



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 24, 2025 – 12:45 PM EST

PDB ID : 8SSK
Title : *Citrobacter rodentium* contact dependent growth inhibition (CDI) entry and toxin (CdiA-CT) domains
Authors : Cuthbert, B.J.; Goulding, C.W.; Hayes, C.S.; Nhan, D.Q.
Deposited on : 2023-05-08
Resolution : 1.90 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

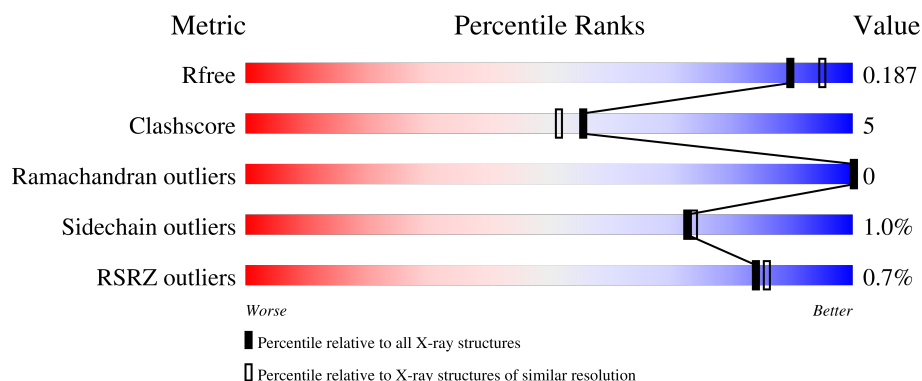
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	318	
1	B	318	
1	C	318	
1	D	318	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	411	-	-	X	-
4	ACT	A	405	-	-	X	-
4	ACT	C	408	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19024 atoms, of which 8697 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 Contact-dependent inhibitor A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	304	Total	C	H	N	O	S	0	7	0
			4330	1385	2119	376	439	11			
1	B	305	Total	C	H	N	O	S	0	8	0
			4351	1396	2121	375	447	12			
1	C	305	Total	C	H	N	O	S	0	7	0
			4436	1409	2188	382	445	12			
1	D	306	Total	C	H	N	O	S	0	11	0
			4386	1403	2144	377	450	12			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	expression tag	UNP A0A482PFX0
A	-32	HIS	-	expression tag	UNP A0A482PFX0
A	-31	HIS	-	expression tag	UNP A0A482PFX0
A	-30	HIS	-	expression tag	UNP A0A482PFX0
A	-29	HIS	-	expression tag	UNP A0A482PFX0
A	-28	HIS	-	expression tag	UNP A0A482PFX0
A	-27	HIS	-	expression tag	UNP A0A482PFX0
A	-26	SER	-	expression tag	UNP A0A482PFX0
A	-25	SER	-	expression tag	UNP A0A482PFX0
A	-24	GLY	-	expression tag	UNP A0A482PFX0
A	-23	VAL	-	expression tag	UNP A0A482PFX0
A	-22	ASP	-	expression tag	UNP A0A482PFX0
A	-21	LEU	-	expression tag	UNP A0A482PFX0
A	-20	GLY	-	expression tag	UNP A0A482PFX0
A	-19	THR	-	expression tag	UNP A0A482PFX0
A	-18	GLU	-	expression tag	UNP A0A482PFX0
A	-17	ASN	-	expression tag	UNP A0A482PFX0
A	-16	LEU	-	expression tag	UNP A0A482PFX0
A	-15	TYR	-	expression tag	UNP A0A482PFX0
A	-14	PHE	-	expression tag	UNP A0A482PFX0
A	-13	GLN	-	expression tag	UNP A0A482PFX0

