



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:48 am BST

PDB ID : 5CCJ  
Title : Crystal structure of the quintuple mutant of the synaptotagmin-1 C2B domain  
Authors : Zhou, Q.; Zhao, M.; Brunger, A.T.  
Deposited on : 2015-07-02  
Resolution : 1.65 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

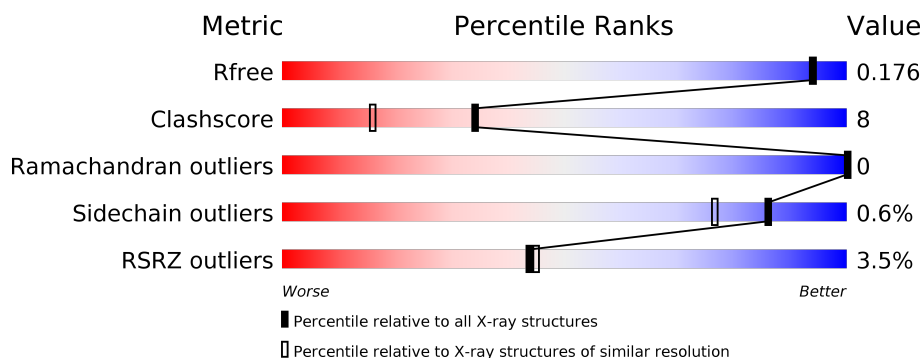
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	152	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 86%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>86%</span> <span>11%</span> <span>•</span> </div> </div>
1	B	152	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 11%, green 88%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>5%</span> <span>88%</span> <span>11%</span> <span>••</span> </div> </div>
1	C	152	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 11%, green 87%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>87%</span> <span>11%</span> <span>•</span> </div> </div>
1	D	152	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 12%, green 88%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>5%</span> <span>88%</span> <span>12%</span> <span>•</span> </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
2	GOL	A	506	-	X	X	-
2	GOL	B	503	-	-	-	X
2	GOL	C	501	-	-	X	-
2	GOL	D	503	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6054 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 Synaptotagmin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	12	0
			1249	807	208	228	6			
1	B	151	Total	C	N	O	S	0	16	0
			1297	841	214	235	7			
1	C	148	Total	C	N	O	S	0	7	0
			1195	771	195	223	6			
1	D	152	Total	C	N	O	S	0	12	0
			1273	823	211	233	6			

There are 24 discrepancies between the modelled and reference sequences:

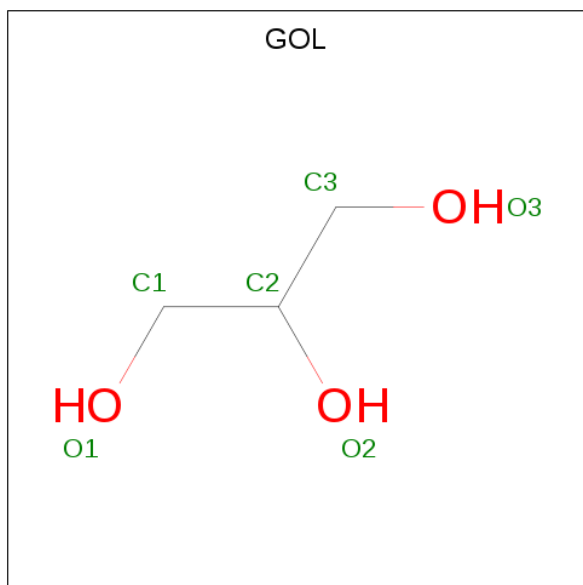
Chain	Residue	Modelled	Actual	Comment	Reference
A	270	SER	-	expression tag	UNP P21707
A	281	ALA	ARG	engineered mutation	UNP P21707
A	295	ALA	GLU	engineered mutation	UNP P21707
A	338	TRP	TYR	engineered mutation	UNP P21707
A	398	ALA	ARG	engineered mutation	UNP P21707
A	399	ALA	ARG	engineered mutation	UNP P21707
B	270	SER	-	expression tag	UNP P21707
B	281	ALA	ARG	engineered mutation	UNP P21707
B	295	ALA	GLU	engineered mutation	UNP P21707
B	338	TRP	TYR	engineered mutation	UNP P21707
B	398	ALA	ARG	engineered mutation	UNP P21707
B	399	ALA	ARG	engineered mutation	UNP P21707
C	270	SER	-	expression tag	UNP P21707
C	281	ALA	ARG	engineered mutation	UNP P21707
C	295	ALA	GLU	engineered mutation	UNP P21707
C	338	TRP	TYR	engineered mutation	UNP P21707
C	398	ALA	ARG	engineered mutation	UNP P21707
C	399	ALA	ARG	engineered mutation	UNP P21707
D	270	SER	-	expression tag	UNP P21707
D	281	ALA	ARG	engineered mutation	UNP P21707
D	295	ALA	GLU	engineered mutation	UNP P21707

