



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:29 PM EDT

PDB ID : 7BOO / pdb_00007boo
Title : Crystal Structure of Core-mannan synthase A (CmsA/Ktr4) from *Aspergillus fumigatus*, apo form
Authors : Hira, D.; Onoue, T.; Oka, T.
Deposited on : 2020-03-19
Resolution : 1.95 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

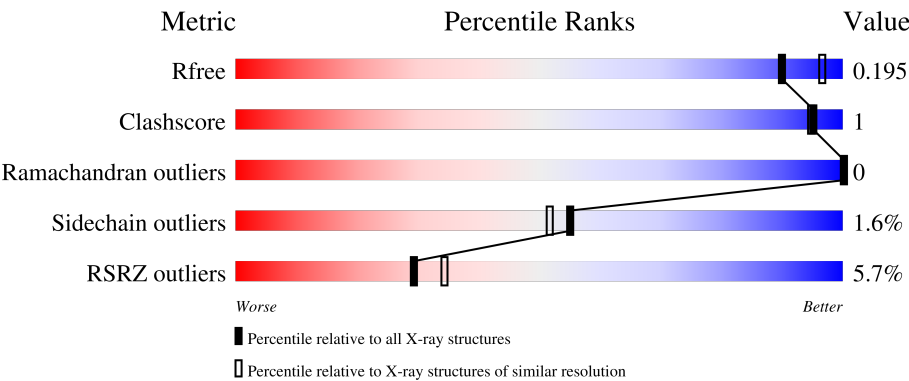
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	386	3% 90% 5% 5%
1	B	386	4% 90% 5% 5%
1	C	386	6% 92% 5% 5%
1	D	386	7% 91% 5% 5%
1	E	386	6% 92% 5% 5%

