



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:17 AM UTC

PDB ID : 6T8F / pdb_00006t8f
Title : Crystal structure of mutant xylose isomerase (V270A/A273G) from *Piromyces*
E2 grown in yeast, in complex with xylose
Authors : Rozeboom, H.J.; Janssen, D.B.
Deposited on : 2019-10-24
Resolution : 2.00 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

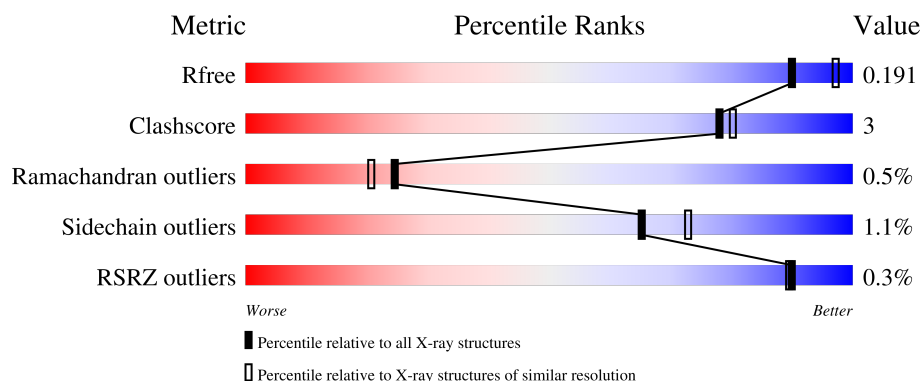
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

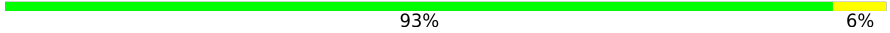
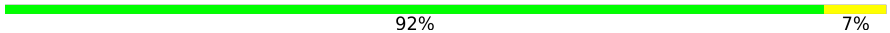
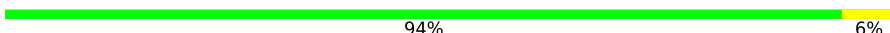
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	437	 93% 6%
1	B	437	 92% 7%
1	C	437	 95% 5%
1	D	437	 94% 6%

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
3	XLS	A	503	-	X	-	-
3	XLS	B	503	-	X	-	-
3	XLS	C	503	-	X	-	-
3	XLS	D	503	-	X	-	-
6	SO4	A	508	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15847 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 Xylose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	1	0
			3471	2202	582	667	20			
1	B	436	Total	C	N	O	S	0	1	0
			3471	2202	582	667	20			
1	C	436	Total	C	N	O	S	0	1	0
			3471	2202	582	667	20			
1	D	436	Total	C	N	O	S	0	4	0
			3495	2217	585	670	23			

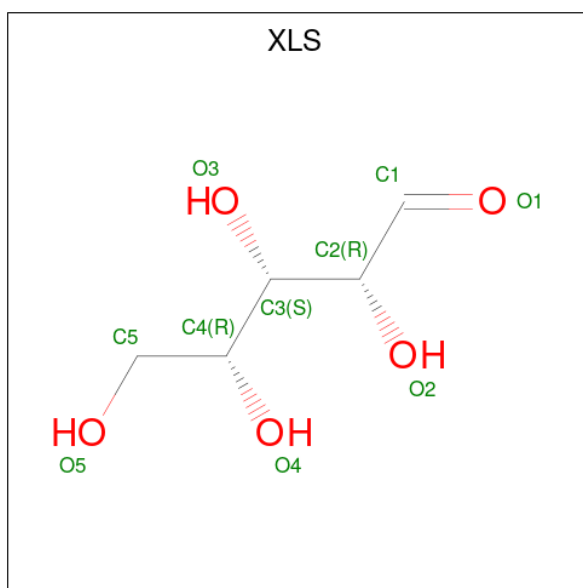
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	270	ALA	VAL	engineered mutation	UNP Q9P8C9
A	273	GLY	ALA	engineered mutation	UNP Q9P8C9
B	270	ALA	VAL	engineered mutation	UNP Q9P8C9
B	273	GLY	ALA	engineered mutation	UNP Q9P8C9
C	270	ALA	VAL	engineered mutation	UNP Q9P8C9
C	273	GLY	ALA	engineered mutation	UNP Q9P8C9
D	270	ALA	VAL	engineered mutation	UNP Q9P8C9
D	273	GLY	ALA	engineered mutation	UNP Q9P8C9

