



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:12 pm GMT

PDB ID : 4ZRQ  
Title : E88 deletion mutant of CD320 in complex with TC2  
Authors : Alam, A.; Locher, K.P.  
Deposited on : 2015-05-12  
Resolution : 2.60 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

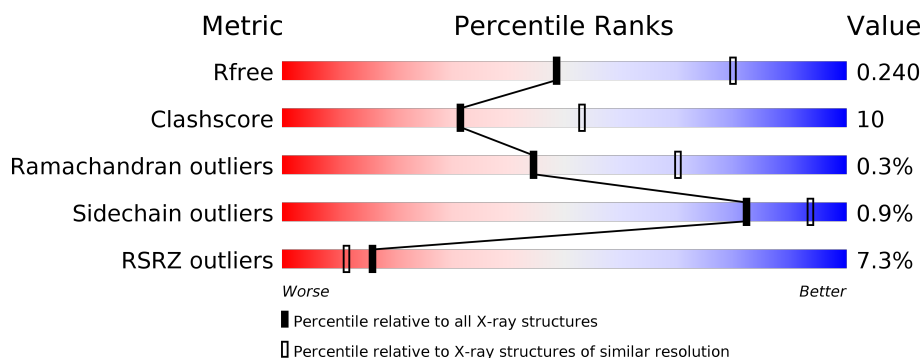
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	409	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>.</div> </div> </div>
1	B	409	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div> </div>
2	C	118	<div> <div>19%</div> <div> <div></div> <div>41%</div> <div>20%</div> <div>..</div> <div>36%</div> </div> </div>
2	D	118	<div> <div>17%</div> <div> <div></div> <div>44%</div> <div>18%</div> <div>.</div> <div>36%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CNC	A	501	X	-	X	-
3	CNC	B	501	X	-	X	-
4	GOL	A	503	-	-	-	X
4	GOL	A	504	-	-	-	X
4	GOL	B	502	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7560 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 Transcobalamin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3119	1989	542	569	19			
1	B	399	Total	C	N	O	S	0	0	0
			3119	1989	543	568	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	GLN	ARG	conflict	UNP P20062
B	209	GLN	ARG	conflict	UNP P20062

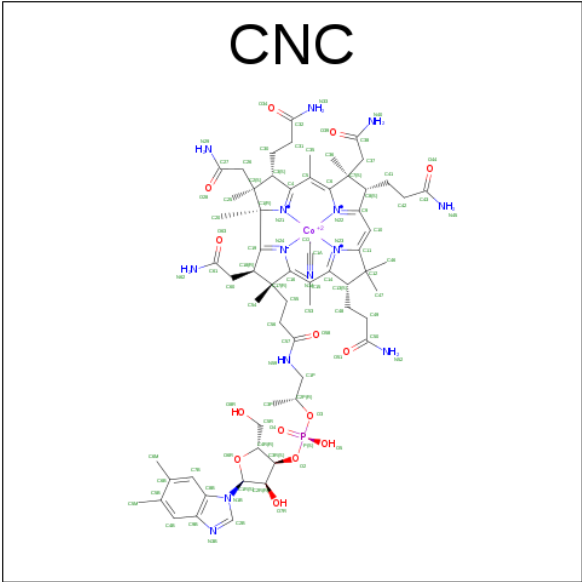
- Molecule 2 is a protein called CD320 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	76	Total	C	N	O	S	0	0	0
			530	316	87	116	11			
2	D	75	Total	C	N	O	S	0	0	0
			534	319	89	115	11			

There are 2 discrepancies between the modelled and reference sequences:

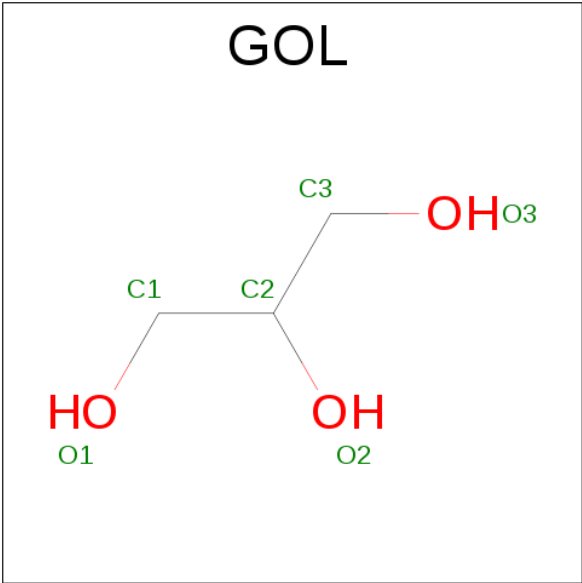
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	deletion	UNP Q9NPF0
D	?	-	GLU	deletion	UNP Q9NPF0