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Chain	Residue	Modelled	Actual	Comment	Reference
D	338	TRP	TYR	engineered mutation	UNP P21707
D	398	ALA	ARG	engineered mutation	UNP P21707
D	399	ALA	ARG	engineered mutation	UNP P21707

- Molecule 2 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
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- 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	B	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		

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

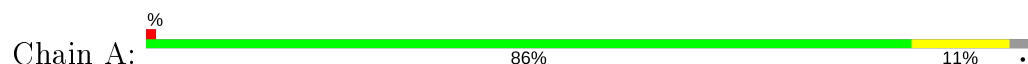
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	203	Total	O	0	0
			203	203		
4	B	196	Total	O	0	0
			196	196		
4	C	165	Total	O	0	0
			165	165		
4	D	204	Total	O	0	0
			204	204		

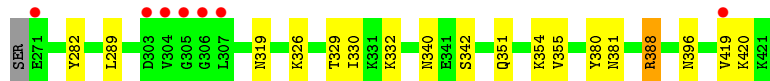
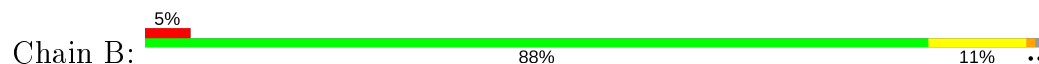
### 3 Residue-property plots [i](#)

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.

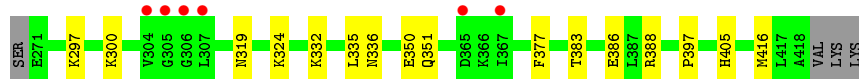
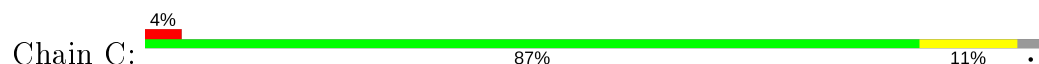
#### • Molecule 1: Synaptotagmin-1



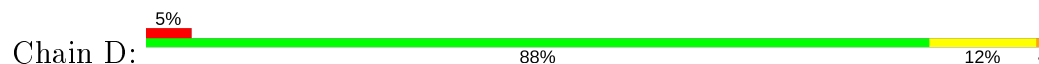
#### • Molecule 1: Synaptotagmin-1



#### • Molecule 1: Synaptotagmin-1



#### • Molecule 1: Synaptotagmin-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.92Å 107.59Å 110.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.65 77.19 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-1.65) 99.0 (77.19-1.65)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.150 , 0.178 0.150 , 0.176	Depositor DCC
$R_{free}$ test set	4930 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 55.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6054	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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, SO4

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	0.86	0/1280	0.83	0/1729
1	B	0.92	0/1339	0.90	1/1808 (0.1%)
1	C	0.82	0/1222	0.79	0/1657
1	D	0.90	2/1304 (0.2%)	0.86	0/1764
All	All	0.88	2/5145 (0.0%)	0.85	1/6958 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	338	TRP	CB-CG	5.09	1.59	1.50
1	D	282	TYR	CZ-OH	5.03	1.46	1.37

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	388	ARG	NE-CZ-NH2	-6.33	117.14	120.30

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	1249	0	1284	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1297	0	1355	17	1
1	C	1195	0	1194	23	0
1	D	1273	0	1298	21	0
2	A	36	0	48	10	0
2	B	42	0	56	11	0
2	C	36	0	48	13	0
2	D	48	0	64	8	0
3	A	25	0	0	1	0
3	B	40	0	0	0	0
3	C	15	0	0	0	0
3	D	30	0	0	1	0
4	A	203	0	0	10	4
4	B	196	0	0	9	0
4	C	165	0	0	8	3
4	D	204	0	0	8	2
All	All	6054	0	5347	90	5

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 8.