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

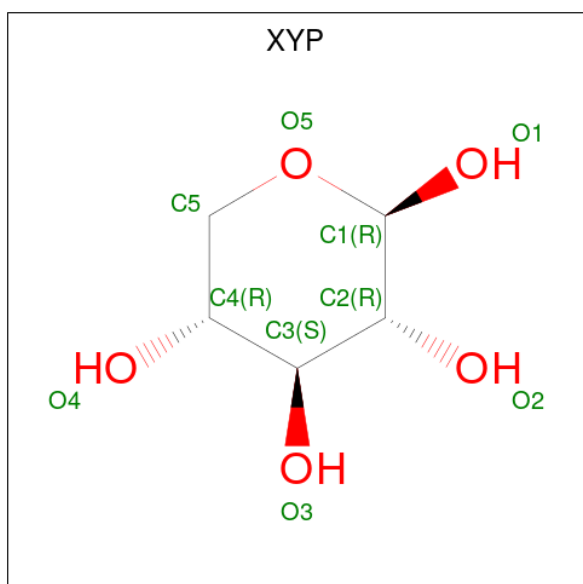
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		
2	C	2	Total	Ca	0	0
			2	2		
2	D	2	Total	Ca	0	0
			2	2		

- Molecule 3 is D-xylose (CCD ID: XLS) (formula: $C_5H_{10}O_5$).



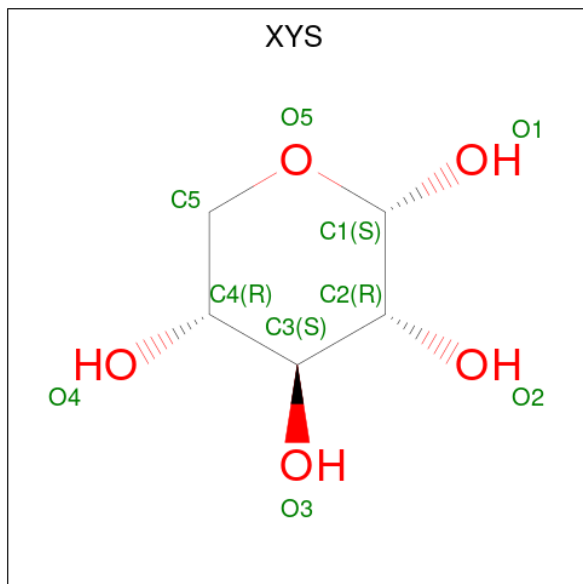
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is beta-D-xylopyranose (CCD ID: XYP) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		
4	B	1	Total	C	O	0	0
			10	5	5		
4	C	1	Total	C	O	0	0
			10	5	5		
4	C	1	Total	C	O	0	0
			10	5	5		
4	D	1	Total	C	O	0	0
			10	5	5		
4	D	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is alpha-D-xylopyranose (CCD ID: YYS) (formula: C₅H₁₀O₅).



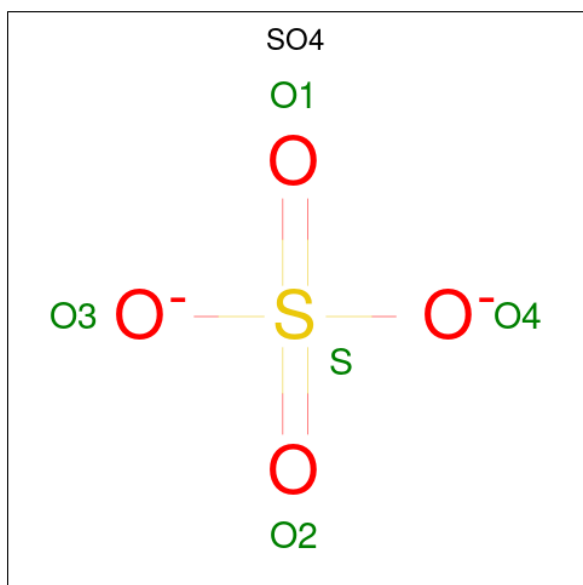
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	5	5		
5	A	1	Total	C	O	0	0
			10	5	5		
5	B	1	Total	C	O	0	0
			10	5	5		
5	B	1	Total	C	O	0	0
			10	5	5		
5	B	1	Total	C	O	0	0
			10	5	5		
5	C	1	Total	C	O	0	0
			10	5	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			10	5	5		
5	D	1	Total	C	O	0	0
			10	5	5		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	415	Total	O	0	0
			415	415		

