



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:45 PM EDT

PDB ID : 3WN6 / pdb_00003wn6
Title : Crystal structure of alpha-amylase AmyI-1 from Oryza sativa
Authors : Ochiai, A.; Sugai, H.; Harada, K.; Tanaka, S.; Ishiyama, Y.; Ito, K.; Tanaka, T.; Uchiumi, T.; Taniguchi, M.; Mitsui, T.
Deposited on : 2013-12-05
Resolution : 2.16 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

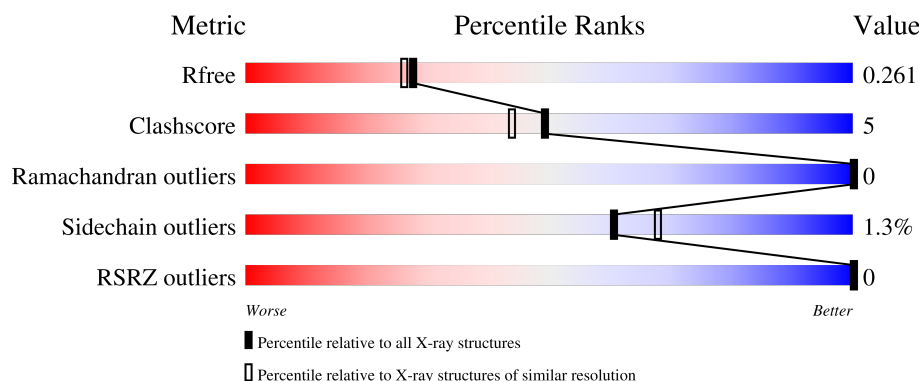
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	404	90% 10%
1	B	404	92% 7%
1	C	404	91% 8%
1	D	404	88% 11%

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
4	TAR	C	506	-	X	X	-
4	TAR	C	507	-	-	X	-
5	PEG	D	508	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14765 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 Alpha-amylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	3	0
			3222	2058	552	598	14			
1	B	404	Total	C	N	O	S	0	10	0
			3280	2087	564	616	13			
1	C	404	Total	C	N	O	S	0	1	0
			3209	2047	550	599	13			
1	D	404	Total	C	N	O	S	0	6	0
			3249	2071	559	606	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	GLY	engineered mutation	UNP P17654
B	25	MET	GLY	engineered mutation	UNP P17654
C	25	MET	GLY	engineered mutation	UNP P17654
D	25	MET	GLY	engineered mutation	UNP P17654

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

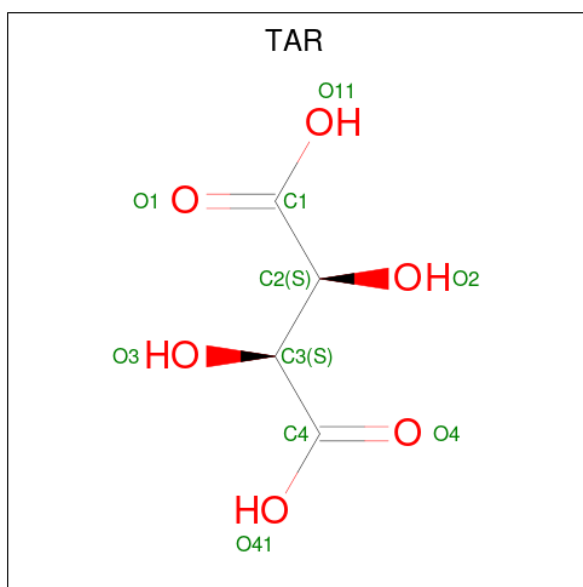
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ca	0	0
			3	3		
2	B	3	Total	Ca	0	0
			3	3		
2	C	3	Total	Ca	0	0
			3	3		
2	D	3	Total	Ca	0	0
			3	3		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	4	6		
4	A	1	Total	C	O	0	0
			10	4	6		
4	B	1	Total	C	O	0	0
			10	4	6		
4	C	1	Total	C	O	0	0
			10	4	6		
4	C	1	Total	C	O	0	0
			10	4	6		
4	D	1	Total	C	O	0	0
			10	4	6		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