- Molecule 3 is CO-CYANOCOBALAMIN (three-letter code: CNC) (formula: C<sub>63</sub>H<sub>88</sub>CoN<sub>14</sub>O<sub>14</sub>P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	0
			93	63	1	14	14	1		
3	B	1	Total	C	Co	N	O	P	0	0
			93	63	1	14	14	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

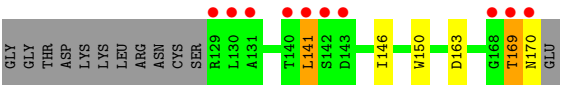
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	2	Total	Ca	0	0
			2	2		
5	C	2	Total	Ca	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	25	Total	O	0	0
			25	25		
6	B	19	Total	O	0	0
			19	19		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.40Å 98.40Å 356.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.43 – 2.60 29.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.43-2.60) 93.7 (29.43-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.199 , 0.231 0.213 , 0.240	Depositor DCC
$R_{free}$ test set	2732 reflections (5.58%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.9	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7560	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: GOL, CA, CNC

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	1/3187 (0.0%)	0.44	0/4320
1	B	0.29	0/3187	0.55	3/4320 (0.1%)
2	C	0.45	0/540	1.08	3/740 (0.4%)
2	D	0.37	0/544	0.87	2/744 (0.3%)
All	All	0.33	1/7458 (0.0%)	0.59	8/10124 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	1
2	D	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	CYS	CB-SG	11.77	2.02	1.82

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329	ILE	CG1-CB-CG2	-12.52	83.85	111.40
2	C	70	LEU	CA-CB-CG	10.03	138.36	115.30
1	B	343	LYS	CD-CE-NZ	-8.12	93.02	111.70
2	C	81	SER	N-CA-C	7.27	130.64	111.00
1	B	382	ASP	CB-CG-OD1	6.93	124.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	141	LEU	CA-CB-CG	5.59	128.16	115.30
2	C	81	SER	N-CA-CB	-5.46	102.30	110.50
2	D	62	ARG	N-CA-C	5.18	124.98	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	166	GLU	Peptide
2	C	80	CYS	Peptide
2	D	169	THR	Peptide
2	D	57	THR	Peptide

## 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	3119	0	3131	31	0
1	B	3119	0	3136	38	0
2	C	530	0	438	30	0
2	D	534	0	456	13	0
3	A	93	0	84	23	0
3	B	93	0	84	24	0
4	A	18	0	24	3	0
4	B	6	0	8	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	25	0	0	4	0
6	B	19	0	0	5	0
All	All	7560	0	7361	152	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 10.