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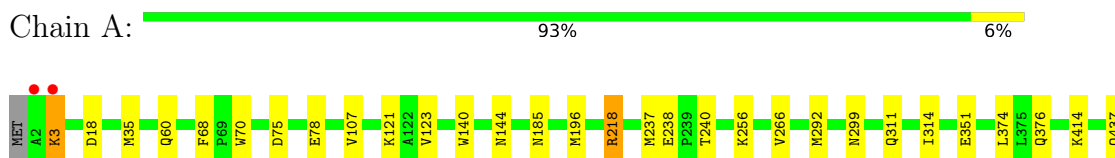
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	433	Total 433	O 433	0	0
7	C	424	Total 424	O 424	0	0
7	D	449	Total 449	O 449	0	0

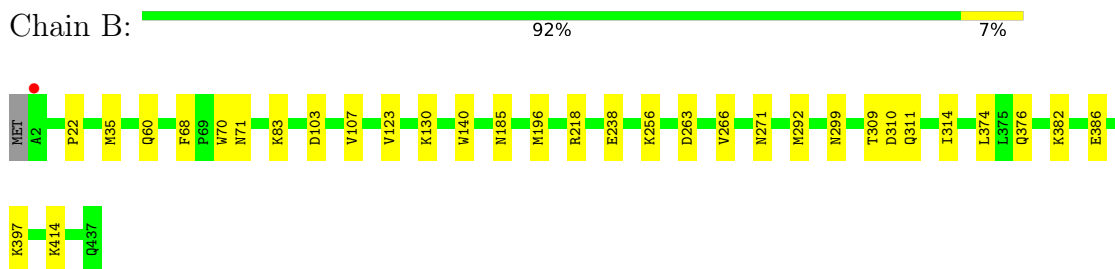
3 Residue-property plots [i](#)

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.

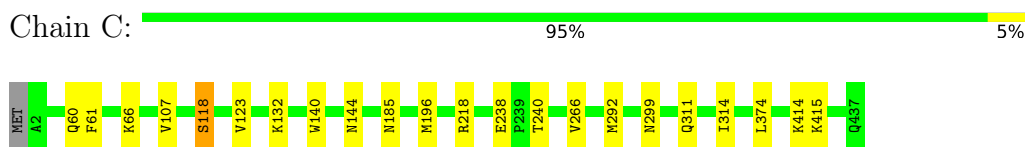
- Molecule 1: Xylose isomerase



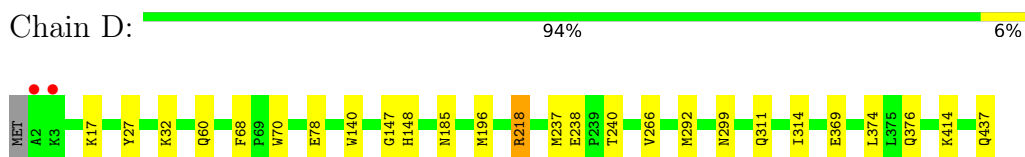
- Molecule 1: Xylose isomerase



- Molecule 1: Xylose isomerase



- Molecule 1: Xylose isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.60Å 79.37Å 91.98Å 115.46° 89.98° 117.13°	Depositor
Resolution (Å)	46.60 – 2.00 46.60 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.3 (46.60-2.00) 95.3 (46.60-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.149 , 0.185 0.158 , 0.191	Depositor DCC
R_{free} test set	5562 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.003 for k,h,-h-k-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15847	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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: XYP, YYS, CA, SO4, XLS

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	1.03	0/3552	1.27	0/4780
1	B	1.02	0/3552	1.25	1/4780 (0.0%)
1	C	1.02	0/3552	1.26	1/4780 (0.0%)
1	D	1.03	1/3576 (0.0%)	1.25	0/4810
All	All	1.03	1/14232 (0.0%)	1.26	2/19150 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	148	HIS	CE1-NE2	5.55	1.38	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	ASP	CA-CB-CG	5.04	117.64	112.60
1	C	415	LYS	CB-CA-C	-5.02	99.58	109.67

