



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:48 PM UTC

PDB ID : 8QME / pdb_00008qme
Title : Structural characterization of beta-xylooxidase XynB2 from Geobacillus stearothermophilus CECT43
Authors : Gavira, J.A.; Martinez-Rodriguez, S.
Deposited on : 2023-09-22
Resolution : 2.25 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

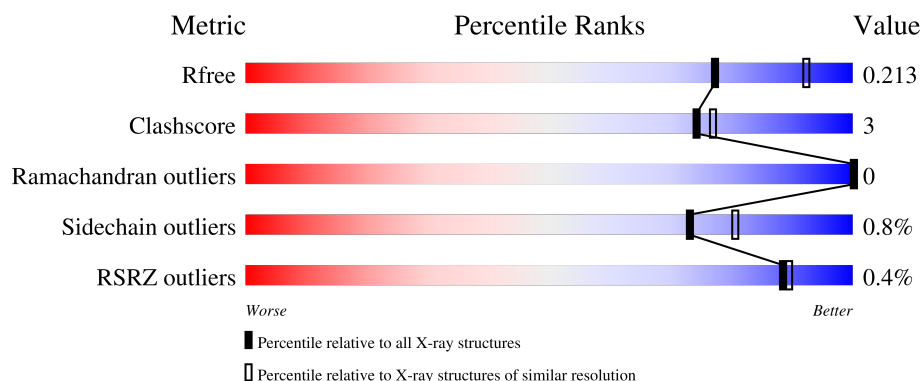
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	711	87% 9% .
1	B	711	88% 8% .
1	C	711	% 87% 8% .
1	D	711	89% 7% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23817 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-xylosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	683	Total	C	N	O	S	0	15	0
			5556	3551	937	1041	27			
1	B	682	Total	C	N	O	S	0	10	0
			5517	3524	933	1032	28			
1	C	681	Total	C	N	O	S	0	16	0
			5562	3553	943	1039	27			
1	D	683	Total	C	N	O	S	0	10	0
			5534	3529	938	1040	27			

There are 36 discrepancies between the modelled and reference sequences:

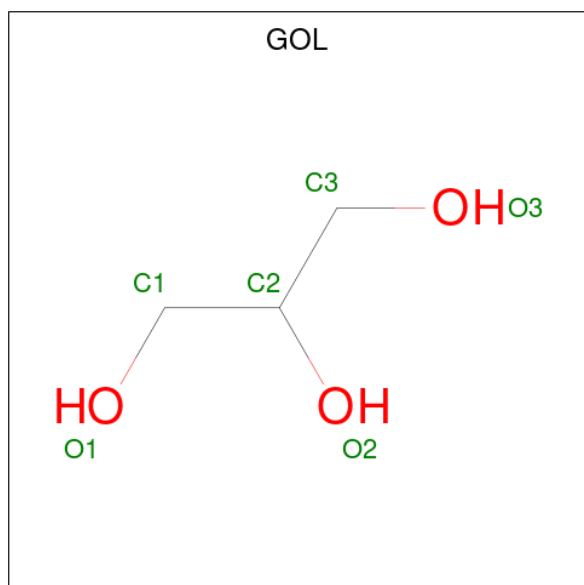
Chain	Residue	Modelled	Actual	Comment	Reference
A	5	LEU	VAL	variant	UNP A0A7U9HVVH2
A	73	CYS	TYR	variant	UNP A0A7U9HVVH2
A	511	THR	ALA	variant	UNP A0A7U9HVVH2
A	706	HIS	-	expression tag	UNP A0A7U9HVVH2
A	707	HIS	-	expression tag	UNP A0A7U9HVVH2
A	708	HIS	-	expression tag	UNP A0A7U9HVVH2
A	709	HIS	-	expression tag	UNP A0A7U9HVVH2
A	710	HIS	-	expression tag	UNP A0A7U9HVVH2
A	711	HIS	-	expression tag	UNP A0A7U9HVVH2
B	5	LEU	VAL	variant	UNP A0A7U9HVVH2
B	73	CYS	TYR	variant	UNP A0A7U9HVVH2
B	511	THR	ALA	variant	UNP A0A7U9HVVH2
B	706	HIS	-	expression tag	UNP A0A7U9HVVH2
B	707	HIS	-	expression tag	UNP A0A7U9HVVH2
B	708	HIS	-	expression tag	UNP A0A7U9HVVH2
B	709	HIS	-	expression tag	UNP A0A7U9HVVH2
B	710	HIS	-	expression tag	UNP A0A7U9HVVH2
B	711	HIS	-	expression tag	UNP A0A7U9HVVH2
C	5	LEU	VAL	variant	UNP A0A7U9HVVH2
C	73	CYS	TYR	variant	UNP A0A7U9HVVH2
C	511	THR	ALA	variant	UNP A0A7U9HVVH2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	706	HIS	-	expression tag	UNP A0A7U9HVVH2
C	707	HIS	-	expression tag	UNP A0A7U9HVVH2
C	708	HIS	-	expression tag	UNP A0A7U9HVVH2
C	709	HIS	-	expression tag	UNP A0A7U9HVVH2
C	710	HIS	-	expression tag	UNP A0A7U9HVVH2
C	711	HIS	-	expression tag	UNP A0A7U9HVVH2
D	5	LEU	VAL	variant	UNP A0A7U9HVVH2
D	73	CYS	TYR	variant	UNP A0A7U9HVVH2
D	511	THR	ALA	variant	UNP A0A7U9HVVH2
D	706	HIS	-	expression tag	UNP A0A7U9HVVH2
D	707	HIS	-	expression tag	UNP A0A7U9HVVH2
D	708	HIS	-	expression tag	UNP A0A7U9HVVH2
D	709	HIS	-	expression tag	UNP A0A7U9HVVH2
D	710	HIS	-	expression tag	UNP A0A7U9HVVH2
D	711	HIS	-	expression tag	UNP A0A7U9HVVH2