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Mol	Chain	Length	Quality of chain
1	F	386	8% 91%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20498 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-1,2-mannosyltransferase (Ktr4), putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	3	0
			3060	1969	511	563	17			
1	B	366	Total	C	N	O	S	0	4	0
			3073	1979	512	565	17			
1	C	372	Total	C	N	O	S	0	9	0
			3151	2025	531	577	18			
1	D	367	Total	C	N	O	S	0	9	0
			3111	2002	520	571	18			
1	E	372	Total	C	N	O	S	0	5	0
			3118	2004	521	575	18			
1	F	372	Total	C	N	O	S	0	4	0
			3114	2001	523	572	18			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP B0Y2F5
A	13	GLY	-	expression tag	UNP B0Y2F5
A	14	SER	-	expression tag	UNP B0Y2F5
A	15	SER	-	expression tag	UNP B0Y2F5
A	16	HIS	-	expression tag	UNP B0Y2F5
A	17	HIS	-	expression tag	UNP B0Y2F5
A	18	HIS	-	expression tag	UNP B0Y2F5
A	19	HIS	-	expression tag	UNP B0Y2F5
A	20	HIS	-	expression tag	UNP B0Y2F5
A	21	HIS	-	expression tag	UNP B0Y2F5
A	22	SER	-	expression tag	UNP B0Y2F5
A	23	SER	-	expression tag	UNP B0Y2F5
A	24	GLY	-	expression tag	UNP B0Y2F5
A	25	HIS	-	expression tag	UNP B0Y2F5
A	26	SER	-	expression tag	UNP B0Y2F5
B	12	MET	-	initiating methionine	UNP B0Y2F5
B	13	GLY	-	expression tag	UNP B0Y2F5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	14	SER	-	expression tag	UNP B0Y2F5
B	15	SER	-	expression tag	UNP B0Y2F5
B	16	HIS	-	expression tag	UNP B0Y2F5
B	17	HIS	-	expression tag	UNP B0Y2F5
B	18	HIS	-	expression tag	UNP B0Y2F5
B	19	HIS	-	expression tag	UNP B0Y2F5
B	20	HIS	-	expression tag	UNP B0Y2F5
B	21	HIS	-	expression tag	UNP B0Y2F5
B	22	SER	-	expression tag	UNP B0Y2F5
B	23	SER	-	expression tag	UNP B0Y2F5
B	24	GLY	-	expression tag	UNP B0Y2F5
B	25	HIS	-	expression tag	UNP B0Y2F5
B	26	SER	-	expression tag	UNP B0Y2F5
C	12	MET	-	initiating methionine	UNP B0Y2F5
C	13	GLY	-	expression tag	UNP B0Y2F5
C	14	SER	-	expression tag	UNP B0Y2F5
C	15	SER	-	expression tag	UNP B0Y2F5
C	16	HIS	-	expression tag	UNP B0Y2F5
C	17	HIS	-	expression tag	UNP B0Y2F5
C	18	HIS	-	expression tag	UNP B0Y2F5
C	19	HIS	-	expression tag	UNP B0Y2F5
C	20	HIS	-	expression tag	UNP B0Y2F5
C	21	HIS	-	expression tag	UNP B0Y2F5
C	22	SER	-	expression tag	UNP B0Y2F5
C	23	SER	-	expression tag	UNP B0Y2F5
C	24	GLY	-	expression tag	UNP B0Y2F5
C	25	HIS	-	expression tag	UNP B0Y2F5
C	26	SER	-	expression tag	UNP B0Y2F5
D	12	MET	-	initiating methionine	UNP B0Y2F5
D	13	GLY	-	expression tag	UNP B0Y2F5
D	14	SER	-	expression tag	UNP B0Y2F5
D	15	SER	-	expression tag	UNP B0Y2F5
D	16	HIS	-	expression tag	UNP B0Y2F5
D	17	HIS	-	expression tag	UNP B0Y2F5
D	18	HIS	-	expression tag	UNP B0Y2F5
D	19	HIS	-	expression tag	UNP B0Y2F5
D	20	HIS	-	expression tag	UNP B0Y2F5
D	21	HIS	-	expression tag	UNP B0Y2F5
D	22	SER	-	expression tag	UNP B0Y2F5
D	23	SER	-	expression tag	UNP B0Y2F5
D	24	GLY	-	expression tag	UNP B0Y2F5
D	25	HIS	-	expression tag	UNP B0Y2F5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	26	SER	-	expression tag	UNP B0Y2F5
E	12	MET	-	initiating methionine	UNP B0Y2F5
E	13	GLY	-	expression tag	UNP B0Y2F5
E	14	SER	-	expression tag	UNP B0Y2F5
E	15	SER	-	expression tag	UNP B0Y2F5
E	16	HIS	-	expression tag	UNP B0Y2F5
E	17	HIS	-	expression tag	UNP B0Y2F5
E	18	HIS	-	expression tag	UNP B0Y2F5
E	19	HIS	-	expression tag	UNP B0Y2F5
E	20	HIS	-	expression tag	UNP B0Y2F5
E	21	HIS	-	expression tag	UNP B0Y2F5
E	22	SER	-	expression tag	UNP B0Y2F5
E	23	SER	-	expression tag	UNP B0Y2F5
E	24	GLY	-	expression tag	UNP B0Y2F5
E	25	HIS	-	expression tag	UNP B0Y2F5
E	26	SER	-	expression tag	UNP B0Y2F5
F	12	MET	-	initiating methionine	UNP B0Y2F5
F	13	GLY	-	expression tag	UNP B0Y2F5
F	14	SER	-	expression tag	UNP B0Y2F5
F	15	SER	-	expression tag	UNP B0Y2F5
F	16	HIS	-	expression tag	UNP B0Y2F5
F	17	HIS	-	expression tag	UNP B0Y2F5
F	18	HIS	-	expression tag	UNP B0Y2F5
F	19	HIS	-	expression tag	UNP B0Y2F5
F	20	HIS	-	expression tag	UNP B0Y2F5
F	21	HIS	-	expression tag	UNP B0Y2F5
F	22	SER	-	expression tag	UNP B0Y2F5
F	23	SER	-	expression tag	UNP B0Y2F5
F	24	GLY	-	expression tag	UNP B0Y2F5
F	25	HIS	-	expression tag	UNP B0Y2F5
F	26	SER	-	expression tag	UNP B0Y2F5

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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	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		
3	D	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

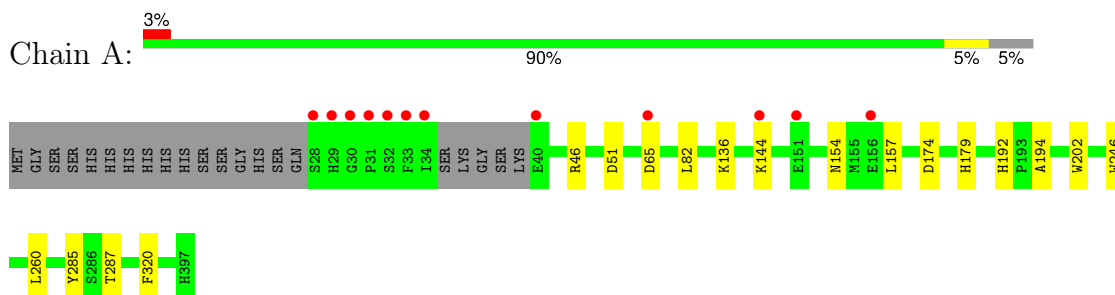
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	319	Total O 319 319	0	0
4	B	316	Total O 316 316	0	0
4	C	280	Total O 280 280	0	0
4	D	302	Total O 302 302	0	0
4	E	266	Total O 266 266	0	0
4	F	255	Total O 255 255	0	0

