



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 03:34 PM BST

PDB ID : 7BOO
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.2

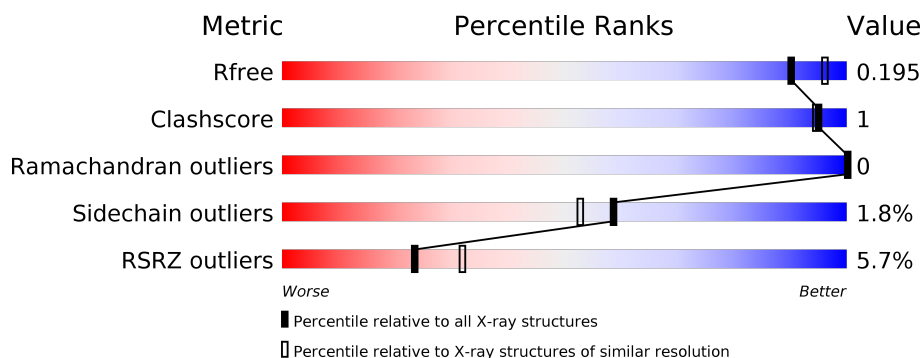
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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 on 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	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>5%</div> </div> </div>
1	B	386	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div>5%</div> </div> </div>
1	C	386	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div></div> <div></div> </div> </div>
1	D	386	<div> <div>9%</div> <div> <div></div> <div>90%</div> <div></div> <div>5%</div> </div> </div>
1	E	386	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div></div> </div> </div>
1	F	386	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div></div> </div> </div>

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 (three-letter code: NA) (formula: Na).

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

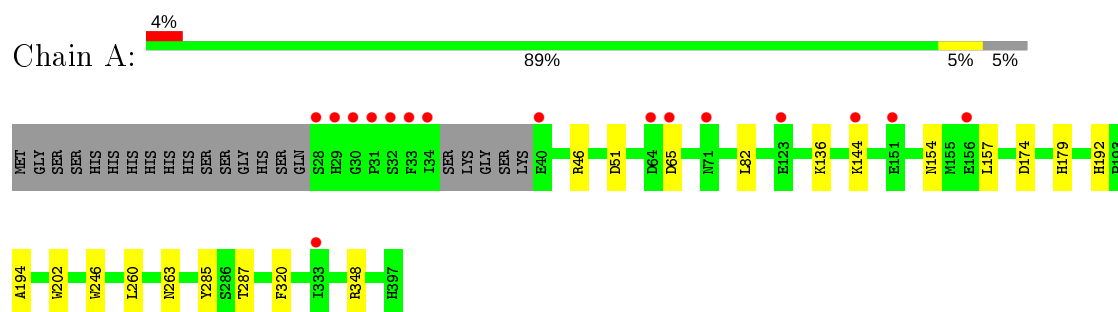
- Molecule 4 is water.

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

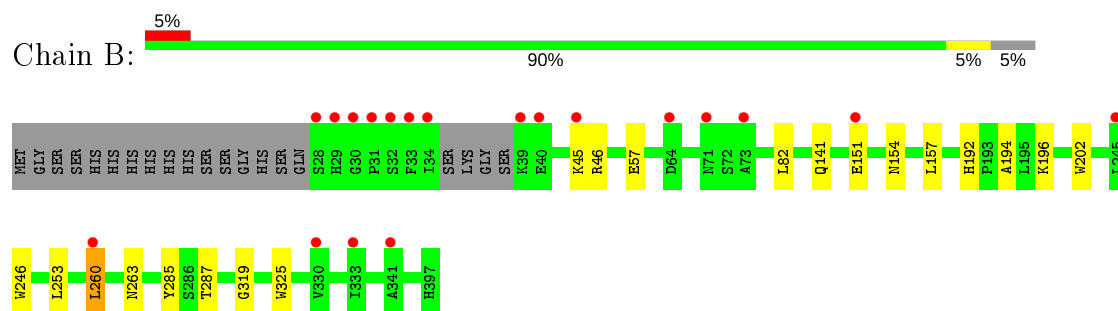
3 Residue-property plots [i](#)

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.

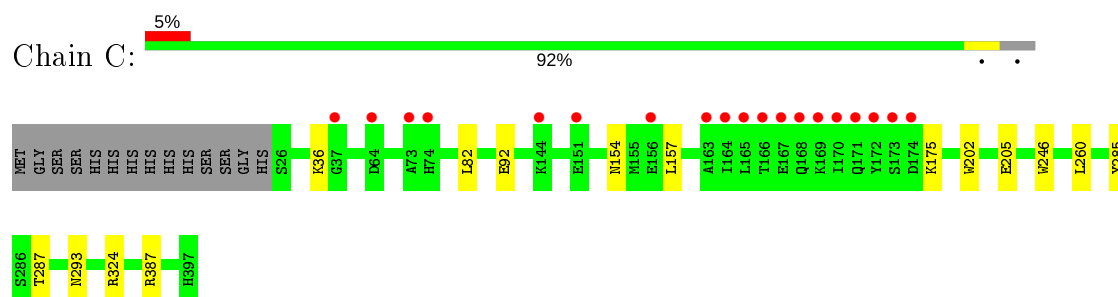
- Molecule 1: Alpha-1,2-mannosyltransferase (Ktr4), putative