All (90) 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:C:377:PHE:H	2:C:501:GOL:H32	1.16	1.08
1:C:332:LYS:H	2:C:503:GOL:H31	1.28	0.99
1:D:419[A]:VAL:O	4:D:601:HOH:O	1.80	0.97
4:B:632:HOH:O	1:D:419[B]:VAL:HG23	1.77	0.84
1:B:351[B]:GLN:NE2	4:B:602:HOH:O	2.09	0.84
1:C:386:GLU:HG2	2:C:501:GOL:H31	1.62	0.82
1:B:381[B]:ASN:OD1	4:B:601:HOH:O	2.03	0.76
3:D:509:SO4:O4	4:D:602:HOH:O	2.05	0.75
1:A:400[A]:PRO:HD2	2:A:506:GOL:H12	1.70	0.74
1:B:380:TYR:OH	1:B:420[B]:LYS:HE2	1.89	0.72
1:C:377:PHE:N	2:C:501:GOL:H32	2.01	0.71
1:A:303[B]:ASP:OD2	4:A:601:HOH:O	2.08	0.71
1:D:381[B]:ASN:OD1	4:D:603:HOH:O	2.09	0.71
1:C:319:ASN:OD1	4:C:601:HOH:O	2.10	0.70
1:D:348[A]:PRO:HB2	1:D:350[A]:GLU:HG2	1.75	0.69
1:D:412:GLU:HA	2:D:503:GOL:H32	1.77	0.67
1:D:358:VAL:HG11	1:D:375[A]:LYS:HE3	1.77	0.66
1:C:336:ASN:HD22	2:C:502:GOL:H11	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:LEU:H	2:C:502:GOL:H12	1.63	0.64
1:B:319:ASN:OD1	4:B:603:HOH:O	2.15	0.64
1:C:350[B]:GLU:HG2	1:C:351:GLN:HG2	1.82	0.62
1:C:324:LYS:HA	2:C:505:GOL:H2	1.80	0.61
2:A:506:GOL:H2	1:B:388:ARG:HD2	1.81	0.61
1:C:416:MET:HE1	4:C:603:HOH:O	2.00	0.61
1:D:358:VAL:CG1	1:D:375[A]:LYS:HE3	2.31	0.61
1:A:288:LYS:HG3	4:A:693:HOH:O	2.00	0.61
1:A:400[A]:PRO:HD2	2:A:506:GOL:H31	1.84	0.60
1:D:412:GLU:CA	2:D:503:GOL:H32	2.32	0.60
1:D:349:PHE:HB2	4:D:618:HOH:O	2.02	0.59
1:C:297[A]:LYS:HD3	1:D:349:PHE:CD2	2.38	0.59
1:C:335:LEU:H	2:C:502:GOL:C1	2.16	0.58
2:C:503:GOL:O3	4:C:602:HOH:O	2.17	0.58
1:A:297[B]:LYS:HE2	4:A:697:HOH:O	2.02	0.58
1:B:396:ASN:OD1	2:C:504:GOL:H2	2.04	0.58
2:D:504:GOL:H31	4:D:669:HOH:O	2.03	0.58
1:A:288:LYS:HE3	4:A:664:HOH:O	2.04	0.58
1:B:342:SER:HB2	2:B:503:GOL:H12	1.84	0.58
2:B:501:GOL:H31	4:B:646:HOH:O	2.04	0.57
2:B:507:GOL:H2	1:C:397:PRO:HG2	1.85	0.57
2:B:501:GOL:O1	2:B:501:GOL:O3	2.18	0.56
1:A:336:ASN:HB2	2:A:503:GOL:H2	1.86	0.56
2:A:506:GOL:H32	4:C:650:HOH:O	2.06	0.56
1:C:332:LYS:N	2:C:503:GOL:H31	2.10	0.56
1:C:383:THR:OG1	4:C:603:HOH:O	2.18	0.56
1:A:303[A]:ASP:OD2	4:A:602:HOH:O	2.18	0.55