All (152) 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:B:501:CNC:C30	3:B:501:CNC:C31	1.79	1.59
3:A:501:CNC:C30	3:A:501:CNC:C31	1.78	1.53
3:B:501:CNC:C3	3:B:501:CNC:C31	1.84	1.52
1:A:78:CYS:CB	1:A:78:CYS:SG	2.02	1.46
3:A:501:CNC:C19	3:A:501:CNC:C1	1.77	1.43
3:A:501:CNC:C3	3:A:501:CNC:C31	1.91	1.41
3:B:501:CNC:H3	3:B:501:CNC:C31	1.45	1.41
3:B:501:CNC:C1	3:B:501:CNC:C19	1.78	1.35
1:A:65:CYS:SG	1:A:78:CYS:CB	2.18	1.31
3:A:501:CNC:H3	3:A:501:CNC:C31	1.51	1.28
1:A:65:CYS:SG	1:A:78:CYS:HB3	1.74	1.21
3:A:501:CNC:C19	3:A:501:CNC:H262	1.85	1.06
1:B:331:VAL:HB	1:B:343:LYS:HE2	1.45	0.99
3:A:501:CNC:C19	3:A:501:CNC:C26	2.42	0.97
3:B:501:CNC:C19	3:B:501:CNC:H262	1.95	0.96
3:B:501:CNC:C26	3:B:501:CNC:C19	2.48	0.92
1:B:389:GLN:NE2	6:B:603:HOH:O	1.94	0.91
3:A:501:CNC:C1	3:A:501:CNC:C18	2.51	0.88
2:C:82:ASP:OD2	2:C:84:SER:OG	1.92	0.88
3:A:501:CNC:C20	3:A:501:CNC:H18	2.04	0.88
1:A:104:HIS:ND1	2:C:77:ASP:OD2	2.10	0.84
3:B:501:CNC:C18	3:B:501:CNC:C1	2.55	0.84
1:A:64:GLN:HE21	2:C:69:PRO:HG3	1.42	0.83
1:B:331:VAL:HB	1:B:343:LYS:CE	2.08	0.83
3:A:501:CNC:H2B	3:A:501:CNC:C14	2.08	0.82
3:A:501:CNC:C6	3:A:501:CNC:C1A	2.56	0.82
3:B:501:CNC:H2B	3:B:501:CNC:C14	2.10	0.82
3:B:501:CNC:C20	3:B:501:CNC:H18	2.12	0.80
1:B:330:SER:C	1:B:343:LYS:HZ3	1.87	0.77
1:A:305:ILE:HD12	1:A:306:PRO:HD2	1.68	0.75
2:C:81:SER:OG	2:C:82:ASP:N	2.19	0.74
3:B:501:CNC:C32	3:B:501:CNC:H3	2.18	0.74
3:A:501:CNC:H3	3:A:501:CNC:H311	1.68	0.71
1:B:1:GLU:OE2	6:B:601:HOH:O	2.09	0.69
2:C:63:THR:OG1	2:C:81:SER:HB2	1.93	0.69
2:C:70:LEU:HD22	2:C:73:ARG:CB	2.23	0.69
1:B:46:GLN:HG2	1:B:48:GLY:H	1.57	0.68
1:A:46:GLN:HG2	1:A:48:GLY:H	1.58	0.68
1:A:209:GLN:NE2	1:A:240:MET:SD	2.68	0.67
1:A:240:MET:HG2	1:A:243:ALA:HB3	1.77	0.67
1:B:353:GLU:OE1	6:B:604:HOH:O	2.12	0.67
3:A:501:CNC:H18	3:A:501:CNC:H201	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:501:CNC:H4B	3:A:501:CNC:C4	2.25	0.66
1:A:174:SER:HB3	4:A:502:GOL:H2	1.78	0.66
1:B:166:GLU:HB3	1:B:167:PRO:HD3	1.77	0.65
1:A:64:GLN:NE2	2:C:69:PRO:HG3	2.12	0.65
1:B:330:SER:C	1:B:343:LYS:NZ	2.50	0.64
2:D:78:LEU:O	2:D:78:LEU:HD12	1.98	0.64
3:B:501:CNC:H201	3:B:501:CNC:H18	1.81	0.63
2:C:80:CYS:HB2	2:C:85:ASP:HB2	1.81	0.61
1:B:353:GLU:HB2	1:B:365:SER:HB3	1.83	0.61
1:B:292:LEU:HD22	2:C:167:CYS:HB3	1.80	0.61
3:B:501:CNC:C4	3:B:501:CNC:H4B	2.30	0.61
3:B:501:CNC:O63	6:B:605:HOH:O	2.16	0.61
2:C:79:ASP:N	2:C:85:ASP:OD2	2.31	0.61
2:D:59:PHE:N	2:D:68:VAL:O	2.29	0.61
1:B:166:GLU:HB3	1:B:167:PRO:CD	2.31	0.60
1:A:353:GLU:HB2	1:A:365:SER:HB3	1.84	0.60
1:B:329:ILE:HG22	1:B:343:LYS:HZ2	1.66	0.60
1:B:104:HIS:ND1	2:D:77:ASP:OD2	2.35	0.60
1:B:5:ILE:HD11	1:B:232:LEU:HD22	1.85	0.59
3:B:501:CNC:O44	6:B:606:HOH:O	2.17	0.58
2:C:82:ASP:OD1	2:C:83:GLY:N	2.37	0.57
1:A:173:HIS:H	4:A:503:GOL:H2	1.70	0.57
3:A:501:CNC:C2B	3:A:501:CNC:C14	2.83	0.56
1:A:372:GLY:HA3	4:A:504:GOL:H11	1.88	0.56
2:D:60:GLN:HA	2:D:67:CYS:HA	1.88	0.56
2:D:79:ASP:N	2:D:85:ASP:OD2	2.28	0.56
3:B:501:CNC:N23	3:B:501:CNC:C2B	2.69	0.55
2:D:74:CYS:SG	2:D:85:ASP:HA	2.47	0.55
2:C:80:CYS:HB2	2:C:85:ASP:CB	2.38	0.54
2:D:82:ASP:OD1	2:D:83:GLY:N	2.42	0.53
3:A:501:CNC:C19	3:A:501:CNC:H261	2.38	0.53
1:B:219:GLU:N	1:B:219:GLU:OE1	2.41	0.53
2:C:54:CYS:HB3	2:C:55:PRO:HD2	1.90	0.53
2:C:169:THR:HG22	2:C:170:ASN:N	2.23	0.53
3:A:501:CNC:C19	3:A:501:CNC:C2	2.81	0.52
1:B:241:ARG:HG2	1:B:242:GLY:HA2	1.91	0.52
2:C:61:CYS:SG	2:C:81:SER:OG	2.52	0.51
2:C:83:GLY:O	2:C:85:ASP:N	2.43	0.51