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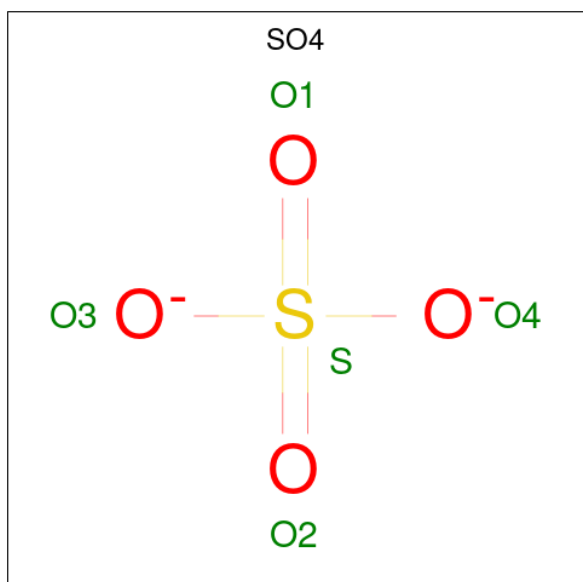
Chain	Residue	Modelled	Actual	Comment	Reference
A	166	ALA	CYS	engineered mutation	UNP A0A482PFX0
B	-33	MET	-	expression tag	UNP A0A482PFX0
B	-32	HIS	-	expression tag	UNP A0A482PFX0
B	-31	HIS	-	expression tag	UNP A0A482PFX0
B	-30	HIS	-	expression tag	UNP A0A482PFX0
B	-29	HIS	-	expression tag	UNP A0A482PFX0
B	-28	HIS	-	expression tag	UNP A0A482PFX0
B	-27	HIS	-	expression tag	UNP A0A482PFX0
B	-26	SER	-	expression tag	UNP A0A482PFX0
B	-25	SER	-	expression tag	UNP A0A482PFX0
B	-24	GLY	-	expression tag	UNP A0A482PFX0
B	-23	VAL	-	expression tag	UNP A0A482PFX0
B	-22	ASP	-	expression tag	UNP A0A482PFX0
B	-21	LEU	-	expression tag	UNP A0A482PFX0
B	-20	GLY	-	expression tag	UNP A0A482PFX0
B	-19	THR	-	expression tag	UNP A0A482PFX0
B	-18	GLU	-	expression tag	UNP A0A482PFX0
B	-17	ASN	-	expression tag	UNP A0A482PFX0
B	-16	LEU	-	expression tag	UNP A0A482PFX0
B	-15	TYR	-	expression tag	UNP A0A482PFX0
B	-14	PHE	-	expression tag	UNP A0A482PFX0
B	-13	GLN	-	expression tag	UNP A0A482PFX0
B	166	ALA	CYS	engineered mutation	UNP A0A482PFX0
C	-33	MET	-	expression tag	UNP A0A482PFX0
C	-32	HIS	-	expression tag	UNP A0A482PFX0
C	-31	HIS	-	expression tag	UNP A0A482PFX0
C	-30	HIS	-	expression tag	UNP A0A482PFX0
C	-29	HIS	-	expression tag	UNP A0A482PFX0
C	-28	HIS	-	expression tag	UNP A0A482PFX0
C	-27	HIS	-	expression tag	UNP A0A482PFX0
C	-26	SER	-	expression tag	UNP A0A482PFX0
C	-25	SER	-	expression tag	UNP A0A482PFX0
C	-24	GLY	-	expression tag	UNP A0A482PFX0
C	-23	VAL	-	expression tag	UNP A0A482PFX0
C	-22	ASP	-	expression tag	UNP A0A482PFX0
C	-21	LEU	-	expression tag	UNP A0A482PFX0
C	-20	GLY	-	expression tag	UNP A0A482PFX0
C	-19	THR	-	expression tag	UNP A0A482PFX0
C	-18	GLU	-	expression tag	UNP A0A482PFX0
C	-17	ASN	-	expression tag	UNP A0A482PFX0
C	-16	LEU	-	expression tag	UNP A0A482PFX0
C	-15	TYR	-	expression tag	UNP A0A482PFX0