1:B:340[A]:ASN:OD1	2:B:503:GOL:H11	2.07	0.55
1:B:330:ILE:HG13	2:B:502:GOL:H31	1.88	0.54
1:D:348[A]:PRO:HG2	1:D:351[A]:GLN:HG2	1.88	0.54
1:A:330:ILE:HD11	2:A:502:GOL:H2	1.88	0.54
2:B:505:GOL:H32	4:B:627:HOH:O	2.08	0.54
1:D:351[B]:GLN:O	1:D:355[B]:VAL:HG13	2.08	0.52
1:B:319:ASN:ND2	1:B:420[B]:LYS:HE3	2.24	0.52
2:B:504:GOL:H11	4:B:737:HOH:O	2.10	0.52
1:A:376[B]:VAL:HG23	1:A:407:LEU:HD23	1.93	0.51
1:B:326:LYS:HD3	2:B:501:GOL:H11	1.92	0.51
1:C:377:PHE:H	2:C:501:GOL:C3	2.06	0.51
1:A:271:GLU:N	4:A:614:HOH:O	2.44	0.50
1:C:350[B]:GLU:CG	1:C:351:GLN:HE21	2.24	0.49
1:B:351[B]:GLN:O	1:B:355[B]:VAL:HG13	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:ILE:HG13	2:D:501:GOL:H31	1.93	0.49
1:C:297[A]:LYS:HD3	1:D:349:PHE:CG	2.47	0.49
2:A:505:GOL:H31	4:A:723:HOH:O	2.13	0.49
1:A:327[A]:LYS:NZ	2:A:502:GOL:O2	2.21	0.49
2:D:503:GOL:H11	4:D:767:HOH:O	2.11	0.49
1:C:300:LYS:HE2	4:C:617:HOH:O	2.12	0.48
2:D:507:GOL:H11	4:D:783:HOH:O	2.13	0.48
1:A:303[A]:ASP:OD1	4:A:603:HOH:O	2.20	0.48
1:C:388:ARG:NH1	4:C:607:HOH:O	2.43	0.47
1:B:332:LYS:NZ	4:B:609:HOH:O	2.35	0.47
1:A:366:LYS:HB3	4:A:735:HOH:O	2.15	0.46
1:A:399:ALA:HB1	2:A:506:GOL:H11	1.96	0.46
1:D:350[A]:GLU:H	1:D:350[A]:GLU:CD	2.19	0.46
1:C:377:PHE:O	2:C:501:GOL:H11	2.17	0.45
1:D:419[A]:VAL:O	1:D:420:LYS:HB2	2.16	0.45
1:B:351[A]:GLN:O	1:B:355[A]:VAL:HG23	2.17	0.44
1:A:317[A]:MET:SD	1:A:322:ARG:HG2	2.57	0.44
1:C:386:GLU:OE2	1:C:405:HIS:ND1	2.50	0.43
1:A:386:GLU:OE2	1:A:405:HIS:ND1	2.47	0.43
1:D:340:ASN:ND2	2:D:504:GOL:H12	2.34	0.43
3:A:511:SO4:O3	4:A:604:HOH:O	2.21	0.42
1:B:282:TYR:HB2	1:B:289[B]:LEU:HD23	2.00	0.42
1:B:329:THR:HB	2:B:505:GOL:H2	2.02	0.42
1:B:354:LYS:NZ	1:B:420[B]:LYS:NZ	2.67	0.42
2:B:503:GOL:H2	4:B:734:HOH:O	2.19	0.42
1:D:412:GLU:HG2	2:D:503:GOL:H12	2.02	0.41
1:C:350[B]:GLU:HB3	4:C:604:HOH:O	2.21	0.41
1:D:280:LEU:HD11	1:D:378:VAL:HG21	2.03	0.41
1:A:327[A]:LYS:HD2	2:A:502:GOL:H32	2.02	0.40
1:D:419[A]:VAL:C	4:D:601:HOH:O	2.47	0.40
1:D:318:GLN:HB2	1:D:323:LEU:HD11	2.03	0.40