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



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

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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	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		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



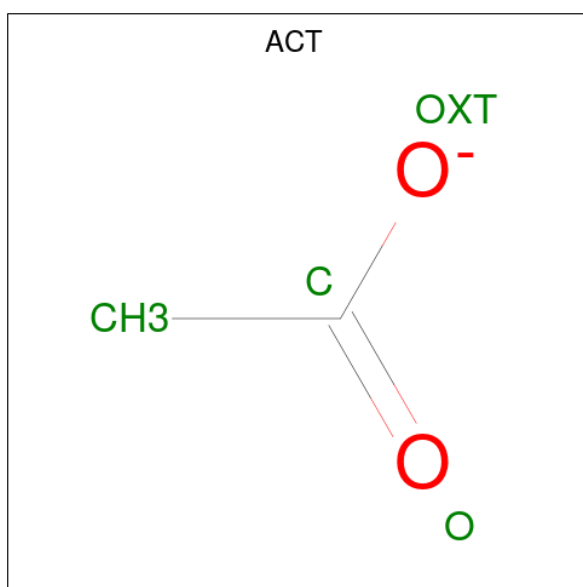
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		
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 ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

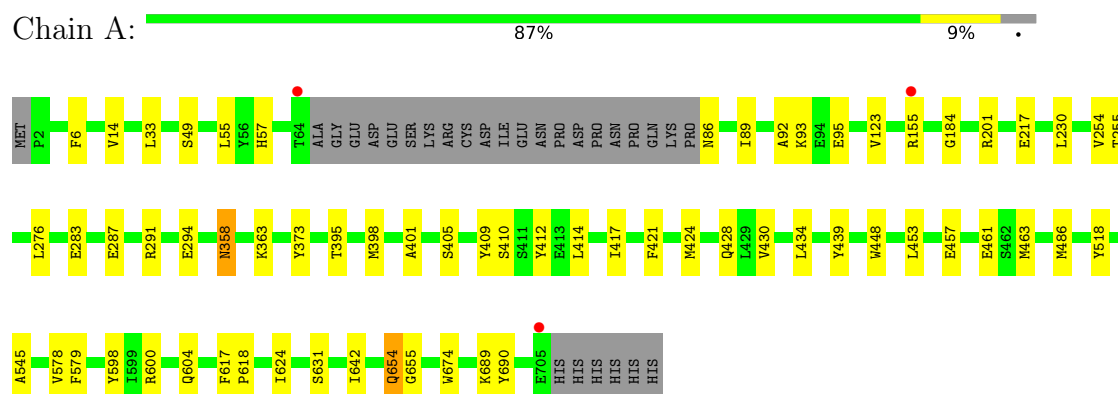
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	394	Total O 394 394	0	0
5	B	365	Total O 365 365	0	0
5	C	372	Total O 372 372	0	0
5	D	356	Total O 356 356	0	0