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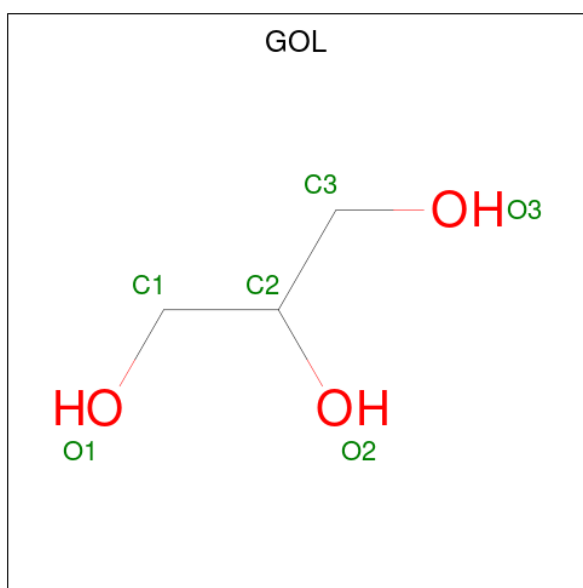
Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	PHE	-	expression tag	UNP A0A482PFX0
C	-13	GLN	-	expression tag	UNP A0A482PFX0
C	166	ALA	CYS	engineered mutation	UNP A0A482PFX0
D	-33	MET	-	expression tag	UNP A0A482PFX0
D	-32	HIS	-	expression tag	UNP A0A482PFX0
D	-31	HIS	-	expression tag	UNP A0A482PFX0
D	-30	HIS	-	expression tag	UNP A0A482PFX0
D	-29	HIS	-	expression tag	UNP A0A482PFX0
D	-28	HIS	-	expression tag	UNP A0A482PFX0
D	-27	HIS	-	expression tag	UNP A0A482PFX0
D	-26	SER	-	expression tag	UNP A0A482PFX0
D	-25	SER	-	expression tag	UNP A0A482PFX0
D	-24	GLY	-	expression tag	UNP A0A482PFX0
D	-23	VAL	-	expression tag	UNP A0A482PFX0
D	-22	ASP	-	expression tag	UNP A0A482PFX0
D	-21	LEU	-	expression tag	UNP A0A482PFX0
D	-20	GLY	-	expression tag	UNP A0A482PFX0
D	-19	THR	-	expression tag	UNP A0A482PFX0
D	-18	GLU	-	expression tag	UNP A0A482PFX0
D	-17	ASN	-	expression tag	UNP A0A482PFX0
D	-16	LEU	-	expression tag	UNP A0A482PFX0
D	-15	TYR	-	expression tag	UNP A0A482PFX0
D	-14	PHE	-	expression tag	UNP A0A482PFX0
D	-13	GLN	-	expression tag	UNP A0A482PFX0
D	166	ALA	CYS	engineered mutation	UNP A0A482PFX0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



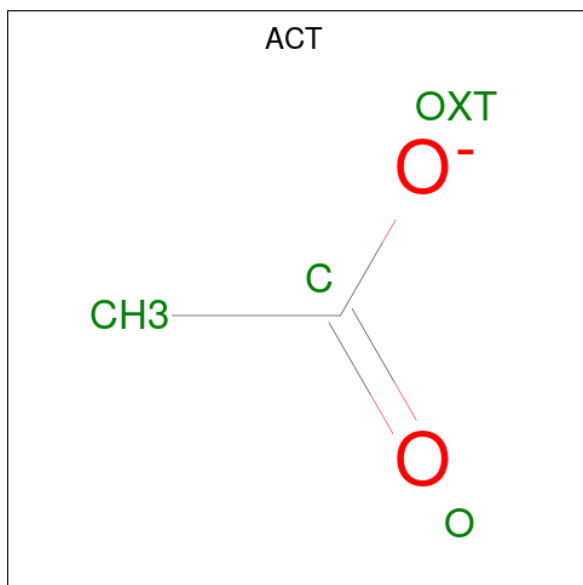
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 13 3 7 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	B	1	Total C H O 13 3 7 3	0	0
3	B	1	Total C H O 12 3 6 3	0	0
3	B	1	Total C H O 14 3 8 3	0	0
3	C	1	Total C H O 14 3 8 3	0	0
3	C	1	Total C H O 14 3 8 3	0	0
3	D	1	Total C H O 13 3 7 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	B	1	Total	C	H	O	0	0
			7	2	3	2		
4	B	1	Total	C	H	O	0	0
			7	2	3	2		
4	C	1	Total	C	H	O	0	0
			7	2	3	2		
4	C	1	Total	C	H	O	0	0
			7	2	3	2		
4	C	1	Total	C	H	O	0	0
			7	2	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			7	2	3	2		
4	C	1	Total	C	H	O	0	0
			7	2	3	2		
4	C	1	Total	C	H	O	0	0
			7	2	3	2		
4	D	1	Total	C	H	O	0	0
			7	2	3	2		
4	D	1	Total	C	H	O	0	0
			7	2	3	2		
4	D	1	Total	C	H	O	0	0
			7	2	3	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		

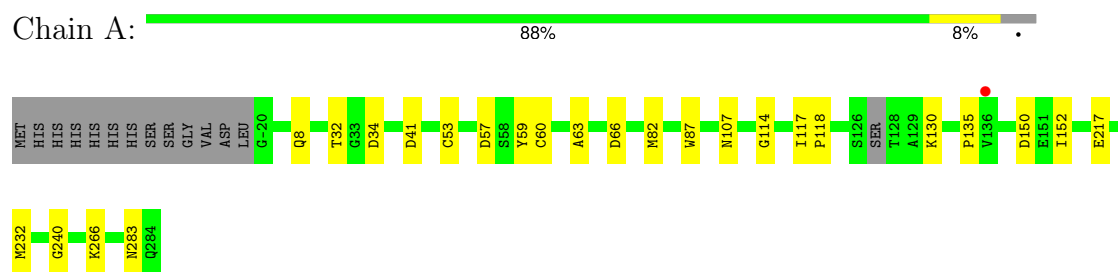
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	299	Total	O	0	0
			299	299		
6	B	299	Total	O	0	0
			299	299		
6	C	334	Total	O	0	0
			334	334		
6	D	318	Total	O	0	0
			318	318		