All (5) 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)
4:A:800:HOH:O	4:C:728:HOH:O[2_554]	1.94	0.26
4:A:756:HOH:O	4:D:677:HOH:O[2_554]	2.03	0.17
4:A:800:HOH:O	4:D:617:HOH:O[2_554]	2.12	0.08
4:A:616:HOH:O	4:C:762:HOH:O[2_554]	2.12	0.08
1:B:420[A]:LYS:NZ	4:C:729:HOH:O[2_554]	2.13	0.07

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	158/152 (104%)	154 (98%)	4 (2%)	0	100	100
1	B	166/152 (109%)	162 (98%)	4 (2%)	0	100	100
1	C	153/152 (101%)	149 (97%)	4 (3%)	0	100	100
1	D	162/152 (107%)	160 (99%)	2 (1%)	0	100	100
All	All	639/608 (105%)	625 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	138/131 (105%)	137 (99%)	1 (1%)	84	73
1	B	146/131 (112%)	144 (99%)	2 (1%)	67	46
1	C	128/131 (98%)	128 (100%)	0	100	100
1	D	139/131 (106%)	137 (99%)	2 (1%)	67	46
All	All	551/524 (105%)	546 (99%)	5 (1%)	86	66

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	301	LYS
1	B	419[A]	VAL

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Mol	Chain	Res	Type
1	B	419[B]	VAL
1	D	350[A]	GLU
1	D	350[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