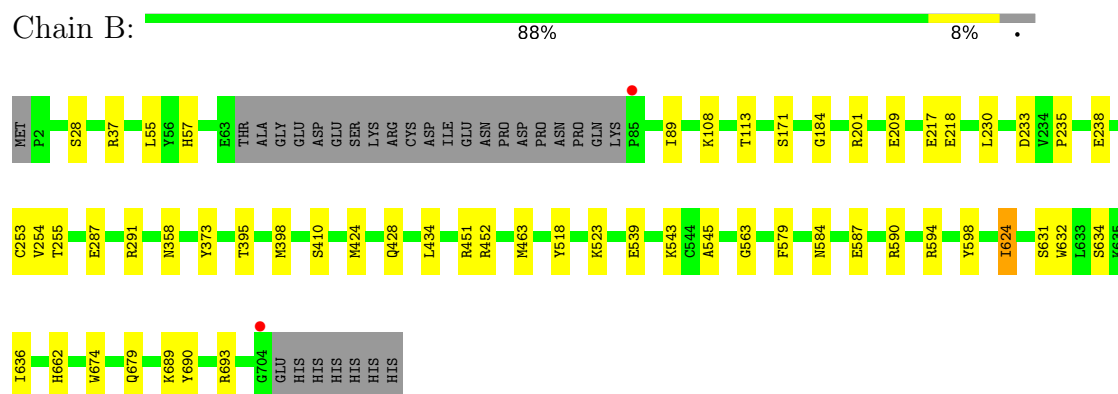
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

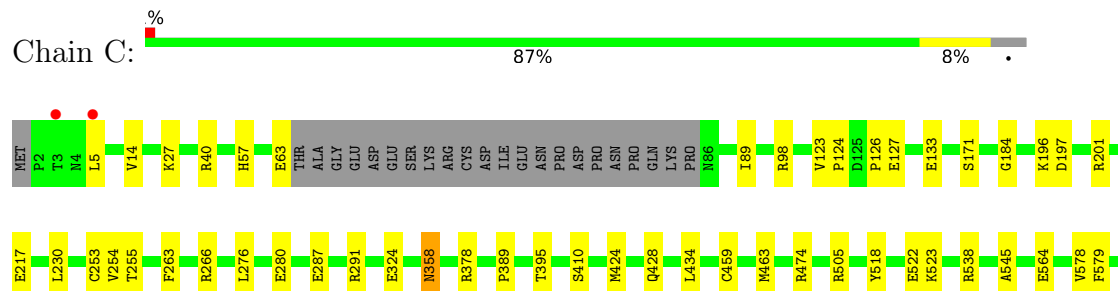
• Molecule 1: Beta-xylosidase

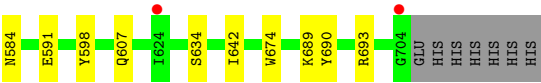


• Molecule 1: Beta-xylosidase

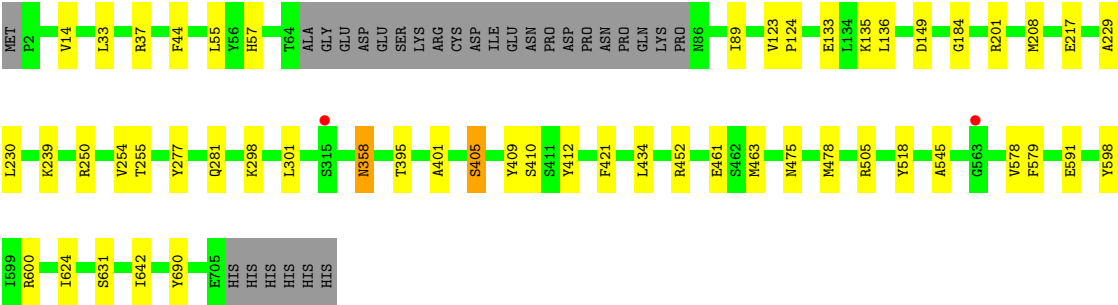
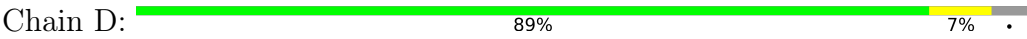