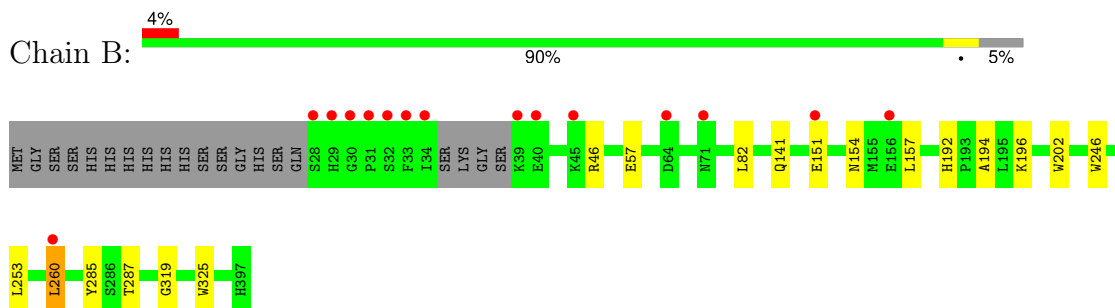
3 Residue-property plots [i](#)

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.

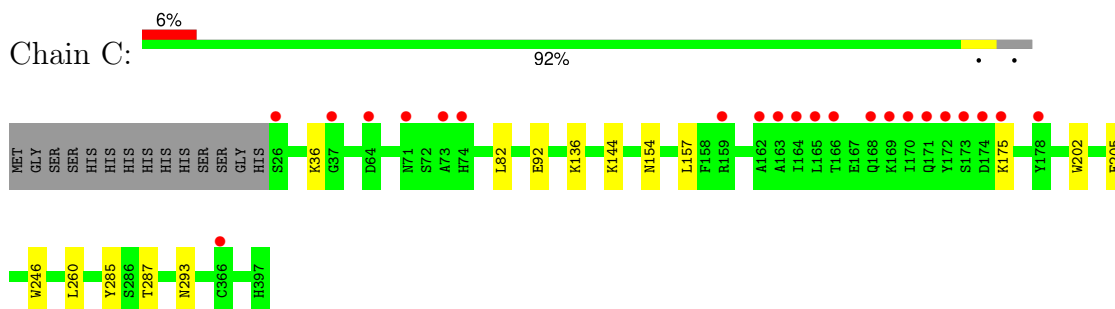
- Molecule 1: Alpha-1,2-mannosyltransferase (Ktr4), putative



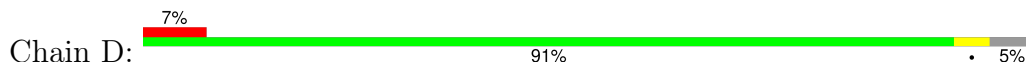
- Molecule 1: Alpha-1,2-mannosyltransferase (Ktr4), putative

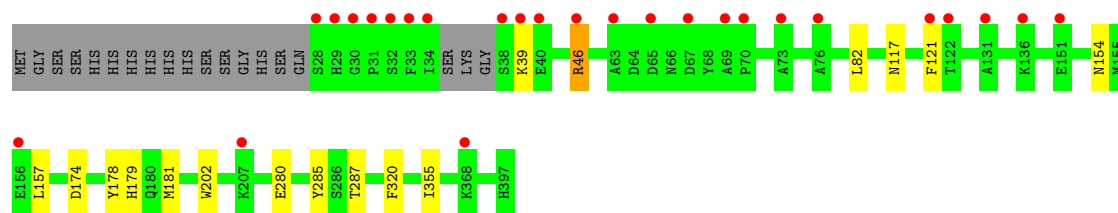


- Molecule 1: Alpha-1,2-mannosyltransferase (Ktr4), putative

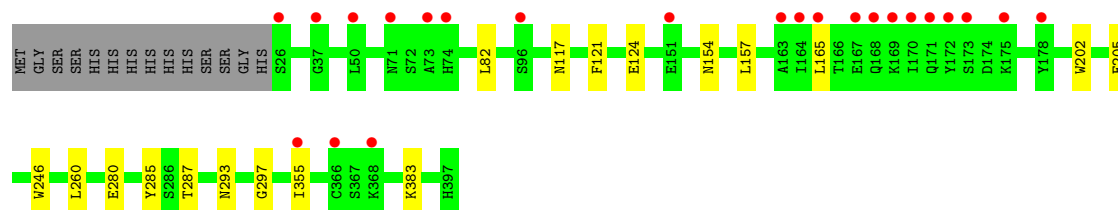
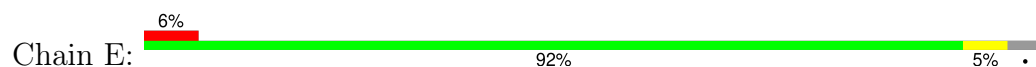