3:B:501:CNC:H261	3:B:501:CNC:C19	2.39	0.51
3:A:501:CNC:N1A	6:A:608:HOH:O	2.34	0.51
2:C:69:PRO:HG2	2:C:72:TRP:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ILE:HD12	1:A:306:PRO:CD	2.38	0.50
1:B:67:LEU:HB3	1:B:108:ARG:HH21	1.77	0.50
3:A:501:CNC:C1A	6:A:608:HOH:O	2.60	0.50
1:B:13:VAL:HG12	1:B:45:LEU:HD11	1.93	0.49
2:D:54:CYS:SG	2:D:55:PRO:HD2	2.52	0.49
1:A:6:PRO:HD2	1:A:253:ARG:HD2	1.93	0.49
3:B:501:CNC:H2B	3:B:501:CNC:N23	2.27	0.49
3:A:501:CNC:C20	3:A:501:CNC:C18	2.81	0.49
1:A:104:HIS:CE1	2:C:77:ASP:OD2	2.66	0.48
2:D:169:THR:HG22	2:D:170:ASN:HB2	1.95	0.48
1:B:170:GLN:N	1:B:170:GLN:OE1	2.47	0.47
1:B:394:TYR:OH	1:B:400:GLU:OE2	2.31	0.47
3:A:501:CNC:H18	3:A:501:CNC:C1	2.31	0.47
1:A:173:HIS:ND1	6:A:607:HOH:O	2.35	0.47
1:B:67:LEU:HD22	1:B:108:ARG:HH21	1.81	0.46
2:C:169:THR:CG2	2:C:170:ASN:N	2.78	0.46
2:D:146:ILE:HD12	2:D:150:TRP:CE3	2.50	0.46
1:B:331:VAL:HB	1:B:343:LYS:NZ	2.31	0.46
1:B:25:ASP:OD1	1:B:50:LYS:HE3	2.15	0.45
1:B:241:ARG:CG	1:B:242:GLY:HA2	2.46	0.45
2:C:68:VAL:HG13	2:C:72:TRP:CE3	2.51	0.45
2:D:73:ARG:HA	2:D:74:CYS:HA	1.66	0.45
1:A:256:LEU:HD21	1:A:274:LEU:HD11	1.99	0.45
1:B:134:THR:OG1	1:B:135:SER:N	2.49	0.44
1:B:205:ILE:O	1:B:209:GLN:HG2	2.17	0.44
2:C:167:CYS:HA	2:C:168:GLY:HA2	1.55	0.44
1:A:13:VAL:HG12	1:A:45:LEU:HD11	1.98	0.44
1:B:67:LEU:HD22	1:B:108:ARG:NH2	2.33	0.43
1:B:217:THR:OG1	1:B:219:GLU:HG2	2.19	0.43
3:B:501:CNC:H491	3:B:501:CNC:C46	2.49	0.43
2:C:141:LEU:HB2	2:C:160:ASP:OD2	2.18	0.43
3:B:501:CNC:N23	3:B:501:CNC:N3B	2.66	0.43
1:B:7:GLU:OE1	1:B:8:MET:N	2.52	0.43
2:C:147:PRO:HD2	2:C:150:TRP:CD2	2.53	0.43
1:B:230:LEU:HD12	1:B:230:LEU:HA	1.83	0.42
3:A:501:CNC:H541	3:A:501:CNC:H602	1.63	0.42
2:C:68:VAL:HG12	2:C:69:PRO:O	2.19	0.42
2:C:160:ASP:N	2:C:160:ASP:OD1	2.52	0.42
3:A:501:CNC:O5	6:A:603:HOH:O	2.21	0.42
2:C:59:PHE:HB3	2:C:68:VAL:O	2.19	0.42
2:C:69:PRO:HG2	2:C:72:TRP:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLU:OE1	1:A:214:LYS:NZ	2.51	0.42
1:A:65:CYS:HB3	1:A:81:LYS:HB3	2.02	0.42
1:B:329:ILE:C	1:B:343:LYS:NZ	2.74	0.41
2:D:59:PHE:CG	2:D:60:GLN:N	2.88	0.41
1:B:170:GLN:H	1:B:170:GLN:CD	2.24	0.41
1:A:381:ARG:HD2	1:A:400:GLU:OE2	2.20	0.41
1:A:46:GLN:HG2	1:A:47:ALA:N	2.36	0.41
3:A:501:CNC:H461	3:A:501:CNC:H491	2.02	0.41
1:B:329:ILE:HG23	1:B:329:ILE:HD12	1.35	0.41
3:B:501:CNC:C1	3:B:501:CNC:H18	2.37	0.41
3:B:501:CNC:H361	3:B:501:CNC:H422	2.02	0.41
1:A:104:HIS:CE1	2:C:75:ASP:HB2	2.56	0.41
1:A:120:GLU:OE2	1:A:133:HIS:N	2.53	0.41
1:B:372:GLY:N	1:B:375:GLU:HG3	2.34	0.41
1:B:32:LEU:HD23	1:B:58:LEU:HD23	2.02	0.41
3:B:501:CNC:H252	3:B:501:CNC:N29	2.32	0.41
1:A:134:THR:OG1	1:A:135:SER:N	2.52	0.41
2:C:163:ASP:N	2:C:163:ASP:OD1	2.53	0.41
3:B:501:CNC:H602	3:B:501:CNC:H541	1.62	0.41
1:A:32:LEU:HD12	1:A:32:LEU:HA	1.77	0.41
3:B:501:CNC:N21	3:B:501:CNC:N3B	2.68	0.41
2:C:69:PRO:O	2:C:72:TRP:HB2	2.21	0.41
2:D:163:ASP:N	2:D:163:ASP:OD1	2.53	0.41
1:B:318:VAL:HG22	1:B:404:LEU:HB2	2.03	0.40
1:A:86:GLN:HG2	1:A:358:LEU:HD11	2.04	0.40
1:A:382:ASP:HA	1:A:383:PRO:HA	1.91	0.40
1:B:329:ILE:HG22	1:B:343:LYS:HG3	2.03	0.40
1:A:99:GLU:HB3	1:A:102:ARG:HH12	1.87	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	396/409 (97%)	389 (98%)	7 (2%)	0	100	100
1	B	395/409 (97%)	385 (98%)	9 (2%)	1 (0%)	44	70
2	C	72/118 (61%)	65 (90%)	6 (8%)	1 (1%)	13	26
2	D	71/118 (60%)	63 (89%)	7 (10%)	1 (1%)	13	26
All	All	934/1054 (89%)	902 (97%)	29 (3%)	3 (0%)	44	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	81	SER
2	D	56	PRO
1	B	80	GLY