• Molecule 1: Beta-xylosidase





● Molecule 1: Beta-xylosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.12Å 97.51Å 107.40Å 107.45° 98.48° 106.55°	Depositor
Resolution (Å)	81.67 – 2.25 81.67 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.2 (81.67-2.25) 97.2 (81.67-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.25Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.178 , 0.213 0.177 , 0.213	Depositor DCC
R_{free} test set	6754 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23817	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, 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	0.12	0/5739	0.32	0/7780
1	B	0.12	0/5683	0.33	0/7709
1	C	0.11	0/5739	0.32	0/7780
1	D	0.12	0/5687	0.32	0/7713
All	All	0.11	0/22848	0.32	0/30982

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	690	TYR	Peptide
1	B	690	TYR	Peptide
1	C	690	TYR	Peptide
1	D	690	TYR	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	5556	0	5385	41	0
1	B	5517	0	5330	31	0
1	C	5562	0	5389	37	0
1	D	5534	0	5326	30	0
2	A	18	0	24	2	0
2	B	18	0	24	2	0
2	C	18	0	24	1	0
2	D	12	0	16	1	0
3	A	20	0	0	0	0
3	B	15	0	0	0	0
3	C	10	0	0	0	0
3	D	30	0	0	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	8	0	6	0	0
4	D	4	0	3	0	0
5	A	394	0	0	3	0
5	B	365	0	0	2	0
5	C	372	0	0	6	0
5	D	356	0	0	3	0
All	All	23817	0	21533	136	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 3.