- Molecule 1: Alpha-1,2-mannosyltransferase (Ktr4), putative

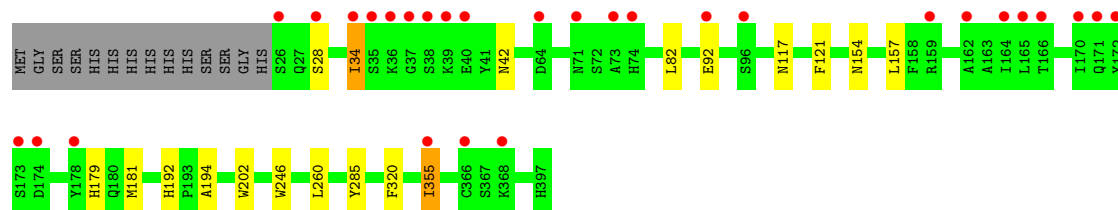
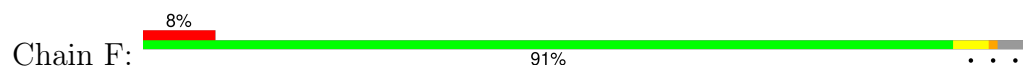




- Molecule 1: Alpha-1,2-mannosyltransferase (Ktr4), putative



- Molecule 1: Alpha-1,2-mannosyltransferase (Ktr4), putative



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	154.72Å 274.30Å 185.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.99 – 1.95 45.99 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.99-1.95) 99.8 (45.99-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.163 , 0.186 0.172 , 0.195	Depositor DCC
R_{free} test set	14177 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.010 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20498	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	0.57	0/3179	0.75	0/4314
1	B	0.56	0/3195	0.74	0/4335
1	C	0.55	0/3289	0.76	0/4457
1	D	0.56	0/3248	0.75	0/4403
1	E	0.56	0/3244	0.75	1/4399 (0.0%)
1	F	0.58	0/3237	0.77	0/4389
All	All	0.56	0/19392	0.75	1/26297 (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	E	297	GLY	N-CA-C	5.05	118.49	110.96

There are no chirality outliers.

There are no planarity outliers.

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	3060	0	2824	8	0
1	B	3073	0	2844	9	0
1	C	3151	0	2941	5	0
1	D	3111	0	2894	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3118	0	2893	6	0
1	F	3114	0	2892	8	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	24	0	32	0	0
3	B	18	0	24	0	0
3	C	12	0	16	0	0
3	D	24	0	32	0	0
3	E	30	0	40	0	0
3	F	18	0	24	0	0
4	A	319	0	0	0	0
4	B	316	0	0	0	0
4	C	280	0	0	0	0
4	D	302	0	0	0	0
4	E	266	0	0	0	0
4	F	255	0	0	1	0
All	All	20498	0	17456	44	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 1.