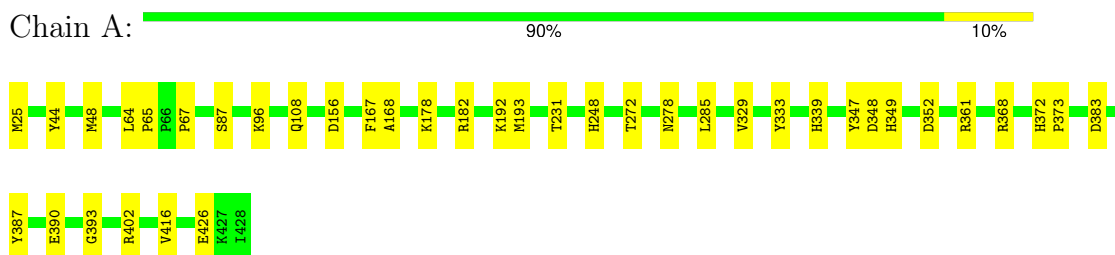
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	405	Total	O	0	0
			405	405		
6	B	420	Total	O	0	0
			420	420		
6	C	393	Total	O	0	0
			393	393		
6	D	412	Total	O	0	0
			412	412		

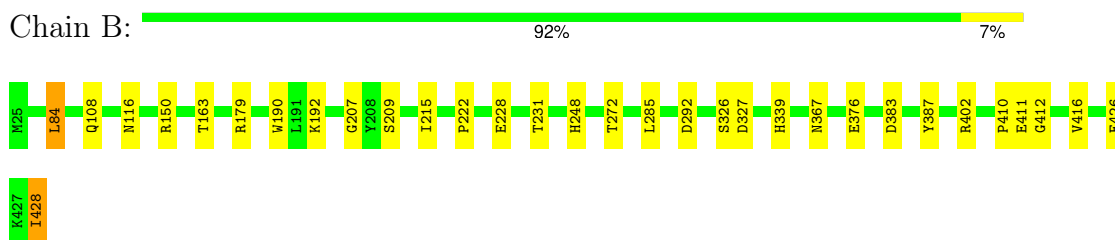
3 Residue-property plots

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.

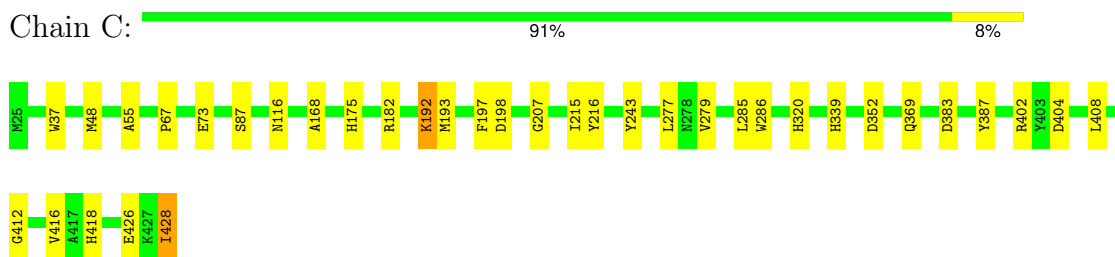
- Molecule 1: Alpha-amylase



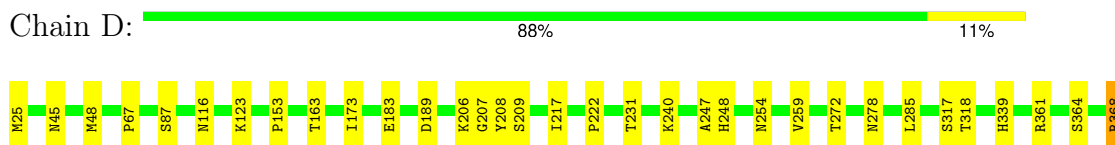
- Molecule 1: Alpha-amylase



- Molecule 1: Alpha-amylase



- Molecule 1: Alpha-amylase



I371	H372	P373	E376	D383	Y387	R402	P410	E411	G412	V416	A417	H418	E426	K427	I428
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.92Å 125.28Å 96.64Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	48.32 – 2.16 48.32 – 2.16	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.32-2.16) 98.7 (48.32-2.16)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.199 , 0.243 0.219 , 0.261	Depositor DCC
R_{free} test set	4462 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.288 for h,-k,-l	Xtriage
Reported twinning fraction	0.551 for H, K, L 0.449 for h,-k,-l	Depositor
Outliers	18 of 88953 reflections (0.020%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14765	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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 61.61 % 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 1.2758e-05. 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: CA, PEG, TAR, 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	0.90	0/3326	0.91	0/4520
1	B	0.89	0/3378	0.90	0/4592
1	C	0.92	0/3307	0.92	0/4496
1	D	0.93	0/3347	0.92	2/4548 (0.0%)
All	All	0.91	0/13358	0.91	2/18156 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	368	ARG	CB-CA-C	-6.40	98.80	110.63
1	D	368	ARG	CG-CD-NE	5.12	123.25	112.00