All (136) 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:123:VAL:H	1:A:358:ASN:HD22	1.26	0.83
1:D:208:MET:HE1	1:D:229:ALA:HB2	1.61	0.81
1:C:266:ARG:NH1	1:C:324:GLU:OE2	2.20	0.75
1:C:201:ARG:NH1	1:C:217:GLU:OE1	2.22	0.73
1:B:201:ARG:NH1	1:B:217:GLU:OE1	2.24	0.71
1:B:235:PRO:HG2	1:B:238:GLU:OE1	1.93	0.69
1:C:607:GLN:HE22	2:C:801:GOL:H2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ARG:NH2	5:C:901:HOH:O	2.29	0.66
1:C:505:ARG:NH1	5:C:903:HOH:O	2.30	0.65
1:C:123:VAL:H	1:C:358:ASN:HD22	1.46	0.64
1:D:201:ARG:NH1	1:D:217:GLU:OE1	2.31	0.64
1:A:395:THR:HB	1:A:410[B]:SER:HB3	1.82	0.62
1:A:201:ARG:NH1	1:A:217:GLU:OE2	2.33	0.61
1:A:291[A]:ARG:NH1	5:A:905:HOH:O	2.25	0.61
1:A:283:GLU:O	1:A:287[B]:GLU:HG2	2.00	0.60
1:C:291:ARG:NH1	5:C:904:HOH:O	2.31	0.60
1:D:37[A]:ARG:NH1	5:D:907:HOH:O	2.35	0.60
1:A:414:LEU:HD13	2:B:801:GOL:H12	1.84	0.59
1:D:123:VAL:H	1:D:358:ASN:HD22	1.50	0.59
1:D:591:GLU:O	1:D:600[A]:ARG:NH1	2.37	0.57
1:A:49:SER:O	1:A:155[A]:ARG:NH2	2.36	0.57
1:B:254:VAL:HG23	1:B:255:THR:HG23	1.86	0.57
1:A:618:PRO:HD2	2:A:803:GOL:H11	1.86	0.57
1:A:395:THR:HB	1:A:410[A]:SER:HB2	1.88	0.56
1:B:590:ARG:HG2	1:B:590:ARG:HH11	1.71	0.56
1:D:478:MET:HG2	1:D:505:ARG:HA	1.87	0.55
1:B:523:LYS:HE3	1:B:584:ASN:HB3	1.89	0.55
1:C:184:GLY:HA2	1:C:230:LEU:HD21	1.88	0.55
1:A:254:VAL:HG23	1:A:255:THR:HG23	1.88	0.55
1:C:395:THR:HB	1:C:410:SER:HB3	1.89	0.55
1:D:184:GLY:HA2	1:D:230:LEU:HD21	1.89	0.55
1:D:149:ASP:HA	1:D:239:LYS:HG3	1.88	0.55
1:D:545:ALA:HB1	1:D:598:TYR:HB2	1.90	0.54
1:D:254:VAL:HG23	1:D:255:THR:HG23	1.89	0.54
1:C:591:GLU:CD	1:C:591:GLU:H	2.15	0.54
1:A:674:TRP:CG	1:A:689:LYS:HD2	2.42	0.54
1:B:545:ALA:HB1	1:B:598:TYR:HB2	1.89	0.54
1:B:184:GLY:HA2	1:B:230:LEU:HD21	1.90	0.53
1:B:674:TRP:CG	1:B:689:LYS:HD2	2.44	0.53
1:B:395:THR:HB	1:B:410:SER:HB3	1.91	0.53
1:A:184:GLY:HA2	1:A:230:LEU:HD21	1.90	0.53
1:D:395:THR:HB	1:D:410:SER:HB3	1.91	0.53
1:A:363:LYS:HD2	1:A:448:TRP:CD1	2.44	0.52
1:A:654[B]:GLN:NE2	5:A:907:HOH:O	2.26	0.52
1:C:27:LYS:HB2	1:C:63:GLU:HG3	1.91	0.52
1:A:123:VAL:H	1:A:358:ASN:ND2	2.01	0.52
1:C:459:CYS:O	1:C:463:MET:HG3	2.12	0.50
1:D:405:SER:OG	1:D:409:TYR:O	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287[A]:GLU:HG3	1:A:291[A]:ARG:NH1	2.27	0.49
1:D:281:GLN:NE2	5:D:916:HOH:O	2.42	0.49
1:A:545:ALA:HB1	1:A:598:TYR:HB2	1.94	0.49
1:A:92:ALA:HB3	1:A:95:GLU:HG3	1.93	0.49
1:C:123:VAL:H	1:C:358:ASN:ND2	2.08	0.49
1:C:254:VAL:HG23	1:C:255:THR:HG23	1.93	0.49
1:B:587:GLU:OE2	1:B:594:ARG:NH2	2.45	0.49
1:B:624[B]:ILE:HG12	1:B:631:SER:HA	1.95	0.49
1:B:539:GLU:HG3	1:B:543:LYS:HE2	1.95	0.49
1:C:5:LEU:HD13	1:C:98:ARG:HB2	1.95	0.49
1:C:545:ALA:HB1	1:C:598:TYR:HB2	1.95	0.49
1:A:417:ILE:HG21	2:B:801:GOL:H31	1.95	0.48
1:D:33:LEU:HD21	1:D:250:ARG:HG2	1.95	0.48
1:D:123:VAL:H	1:D:358:ASN:ND2	2.10	0.48
1:D:136:LEU:HD13	1:D:281:GLN:HG2	1.96	0.48
1:B:37[A]:ARG:NH2	5:B:917:HOH:O	2.46	0.48
1:A:461:GLU:OE2	5:A:901:HOH:O	2.20	0.48
1:C:276:LEU:O	1:C:280:GLU:HG3	2.14	0.48
1:B:563:GLY:O	5:B:901:HOH:O	2.20	0.47
1:D:578:VAL:HB	1:D:642:ILE:HD11	1.96	0.47
1:C:57:HIS:HA	1:C:89:ILE:O	2.15	0.47
1:C:287:GLU:O	1:C:291:ARG:HG3	2.15	0.47
1:C:40[A]:ARG:NH2	5:C:905:HOH:O	2.31	0.47
1:D:298:LYS:HB2	1:D:301:LEU:HD12	1.96	0.46
1:C:197:ASP:HB3	5:C:1151:HOH:O	2.15	0.46
1:B:590:ARG:HG2	1:B:590:ARG:NH1	2.31	0.46