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	3471	0	3354	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3471	0	3354	19	0
1	C	3471	0	3354	11	0
1	D	3495	0	3378	19	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	10	0	8	2	0
3	B	10	0	8	2	0
3	C	10	0	8	1	0
3	D	10	0	8	1	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	20	0	0	0	0
4	D	20	0	0	0	0
5	A	20	0	20	0	0
5	B	30	0	30	1	0
5	C	10	0	10	0	0
5	D	20	0	20	0	0
6	A	10	0	0	3	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	10	0	0	1	0
7	A	415	0	0	13	0
7	B	433	0	0	5	0
7	C	424	0	0	3	0
7	D	449	0	0	6	0
All	All	15847	0	13552	78	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 (78) 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:437:GLN:OE1	7:A:601:HOH:O	1.71	1.06
1:B:196:MET:CE	7:B:944:HOH:O	2.14	0.96
1:A:196:MET:CE	7:A:921:HOH:O	2.20	0.89
1:B:271:ASN:HD21	1:B:309:THR:H	1.26	0.80
1:D:32:LYS:HE2	1:D:369:GLU:OE2	1.84	0.78
1:D:437:GLN:OE1	7:D:601:HOH:O	2.05	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:508:SO4:O4	7:A:602:HOH:O	2.11	0.66
1:A:196:MET:HE3	7:A:921:HOH:O	1.88	0.66
1:A:60:GLN:HG2	1:B:60:GLN:HG2	1.76	0.66
1:B:256:LYS:NZ	7:B:602:HOH:O	2.26	0.65
1:C:60:GLN:HG2	1:D:60:GLN:HG2	1.79	0.65
1:D:196[A]:MET:HE1	1:D:240:THR:HG22	1.79	0.64
6:A:508:SO4:O3	7:A:603:HOH:O	2.15	0.64
1:D:32:LYS:CE	1:D:369:GLU:OE2	2.45	0.64
1:B:196:MET:HE3	7:B:944:HOH:O	1.89	0.63
3:B:503:XLS:H1	7:B:610:HOH:O	1.98	0.63
1:A:196:MET:HE1	1:A:240:THR:HA	1.81	0.63
1:D:196[A]:MET:HE2	1:D:196[A]:MET:N	2.14	0.61
1:D:196[A]:MET:SD	1:D:240:THR:HA	2.42	0.59
6:D:509:SO4:O1	7:D:602:HOH:O	2.15	0.59
3:D:503:XLS:C1	7:D:806:HOH:O	2.50	0.58
1:A:3:LYS:C	1:A:3:LYS:HD3	2.29	0.58
1:C:196:MET:SD	1:C:240:THR:HA	2.44	0.57
1:A:107:VAL:HB	1:A:123:VAL:HG21	1.86	0.57
1:C:107:VAL:HB	1:C:123:VAL:HG21	1.87	0.56
1:B:263:ASP:OD2	7:B:601:HOH:O	2.18	0.56
7:A:656:HOH:O	1:D:237:MET:HE1	2.06	0.55
1:B:107:VAL:HB	1:B:123:VAL:HG21	1.86	0.55
1:A:18:ASP:OD2	7:A:604:HOH:O	2.18	0.54
1:A:437:GLN:CD	7:A:601:HOH:O	2.35	0.54
1:A:376:GLN:HG2	7:A:975:HOH:O	2.06	0.54
1:D:376:GLN:HG3	7:D:973:HOH:O	2.07	0.54
1:A:256:LYS:NZ	7:A:606:HOH:O	2.40	0.54
3:C:503:XLS:H1	7:C:732:HOH:O	2.09	0.52
1:B:382:LYS:HE2	1:B:386:GLU:OE2	2.11	0.51
1:C:66:LYS:NZ	7:C:607:HOH:O	2.42	0.49
3:A:503:XLS:H3	7:A:624:HOH:O	2.13	0.48
3:A:503:XLS:C1	7:A:675:HOH:O	2.61	0.48
3:B:503:XLS:O1	3:B:503:XLS:O3	2.24	0.48
1:C:118:SER:OG	7:C:601:HOH:O	2.19	0.47
1:C:299:ASN:HB2	1:C:311:GLN:O	2.15	0.47
1:D:437:GLN:CD	7:D:601:HOH:O	2.54	0.47
1:B:271:ASN:HD22	1:B:310:ASP:H	1.61	0.47
1:A:299:ASN:HB2	1:A:311:GLN:O	2.15	0.47
1:D:299:ASN:HB2	1:D:311:GLN:O	2.16	0.46
1:B:140:TRP:HB3	1:B:185:ASN:HB2	1.98	0.46
1:B:35:MET:HE3	1:B:376:GLN:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ASN:HB2	1:B:311:GLN:O	2.16	0.45
1:C:374:LEU:C	1:C:374:LEU:HD23	2.41	0.45
1:B:374:LEU:C	1:B:374:LEU:HD23	2.41	0.45
1:D:140:TRP:HB3	1:D:185:ASN:HB2	1.99	0.44
1:A:140:TRP:HB3	1:A:185:ASN:HB2	1.99	0.44
1:D:374:LEU:C	1:D:374:LEU:HD23	2.42	0.44
1:C:140:TRP:HB3	1:C:185:ASN:HB2	2.00	0.44
1:D:196[B]:MET:H	1:D:196[B]:MET:HG2	1.59	0.44
1:A:374:LEU:C	1:A:374:LEU:HD23	2.43	0.44
1:B:71:ASN:ND2	1:B:83:LYS:HD2	2.33	0.44
1:A:237:MET:HE1	7:D:610:HOH:O	2.18	0.43
1:A:266:VAL:HG22	1:A:292:MET:O	2.20	0.42
1:A:437:GLN:NE2	7:A:601:HOH:O	2.51	0.42
1:A:218:ARG:HH21	1:A:218:ARG:HD3	1.66	0.42
1:B:22:PRO:HG2	5:B:507:XYS:H1	2.01	0.42
1:D:266:VAL:HG22	1:D:292[A]:MET:O	2.20	0.42
1:A:35:MET:HE3	1:A:376:GLN:HG3	2.01	0.41
1:C:144:ASN:OD1	1:C:144:ASN:C	2.63	0.41
1:B:68:PHE:HB3	1:B:70:TRP:CE2	2.55	0.41
1:B:266:VAL:HG22	1:B:292:MET:O	2.21	0.41
1:C:266:VAL:HG22	1:C:292:MET:O	2.21	0.41
1:D:17:LYS:HG3	1:D:27:TYR:OH	2.21	0.41
1:A:68:PHE:HB3	1:A:70:TRP:CE2	2.56	0.41
1:C:61:PHE:O	1:D:147:GLY:HA2	2.21	0.41
1:D:68:PHE:HB3	1:D:70:TRP:CE2	2.56	0.41
1:A:75:ASP:HB3	1:A:78:GLU:HB2	2.03	0.40
1:A:351:GLU:N	6:A:508:SO4:O2	2.38	0.40
1:B:271:ASN:HD21	1:B:309:THR:N	2.05	0.40
1:B:271:ASN:ND2	1:B:309:THR:H	2.04	0.40
1:A:144:ASN:OD1	1:A:144:ASN:C	2.64	0.40
1:D:218:ARG:HH11	1:D:218:ARG:HD3	1.71	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	435/437 (100%)	429 (99%)	4 (1%)	2 (0%)	24	21
1	B	435/437 (100%)	428 (98%)	5 (1%)	2 (0%)	24	21
1	C	435/437 (100%)	425 (98%)	8 (2%)	2 (0%)	24	21
1	D	438/437 (100%)	429 (98%)	7 (2%)	2 (0%)	24	21
All	All	1743/1748 (100%)	1711 (98%)	24 (1%)	8 (0%)	24	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	GLU
1	B	238	GLU
1	C	238	GLU
1	D	238	GLU
1	A	314	ILE
1	C	314	ILE
1	D	314	ILE
1	B	314	ILE