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	3222	0	3045	33	0
1	B	3280	0	3081	23	0
1	C	3209	0	3020	32	0
1	D	3249	0	3064	39	2
2	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	12	0	16	1	0
3	B	18	0	24	2	0
3	C	12	0	16	5	0
3	D	12	0	16	4	0
4	A	20	0	8	1	0
4	B	10	0	4	0	0
4	C	20	0	8	5	0
4	D	10	0	4	1	0
5	A	14	0	20	3	0
5	B	7	0	10	0	0
5	D	28	0	40	5	0
6	A	405	0	0	22	2
6	B	420	0	0	10	0
6	C	393	0	0	20	0
6	D	412	0	0	21	0
All	All	14765	0	12376	139	2

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 (139) 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:348:ASP:HA	6:A:946:HOH:O	1.41	1.15
1:B:150[B]:ARG:HH11	1:B:150[B]:ARG:HG2	0.96	1.08
1:D:217:ILE:HA	6:D:827:HOH:O	1.62	0.96
1:D:418:HIS:CG	6:D:856:HOH:O	2.18	0.95
1:B:150[B]:ARG:HH11	1:B:150[B]:ARG:CG	1.80	0.93
1:B:150[B]:ARG:HG2	1:B:150[B]:ARG:NH1	1.76	0.92
1:D:318:THR:HG23	6:D:875:HOH:O	1.74	0.87
4:C:506:TAR:O4	4:C:507:TAR:O1	1.93	0.86
4:C:506:TAR:H2	6:C:603:HOH:O	1.75	0.85
1:C:73:GLU:HB2	6:C:869:HOH:O	1.81	0.81
3:D:505:GOL:H32	6:D:602:HOH:O	1.82	0.79
1:C:37:TRP:CE2	6:C:869:HOH:O	2.37	0.77
1:D:418:HIS:CD2	6:D:856:HOH:O	2.37	0.75
1:A:96[B]:LYS:NZ	6:A:809:HOH:O	2.17	0.74
1:D:418:HIS:CE1	6:D:856:HOH:O	2.41	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ASP:OD2	6:A:946:HOH:O	2.06	0.73
1:A:361:ARG:HD3	6:A:850:HOH:O	1.87	0.73
1:D:418:HIS:ND1	6:D:856:HOH:O	2.22	0.70
1:C:418:HIS:CE1	3:C:505:GOL:H2	2.26	0.69
1:A:368:ARG:HD3	6:A:848:HOH:O	1.91	0.69
1:C:192:LYS:HD2	1:C:197:PHE:O	1.93	0.69
1:B:327:ASP:OD2	6:B:755:HOH:O	2.12	0.68
1:A:182:ARG:NH2	6:A:997:HOH:O	2.27	0.66
1:A:156:ASP:OD2	6:A:936:HOH:O	2.13	0.66
3:D:504:GOL:H2	6:D:604:HOH:O	1.97	0.65
1:A:178:LYS:NZ	6:A:974:HOH:O	2.26	0.65
1:C:404:ASP:OD2	6:C:716:HOH:O	2.15	0.65
4:C:506:TAR:C4	4:C:507:TAR:O1	2.46	0.64
1:C:55:ALA:O	6:C:671:HOH:O	2.15	0.63
1:C:418:HIS:CD2	6:C:923:HOH:O	2.51	0.63
1:C:37:TRP:NE1	6:C:869:HOH:O	2.32	0.62
1:C:175:HIS:HD2	1:C:216:TYR:OH	1.81	0.62
1:B:410:PRO:HB3	6:B:1015:HOH:O	1.99	0.62
1:A:182:ARG:NE	6:A:955:HOH:O	2.34	0.61
1:C:192:LYS:HG3	1:C:193:MET:N	2.12	0.61
1:C:182:ARG:HB2	6:C:760:HOH:O	2.01	0.60
1:B:179:ARG:HH12	3:B:506:GOL:H31	1.66	0.60
1:D:364[B]:SER:O	1:D:368:ARG:HG3	2.02	0.60
4:D:506:TAR:C1	6:D:948:HOH:O	2.50	0.60
1:D:318:THR:N	6:D:875:HOH:O	2.35	0.60
4:C:506:TAR:O41	4:C:507:TAR:C1	2.50	0.59
1:D:25:MET:HG3	1:D:371:ILE:O	2.01	0.59
3:D:504:GOL:C2	6:D:604:HOH:O	2.49	0.59
1:A:25:MET:HE1	6:D:858:HOH:O	2.03	0.59
1:A:108:GLN:NE2	6:A:719:HOH:O	2.37	0.58
1:D:317:SER:C	6:D:875:HOH:O	2.46	0.58
1:C:198:ASP:O	6:C:724:HOH:O	2.17	0.57
1:B:248:HIS:HD2	1:B:272:THR:OG1	1.87	0.57
1:A:352:ASP:CG	6:A:946:HOH:O	2.47	0.57
1:A:248:HIS:HD2	1:A:272:THR:OG1	1.87	0.56
1:B:192:LYS:HD3	6:B:987:HOH:O	2.06	0.56
1:D:248:HIS:HD2	1:D:272:THR:OG1	1.88	0.55
1:B:411:GLU:H	1:B:411:GLU:CD	2.14	0.55
1:C:182:ARG:NE	6:C:873:HOH:O	2.28	0.54
1:C:352:ASP:OD2	6:C:749:HOH:O	2.18	0.54
1:D:411:GLU:CD	1:D:411:GLU:H	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:506:TAR:C4	4:C:507:TAR:C1	2.87	0.53
3:D:505:GOL:C3	6:D:602:HOH:O	2.48	0.53
1:D:45:ASN:O	1:D:48:MET:HB2	2.09	0.53
1:B:231:THR:O	1:B:248:HIS:HE1	1.93	0.52
1:B:222:PRO:HA	6:B:987:HOH:O	2.09	0.52
1:C:37:TRP:CZ2	6:C:869:HOH:O	2.61	0.52
1:D:206:LYS:HA	5:D:508:PEG:C1	2.40	0.52