### 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	336/348 (97%)	335 (100%)	1 (0%)	94	98
1	B	337/348 (97%)	335 (99%)	2 (1%)	89	96
2	C	60/105 (57%)	57 (95%)	3 (5%)	28	53
2	D	62/105 (59%)	61 (98%)	1 (2%)	68	87
All	All	795/906 (88%)	788 (99%)	7 (1%)	82	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	CYS
1	B	241	ARG
1	B	382	ASP
2	C	63	THR
2	C	70	LEU
2	C	80	CYS
2	D	141	LEU



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	209	GLN
2	D	170	ASN

### 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](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	CNC	A	501	-	74,103,103	10.74	30 (40%)	104,171,171	3.40	29 (27%)
4	GOL	A	502	-	5,5,5	0.31	0	5,5,5	0.27	0
4	GOL	A	503	-	5,5,5	0.35	0	5,5,5	0.21	0
4	GOL	A	504	-	5,5,5	0.33	0	5,5,5	0.21	0
3	CNC	B	501	-	74,103,103	11.73	30 (40%)	104,171,171	3.47	31 (29%)
4	GOL	B	502	-	5,5,5	0.35	0	5,5,5	0.27	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	CNC	A	501	-	1/1/36/38	0/51/235/235	0/3/11/11
4	GOL	A	502	-	-	0/4/4/4	0/0/0/0
4	GOL	A	503	-	-	0/4/4/4	0/0/0/0
4	GOL	A	504	-	-	0/4/4/4	0/0/0/0
3	CNC	B	501	-	1/1/36/38	0/51/235/235	0/3/11/11
4	GOL	B	502	-	-	0/4/4/4	0/0/0/0