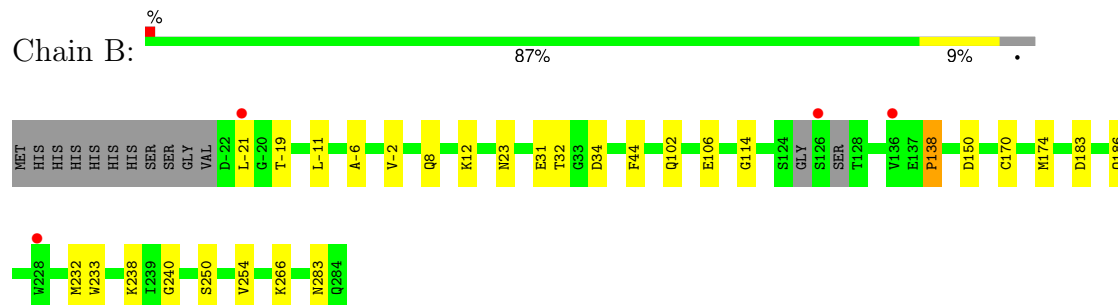
3 Residue-property plots [i](#)

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.

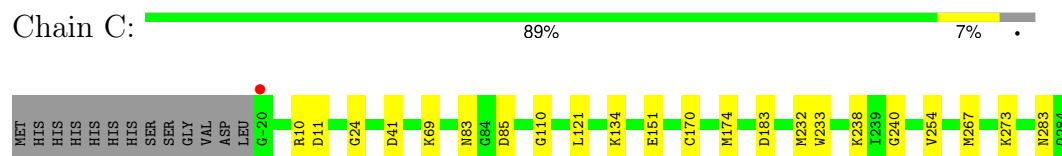
• Molecule 1: Contact-dependent inhibitor A



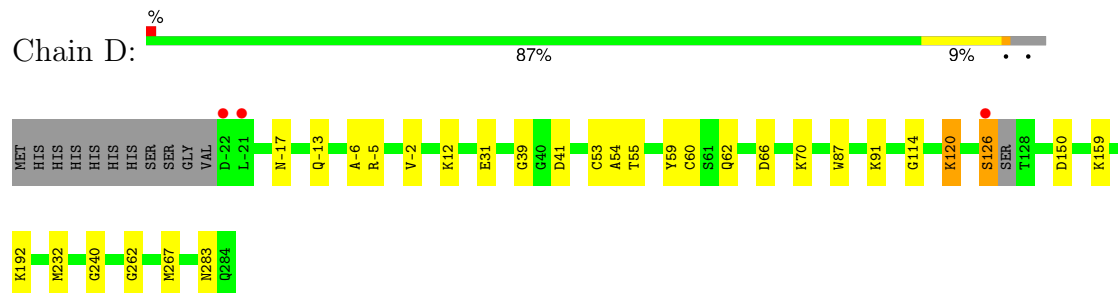
• Molecule 1: Contact-dependent inhibitor A



• Molecule 1: Contact-dependent inhibitor A



• Molecule 1: Contact-dependent inhibitor A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.87Å 113.98Å 87.35Å 90.00° 92.39° 90.00°	Depositor
Resolution (Å)	39.26 – 1.90 39.26 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (39.26-1.90) 98.4 (39.26-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.162 , 0.186 0.163 , 0.187	Depositor DCC
R_{free} test set	92776 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19024	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.21 % 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 8.2946e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, CA, ACT, GOL

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	0.36	0/2272	0.58	0/3083
1	B	0.37	0/2293	0.60	1/3111 (0.0%)
1	C	0.36	0/2310	0.61	0/3129
1	D	0.35	0/2314	0.59	0/3142
All	All	0.36	0/9189	0.59	1/12465 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	PRO	CA-N-CD	-5.77	103.42	111.50