1:A:57:HIS:HA	1:A:89:ILE:O	2.16	0.46
1:A:463:MET:HE2	1:A:518:TYR:CZ	2.51	0.46
1:A:654[A]:GLN:HG3	1:A:655:GLY:N	2.30	0.46
1:B:209:GLU:OE2	1:B:209:GLU:N	2.43	0.46
1:C:463:MET:HE2	1:C:518:TYR:CZ	2.51	0.45
1:B:287:GLU:HG3	1:B:291:ARG:HH11	1.81	0.45
1:C:634:SER:CB	1:C:693:ARG:HG2	2.46	0.45
1:D:461[B]:GLU:OE2	5:D:901:HOH:O	2.21	0.45
1:A:363:LYS:HD3	1:A:439:TYR:OH	2.17	0.45
1:C:522:GLU:OE1	1:C:538:ARG:NH1	2.50	0.45
1:A:578:VAL:HB	1:A:642:ILE:HD11	1.99	0.45
1:A:405:SER:OG	1:A:409:TYR:O	2.34	0.45
1:B:57:HIS:HA	1:B:89:ILE:O	2.17	0.45
1:C:474:ARG:NH1	5:C:902:HOH:O	2.29	0.45
1:C:378[B]:ARG:HD2	1:C:389:PRO:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:MET:HE1	1:B:218:GLU:CD	2.42	0.44
1:A:373:TYR:CD2	1:A:398:MET:HG2	2.53	0.44
1:B:373:TYR:CD2	1:B:398:MET:HG2	2.52	0.44
1:C:424:MET:O	1:C:428:GLN:HG2	2.18	0.44
1:A:6:PHE:CE2	1:A:93:LYS:HG2	2.53	0.43
1:D:624:ILE:HG12	1:D:631:SER:HA	2.00	0.43
1:A:453:LEU:O	1:A:457:GLU:HG3	2.18	0.43
1:B:233:ASP:O	1:B:235:PRO:HD3	2.17	0.43
1:C:196:LYS:HB2	1:C:196:LYS:HE3	1.89	0.43
1:D:57:HIS:HA	1:D:89:ILE:O	2.19	0.43
1:C:523:LYS:HE2	1:C:584:ASN:HB3	2.00	0.43
1:A:412:TYR:CE1	1:A:421:PHE:HA	2.54	0.42
1:C:124:PRO:HG2	1:C:133:GLU:HG2	2.01	0.42
1:C:674:TRP:CG	1:C:689:LYS:HD2	2.54	0.42
1:C:171:SER:HB3	1:D:401:ALA:HB3	2.01	0.42
1:D:412:TYR:CE1	1:D:421:PHE:HA	2.54	0.42
1:A:600:ARG:O	1:A:604:GLN:HG3	2.18	0.42
1:A:55:LEU:HD23	1:A:55:LEU:HA	1.87	0.42
1:B:55:LEU:HD12	1:B:55:LEU:HA	1.83	0.42
1:C:505:ARG:NH1	1:C:564:GLU:OE1	2.52	0.42
1:C:578:VAL:HB	1:C:642:ILE:HD11	2.02	0.42
1:D:124:PRO:HG2	1:D:133:GLU:HG2	2.02	0.42
1:A:434:LEU:HD13	1:A:579:PHE:CE2	2.54	0.41
1:A:689:LYS:HB2	1:A:689:LYS:HE2	1.80	0.41
1:C:126:PRO:HB3	1:C:263:PHE:CZ	2.55	0.41
1:D:434:LEU:HD13	1:D:579:PHE:CE2	2.56	0.41
1:D:475:ASN:HD22	2:D:804:GOL:H11	1.85	0.41
1:D:135:LYS:HE2	1:D:277:TYR:CD1	2.55	0.41
1:A:401:ALA:HB3	1:B:171:SER:HB3	2.02	0.41
1:D:55:LEU:HD12	1:D:55:LEU:HA	1.82	0.41
1:B:108:LYS:HE3	1:B:113:THR:OG1	2.20	0.41
1:B:424:MET:O	1:B:428:GLN:HG2	2.20	0.41
1:B:463:MET:HE2	1:B:518:TYR:CZ	2.55	0.41
1:A:617:PHE:CD1	2:A:803:GOL:H31	2.56	0.41
1:B:634:SER:OG	1:B:693:ARG:HD3	2.21	0.41
1:C:434:LEU:HD13	1:C:579:PHE:CE2	2.56	0.41
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.97	0.41
1:A:624:ILE:HG12	1:A:631:SER:HA	2.01	0.41
1:B:451:ARG:HG2	1:B:452:ARG:HD3	2.03	0.41
1:B:632:TRP:NE1	1:B:679:GLN:HG2	2.36	0.41
1:C:689:LYS:HB2	1:C:689:LYS:HE2	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:MET:HE2	1:D:518:TYR:CZ	2.56	0.40
1:D:44:PHE:CG	1:D:208:MET:HE3	2.56	0.40
1:B:434:LEU:HD13	1:B:579:PHE:CE2	2.56	0.40
1:A:424:MET:O	1:A:428:GLN:HG2	2.21	0.40
1:B:636:ILE:HG21	1:B:662:HIS:CE1	2.56	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	694/711 (98%)	676 (97%)	18 (3%)	0	100	100
1	B	688/711 (97%)	671 (98%)	17 (2%)	0	100	100
1	C	693/711 (98%)	676 (98%)	17 (2%)	0	100	100
1	D	688/711 (97%)	671 (98%)	17 (2%)	0	100	100
All	All	2763/2844 (97%)	2694 (98%)	69 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	590/601 (98%)	582 (99%)	8 (1%)	59	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	584/601 (97%)	578 (99%)	6 (1%)	68	77
1	C	589/601 (98%)	584 (99%)	5 (1%)	73	80
1	D	584/601 (97%)	580 (99%)	4 (1%)	76	82
All	All	2347/2404 (98%)	2324 (99%)	23 (1%)	73	77

