347:THR:HG23	2.16	0.45
1:B:281:ASP:OD1	2:B:402:EDO:O1	2.26	0.45
1:A:31:GLN:OE1	1:A:293:GLN:HG3	2.17	0.45
1:F:208:ILE:HD12	1:F:208:ILE:N	2.32	0.45
1:F:96:TYR:OH	1:F:334:ASN:OD1	2.34	0.45
1:D:349:GLN:O	1:D:350:PHE:C	2.54	0.45
1:E:111:GLN:C	1:E:113:LYS:N	2.69	0.45
1:B:34:LEU:HD12	1:B:34:LEU:HA	1.68	0.45
1:E:99:LEU:HB3	1:E:333:PHE:CZ	2.52	0.45
1:E:84:GLU:HG3	1:E:87:ARG:NH2	2.31	0.45
1:A:49:LYS:CD	4:A:695:HOH:O	2.65	0.45
1:C:26:ARG:HD3	1:C:349:GLN:OE1	2.17	0.45
1:F:252:ILE:O	1:F:256:GLN:HG3	2.17	0.45
1:B:13:GLN:OE1	1:B:331:LYS:NZ	2.48	0.44
1:F:326:SER:HB3	4:F:532:HOH:O	2.17	0.44
1:A:134:MET:CE	1:A:301:LEU:N	2.80	0.44
1:D:213:PHE:CE1	1:D:263:ILE:HG21	2.52	0.44
1:H:26:ARG:HH11	1:H:349:GLN:HE22	1.66	0.44
1:D:222:THR:N	1:D:223:LYS:N	2.65	0.44
1:H:135:GLU:HB3	1:H:301:LEU:HD21	2.00	0.44
1:C:324:THR:O	1:C:324:THR:N	2.50	0.44
1:E:225:ILE:CD1	1:E:267:SER:HB3	2.46	0.44
1:F:81:LEU:HA	1:F:81:LEU:HD12	1.85	0.43
1:D:22:SER:OG	1:D:23:ASN:N	2.51	0.43
1:D:75:ASN:HB3	1:D:76:PRO:HD3	2.00	0.43
1:C:113:LYS:C	1:C:115:ASP:N	2.71	0.43
1:A:49:LYS:HD2	4:A:695:HOH:O	2.17	0.43
1:B:8:LYS:HD3	1:B:322:THR:HG21	2.01	0.43
1:C:205:SER:HA	1:C:358:GLU:O	2.19	0.42
1:D:258:GLU:HG3	1:G:261:PRO:HB3	2.01	0.42
1:F:199:GLN:HG2	1:F:201:ILE:O	2.18	0.42
2:E:401:EDO:C1	4:E:539:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:MET:HB3	1:D:301:LEU:HD13	2.00	0.42
1:F:32:SER:N	1:F:33:PRO:CD	2.83	0.42
1:G:92:PHE:CE2	1:G:337:LYS:HA	2.54	0.42
1:D:342:GLU:OE1	1:D:345:LYS:HE3	2.20	0.42
1:G:96:TYR:OH	1:G:334:ASN:OD1	2.37	0.42
1:G:331:LYS:O	1:G:333:PHE:N	2.52	0.42
1:A:75:ASN:N	1:A:76:PRO:CD	2.83	0.42
1:C:81:LEU:HD21	1:C:134:MET:HG3	2.01	0.42
1:D:184:GLN:OE1	1:D:184:GLN:HA	2.18	0.42
1:E:45:GLN:HA	1:E:46:PRO:HD3	1.90	0.42
1:G:123:LEU:HD23	1:G:123:LEU:HA	1.87	0.42
1:D:74:TYR:HB3	1:D:141:LEU:HD23	2.01	0.41
1:F:134:MET:HB3	1:F:301:LEU:HD13	2.02	0.41
1:D:34:LEU:HA	1:D:34:LEU:HD12	1.85	0.41
1:E:106:ILE:O	1:E:106:ILE:HG13	2.20	0.41
1:G:40:LEU:HD23	1:G:208:ILE:HG12	2.02	0.41
1:H:106:ILE:HD12	1:H:113:LYS:HA	2.02	0.41
1:G:193:THR:O	1:G:197:ARG:HG2	2.19	0.41
1:A:96:TYR:OH	1:A:334:ASN:OD1	2.19	0.41
1:D:34:LEU:HD13	1:D:195:LEU:CD1	2.51	0.41
1:G:258:GLU:HG2	4:G:638:HOH:O	2.19	0.41
1:F:182:ARG:HD2	1:G:44:GLN:HG2	2.02	0.41
1:A:134:MET:HB3	1:A:301:LEU:HD13	2.01	0.41
1:F:138:LEU:HD22	1:F:298:GLU:HG3	2.01	0.41
1:G:50:VAL:HG23	1:G:53:MET:O	2.20	0.41
1:D:252:ILE:O	1:D:256:GLN:HG3	2.21	0.41
1:H:32:SER:HB2	1:H:33:PRO:HD3	2.03	0.41
1:B:225:ILE:HD12	1:B:267:SER:HB3	2.03	0.41
1:C:95:TYR:O	1:C:99:LEU:HD12	2.21	0.41
1:B:236:GLU:O	1:B:240:ALA:HB2	2.21	0.41
1:C:205:SER:OG	1:C:234:SER:HB3	2.21	0.41
1:D:138:LEU:HD11	1:D:297:LEU:HG	2.03	0.41
1:A:40:LEU:HD11	1:A:44:GLN:OE1	2.20	0.40
1:B:42:ILE:HD11	1:B:283:VAL:HA	2.02	0.40
1:H:42:ILE:O	1:H:64:LYS:HE2	2.21	0.40
1:B:14:ASN:HA	1:B:335:GLN:HE22	1.86	0.40
1:H:278:PHE:O	1:H:282:GLN:HG3	2.22	0.40
1:A:138:LEU:HD22	1:A:298:GLU:HG2	2.04	0.40
1:H:40:LEU:HD12	1:H:40:LEU:HA	1.94	0.40
1:B:215:ILE:C	1:B:215:ILE:CD1	2.89	0.40
1:G:258:GLU:CG	4:G:638:HOH:O	2.69	0.40