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	357/357 (100%)	353 (99%)	4 (1%)	65	73
1	B	357/357 (100%)	353 (99%)	4 (1%)	65	73
1	C	357/357 (100%)	353 (99%)	4 (1%)	65	73
1	D	360/357 (101%)	357 (99%)	3 (1%)	73	80
All	All	1431/1428 (100%)	1416 (99%)	15 (1%)	65	75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	121	LYS
1	A	218	ARG
1	A	414	LYS
1	B	130	LYS
1	B	218	ARG
1	B	397	LYS
1	B	414	LYS
1	C	118	SER
1	C	132	LYS
1	C	218	ARG
1	C	414	LYS
1	D	78	GLU
1	D	218	ARG
1	D	414	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	203	GLN
1	A	311	GLN
1	A	437	GLN
1	B	71	ASN
1	B	82	GLN
1	B	131	GLN
1	B	203	GLN
1	B	271	ASN
1	B	416	ASN
1	C	8	GLN
1	C	131	GLN
1	C	203	GLN
1	C	243	GLN
1	D	82	GLN
1	D	131	GLN
1	D	203	GLN
1	D	259	ASN
1	D	416	ASN
1	D	437	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 8 are monoatomic - leaving 24 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	$\# Z > 2$
6	SO4	B	508	-	4,4,4	0.31	0	6,6,6	0.11	0
4	XYP	A	504	-	10,10,10	0.80	0	14,14,14	1.44	3 (21%)
4	XYP	D	504	-	10,10,10	0.53	0	14,14,14	1.28	3 (21%)
5	XYS	B	505	-	10,10,10	1.17	0	14,14,14	1.38	1 (7%)
6	SO4	D	508	-	4,4,4	0.28	0	6,6,6	0.16	0
6	SO4	D	509	-	4,4,4	0.35	0	6,6,6	0.10	0
4	XYP	D	507	-	10,10,10	0.50	0	14,14,14	1.77	3 (21%)
3	XLS	D	503	2	8,9,9	0.93	1 (12%)	10,11,11	3.43	8 (80%)
6	SO4	A	507	-	4,4,4	0.31	0	6,6,6	0.09	0
5	XYS	D	506	-	10,10,10	1.23	1 (10%)	14,14,14	0.97	1 (7%)
5	XYS	A	505	-	10,10,10	1.24	1 (10%)	14,14,14	1.00	0
5	XYS	B	507	-	10,10,10	0.87	0	14,14,14	2.33	5 (35%)
3	XLS	A	503	2	8,9,9	1.02	1 (12%)	10,11,11	2.96	7 (70%)
3	XLS	C	503	2	8,9,9	1.56	2 (25%)	10,11,11	3.75	9 (90%)
6	SO4	A	508	-	4,4,4	0.34	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	C	507	-	4,4,4	0.35	0	6,6,6	0.11	0
5	XYS	C	505	-	10,10,10	1.22	1 (10%)	14,14,14	1.24	0
5	XYS	A	506	-	10,10,10	0.45	0	14,14,14	1.80	2 (14%)
5	XYS	D	505	-	10,10,10	1.29	1 (10%)	14,14,14	1.19	2 (14%)
3	XLS	B	503	2	8,9,9	0.99	1 (12%)	10,11,11	3.85	9 (90%)
4	XYP	C	504	-	10,10,10	0.77	0	14,14,14	1.21	1 (7%)
4	XYP	B	504	-	10,10,10	0.85	0	14,14,14	1.17	1 (7%)
4	XYP	C	506	-	10,10,10	0.74	0	14,14,14	1.45	4 (28%)
5	XYS	B	506	-	10,10,10	1.26	1 (10%)	14,14,14	1.24	1 (7%)