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	2211	2119	2121	22	0
1	B	2230	2121	2123	19	0
1	C	2248	2188	2190	19	0
1	D	2242	2144	2138	21	0
2	A	10	0	0	0	0
2	C	10	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	15	15	1	0
3	B	18	21	23	1	0
3	C	12	16	16	1	0
3	D	24	31	31	5	0
4	A	8	6	6	3	0
4	B	8	6	6	0	0
4	C	28	21	21	2	0
4	D	12	9	9	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	299	0	0	2	0
6	B	299	0	0	2	0
6	C	334	0	0	7	0
6	D	318	0	0	5	0
All	All	10327	8697	8699	81	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (81) 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)
2:C:411:SO4:O1	6:C:501:HOH:O	1.98	0.81
1:D:-5:ARG:HH22	3:D:1505:GOL:H2	1.44	0.80
1:C:11[A]:ASP:OD1	6:C:502:HOH:O	2.12	0.68
1:A:53[B]:CYS:HA	1:A:60[B]:CYS:SG	2.35	0.67
4:D:1502:ACT:H3	6:D:1881:HOH:O	1.94	0.67
1:D:192:LYS:NZ	3:D:1504:GOL:H31	2.12	0.65
1:A:135:PRO:HG2	4:A:405:ACT:H1	1.80	0.64
1:B:250:SER:O	6:B:601:HOH:O	2.16	0.61
1:A:57:ASP:O	1:A:60[B]:CYS:SG	2.56	0.60
1:D:62:GLN:NE2	1:D:66:ASP:OD1	2.32	0.60
1:C:170:CYS:O	1:C:174:MET:HG3	2.03	0.58
1:C:24:GLY:HA2	4:C:407:ACT:H1	1.86	0.58
1:D:12:LYS:HD3	1:D:59:TYR:OH	2.04	0.57
1:D:120:LYS:NZ	6:D:1603:HOH:O	2.34	0.57
1:D:159:LYS:HG3	1:D:262:GLY:HA3	1.85	0.57
1:A:34:ASP:HB3	1:B:32:THR:HB	1.87	0.57
1:B:138:PRO:O	1:B:138:PRO:HD2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ASP:HB2	4:C:403:ACT:H1	1.87	0.56
1:D:41:ASP:HB3	1:D:70:LYS:HD3	1.86	0.56
3:A:402:GOL:H2	6:A:582:HOH:O	2.04	0.56
6:B:653:HOH:O	3:D:1503:GOL:H2	2.05	0.56
1:D:192:LYS:HZ3	3:D:1504:GOL:H31	1.72	0.55
1:C:121:LEU:HD12	6:D:1838:HOH:O	2.05	0.55
1:A:8:GLN:HA	1:A:8:GLN:OE1	2.08	0.53
1:B:114:GLY:O	1:B:150[A]:ASP:HA	2.09	0.52
1:A:53[B]:CYS:HB3	1:A:82:MET:HE3	1.90	0.52
1:C:110:GLY:HA2	1:D:31:GLU:O	2.10	0.52
3:D:1504:GOL:O3	6:D:1601:HOH:O	2.19	0.52
1:C:85:ASP:OD2	6:C:505:HOH:O	2.19	0.51
1:C:183:ASP:OD1	6:C:504:HOH:O	2.19	0.51
1:A:217:GLU:CG	6:C:810:HOH:O	2.59	0.51
1:A:232:MET:O	1:A:240:GLY:HA3	2.11	0.50
1:C:134:LYS:HE2	6:C:780:HOH:O	2.09	0.50
1:A:66:ASP:OD1	6:A:501:HOH:O	2.19	0.50
1:A:53[A]:CYS:HB3	1:A:82:MET:HE3	1.94	0.50
1:B:170:CYS:O	1:B:174:MET:HG3	2.12	0.50
1:D:53[B]:CYS:SG	1:D:60[B]:CYS:HB2	2.52	0.49
1:D:-6:ALA:O	1:D:-2:VAL:HG13	2.11	0.49