All (2) 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)
1:A:210:LYS:NZ	1:D:178:GLU:OE2[1_545]	2.12	0.08
4:B:573:HOH:O	4:C:580:HOH:O[3_545]	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	333/360 (92%)	328 (98%)	5 (2%)	0	100	100
1	B	340/360 (94%)	333 (98%)	6 (2%)	1 (0%)	41	31
1	C	317/360 (88%)	306 (96%)	8 (2%)	3 (1%)	17	8
1	D	337/360 (94%)	332 (98%)	5 (2%)	0	100	100
1	E	315/360 (88%)	305 (97%)	8 (2%)	2 (1%)	25	15
1	F	315/360 (88%)	313 (99%)	2 (1%)	0	100	100
1	G	315/360 (88%)	309 (98%)	5 (2%)	1 (0%)	41	31
1	H	330/360 (92%)	322 (98%)	6 (2%)	2 (1%)	25	15
All	All	2602/2880 (90%)	2548 (98%)	45 (2%)	9 (0%)	41	31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	108	GLU
1	C	114	ALA
1	C	115	ASP
1	C	322	THR
1	E	112	SER
1	H	109	ASP
1	H	173	ILE
1	E	106	ILE

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Mol	Chain	Res	Type
1	G	332	HIS

### 5.3.2 Protein sidechains [i](#)

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	302/329 (92%)	298 (99%)	4 (1%)	69 67
1	B	306/329 (93%)	302 (99%)	4 (1%)	69 67
1	C	281/329 (85%)	273 (97%)	8 (3%)	43 37
1	D	304/329 (92%)	300 (99%)	4 (1%)	69 67
1	E	283/329 (86%)	276 (98%)	7 (2%)	47 40
1	F	288/329 (88%)	284 (99%)	4 (1%)	67 65
1	G	283/329 (86%)	276 (98%)	7 (2%)	47 40
1	H	296/329 (90%)	289 (98%)	7 (2%)	49 42
All	All	2343/2632 (89%)	2298 (98%)	45 (2%)	57 53