All (44) 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:D:174:ASP:OD1	1:D:179:HIS:HE1	1.89	0.55
1:A:154:ASN:HD22	1:A:157:LEU:H	1.56	0.54
1:D:178:TYR:HA	1:D:181[B]:MET:HE2	1.89	0.53
1:A:179:HIS:HD2	1:A:320:PHE:O	1.91	0.53
1:B:253:LEU:HD22	1:B:260[B]:LEU:HD11	1.91	0.52
1:D:82:LEU:HD23	1:D:202:TRP:HB3	1.92	0.52
1:C:82:LEU:HD23	1:C:202:TRP:HB3	1.91	0.51
1:A:82:LEU:HD23	1:A:202:TRP:HB3	1.92	0.51
1:F:192:HIS:HD2	1:F:194:ALA:H	1.59	0.51
1:B:154:ASN:HD22	1:B:157:LEU:H	1.58	0.51
1:E:82:LEU:HD23	1:E:202:TRP:HB3	1.92	0.50
1:A:174:ASP:OD2	1:A:179:HIS:HE1	1.94	0.50
1:F:82:LEU:HD23	1:F:202:TRP:HB3	1.94	0.49
1:B:246:TRP:HB2	1:B:285:TYR:HB2	1.95	0.48
1:A:46:ARG:NH1	1:A:51:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:TRP:HB2	1:C:285:TYR:HB2	1.96	0.47
1:D:285:TYR:CE2	1:D:287:THR:HA	2.50	0.46
1:D:154:ASN:HD22	1:D:157:LEU:H	1.63	0.46
1:D:179:HIS:HD2	1:D:320:PHE:O	1.98	0.46
1:F:154:ASN:HD22	1:F:157:LEU:H	1.65	0.44
1:C:154:ASN:HD22	1:C:157:LEU:H	1.63	0.44
1:C:205:GLU:HG3	1:C:293:ASN:HB2	2.00	0.43
1:F:179:HIS:HD2	1:F:320:PHE:O	2.02	0.43
1:E:246:TRP:HB2	1:E:285:TYR:HB2	1.98	0.43
1:B:141:GLN:O	1:B:192:HIS:HE1	2.02	0.43
1:F:34:ILE:HD13	1:F:42:ASN:HB2	2.01	0.43
1:F:117:ASN:HB2	1:F:121:PHE:CZ	2.54	0.42
1:A:192:HIS:HD2	1:A:194:ALA:H	1.67	0.42
1:F:246:TRP:HB2	1:F:285:TYR:HB2	2.01	0.42
1:E:154:ASN:HD22	1:E:157:LEU:H	1.67	0.42
1:E:285:TYR:CE2	1:E:287:THR:HA	2.55	0.42
1:B:192:HIS:HD2	1:B:194:ALA:H	1.67	0.42
1:B:285:TYR:CE2	1:B:287:THR:HA	2.55	0.42
1:B:319:GLY:HA3	1:B:325:TRP:CZ2	2.55	0.42
1:E:117:ASN:HB2	1:E:121:PHE:CZ	2.55	0.42
1:E:205:GLU:HG3	1:E:293:ASN:HB2	2.02	0.41
1:B:253:LEU:HD22	1:B:260[B]:LEU:CD1	2.50	0.41
1:A:285:TYR:CE2	1:A:287:THR:HA	2.55	0.41
1:C:285:TYR:CE2	1:C:287:THR:HA	2.54	0.41
1:F:355:ILE:HG23	4:F:502:HOH:O	2.21	0.41
1:A:246:TRP:HB2	1:A:285:TYR:HB2	2.03	0.41
1:D:46[A]:ARG:HE	1:D:46[A]:ARG:HB3	1.62	0.41
1:D:117:ASN:HB2	1:D:121:PHE:CZ	2.56	0.40
1:B:82:LEU:HD23	1:B:202:TRP:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	364/386 (94%)	356 (98%)	8 (2%)	0	100	100
1	B	366/386 (95%)	358 (98%)	8 (2%)	0	100	100
1	C	379/386 (98%)	372 (98%)	7 (2%)	0	100	100
1	D	372/386 (96%)	360 (97%)	12 (3%)	0	100	100
1	E	375/386 (97%)	368 (98%)	7 (2%)	0	100	100
1	F	374/386 (97%)	363 (97%)	11 (3%)	0	100	100
All	All	2230/2316 (96%)	2177 (98%)	53 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	325/340 (96%)	321 (99%)	4 (1%)	63	61
1	B	327/340 (96%)	321 (98%)	6 (2%)	51	47
1	C	337/340 (99%)	331 (98%)	6 (2%)	51	47
1	D	333/340 (98%)	327 (98%)	6 (2%)	51	47
1	E	333/340 (98%)	326 (98%)	7 (2%)	47	41
1	F	332/340 (98%)	325 (98%)	7 (2%)	47	41
All	All	1987/2040 (97%)	1951 (98%)	36 (2%)	55	47

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ASP
1	A	136	LYS
1	A	144	LYS
1	A	260	LEU
1	B	46	ARG
1	B	57	GLU
1	B	151	GLU

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Mol	Chain	Res	Type
1	B	196	LYS
1	B	260[A]	LEU
1	B	260[B]	LEU
1	C	36	LYS
1	C	92	GLU
1	C	136	LYS
1	C	144	LYS
1	C	175	LYS
1	C	260	LEU
1	D	39	LYS
1	D	46[A]	ARG
1	D	46[B]	ARG
1	D	280[A]	GLU
1	D	280[B]	GLU
1	D	355	ILE
1	E	124	GLU
1	E	165	LEU
1	E	260	LEU
1	E	280[A]	GLU
1	E	280[B]	GLU
1	E	355	ILE
1	E	383	LYS
1	F	28	SER
1	F	34	ILE
1	F	92	GLU
1	F	181[A]	MET
1	F	181[B]	MET
1	F	260	LEU
1	F	355	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	74	HIS
1	A	130	GLN
1	A	154	ASN
1	A	171	GLN
1	A	179	HIS
1	A	185	ASN
1	A	192	HIS
1	A	263	ASN