1:D:116:ASN:ND2	1:D:207:GLY:HA3	2.25	0.52
1:C:286:TRP:HB2	1:D:247:ALA:HB2	1.92	0.51
1:C:48:MET:HE2	6:C:976:HOH:O	2.09	0.51
1:D:412:GLY:O	1:D:428:ILE:N	2.35	0.51
1:B:367[B]:ASN:ND2	6:B:802:HOH:O	2.43	0.50
1:C:243:TYR:H	1:D:254:ASN:HD21	1.58	0.50
1:A:231:THR:O	1:A:248:HIS:HE1	1.95	0.49
1:A:48:MET:HE2	6:A:834:HOH:O	2.11	0.49
1:D:231:THR:O	1:D:248:HIS:HE1	1.95	0.49
1:B:163:THR:HB	1:B:209[A]:SER:OG	2.13	0.49
1:C:412:GLY:O	1:C:428:ILE:N	2.35	0.49
1:D:410:PRO:HB3	6:D:959:HOH:O	2.12	0.48
1:A:48:MET:CE	6:A:834:HOH:O	2.61	0.48
1:A:339:HIS:HE1	1:A:387:TYR:OH	1.95	0.48
1:C:416:VAL:HG21	1:C:426:GLU:HG3	1.96	0.48
1:A:193[A]:MET:HG2	6:A:878:HOH:O	2.13	0.48
1:B:339:HIS:HE1	1:B:387:TYR:OH	1.96	0.48
1:D:416:VAL:HG21	1:D:426:GLU:HG3	1.96	0.48
1:A:416:VAL:HG21	1:A:426:GLU:HG3	1.96	0.48
1:B:412:GLY:O	1:B:428:ILE:N	2.34	0.48
1:C:168:ALA:HB1	6:C:802:HOH:O	2.13	0.47
1:D:163:THR:O	5:D:508:PEG:H41	2.15	0.47
1:B:326:SER:N	6:B:716:HOH:O	2.22	0.47
1:B:416:VAL:HG21	1:B:426:GLU:HG3	1.96	0.47
1:D:361:ARG:NH2	6:D:977:HOH:O	2.37	0.47
1:C:243:TYR:H	1:D:254:ASN:ND2	2.13	0.47
1:D:339:HIS:HE1	1:D:387:TYR:OH	1.97	0.47
1:A:278:ASN:HB3	5:A:509:PEG:C4	2.44	0.47
1:C:116:ASN:ND2	1:C:207:GLY:HA3	2.30	0.47
1:C:339:HIS:HE1	1:C:387:TYR:OH	1.97	0.47
3:C:504:GOL:C1	6:C:602:HOH:O	2.62	0.47
1:A:347:TYR:HD1	6:A:946:HOH:O	1.98	0.46
1:C:320:HIS:CG	6:C:658:HOH:O	2.67	0.46
1:B:228:GLU:HG3	6:B:635:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:506:GOL:H2	6:B:771:HOH:O	2.14	0.46
1:A:278:ASN:HB3	5:A:509:PEG:H41	1.98	0.45
1:B:116:ASN:ND2	1:B:207:GLY:HA3	2.31	0.45
3:C:504:GOL:H11	6:C:602:HOH:O	2.16	0.45
1:D:163:THR:HB	1:D:209[B]:SER:OG	2.16	0.45
4:A:506:TAR:O11	4:A:506:TAR:C4	2.65	0.45
1:A:333:TYR:OH	1:A:349:HIS:HD2	1.99	0.44
6:A:713:HOH:O	1:D:240:LYS:HD3	2.17	0.44
1:B:108:GLN:OE1	6:B:950:HOH:O	2.21	0.44
3:A:505:GOL:H2	6:A:603:HOH:O	2.18	0.43
1:D:372:HIS:HB2	1:D:373:PRO:CD	2.49	0.43
1:D:123:LYS:HE2	6:D:794:HOH:O	2.18	0.43
1:D:163:THR:O	5:D:508:PEG:C4	2.67	0.43
1:C:408:LEU:HD21	6:C:824:HOH:O	2.18	0.42
1:A:168:ALA:HB1	6:A:779:HOH:O	2.18	0.42
1:C:418:HIS:HE1	3:C:505:GOL:H2	1.77	0.42
1:D:217:ILE:HG12	6:D:827:HOH:O	2.18	0.42
1:C:285:LEU:HB2	1:C:383:ASP:O	2.20	0.42
1:C:67:PRO:O	1:C:87:SER:HB2	2.20	0.41
1:A:167:PHE:CD1	6:A:798:HOH:O	2.72	0.41
1:C:418:HIS:CE1	3:C:505:GOL:H12	2.56	0.41
1:B:285:LEU:HB2	1:B:383:ASP:O	2.20	0.41
1:A:372:HIS:HB2	1:A:373:PRO:CD	2.50	0.41
1:C:279:VAL:CG2	6:C:781:HOH:O	2.69	0.41
1:D:153:PRO:HA	5:D:510:PEG:H21	2.02	0.41
1:D:173:ILE:HG13	6:D:611:HOH:O	2.21	0.41
1:D:278:ASN:HB3	6:D:885:HOH:O	2.21	0.41
1:A:67:PRO:O	1:A:87:SER:HB2	2.21	0.41
1:D:285:LEU:HB2	1:D:383:ASP:O	2.20	0.41
1:A:44:TYR:OH	6:A:610:HOH:O	2.22	0.41
1:A:285:LEU:HB2	1:A:383:ASP:O	2.20	0.41
1:A:390:GLU:OE2	1:A:393:GLY:HA2	2.21	0.41
1:C:369:GLN:NE2	6:C:971:HOH:O	2.54	0.41
6:A:713:HOH:O	1:D:240:LYS:HE2	2.20	0.40
1:D:67:PRO:O	1:D:87:SER:HB2	2.21	0.40
1:D:208:TYR:O	5:D:508:PEG:H11	2.21	0.40
1:B:84:LEU:HD22	1:B:190:TRP:CH2	2.56	0.40
1:B:292:ASP:OD2	6:B:966:HOH:O	2.21	0.40
1:A:64:LEU:HB3	1:A:65:PRO:HD2	2.02	0.40
1:A:168:ALA:HB2	6:A:771:HOH:O	2.21	0.40
1:A:278:ASN:HB3	5:A:509:PEG:H32	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:PRO:HG3	6:D:827:HOH:O	2.22	0.40