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ASP
1	A	125	LEU
1	A	134	MET
1	A	322	THR
1	B	97	SER
1	B	102	LEU
1	B	203	LYS
1	B	284	SER
1	C	50	VAL
1	C	54	SER
1	C	99	LEU
1	C	208	ILE
1	C	216	THR
1	C	328	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	337	LYS
1	C	345	LYS
1	D	102	LEU
1	D	167	GLN
1	D	235	ASN
1	D	358	GLU
1	E	91	ARG
1	E	106	ILE
1	E	129	SER
1	E	173	ILE
1	E	235	ASN
1	E	243	SER
1	E	328	LEU
1	F	167	GLN
1	F	324	THR
1	F	331	LYS
1	F	340	SER
1	G	20	THR
1	G	26	ARG
1	G	106	ILE
1	G	164	LYS
1	G	205	SER
1	G	225	ILE
1	G	232	THR
1	H	136	GLN
1	H	139	LEU
1	H	235	ASN
1	H	284	SER
1	H	292	ARG
1	H	324	THR
1	H	350	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	111	GLN
1	C	235	ASN
1	C	239	ASN
1	E	58	ASN
1	H	211	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	$\# Z  > 2$
2	EDO	B	402	-	3,3,3	0.49	0	2,2,2	0.24	0
2	EDO	G	401	-	3,3,3	0.42	0	2,2,2	0.41	0
3	SO4	B	401	-	4,4,4	0.33	0	6,6,6	0.13	0
2	EDO	D	401	-	3,3,3	0.48	0	2,2,2	0.26	0
2	EDO	A	401	-	3,3,3	0.35	0	2,2,2	0.52	0
2	EDO	E	401	-	2,2,3	0.51	0	1,1,2	0.29	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
2	EDO	B	402	-	-	0/1/1/1	-
2	EDO	D	401	-	-	1/1/1/1	-
2	EDO	G	401	-	-	0/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	EDO	1	0
2	E	401	EDO	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	339/360 (94%)	-0.21	3 (0%) 84 86	14, 27, 49, 63	0
1	B	346/360 (96%)	-0.13	6 (1%) 70 73	16, 30, 53, 66	0
1	C	330/360 (91%)	-0.11	7 (2%) 63 67	14, 28, 51, 72	0
1	D	346/360 (96%)	-0.20	4 (1%) 79 81	14, 27, 50, 67	0
1	E	325/360 (90%)	-0.02	9 (2%) 53 58	15, 31, 59, 74	0
1	F	325/360 (90%)	-0.05	6 (1%) 68 71	14, 30, 56, 75	0
1	G	325/360 (90%)	-0.01	5 (1%) 73 76	15, 33, 60, 73	0
1	H	336/360 (93%)	-0.08	5 (1%) 73 76	19, 35, 59, 71	0
All	All	2672/2880 (92%)	-0.10	45 (1%) 70 73	14, 30, 56, 75	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	323	TYR	5.4
1	C	318	VAL	4.7
1	C	323	TYR	3.6
1	F	324	THR	3.6
1	E	314	ILE	3.4
1	B	116	PHE	3.3
1	F	322	THR	3.2
1	E	119	ALA	3.1
1	B	112	SER	2.9
1	E	336	ILE	2.8
1	F	314	ILE	2.8
1	B	118	ASN	2.7
1	G	336	ILE	2.7
1	C	314	ILE	2.6
1	G	318	VAL	2.6
1	E	328	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	333	PHE	2.5
1	F	336	ILE	2.4
1	D	238	VAL	2.4
1	G	313	GLN	2.4
1	G	314	ILE	2.4
1	A	171	GLY	2.4
1	A	235	ASN	2.4
1	C	130	ILE	2.4
1	C	336	ILE	2.3
1	H	106	ILE	2.3
1	H	15	VAL	2.3
1	E	326	SER	2.3
1	E	118	ASN	2.2
1	D	112	SER	2.2
1	H	243	SER	2.2
1	G	329	LEU	2.2
1	D	7	VAL	2.2
1	D	95	TYR	2.2
1	B	12	ALA	2.1
1	B	198	PRO	2.1
1	C	123	LEU	2.1
1	E	123	LEU	2.1
1	H	114	ALA	2.1
1	F	102	LEU	2.0
1	B	114	ALA	2.0
1	C	322	THR	2.0
1	A	125	LEU	2.0
1	H	198	PRO	2.0
1	E	216	THR	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, 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
2	EDO	E	401	3/4	0.82	0.26	37,37,46,53	0
2	EDO	G	401	4/4	0.87	0.17	36,37,54,55	0
2	EDO	B	402	4/4	0.90	0.14	37,44,55,65	0
2	EDO	D	401	4/4	0.91	0.13	42,47,51,64	0
2	EDO	A	401	4/4	0.93	0.17	30,30,52,56	0
3	SO4	B	401	5/5	0.94	0.15	49,51,66,89	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.