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Mol	Chain	Res	Type
1	A	312	ASN
1	A	359	ASN
1	B	59	HIS
1	B	74	HIS
1	B	192	HIS
1	B	197	ASN
1	B	263	ASN
1	B	312	ASN
1	B	359	ASN
1	C	42	ASN
1	C	154	ASN
1	C	185	ASN
1	C	263	ASN
1	C	312	ASN
1	C	353	ASN
1	C	354	HIS
1	D	130	GLN
1	D	154	ASN
1	D	179	HIS
1	D	185	ASN
1	D	263	ASN
1	D	312	ASN
1	D	313	HIS
1	D	353	ASN
1	D	359	ASN
1	E	42	ASN
1	E	154	ASN
1	E	185	ASN
1	E	192	HIS
1	E	197	ASN
1	E	263	ASN
1	E	312	ASN
1	F	42	ASN
1	F	59	HIS
1	F	154	ASN
1	F	168	GLN
1	F	179	HIS
1	F	185	ASN
1	F	192	HIS
1	F	197	ASN
1	F	263	ASN
1	F	312	ASN

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Mol	Chain	Res	Type
1	F	313	HIS
1	F	353	ASN

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 28 ligands modelled in this entry, 7 are monoatomic - leaving 21 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	$\# Z > 2$
3	GOL	E	403	-	5,5,5	0.46	0	5,5,5	0.44	0
3	GOL	C	402	-	5,5,5	0.28	0	5,5,5	0.23	0
3	GOL	E	401	-	5,5,5	0.28	0	5,5,5	0.55	0
3	GOL	F	403	-	5,5,5	0.50	0	5,5,5	0.93	0
3	GOL	A	404	-	5,5,5	0.32	0	5,5,5	0.23	0
3	GOL	D	405	-	5,5,5	0.23	0	5,5,5	0.50	0
3	GOL	D	404	-	5,5,5	0.35	0	5,5,5	0.52	0
3	GOL	A	406	-	5,5,5	0.37	0	5,5,5	0.32	0
3	GOL	E	405	-	5,5,5	0.27	0	5,5,5	0.39	0
3	GOL	E	404	-	5,5,5	0.44	0	5,5,5	0.48	0
3	GOL	C	403	-	5,5,5	0.41	0	5,5,5	0.44	0
3	GOL	A	403	-	5,5,5	0.45	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	D	406	-	5,5,5	0.32	0	5,5,5	0.51	0
3	GOL	E	402	-	5,5,5	0.39	0	5,5,5	0.23	0
3	GOL	F	402	-	5,5,5	0.37	0	5,5,5	0.37	0
3	GOL	A	405	-	5,5,5	0.33	0	5,5,5	0.42	0
3	GOL	F	401	-	5,5,5	0.34	0	5,5,5	0.83	0
3	GOL	B	405	-	5,5,5	0.32	0	5,5,5	0.30	0
3	GOL	B	403	-	5,5,5	0.19	0	5,5,5	0.75	0
3	GOL	B	404	-	5,5,5	0.31	0	5,5,5	0.51	0
3	GOL	D	403	-	5,5,5	0.36	0	5,5,5	0.76	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
3	GOL	E	403	-	-	4/4/4/4	-
3	GOL	C	402	-	-	0/4/4/4	-
3	GOL	E	401	-	-	0/4/4/4	-
3	GOL	F	403	-	-	2/4/4/4	-
3	GOL	A	404	-	-	3/4/4/4	-
3	GOL	D	405	-	-	2/4/4/4	-
3	GOL	D	404	-	-	2/4/4/4	-
3	GOL	A	406	-	-	2/4/4/4	-
3	GOL	E	405	-	-	2/4/4/4	-
3	GOL	E	404	-	-	2/4/4/4	-
3	GOL	C	403	-	-	0/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-
3	GOL	D	406	-	-	2/4/4/4	-
3	GOL	E	402	-	-	2/4/4/4	-
3	GOL	F	402	-	-	2/4/4/4	-
3	GOL	A	405	-	-	2/4/4/4	-
3	GOL	F	401	-	-	2/4/4/4	-
3	GOL	B	405	-	-	2/4/4/4	-
3	GOL	B	403	-	-	2/4/4/4	-
3	GOL	B	404	-	-	1/4/4/4	-
3	GOL	D	403	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	GOL	O1-C1-C2-C3