All (2) 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)
1:D:189:ASP:OD2	6:A:955:HOH:O[2_645]	2.14	0.06
1:D:183:GLU:OE2	6:A:884:HOH:O[2_645]	2.16	0.04

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	405/404 (100%)	388 (96%)	17 (4%)	0	100	100
1	B	412/404 (102%)	395 (96%)	17 (4%)	0	100	100
1	C	403/404 (100%)	387 (96%)	16 (4%)	0	100	100
1	D	408/404 (101%)	386 (95%)	22 (5%)	0	100	100
All	All	1628/1616 (101%)	1556 (96%)	72 (4%)	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	329/326 (101%)	326 (99%)	3 (1%)	70	77
1	B	336/326 (103%)	330 (98%)	6 (2%)	51	58
1	C	327/326 (100%)	322 (98%)	5 (2%)	57	64
1	D	332/326 (102%)	328 (99%)	4 (1%)	63	70
All	All	1324/1304 (102%)	1306 (99%)	18 (1%)	61	66

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	LYS
1	A	329	VAL
1	A	402	ARG
1	B	84	LEU
1	B	215[A]	ILE
1	B	215[B]	ILE
1	B	376	GLU
1	B	402	ARG
1	B	428	ILE
1	C	192	LYS
1	C	215	ILE
1	C	277	LEU
1	C	402	ARG
1	C	428	ILE
1	D	259	VAL
1	D	376	GLU
1	D	402	ARG
1	D	428	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	235	ASN
1	A	248	HIS
1	A	265	ASN
1	A	278	ASN
1	A	339	HIS
1	A	349	HIS
1	B	108	GLN
1	B	181	GLN