49 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	GOL	B	501	-	5,5,5	0.28	0	5,5,5	0.38	0
2	GOL	A	501	-	5,5,5	0.56	0	5,5,5	0.70	0
3	SO4	B	514	-	4,4,4	0.14	0	6,6,6	0.17	0
2	GOL	C	501	-	5,5,5	0.60	0	5,5,5	0.73	0
3	SO4	D	510	-	4,4,4	0.19	0	6,6,6	0.45	0
2	GOL	B	507	-	5,5,5	0.42	0	5,5,5	0.70	0
2	GOL	A	503	-	5,5,5	0.68	0	5,5,5	1.32	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	B	509	-	4,4,4	0.09	0	6,6,6	0.44	0
2	GOL	D	505	-	5,5,5	0.46	0	5,5,5	0.63	0
2	GOL	D	502	-	5,5,5	0.46	0	5,5,5	1.02	0
3	SO4	C	507	-	4,4,4	0.24	0	6,6,6	0.37	0
3	SO4	A	508	-	4,4,4	0.15	0	6,6,6	0.58	0
3	SO4	C	508	-	4,4,4	0.18	0	6,6,6	0.40	0
2	GOL	A	505	-	5,5,5	0.39	0	5,5,5	0.31	0
2	GOL	C	502	-	5,5,5	0.47	0	5,5,5	0.29	0
3	SO4	D	511	-	4,4,4	0.09	0	6,6,6	0.29	0
3	SO4	A	510	-	4,4,4	0.15	0	6,6,6	0.20	0
3	SO4	B	515	-	4,4,4	0.09	0	6,6,6	0.24	0
2	GOL	D	507	-	5,5,5	0.38	0	5,5,5	1.97	2 (40%)
2	GOL	D	503	-	5,5,5	0.28	0	5,5,5	0.99	0
2	GOL	D	508	-	5,5,5	0.64	0	5,5,5	1.23	1 (20%)
2	GOL	A	504	-	5,5,5	0.35	0	5,5,5	0.50	0
3	SO4	D	513	-	4,4,4	0.13	0	6,6,6	0.18	0
3	SO4	C	509	-	4,4,4	0.13	0	6,6,6	0.10	0
3	SO4	D	514	-	4,4,4	0.15	0	6,6,6	0.62	0
2	GOL	D	501	-	5,5,5	0.47	0	5,5,5	0.65	0
3	SO4	B	513	-	4,4,4	0.15	0	6,6,6	0.66	0
2	GOL	B	505	-	5,5,5	0.46	0	5,5,5	0.40	0
2	GOL	C	505	-	5,5,5	0.30	0	5,5,5	0.52	0
2	GOL	A	502	-	5,5,5	0.73	0	5,5,5	0.45	0
2	GOL	D	504	-	5,5,5	0.24	0	5,5,5	1.07	0
2	GOL	A	506	-	5,5,5	0.83	0	5,5,5	1.91	2 (40%)
3	SO4	A	509	-	4,4,4	0.25	0	6,6,6	0.36	0
3	SO4	D	512	-	4,4,4	0.17	0	6,6,6	0.59	0
3	SO4	D	509	-	4,4,4	0.49	0	6,6,6	0.63	0
2	GOL	B	502	-	5,5,5	0.33	0	5,5,5	0.82	0
2	GOL	D	506	-	5,5,5	0.48	0	5,5,5	0.43	0
2	GOL	B	506	-	5,5,5	0.33	0	5,5,5	0.34	0
3	SO4	B	510	-	4,4,4	0.25	0	6,6,6	0.88	0
3	SO4	B	511	-	4,4,4	0.15	0	6,6,6	0.88	0
2	GOL	C	506	-	5,5,5	0.41	0	5,5,5	0.42	0
3	SO4	A	507	-	4,4,4	0.23	0	6,6,6	0.20	0
2	GOL	B	503	-	5,5,5	0.35	0	5,5,5	0.88	0
2	GOL	B	504	-	5,5,5	0.53	0	5,5,5	0.78	0
3	SO4	B	512	-	4,4,4	0.37	0	6,6,6	1.10	0
2	GOL	C	503	-	5,5,5	0.31	0	5,5,5	0.37	0
3	SO4	A	511	-	4,4,4	0.17	0	6,6,6	0.25	0
2	GOL	C	504	-	5,5,5	0.52	0	5,5,5	1.71	2 (40%)
3	SO4	B	508	-	4,4,4	0.20	0	6,6,6	0.74	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	GOL	B	501	-	-	2/4/4/4	-
2	GOL	A	501	-	-	1/4/4/4	-
2	GOL	C	501	-	-	3/4/4/4	-
2	GOL	B	507	-	-	2/4/4/4	-
2	GOL	A	503	-	-	4/4/4/4	-
2	GOL	D	505	-	-	4/4/4/4	-
2	GOL	D	502	-	-	4/4/4/4	-
2	GOL	A	505	-	-	4/4/4/4	-
2	GOL	C	502	-	-	4/4/4/4	-
2	GOL	D	507	-	-	2/4/4/4	-
2	GOL	D	503	-	-	2/4/4/4	-
2	GOL	D	508	-	-	2/4/4/4	-
2	GOL	A	504	-	-	4/4/4/4	-
2	GOL	D	501	-	-	1/4/4/4	-
2	GOL	B	505	-	-	0/4/4/4	-
2	GOL	C	505	-	-	0/4/4/4	-
2	GOL	A	502	-	-	2/4/4/4	-
2	GOL	D	504	-	-	4/4/4/4	-
2	GOL	A	506	-	-	4/4/4/4	-
2	GOL	B	502	-	-	1/4/4/4	-
2	GOL	D	506	-	-	2/4/4/4	-
2	GOL	B	506	-	-	3/4/4/4	-
2	GOL	C	506	-	-	0/4/4/4	-
2	GOL	B	503	-	-	3/4/4/4	-
2	GOL	B	504	-	-	2/4/4/4	-
2	GOL	C	503	-	-	0/4/4/4	-
2	GOL	C	504	-	-	2/4/4/4	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	506	GOL	O2-C2-C1	2.97	122.18	109.12
2	C	504	GOL	O2-C2-C1	2.95	122.12	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	507	GOL	C3-C2-C1	-2.78	100.91	111.70
2	D	507	GOL	O2-C2-C3	2.63	120.70	109.12
2	A	506	GOL	O1-C1-C2	2.56	122.49	110.20
2	A	503	GOL	O2-C2-C1	-2.40	98.56	109.12
2	D	508	GOL	C3-C2-C1	2.30	120.63	111.70
2	C	504	GOL	O3-C3-C2	-2.20	99.67	110.20