3	A	405	GOL	O1-C1-C2-C3
3	B	403	GOL	C1-C2-C3-O3
3	B	403	GOL	O2-C2-C3-O3
3	D	405	GOL	O1-C1-C2-C3
3	E	402	GOL	C1-C2-C3-O3
3	E	403	GOL	O1-C1-C2-C3
3	E	403	GOL	C1-C2-C3-O3
3	E	404	GOL	O1-C1-C2-C3
3	E	405	GOL	C1-C2-C3-O3
3	F	401	GOL	O1-C1-C2-O2
3	F	401	GOL	O1-C1-C2-C3
3	F	403	GOL	C1-C2-C3-O3
3	D	405	GOL	O1-C1-C2-O2
3	A	406	GOL	O1-C1-C2-C3
3	B	404	GOL	O1-C1-C2-C3
3	B	405	GOL	O1-C1-C2-C3
3	D	403	GOL	O1-C1-C2-C3
3	D	406	GOL	O1-C1-C2-C3
3	F	402	GOL	C1-C2-C3-O3
3	A	404	GOL	O1-C1-C2-O2
3	A	405	GOL	O1-C1-C2-O2
3	A	406	GOL	O1-C1-C2-O2
3	E	403	GOL	O1-C1-C2-O2
3	E	404	GOL	O1-C1-C2-O2
3	E	405	GOL	O2-C2-C3-O3
3	E	403	GOL	O2-C2-C3-O3
3	F	402	GOL	O2-C2-C3-O3
3	F	403	GOL	O2-C2-C3-O3
3	A	404	GOL	O2-C2-C3-O3
3	E	402	GOL	O2-C2-C3-O3
3	D	403	GOL	O2-C2-C3-O3
3	D	403	GOL	C1-C2-C3-O3
3	D	404	GOL	C1-C2-C3-O3
3	D	404	GOL	O2-C2-C3-O3
3	D	406	GOL	O1-C1-C2-O2
3	B	405	GOL	O1-C1-C2-O2
3	D	403	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	365/386 (94%)	0.03	12 (3%)	49	55	17, 30, 50, 93	3 (0%)
1	B	366/386 (94%)	0.05	15 (4%)	41	48	19, 30, 49, 104	4 (1%)
1	C	372/386 (96%)	0.13	22 (5%)	28	32	18, 32, 58, 93	9 (2%)
1	D	367/386 (95%)	0.28	26 (7%)	22	25	16, 32, 56, 111	9 (2%)
1	E	372/386 (96%)	0.40	23 (6%)	26	31	21, 36, 60, 97	5 (1%)
1	F	372/386 (96%)	0.39	29 (7%)	19	22	22, 35, 56, 98	4 (1%)
All	All	2214/2316 (95%)	0.21	127 (5%)	29	34	16, 32, 56, 111	34 (1%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	34	ILE	9.4
1	A	34	ILE	8.1
1	B	34	ILE	7.7
1	C	170	ILE	6.9
1	C	165	LEU	6.4
1	B	33	PHE	5.5
1	E	172	TYR	5.3
1	E	170	ILE	5.1
1	A	28	SER	4.9
1	B	32	SER	4.9
1	B	29	HIS	4.8
1	B	31	PRO	4.7
1	A	33	PHE	4.7
1	C	172	TYR	4.7
1	D	29	HIS	4.7
1	B	28	SER	4.6
1	D	38	SER	4.3
1	E	165	LEU	4.2
1	C	74	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	172	TYR	4.0
1	F	165	LEU	4.0
1	A	29	HIS	4.0
1	B	39	LYS	4.0
1	F	39	LYS	4.0
1	D	33	PHE	4.0
1	E	74	HIS	3.9
1	D	65	ASP	3.9
1	F	38	SER	3.8
1	F	173	SER	3.8
1	D	39	LYS	3.8
1	D	28	SER	3.8
1	F	366	CYS	3.7
1	F	170	ILE	3.7
1	A	32	SER	3.7
1	F	64	ASP	3.5
1	E	173	SER	3.5
1	B	40	GLU	3.5
1	A	30	GLY	3.4
1	B	30	GLY	3.4
1	F	178	TYR	3.3
1	C	73	ALA	3.3
1	F	34	ILE	3.3
1	E	171	GLN	3.3
1	B	71	ASN	3.3
1	D	32	SER	3.3
1	F	74	HIS	3.2
1	C	173	SER	3.2
1	D	136	LYS	3.2
1	B	156	GLU	3.2
1	F	73	ALA	3.1
1	D	156	GLU	3.0
1	E	163	ALA	3.0
1	C	171	GLN	3.0
1	C	37	GLY	2.9
1	B	260[A]	LEU	2.9
1	D	131	ALA	2.9
1	B	45	LYS	2.9
1	F	71	ASN	2.8
1	E	178	TYR	2.8