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Mol	Chain	Res	Type
1	B	235	ASN
1	B	246	ASN
1	B	248	HIS
1	B	265	ASN
1	B	278	ASN
1	B	339	HIS
1	B	372	HIS
1	B	407	HIS
1	C	108	GLN
1	C	175	HIS
1	C	235	ASN
1	C	278	ASN
1	C	339	HIS
1	C	418	HIS
1	D	108	GLN
1	D	116	ASN
1	D	242	ASN
1	D	248	HIS
1	D	250	GLN
1	D	254	ASN
1	D	278	ASN
1	D	339	HIS

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](#)

Of 34 ligands modelled in this entry, 12 are monoatomic - leaving 22 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	TAR	C	506	-	9,9,9	1.46	1 (11%)	12,12,12	1.71	4 (33%)
3	GOL	B	504	-	5,5,5	0.54	0	5,5,5	0.54	0
4	TAR	C	507	-	9,9,9	1.91	2 (22%)	12,12,12	1.96	5 (41%)
5	PEG	D	510	-	6,6,6	0.61	0	5,5,5	0.45	0
3	GOL	A	504	-	5,5,5	0.91	0	5,5,5	1.43	0
5	PEG	D	509	-	6,6,6	0.53	0	5,5,5	0.41	0
5	PEG	B	508	-	6,6,6	0.46	0	5,5,5	0.46	0
5	PEG	A	509	-	6,6,6	0.75	0	5,5,5	0.14	0
5	PEG	D	508	-	6,6,6	0.52	0	5,5,5	0.36	0
3	GOL	C	505	-	5,5,5	0.76	0	5,5,5	0.91	0
4	TAR	A	507	-	9,9,9	1.16	0	12,12,12	1.13	1 (8%)
3	GOL	B	506	-	5,5,5	0.48	0	5,5,5	0.94	0
3	GOL	B	505	-	5,5,5	0.73	0	5,5,5	0.33	0
4	TAR	D	506	-	9,9,9	1.18	0	12,12,12	0.96	1 (8%)
3	GOL	D	505	-	5,5,5	0.28	0	5,5,5	0.70	0
3	GOL	C	504	-	5,5,5	0.55	0	5,5,5	0.50	0
4	TAR	B	507	-	9,9,9	1.12	0	12,12,12	0.96	1 (8%)
5	PEG	D	507	-	6,6,6	0.63	0	5,5,5	0.46	0
3	GOL	A	505	-	5,5,5	0.66	0	5,5,5	0.58	0
5	PEG	A	508	-	6,6,6	0.58	0	5,5,5	0.71	0
3	GOL	D	504	-	5,5,5	0.44	0	5,5,5	0.50	0
4	TAR	A	506	-	9,9,9	1.38	1 (11%)	12,12,12	1.25	1 (8%)

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
4	TAR	C	506	-	-	10/12/12/12	-
3	GOL	B	504	-	-	4/4/4/4	-
4	TAR	C	507	-	-	4/12/12/12	-
5	PEG	D	510	-	-	1/4/4/4	-
3	GOL	A	504	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	D	509	-	-	2/4/4/4	-
5	PEG	B	508	-	-	3/4/4/4	-
5	PEG	A	509	-	-	3/4/4/4	-
5	PEG	D	508	-	-	2/4/4/4	-
3	GOL	C	505	-	-	4/4/4/4	-
4	TAR	A	507	-	-	8/12/12/12	-
3	GOL	B	506	-	-	4/4/4/4	-
3	GOL	B	505	-	-	4/4/4/4	-
4	TAR	D	506	-	-	6/12/12/12	-
3	GOL	D	505	-	-	0/4/4/4	-
3	GOL	C	504	-	-	2/4/4/4	-
4	TAR	B	507	-	-	6/12/12/12	-
5	PEG	D	507	-	-	4/4/4/4	-
3	GOL	A	505	-	-	4/4/4/4	-
5	PEG	A	508	-	-	3/4/4/4	-
3	GOL	D	504	-	-	3/4/4/4	-
4	TAR	A	506	-	-	5/12/12/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	507	TAR	C3-C4	-3.56	1.47	1.52
4	C	507	TAR	C2-C1	-3.14	1.48	1.52
4	C	506	TAR	C3-C4	-2.98	1.48	1.52
4	A	506	TAR	C3-C4	-2.57	1.49	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	506	TAR	C2-C3-C4	-3.94	101.09	109.82
4	C	507	TAR	O2-C2-C1	-3.25	103.74	110.69
4	C	507	TAR	O4-C4-C3	-2.64	114.58	121.62
4	A	507	TAR	O11-C1-C2	2.53	120.34	113.31
4	B	507	TAR	O41-C4-C3	2.30	119.71	113.31
4	D	506	TAR	O41-C4-C3	2.26	119.60	113.31
4	C	507	TAR	C2-C3-C4	-2.24	104.86	109.82
4	C	506	TAR	O11-C1-C2	2.16	119.30	113.31
4	A	506	TAR	O11-C1-C2	2.14	119.26	113.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	507	TAR	O11-C1-C2	2.13	119.24	113.31
4	C	506	TAR	O3-C3-C2	2.12	114.48	110.17
4	C	507	TAR	O3-C3-C4	-2.09	106.22	110.69
4	C	506	TAR	O4-C4-C3	-2.06	116.14	121.62