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	CNC	C30-C3	-93.04	0.11	1.54
3	A	501	CNC	C30-C3	-84.15	0.25	1.54
3	A	501	CNC	C2R-C3R	-10.55	1.29	1.53
3	B	501	CNC	C2R-C3R	-10.52	1.29	1.53
3	B	501	CNC	C1-N21	-6.38	1.39	1.50
3	A	501	CNC	C1-N21	-6.32	1.39	1.50
3	B	501	CNC	O6R-C4R	-5.72	1.32	1.45
3	A	501	CNC	O6R-C4R	-5.45	1.32	1.45
3	B	501	CNC	C48-C49	-4.71	1.37	1.52
3	A	501	CNC	C48-C49	-4.51	1.38	1.52
3	B	501	CNC	C60-C61	-4.26	1.40	1.51
3	A	501	CNC	C60-C61	-4.10	1.40	1.51
3	A	501	CNC	C25-C2	-3.85	1.46	1.54
3	B	501	CNC	C37-C7	-3.57	1.45	1.56
3	B	501	CNC	C8B-N1B	-3.49	1.34	1.38
3	A	501	CNC	C37-C7	-3.31	1.46	1.56
3	B	501	CNC	C48-C13	-3.01	1.49	1.54
3	B	501	CNC	C49-C50	-2.85	1.40	1.51
3	A	501	CNC	C49-C50	-2.82	1.40	1.51
3	A	501	CNC	C48-C13	-2.67	1.50	1.54
3	A	501	CNC	C8B-N1B	-2.52	1.35	1.38
3	B	501	CNC	C25-C2	-2.46	1.49	1.54
3	A	501	CNC	C1P-C2P	-2.30	1.45	1.51
3	B	501	CNC	C1P-C2P	-2.30	1.45	1.51
3	A	501	CNC	C3R-C4R	2.02	1.58	1.52
3	B	501	CNC	C3R-C4R	2.09	1.58	1.52
3	A	501	CNC	C26-C27	2.12	1.58	1.51
3	B	501	CNC	C26-C27	2.34	1.59	1.51
3	B	501	CNC	O7R-C2R	2.66	1.49	1.43
3	A	501	CNC	O7R-C2R	2.71	1.49	1.43
3	A	501	CNC	C41-C42	2.86	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	CNC	C55-C17	2.99	1.62	1.54
3	A	501	CNC	C55-C17	3.12	1.62	1.54
3	B	501	CNC	C41-C42	3.33	1.63	1.52
3	B	501	CNC	C38-N40	3.45	1.44	1.32
3	A	501	CNC	C38-N40	3.57	1.44	1.32
3	B	501	CNC	C4-N21	3.62	1.42	1.32
3	A	501	CNC	C9-C10	3.64	1.60	1.42
3	B	501	CNC	C9-C10	3.78	1.61	1.42
3	B	501	CNC	C31-C32	3.94	1.67	1.51
3	A	501	CNC	C31-C32	4.54	1.69	1.51
3	A	501	CNC	C4-N21	5.03	1.45	1.32
3	A	501	CNC	C20-C1	5.38	1.66	1.52
3	B	501	CNC	C20-C1	5.53	1.66	1.52
3	B	501	CNC	C56-C57	5.97	1.62	1.51
3	A	501	CNC	C56-C57	5.99	1.63	1.51
3	B	501	CNC	C57-N59	6.11	1.47	1.33
3	A	501	CNC	C57-N59	6.13	1.47	1.33
3	B	501	CNC	C43-N45	7.00	1.55	1.32
3	A	501	CNC	C43-N45	7.03	1.55	1.32
3	B	501	CNC	O6R-C1R	7.28	1.51	1.41
3	A	501	CNC	O6R-C1R	7.46	1.51	1.41
3	A	501	CNC	C30-C31	7.86	1.78	1.52
3	B	501	CNC	C30-C31	8.33	1.79	1.52
3	A	501	CNC	C32-N33	9.35	1.63	1.32
3	B	501	CNC	C32-N33	10.47	1.67	1.32
3	B	501	CNC	C11-C10	11.66	1.61	1.41
3	A	501	CNC	C11-C10	11.99	1.62	1.41
3	A	501	CNC	C1-C19	22.99	1.77	1.51
3	B	501	CNC	C1-C19	24.16	1.78	1.51