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	507	GOL	O1-C1-C2-C3
2	A	503	GOL	C1-C2-C3-O3
2	D	505	GOL	O1-C1-C2-C3
2	D	505	GOL	C1-C2-C3-O3
2	D	502	GOL	O1-C1-C2-C3
2	A	505	GOL	O1-C1-C2-C3
2	C	502	GOL	O1-C1-C2-O2
2	C	502	GOL	O1-C1-C2-C3
2	D	507	GOL	O1-C1-C2-O2
2	D	507	GOL	O1-C1-C2-C3
2	D	503	GOL	O1-C1-C2-C3
2	D	508	GOL	O1-C1-C2-C3
2	A	502	GOL	O1-C1-C2-C3
2	D	504	GOL	C1-C2-C3-O3
2	A	506	GOL	O1-C1-C2-C3
2	D	506	GOL	O1-C1-C2-C3
2	B	506	GOL	O1-C1-C2-C3
2	B	504	GOL	O1-C1-C2-C3
2	D	503	GOL	O1-C1-C2-O2
2	A	506	GOL	O1-C1-C2-O2
2	B	504	GOL	O1-C1-C2-O2
2	B	501	GOL	C1-C2-C3-O3
2	C	501	GOL	O1-C1-C2-C3
2	A	503	GOL	O1-C1-C2-C3
2	A	505	GOL	C1-C2-C3-O3
2	C	502	GOL	C1-C2-C3-O3
2	A	504	GOL	O1-C1-C2-C3
2	A	504	GOL	C1-C2-C3-O3
2	D	504	GOL	O1-C1-C2-C3
2	A	506	GOL	C1-C2-C3-O3
2	B	503	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	C	504	GOL	O1-C1-C2-C3
2	A	503	GOL	O2-C2-C3-O3
2	A	502	GOL	O1-C1-C2-O2
2	D	504	GOL	O2-C2-C3-O3
2	A	506	GOL	O2-C2-C3-O3
2	D	506	GOL	O1-C1-C2-O2
2	B	506	GOL	O1-C1-C2-O2
2	B	503	GOL	O1-C1-C2-O2
2	C	504	GOL	O1-C1-C2-O2
2	C	501	GOL	O1-C1-C2-O2
2	B	507	GOL	O1-C1-C2-O2
2	D	505	GOL	O1-C1-C2-O2
2	D	505	GOL	O2-C2-C3-O3
2	D	502	GOL	O1-C1-C2-O2
2	D	502	GOL	O2-C2-C3-O3
2	A	505	GOL	O1-C1-C2-O2
2	B	501	GOL	O2-C2-C3-O3
2	D	504	GOL	O1-C1-C2-O2
2	A	503	GOL	O1-C1-C2-O2
2	C	502	GOL	O2-C2-C3-O3
2	A	504	GOL	O1-C1-C2-O2
2	B	503	GOL	O2-C2-C3-O3
2	D	508	GOL	O2-C2-C3-O3
2	A	504	GOL	O2-C2-C3-O3
2	D	501	GOL	O2-C2-C3-O3
2	B	502	GOL	O1-C1-C2-O2
2	A	501	GOL	O1-C1-C2-C3
2	D	502	GOL	C1-C2-C3-O3
2	B	506	GOL	C1-C2-C3-O3
2	A	505	GOL	O2-C2-C3-O3
2	C	501	GOL	O2-C2-C3-O3

There are no ring outliers.