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	GOL	O1-C1-C2-C3
3	A	504	GOL	O2-C2-C3-O3
3	A	505	GOL	O1-C1-C2-C3
3	B	504	GOL	C1-C2-C3-O3
3	B	505	GOL	O1-C1-C2-C3
3	B	505	GOL	C1-C2-C3-O3
3	B	506	GOL	O1-C1-C2-C3
3	B	506	GOL	C1-C2-C3-O3
3	C	504	GOL	C1-C2-C3-O3
3	C	505	GOL	O1-C1-C2-C3
3	C	505	GOL	C1-C2-C3-O3
3	C	505	GOL	O2-C2-C3-O3
3	D	504	GOL	O1-C1-C2-C3
4	A	506	TAR	O3-C3-C4-O4
4	A	506	TAR	O3-C3-C4-O41
4	A	507	TAR	O3-C3-C4-O4
4	A	507	TAR	O3-C3-C4-O41
4	C	506	TAR	O2-C2-C3-C4
4	D	506	TAR	C1-C2-C3-O3
4	B	507	TAR	O2-C2-C3-O3
4	C	507	TAR	C1-C2-C3-C4
4	B	507	TAR	C1-C2-C3-O3
4	B	507	TAR	O2-C2-C3-C4
4	D	506	TAR	O2-C2-C3-C4
4	B	507	TAR	O3-C3-C4-O4
4	B	507	TAR	O3-C3-C4-O41
4	C	506	TAR	O3-C3-C4-O4
4	D	506	TAR	O3-C3-C4-O4
4	D	506	TAR	O3-C3-C4-O41
5	D	507	PEG	O1-C1-C2-O2
4	C	506	TAR	C1-C2-C3-O3
4	C	506	TAR	O2-C2-C3-O3
4	D	506	TAR	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	C	506	TAR	O3-C3-C4-O41
3	B	505	GOL	O1-C1-C2-O2
3	C	504	GOL	O2-C2-C3-O3
3	D	504	GOL	O1-C1-C2-O2
5	D	507	PEG	O2-C3-C4-O4
5	D	510	PEG	O1-C1-C2-O2
4	C	507	TAR	C1-C2-C3-O3
4	C	507	TAR	O2-C2-C3-C4
4	A	506	TAR	C1-C2-C3-C4
5	D	509	PEG	O2-C3-C4-O4
3	A	504	GOL	C1-C2-C3-O3
3	A	505	GOL	C1-C2-C3-O3
3	B	504	GOL	O1-C1-C2-C3
4	C	506	TAR	C1-C2-C3-C4
4	A	506	TAR	C1-C2-C3-O3
4	A	506	TAR	O2-C2-C3-C4
3	A	504	GOL	O1-C1-C2-O2
3	A	505	GOL	O1-C1-C2-O2
3	B	504	GOL	O2-C2-C3-O3
3	B	505	GOL	O2-C2-C3-O3
3	B	506	GOL	O1-C1-C2-O2
3	B	506	GOL	O2-C2-C3-O3
3	C	505	GOL	O1-C1-C2-O2
5	A	508	PEG	O1-C1-C2-O2
5	A	509	PEG	O2-C3-C4-O4
5	D	508	PEG	O1-C1-C2-O2
4	B	507	TAR	C1-C2-C3-C4
4	D	506	TAR	C1-C2-C3-C4
5	A	508	PEG	O2-C3-C4-O4
3	A	505	GOL	O2-C2-C3-O3
5	B	508	PEG	O2-C3-C4-O4
4	A	507	TAR	O11-C1-C2-C3
4	A	507	TAR	C1-C2-C3-C4
5	A	509	PEG	O1-C1-C2-O2
4	A	507	TAR	O1-C1-C2-C3
5	D	509	PEG	C1-C2-O2-C3
4	A	507	TAR	O2-C2-C3-O3
4	C	507	TAR	O2-C2-C3-O3
5	D	508	PEG	C1-C2-O2-C3
3	B	504	GOL	O1-C1-C2-O2
5	D	507	PEG	C4-C3-O2-C2
5	D	507	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
5	B	508	PEG	C1-C2-O2-C3
5	A	509	PEG	C1-C2-O2-C3
4	C	506	TAR	O11-C1-C2-O2
4	C	506	TAR	O1-C1-C2-O2
4	C	506	TAR	O1-C1-C2-C3
4	C	506	TAR	O11-C1-C2-C3
5	B	508	PEG	C4-C3-O2-C2
4	A	507	TAR	O11-C1-C2-O2
4	A	507	TAR	O1-C1-C2-O2
3	D	504	GOL	O2-C2-C3-O3
5	A	508	PEG	C1-C2-O2-C3