1:C:10:ARG:HG2	1:C:10:ARG:HH11	1.77	0.49
1:C:10:ARG:HG2	1:C:10:ARG:NH1	2.27	0.49
1:A:152:ILE:HG22	1:B:-11:LEU:HG	1.94	0.48
1:D:54:ALA:HA	1:D:91:LYS:HG2	1.94	0.48
1:A:117:ILE:O	1:A:150[A]:ASP:OD1	2.32	0.48
1:B:232:MET:O	1:B:240:GLY:HA3	2.14	0.47
1:D:87:TRP:NE1	1:D:91:LYS:HD3	2.30	0.47
1:C:232:MET:O	1:C:240:GLY:HA3	2.15	0.47
1:D:232:MET:O	1:D:240:GLY:HA3	2.14	0.47
1:C:41:ASP:OD2	1:D:126:SER:HA	2.16	0.46
1:D:39:GLY:HA3	4:D:1507:ACT:C	2.46	0.46
1:A:32:THR:HB	1:B:34:ASP:HB3	1.98	0.46
1:B:233:TRP:CH2	1:B:238:LYS:HG2	2.51	0.46
1:A:82:MET:HG2	1:A:87:TRP:CZ2	2.51	0.45
1:C:83:ASN:OD1	3:C:410:GOL:H11	2.17	0.45
1:B:8:GLN:HB3	1:B:44:PHE:CE1	2.52	0.45
1:A:59:TYR:CD2	1:A:63:ALA:HB2	2.53	0.44
1:C:273:LYS:HE2	6:C:791:HOH:O	2.18	0.44
1:B:114:GLY:O	1:B:150[B]:ASP:HA	2.16	0.43
1:B:233:TRP:CZ3	1:B:238:LYS:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:GLN:O	1:B:106:GLU:HG3	2.18	0.43
1:B:183[B]:ASP:OD1	1:B:186:GLN:HG3	2.19	0.43
1:D:-17:ASN:O	1:D:-13:GLN:HG3	2.19	0.43
1:A:107:ASN:HA	1:B:31[B]:GLU:OE2	2.19	0.43
3:B:504:GOL:H2	6:D:1692:HOH:O	2.17	0.42
1:C:151:GLU:OE2	2:C:411:SO4:O4	2.37	0.42
1:A:130:LYS:HA	1:A:130:LYS:HD2	1.76	0.42
1:D:87:TRP:CE2	1:D:91:LYS:HD3	2.54	0.42
1:A:135:PRO:HG2	4:A:405:ACT:CH3	2.49	0.42
1:B:254:VAL:O	1:B:266:LYS:HA	2.20	0.42
1:C:233:TRP:CZ3	1:C:238:LYS:HG2	2.54	0.42
1:C:254[A]:VAL:HG13	1:C:267:MET:HB2	2.02	0.41
1:C:254[A]:VAL:CG1	1:C:267:MET:HB2	2.50	0.41
1:D:114:GLY:O	1:D:150[A]:ASP:HA	2.20	0.41
1:A:114:GLY:O	1:A:150[B]:ASP:HA	2.20	0.41
1:B:-21:LEU:O	1:B:-19:THR:HG23	2.21	0.41
1:B:-6:ALA:O	1:B:-2:VAL:HG23	2.21	0.41
1:A:41:ASP:HB2	4:A:403:ACT:O	2.21	0.41
1:B:-21:LEU:HD11	1:B:23:ASN:HB3	2.03	0.41
1:A:118:PRO:HA	1:A:150[A]:ASP:OD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/318 (96%)	303 (99%)	4 (1%)	0	100	100
1	B	308/318 (97%)	305 (99%)	3 (1%)	0	100	100
1	C	310/318 (98%)	307 (99%)	3 (1%)	0	100	100
1	D	313/318 (98%)	310 (99%)	3 (1%)	0	100	100
All	All	1238/1272 (97%)	1225 (99%)	13 (1%)	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	221/243 (91%)	220 (100%)	1 (0%)	86	88
1	B	223/243 (92%)	221 (99%)	2 (1%)	75	77
1	C	229/243 (94%)	227 (99%)	2 (1%)	75	77
1	D	226/243 (93%)	222 (98%)	4 (2%)	54	52
All	All	899/972 (92%)	890 (99%)	9 (1%)	73	74