1	F	40	GLU	2.8
1	C	64	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	164	ILE	2.7
1	D	40	GLU	2.7
1	E	73	ALA	2.7
1	A	31	PRO	2.7
1	F	26	SER	2.7
1	F	164	ILE	2.7
1	A	144	LYS	2.6
1	C	159[A]	ARG	2.6
1	F	35	SER	2.6
1	C	71	ASN	2.6
1	E	71	ASN	2.6
1	C	366	CYS	2.6
1	C	169	LYS	2.6
1	F	355	ILE	2.5
1	F	368	LYS	2.5
1	D	151	GLU	2.5
1	D	30	GLY	2.5
1	A	65	ASP	2.5
1	E	167	GLU	2.4
1	F	28	SER	2.4
1	D	63	ALA	2.4
1	D	76	ALA	2.4
1	D	31	PRO	2.4
1	A	151	GLU	2.4
1	C	178	TYR	2.4
1	C	174	ASP	2.4
1	E	164	ILE	2.4
1	E	37	GLY	2.4
1	C	26	SER	2.4
1	F	37	GLY	2.4
1	D	368	LYS	2.4
1	D	122	THR	2.3
1	E	355	ILE	2.3
1	E	50	LEU	2.3
1	D	73	ALA	2.3
1	A	156	GLU	2.3
1	F	171	GLN	2.3
1	F	159[A]	ARG	2.2
1	D	67	ASP	2.2
1	D	69	ALA	2.2
1	C	175	LYS	2.2
1	F	174	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	40	GLU	2.2
1	F	166	THR	2.2
1	E	368	LYS	2.2
1	B	64	ASP	2.1
1	C	166	THR	2.1
1	F	92	GLU	2.1
1	F	162	ALA	2.1
1	C	168	GLN	2.1
1	E	26	SER	2.1
1	F	36	LYS	2.1
1	B	151	GLU	2.1
1	D	70	PRO	2.1
1	C	162	ALA	2.1
1	F	96	SER	2.1
1	D	207	LYS	2.1
1	C	163	ALA	2.1
1	E	169	LYS	2.0
1	E	175	LYS	2.0
1	E	168	GLN	2.0
1	E	366	CYS	2.0
1	D	46[A]	ARG	2.0
1	E	151	GLU	2.0
1	E	96	SER	2.0
1	D	121	PHE	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($\text{\AA}^2$)	Q<0.9
3	GOL	F	403	6/6	0.71	0.28	51,55,58,64	0
3	GOL	F	401	6/6	0.79	0.19	48,61,66,67	0
3	GOL	B	405	6/6	0.79	0.22	64,66,67,68	0
3	GOL	B	404	6/6	0.82	0.18	39,50,51,55	0
3	GOL	A	405	6/6	0.82	0.19	41,53,57,64	0
3	GOL	C	403	6/6	0.84	0.17	41,54,59,59	0
3	GOL	D	406	6/6	0.85	0.18	51,57,58,59	0
3	GOL	E	403	6/6	0.86	0.15	56,61,62,64	0
3	GOL	E	405	6/6	0.86	0.17	50,55,57,62	0
3	GOL	E	404	6/6	0.87	0.17	62,65,66,67	0
3	GOL	A	406	6/6	0.87	0.17	54,57,60,64	0
3	GOL	E	402	6/6	0.87	0.17	45,57,60,61	0
3	GOL	D	405	6/6	0.87	0.16	41,50,53,61	0
3	GOL	D	403	6/6	0.88	0.16	41,48,52,56	0
3	GOL	D	404	6/6	0.88	0.14	33,38,44,47	0
3	GOL	E	401	6/6	0.90	0.15	41,48,51,56	0
3	GOL	A	403	6/6	0.91	0.14	35,39,45,49	0
3	GOL	B	403	6/6	0.91	0.15	33,37,44,46	0
3	GOL	A	404	6/6	0.91	0.12	47,51,53,55	0
2	NA	D	402	1/1	0.91	0.12	49,49,49,49	0
2	NA	C	401	1/1	0.92	0.15	45,45,45,45	0
3	GOL	F	402	6/6	0.92	0.11	52,54,58,60	0
3	GOL	C	402	6/6	0.92	0.11	43,49,50,52	0
2	NA	B	402	1/1	0.97	0.17	41,41,41,41	0
2	NA	A	401	1/1	0.98	0.09	32,32,32,32	0
2	NA	B	401	1/1	0.99	0.04	26,26,26,26	0
2	NA	D	401	1/1	0.99	0.03	25,25,25,25	0
2	NA	A	402	1/1	0.99	0.04	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.