There are no ring outliers.

13 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	506	TAR	5	0
4	C	507	TAR	4	0
5	D	510	PEG	1	0
5	A	509	PEG	3	0
5	D	508	PEG	4	0
3	C	505	GOL	3	0
3	B	506	GOL	2	0
4	D	506	TAR	1	0
3	D	505	GOL	2	0
3	C	504	GOL	2	0
3	A	505	GOL	1	0
3	D	504	GOL	2	0
4	A	506	TAR	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	404/404 (100%)	-1.24	0 100 100	12, 22, 34, 49	3 (0%)
1	B	404/404 (100%)	-1.27	0 100 100	9, 20, 32, 49	10 (2%)
1	C	404/404 (100%)	-1.24	0 100 100	9, 20, 33, 54	1 (0%)
1	D	404/404 (100%)	-1.28	0 100 100	8, 20, 31, 46	6 (1%)
All	All	1616/1616 (100%)	-1.26	0 100 100	8, 20, 33, 54	20 (1%)

There are no RSRZ outliers to report.

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	GOL	D	504	6/6	0.95	0.09	38,43,44,45	0
5	PEG	D	507	7/7	0.95	0.08	47,54,59,62	0
5	PEG	D	509	7/7	0.95	0.09	46,48,49,50	0
3	GOL	C	505	6/6	0.97	0.09	30,30,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	505	6/6	0.97	0.08	33,38,39,39	0
3	GOL	D	505	6/6	0.97	0.04	32,35,36,37	0
4	TAR	A	507	10/10	0.97	0.06	48,54,56,66	0
3	GOL	B	504	6/6	0.97	0.06	37,41,41,43	0
3	GOL	B	505	6/6	0.97	0.07	36,37,40,42	0
5	PEG	D	510	7/7	0.97	0.06	43,44,47,50	0
3	GOL	A	504	6/6	0.98	0.06	31,37,38,40	0
4	TAR	B	507	10/10	0.98	0.04	49,53,56,56	0
4	TAR	C	506	10/10	0.98	0.04	49,54,55,59	0
4	TAR	D	506	10/10	0.98	0.04	38,45,48,51	0
5	PEG	A	508	7/7	0.98	0.05	30,34,35,37	0
5	PEG	A	509	7/7	0.98	0.05	27,33,36,37	0
5	PEG	B	508	7/7	0.98	0.05	41,44,47,47	0
3	GOL	B	506	6/6	0.98	0.05	32,35,37,41	0
3	GOL	C	504	6/6	0.98	0.06	36,41,42,44	0
4	TAR	A	506	10/10	0.98	0.06	57,65,72,76	0
2	CA	B	501	1/1	0.99	0.01	21,21,21,21	0
5	PEG	D	508	7/7	0.99	0.05	33,38,40,43	0
4	TAR	C	507	10/10	0.99	0.04	39,46,47,50	0
2	CA	D	501	1/1	0.99	0.02	18,18,18,18	0
2	CA	B	502	1/1	1.00	0.03	16,16,16,16	0
2	CA	B	503	1/1	1.00	0.04	21,21,21,21	0
2	CA	C	501	1/1	1.00	0.01	16,16,16,16	0
2	CA	C	502	1/1	1.00	0.01	24,24,24,24	0
2	CA	C	503	1/1	1.00	0.01	28,28,28,28	0
2	CA	A	502	1/1	1.00	0.04	24,24,24,24	0
2	CA	D	502	1/1	1.00	0.01	23,23,23,23	0
2	CA	D	503	1/1	1.00	0.04	26,26,26,26	0
2	CA	A	503	1/1	1.00	0.03	26,26,26,26	0
2	CA	A	501	1/1	1.00	0.01	14,14,14,14	0

6.5 Other polymers ⓘ

There are no such residues in this entry.