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	CNC	C25-C2-C26	-14.75	79.83	109.75
3	A	501	CNC	C25-C2-C26	-13.63	82.12	109.75
3	A	501	CNC	C26-C2-C1	-13.25	89.55	110.01
3	B	501	CNC	C26-C2-C1	-12.84	90.18	110.01
3	A	501	CNC	C9-C10-C11	-9.06	105.50	131.90
3	B	501	CNC	C13-C14-C15	-8.64	101.88	131.85
3	A	501	CNC	C13-C14-C15	-8.61	101.99	131.85
3	A	501	CNC	C3-C4-C5	-8.46	102.50	131.85
3	B	501	CNC	C3-C4-C5	-8.03	103.98	131.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	CNC	C30-C3-C2	-7.39	105.00	119.07
3	A	501	CNC	C54-C17-C55	-7.22	97.42	109.23
3	B	501	CNC	C54-C17-C55	-7.20	97.44	109.23
3	B	501	CNC	C6-C5-C4	-6.16	113.74	124.00
3	B	501	CNC	C47-C12-C46	-6.14	96.11	109.66
3	B	501	CNC	C9-C10-C11	-5.86	114.83	131.90
3	A	501	CNC	C26-C2-C3	-5.77	96.55	107.51
3	A	501	CNC	C6-C5-C4	-5.66	114.58	124.00
3	B	501	CNC	C36-C7-C37	-5.49	101.42	110.80
3	A	501	CNC	C36-C7-C37	-5.31	101.73	110.80
3	A	501	CNC	C47-C12-C46	-5.07	98.47	109.66
3	B	501	CNC	C4R-O6R-C1R	-5.05	104.39	109.77
3	A	501	CNC	C5M-C5B-C4B	-5.05	107.68	120.34
3	A	501	CNC	C5-C6-N22	-4.92	115.68	124.92
3	B	501	CNC	C5M-C5B-C4B	-4.85	108.18	120.34
3	B	501	CNC	C16-C15-C14	-4.43	116.62	124.00
3	A	501	CNC	C16-C15-C14	-4.16	117.07	124.00
3	B	501	CNC	C13-C12-C11	-3.83	95.69	100.87
3	A	501	CNC	C1-C19-N24	-3.34	106.47	114.53
3	B	501	CNC	C55-C17-C18	-3.22	104.65	111.06
3	B	501	CNC	C26-C2-C3	-3.11	101.61	107.51
3	B	501	CNC	C35-C5-C6	-3.10	113.81	117.85
3	B	501	CNC	C1-C19-N24	-2.91	107.52	114.53
3	A	501	CNC	C4R-O6R-C1R	-2.85	106.73	109.77
3	A	501	CNC	C35-C5-C6	-2.79	114.21	117.85
3	A	501	CNC	C55-C17-C18	-2.73	105.62	111.06
3	B	501	CNC	O28-C27-N29	-2.37	115.95	122.47
3	A	501	CNC	C5R-C4R-C3R	-2.25	107.53	114.89
3	A	501	CNC	C56-C57-N59	2.07	120.06	116.49
3	A	501	CNC	C26-C27-N29	2.09	123.37	116.55
3	B	501	CNC	C46-C12-C13	2.38	122.41	112.75
3	B	501	CNC	C26-C27-N29	2.40	124.40	116.55
3	B	501	CNC	C56-C57-N59	2.43	120.68	116.49
3	B	501	CNC	C60-C18-C19	2.47	117.42	112.61
3	A	501	CNC	C2-C26-C27	2.74	123.02	115.29
3	A	501	CNC	C53-C15-C16	2.77	121.47	117.85
3	A	501	CNC	C8-C7-C6	2.86	105.87	101.04
3	A	501	CNC	C60-C18-C19	2.92	118.30	112.61
3	B	501	CNC	C20-C1-C19	3.19	113.37	109.42
3	B	501	CNC	C30-C31-C32	3.22	123.26	112.65
3	B	501	CNC	C2-C26-C27	3.31	124.61	115.29
3	A	501	CNC	C20-C1-C19	3.64	113.93	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	CNC	C53-C15-C16	4.08	123.18	117.85
3	A	501	CNC	C1-C2-C3	4.15	106.92	101.60
3	B	501	CNC	C5M-C5B-C6B	4.92	131.04	120.72
3	A	501	CNC	C5M-C5B-C6B	5.34	131.93	120.72
3	B	501	CNC	C1-C2-C3	5.59	108.77	101.60
3	B	501	CNC	C25-C2-C3	6.98	126.32	115.56
3	A	501	CNC	C25-C2-C3	8.23	128.25	115.56
3	A	501	CNC	C35-C5-C4	10.14	131.09	117.85
3	B	501	CNC	C35-C5-C4	10.44	131.48	117.85