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	33	LEU
1	A	86	ASN
1	A	358	ASN
1	A	430[A]	VAL
1	A	430[B]	VAL
1	A	654[A]	GLN
1	A	654[B]	GLN
1	B	28[A]	SER
1	B	28[B]	SER
1	B	253	CYS
1	B	358	ASN
1	B	624[A]	ILE
1	B	624[B]	ILE
1	C	14	VAL
1	C	127[A]	GLU
1	C	127[B]	GLU
1	C	253	CYS
1	C	358	ASN
1	D	14	VAL
1	D	358	ASN
1	D	405	SER
1	D	452	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	321	GLN
1	A	358	ASN
1	A	442	GLN
1	B	57	HIS

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Mol	Chain	Res	Type
1	B	551	HIS
1	C	57	HIS
1	C	358	ASN
1	D	57	HIS
1	D	321	GLN
1	D	334	ASN
1	D	358	ASN
1	D	442	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

31 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	A	803	-	5,5,5	0.95	0	5,5,5	1.02	0
3	SO4	D	809	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	A	807	-	4,4,4	0.24	0	6,6,6	0.09	0
2	GOL	A	801	-	5,5,5	0.95	0	5,5,5	1.08	0
3	SO4	D	808	-	4,4,4	0.24	0	6,6,6	0.06	0
4	ACT	C	804	-	3,3,3	1.39	1 (33%)	3,3,3	1.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	801	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	D	807	-	4,4,4	0.25	0	6,6,6	0.07	0
2	GOL	C	801	-	5,5,5	0.99	0	5,5,5	1.06	0
4	ACT	D	803	-	3,3,3	1.42	1 (33%)	3,3,3	1.50	0
3	SO4	B	806	-	4,4,4	0.24	0	6,6,6	0.08	0
2	GOL	A	802	-	5,5,5	0.87	0	5,5,5	1.15	0
2	GOL	B	804	-	5,5,5	0.92	0	5,5,5	1.10	0
3	SO4	B	807	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	C	806	-	4,4,4	0.23	0	6,6,6	0.10	0
4	ACT	C	805	-	3,3,3	1.41	1 (33%)	3,3,3	1.36	0
2	GOL	D	802	-	5,5,5	0.87	0	5,5,5	1.15	1 (20%)
3	SO4	A	805	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	D	805	-	4,4,4	0.24	0	6,6,6	0.09	0
4	ACT	A	808	-	3,3,3	1.39	1 (33%)	3,3,3	1.36	0
2	GOL	B	802	-	5,5,5	0.94	0	5,5,5	1.07	0
3	SO4	A	806	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	A	804	-	4,4,4	0.24	0	6,6,6	0.10	0
2	GOL	B	801	-	5,5,5	0.89	0	5,5,5	1.19	1 (20%)
2	GOL	C	802	-	5,5,5	0.92	0	5,5,5	1.10	0
3	SO4	B	805	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	D	806	-	4,4,4	0.24	0	6,6,6	0.06	0
2	GOL	C	803	-	5,5,5	0.93	0	5,5,5	1.06	0
3	SO4	C	807	-	4,4,4	0.24	0	6,6,6	0.07	0
2	GOL	D	804	-	5,5,5	0.95	0	5,5,5	1.02	0
4	ACT	B	803	-	3,3,3	1.36	0	3,3,3	1.37	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	A	803	-	-	2/4/4/4	-
2	GOL	D	802	-	-	4/4/4/4	-
2	GOL	C	803	-	-	0/4/4/4	-
2	GOL	A	801	-	-	0/4/4/4	-
2	GOL	D	804	-	-	2/4/4/4	-
2	GOL	B	802	-	-	0/4/4/4	-
2	GOL	B	801	-	-	0/4/4/4	-
2	GOL	A	802	-	-	0/4/4/4	-
2	GOL	B	804	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	802	-	-	1/4/4/4	-
2	GOL	C	801	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	803	ACT	CH3-C	2.05	1.57	1.49