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	283	ASN
1	B	12	LYS
1	B	283	ASN
1	C	69	LYS
1	C	283	ASN
1	D	120	LYS
1	D	126	SER
1	D	267	MET
1	D	283	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	8	GLN

5.3.3 RNA ⓘ

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](#)

Of 33 ligands modelled in this entry, 4 are monoatomic - leaving 29 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	$\# Z > 2$
4	ACT	C	404	-	3,3,3	0.99	0	3,3,3	1.15	0
2	SO4	A	401	-	4,4,4	0.26	0	6,6,6	0.29	0
4	ACT	D	1502	-	3,3,3	1.08	0	3,3,3	1.48	0
4	ACT	A	405	-	3,3,3	1.30	0	3,3,3	0.96	0
2	SO4	C	401	-	4,4,4	0.30	0	6,6,6	0.19	0
4	ACT	C	405	-	3,3,3	1.02	0	3,3,3	1.66	1 (33%)
4	ACT	B	502	-	3,3,3	0.95	0	3,3,3	1.70	2 (66%)
4	ACT	C	408	-	3,3,3	1.37	1 (33%)	3,3,3	1.84	2 (66%)
3	GOL	C	410	-	5,5,5	1.60	2 (40%)	5,5,5	1.28	1 (20%)
3	GOL	D	1505	-	5,5,5	0.57	0	5,5,5	1.22	0
4	ACT	D	1501	-	3,3,3	1.14	0	3,3,3	1.06	0
4	ACT	C	403	-	3,3,3	0.90	0	3,3,3	1.41	0
3	GOL	B	503	-	5,5,5	0.91	0	5,5,5	1.24	1 (20%)
3	GOL	C	402	-	5,5,5	1.23	1 (20%)	5,5,5	1.38	1 (20%)
4	ACT	C	409	-	3,3,3	0.96	0	3,3,3	1.45	0
3	GOL	A	402	-	5,5,5	1.32	1 (20%)	5,5,5	1.55	1 (20%)
2	SO4	A	406	-	4,4,4	0.12	0	6,6,6	0.17	0
3	GOL	D	1504	-	5,5,5	0.78	0	5,5,5	0.88	0
4	ACT	A	403	-	3,3,3	0.91	0	3,3,3	1.70	1 (33%)
3	GOL	B	504	-	5,5,5	1.45	1 (20%)	5,5,5	1.66	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	D	1507	-	3,3,3	1.27	0	3,3,3	1.04	0
4	ACT	C	407	-	3,3,3	1.08	0	3,3,3	1.42	0
3	GOL	B	505	-	5,5,5	0.93	0	5,5,5	1.14	1 (20%)
3	GOL	D	1506	-	5,5,5	1.11	1 (20%)	5,5,5	1.48	1 (20%)
2	SO4	C	411	-	4,4,4	0.34	0	6,6,6	0.17	0
3	GOL	A	404	-	5,5,5	1.18	1 (20%)	5,5,5	1.25	1 (20%)
4	ACT	B	501	-	3,3,3	0.93	0	3,3,3	1.69	1 (33%)
4	ACT	C	406	-	3,3,3	1.02	0	3,3,3	1.41	0
3	GOL	D	1503	-	5,5,5	1.14	0	5,5,5	1.29	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	402	-	-	1/4/4/4	-
3	GOL	B	504	-	-	0/4/4/4	-
3	GOL	C	410	-	-	2/4/4/4	-
3	GOL	D	1505	-	-	2/4/4/4	-
3	GOL	B	505	-	-	3/4/4/4	-
3	GOL	B	503	-	-	0/4/4/4	-
3	GOL	D	1506	-	-	0/4/4/4	-
3	GOL	A	404	-	-	2/4/4/4	-
3	GOL	C	402	-	-	0/4/4/4	-
3	GOL	D	1504	-	-	2/4/4/4	-
3	GOL	D	1503	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	GOL	O2-C2	-2.43	1.36	1.43
3	B	504	GOL	O2-C2	-2.32	1.36	1.43
3	A	404	GOL	C3-C2	2.30	1.60	1.51
3	C	410	GOL	C3-C2	2.28	1.60	1.51
3	D	1506	GOL	O2-C2	-2.28	1.36	1.43
3	C	410	GOL	C1-C2	2.27	1.60	1.51
3	C	402	GOL	O2-C2	-2.13	1.37	1.43
4	C	408	ACT	O-C	2.02	1.31	1.22

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	504	GOL	C3-C2-C1	-3.34	99.56	111.80
3	A	402	GOL	C3-C2-C1	-3.07	100.52	111.80
3	C	402	GOL	C3-C2-C1	-2.73	101.80	111.80
3	C	410	GOL	C3-C2-C1	-2.66	102.03	111.80
3	D	1503	GOL	C3-C2-C1	-2.54	102.50	111.80
3	D	1506	GOL	C3-C2-C1	-2.52	102.56	111.80
4	C	408	ACT	O-C-CH3	-2.37	112.80	122.53
3	B	503	GOL	C3-C2-C1	-2.31	103.32	111.80
3	B	505	GOL	C3-C2-C1	-2.23	103.62	111.80
3	A	404	GOL	C3-C2-C1	-2.22	103.67	111.80
4	A	403	ACT	O-C-CH3	-2.14	113.75	122.53
4	B	501	ACT	O-C-CH3	-2.12	113.82	122.53
4	B	502	ACT	O-C-CH3	-2.10	113.92	122.53
4	C	408	ACT	OXT-C-O	2.07	129.71	122.03
4	C	405	ACT	O-C-CH3	-2.07	114.05	122.53
4	B	502	ACT	OXT-C-O	2.02	129.52	122.03

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	505	GOL	O1-C1-C2-C3
3	D	1503	GOL	O1-C1-C2-C3
3	D	1505	GOL	C1-C2-C3-O3
3	B	505	GOL	O1-C1-C2-O2
3	A	404	GOL	O1-C1-C2-C3
3	C	410	GOL	C1-C2-C3-O3
3	D	1504	GOL	C1-C2-C3-O3
3	D	1503	GOL	O1-C1-C2-O2
3	D	1504	GOL	O2-C2-C3-O3
3	C	410	GOL	O2-C2-C3-O3
3	D	1505	GOL	O2-C2-C3-O3
3	A	404	GOL	O1-C1-C2-O2
3	B	505	GOL	C1-C2-C3-O3
3	A	402	GOL	O2-C2-C3-O3

There are no ring outliers.