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
5	XYS	A	506	-	-	-	0/1/1/1
5	XYS	C	505	-	-	-	0/1/1/1
3	XLS	D	503	2	-	5/11/12/12	-
3	XLS	B	503	2	-	5/11/12/12	-
5	XYS	D	506	-	-	-	0/1/1/1
4	XYP	A	504	-	-	-	0/1/1/1
4	XYP	D	504	-	-	-	0/1/1/1
5	XYS	A	505	-	-	-	0/1/1/1
5	XYS	B	505	-	-	-	0/1/1/1
5	XYS	B	507	-	-	-	0/1/1/1
3	XLS	A	503	2	-	10/11/12/12	-
4	XYP	C	504	-	-	-	0/1/1/1
5	XYS	D	505	-	-	-	0/1/1/1
4	XYP	B	504	-	-	-	0/1/1/1
3	XLS	C	503	2	-	7/11/12/12	-
4	XYP	C	506	-	-	-	0/1/1/1
5	XYS	B	506	-	-	-	0/1/1/1
4	XYP	D	507	-	-	-	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	505	XYS	C4-C3	3.08	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	XLS	O3-C3	3.05	1.50	1.43
3	A	503	XLS	C3-C2	-2.63	1.49	1.53
5	D	506	XYS	O1-C1	2.43	1.47	1.39
5	B	506	XYS	O5-C1	2.37	1.47	1.43
3	D	503	XLS	C3-C2	-2.35	1.49	1.53
5	C	505	XYS	C4-C3	2.33	1.56	1.52
3	B	503	XLS	O3-C3	2.17	1.48	1.43
3	C	503	XLS	C4-C3	2.10	1.57	1.53
5	A	505	XYS	O1-C1	2.08	1.46	1.39