4	A	808	ACT	CH3-C	2.03	1.57	1.49
4	C	805	ACT	CH3-C	2.03	1.57	1.49
4	C	804	ACT	CH3-C	2.03	1.57	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	GOL	C3-C2-C1	-2.17	103.83	111.80
2	D	802	GOL	C3-C2-C1	-2.09	104.15	111.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	801	GOL	O1-C1-C2-O2
2	C	801	GOL	O1-C1-C2-C3
2	A	803	GOL	C1-C2-C3-O3
2	D	802	GOL	O1-C1-C2-C3
2	D	802	GOL	C1-C2-C3-O3
2	D	804	GOL	O1-C1-C2-C3
2	D	802	GOL	O1-C1-C2-O2
2	A	803	GOL	O2-C2-C3-O3
2	B	804	GOL	O1-C1-C2-O2
2	C	802	GOL	O2-C2-C3-O3
2	D	802	GOL	O2-C2-C3-O3
2	D	804	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	803	GOL	2	0
2	C	801	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	GOL	2	0
2	D	804	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	683/711 (96%)	-0.25	3 (0%) 88 89	17, 32, 49, 107	15 (2%)
1	B	682/711 (95%)	-0.22	2 (0%) 90 90	17, 33, 54, 96	10 (1%)
1	C	681/711 (95%)	-0.25	4 (0%) 85 86	16, 32, 49, 76	16 (2%)
1	D	683/711 (96%)	-0.22	2 (0%) 90 90	15, 34, 54, 104	9 (1%)
All	All	2729/2844 (95%)	-0.23	11 (0%) 88 89	15, 33, 52, 107	50 (1%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	704	GLY	4.0
1	B	85	PRO	3.3
1	C	624	ILE	2.9
1	C	704	GLY	2.8
1	D	563	GLY	2.6
1	C	5	LEU	2.5
1	A	705	GLU	2.5
1	A	64	THR	2.3
1	D	315[A]	SER	2.1
1	A	155[A]	ARG	2.1
1	C	3	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	806	5/5	0.59	0.11	87,93,99,104	0
4	ACT	D	803	4/4	0.68	0.16	55,57,57,59	0
4	ACT	C	804	4/4	0.73	0.17	57,58,59,62	0
2	GOL	A	802	6/6	0.75	0.14	55,67,71,83	0
3	SO4	A	807	5/5	0.78	0.11	77,83,87,88	0
3	SO4	D	805	5/5	0.78	0.10	70,74,79,79	0
3	SO4	C	807	5/5	0.82	0.12	56,64,68,79	0
2	GOL	C	801	6/6	0.82	0.16	44,49,50,51	0
4	ACT	C	805	4/4	0.83	0.13	52,52,53,56	0
2	GOL	D	804	6/6	0.84	0.12	51,58,63,64	0
4	ACT	B	803	4/4	0.85	0.14	34,41,42,50	0
2	GOL	C	802	6/6	0.85	0.13	50,64,69,71	0
2	GOL	B	801	6/6	0.86	0.13	46,49,55,62	0
2	GOL	B	804	6/6	0.87	0.13	55,57,65,66	0
3	SO4	D	806	5/5	0.87	0.14	53,54,64,66	0
4	ACT	A	808	4/4	0.88	0.12	45,46,49,54	0
3	SO4	A	805	5/5	0.89	0.15	50,52,61,62	0
3	SO4	B	807	5/5	0.89	0.17	57,57,63,64	0
2	GOL	A	803	6/6	0.90	0.16	41,48,52,53	0
3	SO4	C	806	5/5	0.91	0.11	57,59,65,65	0
3	SO4	D	809	5/5	0.92	0.22	55,57,63,69	0
3	SO4	D	807	5/5	0.92	0.12	53,56,61,61	0
3	SO4	A	806	5/5	0.93	0.09	48,49,51,56	0
3	SO4	D	808	5/5	0.93	0.11	45,51,56,57	0
3	SO4	B	805	5/5	0.94	0.14	57,57,60,60	0
3	SO4	A	804	5/5	0.94	0.15	55,59,68,74	0
2	GOL	D	802	6/6	0.94	0.09	28,34,36,38	0
2	GOL	C	803	6/6	0.95	0.07	32,33,37,39	0
2	GOL	B	802	6/6	0.95	0.07	28,31,33,35	0
2	GOL	A	801	6/6	0.96	0.08	23,29,33,36	0
3	SO4	D	801	5/5	0.96	0.10	47,53,54,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.