13 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1502	ACT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	ACT	2	0
3	C	410	GOL	1	0
3	D	1505	GOL	1	0
4	C	403	ACT	1	0
3	A	402	GOL	1	0
3	D	1504	GOL	3	0
4	A	403	ACT	1	0
3	B	504	GOL	1	0
4	D	1507	ACT	1	0
4	C	407	ACT	1	0
2	C	411	SO4	2	0
3	D	1503	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	304/318 (95%)	-0.46	1 (0%) 90 91	13, 28, 52, 71	7 (2%)
1	B	305/318 (95%)	-0.36	4 (1%) 74 76	12, 29, 51, 70	8 (2%)
1	C	305/318 (95%)	-0.49	1 (0%) 90 91	12, 26, 50, 75	7 (2%)
1	D	306/318 (96%)	-0.38	3 (0%) 79 81	13, 28, 53, 73	10 (3%)
All	All	1220/1272 (95%)	-0.42	9 (0%) 84 86	12, 28, 52, 75	32 (2%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	SER	5.3
1	D	-22	ASP	4.2
1	D	-21	LEU	3.7
1	B	228	TRP	3.3
1	B	-21	LEU	3.1
1	D	126	SER	3.1
1	C	-20	GLY	2.8
1	A	136	VAL	2.1
1	B	136	VAL	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 monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	ACT	D	1507	4/4	0.60	0.19	51,56,67,67	0
4	ACT	C	404	4/4	0.66	0.17	40,48,49,50	7
4	ACT	C	405	4/4	0.68	0.18	37,39,47,47	0
3	GOL	D	1505	6/6	0.75	0.13	40,54,62,66	0
3	GOL	B	505	6/6	0.75	0.14	39,54,65,65	0
3	GOL	A	404	6/6	0.76	0.13	46,55,65,76	0
3	GOL	D	1506	6/6	0.77	0.17	38,48,58,69	14
3	GOL	C	410	6/6	0.77	0.15	43,62,73,88	0
4	ACT	C	408	4/4	0.79	0.21	34,42,50,50	7
4	ACT	D	1501	4/4	0.80	0.25	30,33,44,44	0
4	ACT	C	407	4/4	0.80	0.20	35,42,43,44	0
4	ACT	A	403	4/4	0.81	0.13	54,56,65,65	0
3	GOL	D	1504	6/6	0.84	0.12	31,49,58,59	0
4	ACT	C	406	4/4	0.85	0.11	46,49,55,55	0
4	ACT	B	502	4/4	0.87	0.12	40,46,55,55	0
4	ACT	D	1502	4/4	0.87	0.11	36,44,51,51	0
4	ACT	B	501	4/4	0.87	0.15	45,46,55,55	0
4	ACT	A	405	4/4	0.89	0.12	47,57,72,72	0
3	GOL	B	504	6/6	0.89	0.10	28,36,41,48	0
4	ACT	C	409	4/4	0.89	0.16	43,50,58,58	0
3	GOL	A	402	6/6	0.91	0.09	26,31,37,37	0
3	GOL	D	1503	6/6	0.91	0.09	29,35,40,43	0
4	ACT	C	403	4/4	0.94	0.09	35,42,53,53	0
3	GOL	B	503	6/6	0.94	0.08	23,32,41,41	0
2	SO4	C	411	5/5	0.96	0.12	17,24,25,30	5
3	GOL	C	402	6/6	0.97	0.06	24,30,37,37	0
2	SO4	A	401	5/5	0.98	0.06	27,27,28,33	0
2	SO4	A	406	5/5	0.98	0.07	24,25,28,33	0
2	SO4	C	401	5/5	0.99	0.05	18,23,25,26	0
5	CA	A	407	1/1	1.00	0.02	20,20,20,20	0
5	CA	B	506	1/1	1.00	0.04	21,21,21,21	0
5	CA	C	412	1/1	1.00	0.02	22,22,22,22	0
5	CA	D	1508	1/1	1.00	0.03	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.