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	503	XLS	C5-C4-C3	-5.85	100.25	112.17
3	B	503	XLS	O4-C4-C3	5.70	122.58	109.25
3	C	503	XLS	O3-C3-C4	5.47	121.35	108.93
3	B	503	XLS	C5-C4-C3	-5.27	101.44	112.17
3	C	503	XLS	O4-C4-C3	4.95	120.84	109.25
3	B	503	XLS	O3-C3-C2	4.92	118.27	109.13
3	D	503	XLS	O4-C4-C5	4.83	120.01	109.03
3	A	503	XLS	O2-C2-C1	4.62	120.99	110.48
3	B	503	XLS	O3-C3-C4	4.38	118.88	108.93
3	C	503	XLS	C5-C4-C3	-4.36	103.28	112.17
3	C	503	XLS	O2-C2-C3	4.34	119.63	109.46
5	B	507	XYS	O4-C4-C3	4.26	118.98	110.15
3	D	503	XLS	O5-C5-C4	-4.15	102.43	111.16
3	A	503	XLS	O4-C4-C5	4.08	118.30	109.03
5	A	506	XYS	C5-O5-C1	4.06	120.89	112.46
3	C	503	XLS	O5-C5-C4	-3.92	102.93	111.16
3	C	503	XLS	O3-C3-C2	3.88	116.35	109.13
5	B	507	XYS	O5-C5-C4	-3.83	101.66	110.79
3	A	503	XLS	O5-C5-C4	-3.82	103.13	111.16
5	A	506	XYS	C5-C4-C3	-3.78	104.15	109.64
3	A	503	XLS	C5-C4-C3	-3.67	104.69	112.17
5	B	507	XYS	C5-C4-C3	-3.64	104.34	109.64
3	B	503	XLS	O2-C2-C3	3.58	117.85	109.46
5	B	507	XYS	O3-C3-C2	-3.56	101.97	110.38
3	D	503	XLS	C3-C2-C1	-3.54	100.26	111.03
4	D	507	XYP	O3-C3-C4	3.36	116.92	110.05
3	B	503	XLS	O2-C2-C1	3.27	117.90	110.48
3	D	503	XLS	O2-C2-C1	3.06	117.44	110.48
4	A	504	XYP	C4-C3-C2	-2.96	105.65	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	XLS	C3-C2-C1	-2.87	102.29	111.03
4	D	507	XYP	C5-C4-C3	-2.87	105.47	109.64
4	D	507	XYP	C4-C3-C2	-2.84	105.87	110.86
5	B	505	XYS	O2-C2-C1	-2.78	102.83	109.25
3	B	503	XLS	O4-C4-C5	2.77	115.32	109.03
4	C	504	XYP	C4-C3-C2	-2.74	106.04	110.86
5	B	507	XYS	C1-C2-C3	2.73	115.91	110.36
3	A	503	XLS	C3-C2-C1	-2.60	103.12	111.03
3	A	503	XLS	C4-C3-C2	-2.59	106.52	112.70
3	A	503	XLS	O3-C3-C4	2.51	114.63	108.93
4	A	504	XYP	O4-C4-C5	2.50	114.95	109.22
4	C	506	XYP	C5-C4-C3	-2.49	106.01	109.64
4	D	504	XYP	C4-C3-C2	-2.49	106.48	110.86
3	D	503	XLS	O4-C4-C3	2.49	115.07	109.25
3	C	503	XLS	C3-C2-C1	-2.45	103.59	111.03
4	C	506	XYP	C4-C3-C2	-2.40	106.65	110.86
3	D	503	XLS	O3-C3-C4	2.36	114.28	108.93
4	D	504	XYP	C5-O5-C1	2.32	117.28	112.46
3	D	503	XLS	O2-C2-C3	2.32	114.89	109.46
3	C	503	XLS	O4-C4-C5	2.31	114.28	109.03
4	D	504	XYP	C1-C2-C3	-2.31	105.65	110.36
5	D	506	XYS	O1-C1-O5	2.27	115.72	109.91
4	B	504	XYP	C5-O5-C1	-2.27	107.75	112.46
3	B	503	XLS	O5-C5-C4	-2.26	106.41	111.16
5	D	505	XYS	O4-C4-C3	2.25	114.81	110.15
4	A	504	XYP	O4-C4-C3	-2.19	105.61	110.15
4	C	506	XYP	O3-C3-C4	2.15	114.44	110.05
5	D	505	XYS	O3-C3-C2	-2.11	105.40	110.38
5	B	506	XYS	O4-C4-C5	2.07	113.97	109.22
4	C	506	XYP	O5-C1-C2	-2.05	103.96	109.94
3	C	503	XLS	O2-C2-C1	2.04	115.11	110.48