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	501	CNC	C3
3	A	501	CNC	C3

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	CNC	23	0
4	A	502	GOL	1	0
4	A	503	GOL	1	0
4	A	504	GOL	1	0
3	B	501	CNC	24	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	400/409 (97%)	-0.16	10 (2%) 58 50	41, 63, 96, 113	0
1	B	399/409 (97%)	-0.12	16 (4%) 39 31	41, 67, 102, 119	0
2	C	76/118 (64%)	1.40	23 (30%) 0 0	66, 119, 158, 166	0
2	D	75/118 (63%)	1.08	20 (26%) 1 0	59, 114, 140, 155	0
All	All	950/1054 (90%)	0.08	69 (7%) 16 11	41, 69, 128, 166	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	171	GLU	7.2
2	C	131	ALA	5.9
2	C	130	LEU	5.6
2	D	129	ARG	5.4
2	D	130	LEU	5.4
2	D	142	SER	5.0
2	D	143	ASP	5.0
2	C	170	ASN	4.8
2	D	57	THR	4.8
2	D	168	GLY	4.8
2	C	129	ARG	4.7
2	C	54	CYS	4.6
1	A	78	CYS	4.5
1	B	170	GLN	4.4
1	A	304	THR	4.4
2	C	82	ASP	4.3
1	A	305	ILE	4.2
1	B	79	GLN	4.2
2	D	170	ASN	4.2
1	B	168	PHE	4.2
2	C	70	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	C	81	SER	3.9
2	D	141	LEU	3.9
2	D	140	THR	3.9
2	C	56	PRO	3.8
2	C	76	ARG	3.8
2	D	56	PRO	3.8
1	B	305	ILE	3.7
1	B	242	GLY	3.7
1	A	303	GLU	3.4
1	B	241	ARG	3.3
2	D	73	ARG	3.3
2	D	59	PHE	3.2
1	A	68	GLY	3.1
2	C	84	SER	3.1
1	B	167	PRO	3.0
1	B	80	GLY	2.9
1	B	78	CYS	2.9
2	C	61	CYS	2.8
2	C	74	CYS	2.8
1	A	80	GLY	2.7
2	D	71	THR	2.7
1	B	244	GLU	2.7
2	C	141	LEU	2.6
1	B	163	TYR	2.6
1	A	241	ARG	2.6
1	A	306	PRO	2.5
2	D	54	CYS	2.5
2	C	169	THR	2.5
2	D	78	LEU	2.5
2	C	59	PHE	2.4
2	C	55	PRO	2.4
2	D	74	CYS	2.4
2	C	133	LEU	2.3
2	C	57	THR	2.3
1	B	128	HIS	2.3
2	C	68	VAL	2.2
1	B	307	GLN	2.2
2	D	131	ALA	2.2
1	A	79	GLN	2.1
1	A	127	ASP	2.1
2	C	167	CYS	2.1
2	D	80	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	169	THR	2.1
2	C	168	GLY	2.1
2	D	63	THR	2.0
1	B	301	ALA	2.0
1	B	169	HIS	2.0
1	B	304	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	A	503	6/6	0.76	0.48	4.30	109,111,112,112	0
4	GOL	A	504	6/6	0.84	0.31	3.46	94,99,101,101	0
4	GOL	B	502	6/6	0.78	0.39	2.79	105,107,107,110	0
3	CNC	A	501	93/93	0.96	0.26	1.66	32,44,72,82	28
3	CNC	B	501	93/93	0.95	0.24	1.46	37,48,80,91	23
5	CA	C	201	1/1	0.99	0.12	-0.54	64,64,64,64	0
5	CA	D	201	1/1	0.99	0.08	-1.27	53,53,53,53	0
5	CA	C	202	1/1	0.94	0.14	-1.99	116,116,116,116	0
5	CA	D	202	1/1	0.88	0.05	-2.29	110,110,110,110	0
4	GOL	A	502	6/6	0.83	0.23	-	90,91,95,95	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.