21 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	GOL	3	0
2	C	501	GOL	5	0
2	B	507	GOL	1	0
2	A	503	GOL	1	0
2	A	505	GOL	1	0
2	C	502	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	507	GOL	1	0
2	D	503	GOL	4	0
2	D	501	GOL	1	0
2	B	505	GOL	2	0
2	C	505	GOL	1	0
2	A	502	GOL	3	0
2	D	504	GOL	2	0
2	A	506	GOL	5	0
3	D	509	SO4	1	0
2	B	502	GOL	1	0
2	B	503	GOL	3	0
2	B	504	GOL	1	0
2	C	503	GOL	3	0
3	A	511	SO4	1	0
2	C	504	GOL	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	148/152 (97%)	-0.16	1 (0%) 87 89	13, 20, 36, 60	1 (0%)
1	B	151/152 (99%)	0.05	7 (4%) 32 31	12, 19, 40, 69	6 (3%)
1	C	148/152 (97%)	-0.01	6 (4%) 37 37	14, 22, 54, 78	1 (0%)
1	D	152/152 (100%)	0.02	7 (4%) 32 31	13, 21, 43, 82	3 (1%)
All	All	599/608 (98%)	-0.03	21 (3%) 44 45	12, 20, 45, 82	11 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	306	GLY	6.4
1	C	307	LEU	6.4
1	D	270	SER	4.5
1	B	306	GLY	4.2
1	B	305	GLY	4.2
1	C	305[A]	GLY	4.1
1	B	304	VAL	4.0
1	B	419[A]	VAL	3.1
1	C	367	ILE	3.0
1	B	307	LEU	2.9
1	D	305	GLY	2.8
1	D	419[A]	VAL	2.8
1	C	304	VAL	2.6
1	D	351[A]	GLN	2.5
1	B	271	GLU	2.4
1	A	322	ARG	2.3
1	B	303	ASP	2.3
1	D	271	GLU	2.3
1	D	307	LEU	2.2
1	C	365[A]	ASP	2.2
1	D	306	GLY	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( $\text{\AA}^2$ )	Q<0.9
2	GOL	D	508	6/6	0.42	0.32	35,45,48,49	6
2	GOL	B	501	6/6	0.47	0.33	69,73,76,77	0
2	GOL	B	507	6/6	0.49	0.35	52,69,73,75	0
2	GOL	B	506	6/6	0.54	0.34	50,57,64,73	6
2	GOL	D	505	6/6	0.55	0.26	34,47,50,52	6
2	GOL	B	503	6/6	0.59	0.41	44,46,51,53	0
2	GOL	D	504	6/6	0.63	0.34	26,33,38,42	6
2	GOL	A	506	6/6	0.65	0.26	28,32,41,47	6
2	GOL	A	505	6/6	0.69	0.20	68,71,73,73	0
2	GOL	D	502	6/6	0.72	0.29	45,55,58,62	0
2	GOL	C	506	6/6	0.74	0.24	70,73,74,76	0
2	GOL	C	505	6/6	0.75	0.26	50,63,68,71	0
2	GOL	C	503	6/6	0.76	0.17	49,56,60,66	0
3	SO4	A	510	5/5	0.79	0.30	96,97,100,101	0
2	GOL	B	502	6/6	0.80	0.11	37,46,49,51	0
2	GOL	D	506	6/6	0.81	0.22	56,63,65,67	0
2	GOL	D	507	6/6	0.83	0.19	21,23,40,40	6
3	SO4	A	511	5/5	0.83	0.17	45,46,53,53	5
2	GOL	A	502	6/6	0.84	0.16	31,38,39,42	0
2	GOL	B	505	6/6	0.85	0.39	28,57,62,67	0
2	GOL	B	504	6/6	0.85	0.27	29,55,62,69	0
3	SO4	B	515	5/5	0.85	0.24	47,55,57,58	5
2	GOL	D	501	6/6	0.85	0.23	38,50,51,58	0
2	GOL	C	502	6/6	0.86	0.18	36,51,54,56	0
2	GOL	D	503	6/6	0.87	0.35	31,47,63,65	0
2	GOL	A	504	6/6	0.87	0.20	29,41,53,56	0
2	GOL	C	504	6/6	0.87	0.18	18,31,37,39	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	B	514	5/5	0.88	0.25	112,112,113,115	0
3	SO4	D	514	5/5	0.90	0.13	54,54,63,68	0
2	GOL	A	503	6/6	0.90	0.16	27,44,44,55	0
2	GOL	C	501	6/6	0.91	0.16	31,35,47,52	0
3	SO4	C	509	5/5	0.91	0.18	105,106,107,107	0
2	GOL	A	501	6/6	0.94	0.12	25,41,46,48	0
3	SO4	C	507	5/5	0.94	0.12	61,65,66,67	0
3	SO4	A	509	5/5	0.94	0.09	43,49,52,59	5
3	SO4	D	509	5/5	0.95	0.18	30,32,46,46	5
3	SO4	B	511	5/5	0.95	0.12	32,35,41,44	5
3	SO4	C	508	5/5	0.95	0.10	78,79,81,85	0
3	SO4	B	513	5/5	0.95	0.11	39,42,48,53	5
3	SO4	D	511	5/5	0.96	0.14	47,50,55,59	0
3	SO4	B	510	5/5	0.96	0.11	27,30,39,40	5
3	SO4	A	508	5/5	0.96	0.10	41,45,51,53	0
3	SO4	A	507	5/5	0.97	0.11	44,46,48,55	0
3	SO4	D	512	5/5	0.97	0.07	39,44,49,57	0
3	SO4	D	513	5/5	0.98	0.09	36,38,48,48	5
3	SO4	D	510	5/5	0.98	0.07	45,48,55,55	0
3	SO4	B	512	5/5	0.98	0.10	27,32,37,37	0
3	SO4	B	508	5/5	0.98	0.08	35,35,39,44	0
3	SO4	B	509	5/5	0.99	0.12	34,39,51,51	0

## 6.5 Other polymers

There are no such residues in this entry.