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	XLS	C1-C2-C3-C4
3	B	503	XLS	C1-C2-C3-O3
3	B	503	XLS	O2-C2-C3-O3
3	C	503	XLS	O1-C1-C2-C3
3	C	503	XLS	C1-C2-C3-O3
3	C	503	XLS	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	D	503	XLS	C1-C2-C3-C4
3	C	503	XLS	C3-C4-C5-O5
3	A	503	XLS	O3-C3-C4-C5
3	A	503	XLS	C2-C3-C4-C5
3	B	503	XLS	O3-C3-C4-O4
3	A	503	XLS	C3-C4-C5-O5
3	B	503	XLS	C3-C4-C5-O5
3	D	503	XLS	C3-C4-C5-O5
3	A	503	XLS	O2-C2-C3-O3
3	A	503	XLS	O3-C3-C4-O4
3	A	503	XLS	O2-C2-C3-C4
3	A	503	XLS	O4-C4-C5-O5
3	A	503	XLS	C1-C2-C3-O3
3	D	503	XLS	C2-C3-C4-C5
3	B	503	XLS	O3-C3-C4-C5
3	C	503	XLS	O4-C4-C5-O5
3	C	503	XLS	O2-C2-C3-C4
3	C	503	XLS	O3-C3-C4-O4
3	D	503	XLS	O3-C3-C4-C5
3	A	503	XLS	C2-C3-C4-O4
3	D	503	XLS	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	509	SO4	1	0
3	D	503	XLS	1	0
5	B	507	XYS	1	0
3	A	503	XLS	2	0
3	C	503	XLS	1	0
6	A	508	SO4	3	0
3	B	503	XLS	2	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	436/437 (99%)	-0.35	2 (0%) 87 87	11, 20, 34, 54	1 (0%)
1	B	436/437 (99%)	-0.37	1 (0%) 91 90	11, 20, 33, 60	1 (0%)
1	C	436/437 (99%)	-0.42	0 100 100	10, 18, 32, 45	1 (0%)
1	D	436/437 (99%)	-0.43	2 (0%) 87 87	8, 19, 33, 62	4 (0%)
All	All	1744/1748 (99%)	-0.39	5 (0%) 90 89	8, 19, 33, 62	7 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	5.1
1	D	2	ALA	4.1
1	B	2	ALA	3.8
1	D	3	LYS	2.7
1	A	3	LYS	2.5

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
6	SO4	C	507	5/5	0.70	0.17	66,68,71,72	0
4	XYP	C	506	10/10	0.76	0.14	58,66,69,70	0
4	XYP	D	507	10/10	0.77	0.14	51,56,59,61	0
5	XYS	B	507	10/10	0.78	0.12	47,49,51,56	0
6	SO4	A	508	5/5	0.79	0.13	62,63,72,74	0
6	SO4	D	509	5/5	0.80	0.12	56,63,67,68	0
4	XYP	B	504	10/10	0.81	0.12	52,58,59,59	0
5	XYS	A	505	10/10	0.81	0.12	41,47,49,50	0
4	XYP	D	504	10/10	0.82	0.11	46,53,55,59	0
5	XYS	A	506	10/10	0.83	0.11	59,62,63,63	0
4	XYP	C	504	10/10	0.85	0.10	45,50,52,54	0
5	XYS	B	505	10/10	0.86	0.11	36,42,43,43	0
5	XYS	D	505	10/10	0.88	0.10	32,37,38,38	0
4	XYP	A	504	10/10	0.88	0.10	42,47,53,54	0
5	XYS	B	506	10/10	0.88	0.09	31,34,37,40	0
3	XLS	D	503	10/10	0.88	0.12	26,32,36,40	0
6	SO4	A	507	5/5	0.89	0.12	69,70,74,77	0
3	XLS	C	503	10/10	0.89	0.09	27,31,36,37	0
3	XLS	A	503	10/10	0.89	0.10	29,32,34,36	0
6	SO4	D	508	5/5	0.89	0.10	47,49,53,56	0
5	XYS	D	506	10/10	0.89	0.09	33,36,38,42	0
3	XLS	B	503	10/10	0.90	0.10	31,35,40,43	0
5	XYS	C	505	10/10	0.91	0.09	32,36,36,37	0
6	SO4	B	508	5/5	0.94	0.17	40,41,46,46	0
2	CA	D	502	1/1	0.99	0.01	20,20,20,20	0
2	CA	A	501	1/1	0.99	0.05	16,16,16,16	0
2	CA	A	502	1/1	0.99	0.03	21,21,21,21	0
2	CA	B	502	1/1	0.99	0.03	21,21,21,21	0
2	CA	C	502	1/1	0.99	0.03	18,18,18,18	0
2	CA	B	501	1/1	1.00	0.02	16,16,16,16	0
2	CA	D	501	1/1	1.00	0.02	15,15,15,15	0
2	CA	C	501	1/1	1.00	0.04	13,13,13,13	0

6.5 Other polymers ⓘ

There are no such residues in this entry.