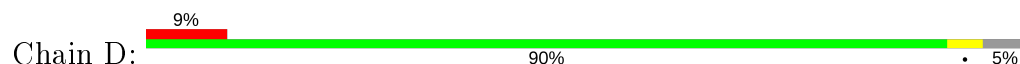
- Molecule 1: Alpha-1,2-mannosyltransferase (Ktr4), putative

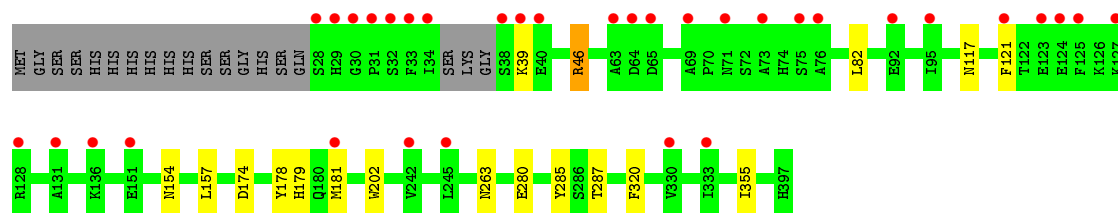


- Molecule 1: Alpha-1,2-mannosyltransferase (Ktr4), putative

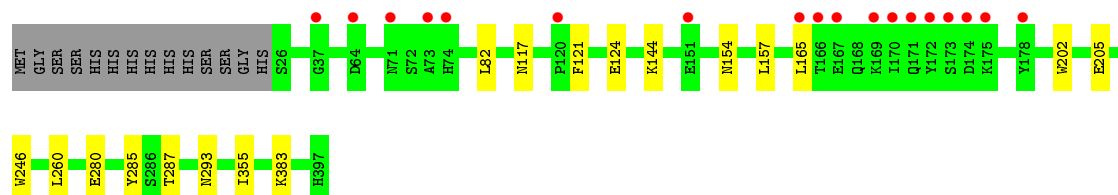
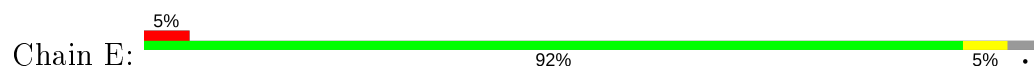


- Molecule 1: Alpha-1,2-mannosyltransferase (Ktr4), putative

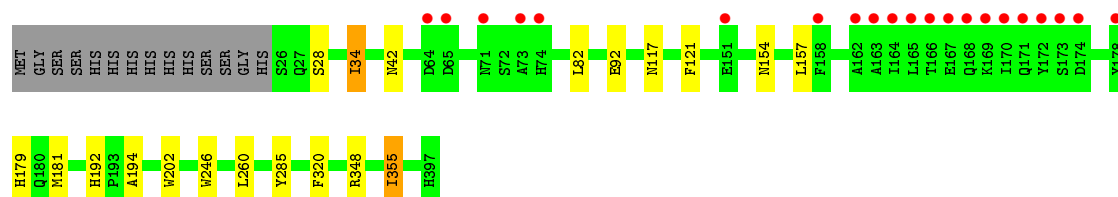
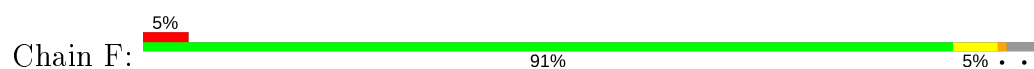




- Molecule 1: Alpha-1,2-mannosyltransferase (Ktr4), putative



- 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 49.47 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.99-1.95) 99.8 (49.47-1.95)	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 (4.98%)	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 , 44.6	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: GOL, NA

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	0.44	0/3179	0.66	2/4314 (0.0%)
1	B	0.43	0/3195	0.63	0/4335
1	C	0.43	0/3289	0.63	1/4457 (0.0%)
1	D	0.44	0/3248	0.63	0/4403
1	E	0.43	0/3244	0.62	0/4399
1	F	0.43	0/3237	0.64	2/4389 (0.0%)
All	All	0.43	0/19392	0.63	5/26297 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	348	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	F	348	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	F	348	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	C	387	ARG	NE-CZ-NH2	-5.12	117.74	120.30

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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:178:TYR:HA	1:D:181[B]:MET:HE2	1.96	0.48
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:HB3	1:D:46[A]:ARG:HE	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%)	320 (98%)	5 (2%)	65	60
1	B	327/340 (96%)	319 (98%)	8 (2%)	49	40
1	C	337/340 (99%)	331 (98%)	6 (2%)	59	53
1	D	333/340 (98%)	326 (98%)	7 (2%)	53	46
1	E	333/340 (98%)	325 (98%)	8 (2%)	49	40
1	F	332/340 (98%)	325 (98%)	7 (2%)	53	46
All	All	1987/2040 (97%)	1946 (98%)	41 (2%)	59	46

All (41) 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

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Mol	Chain	Res	Type
1	A	260	LEU
1	A	263	ASN
1	B	45	LYS
1	B	46	ARG
1	B	57	GLU
1	B	151	GLU
1	B	196	LYS
1	B	260[A]	LEU
1	B	260[B]	LEU
1	B	263	ASN
1	C	36	LYS
1	C	92	GLU
1	C	175	LYS
1	C	260	LEU
1	C	324[A]	ARG
1	C	324[B]	ARG
1	D	39	LYS
1	D	46[A]	ARG
1	D	46[B]	ARG
1	D	263	ASN
1	D	280[A]	GLU
1	D	280[B]	GLU
1	D	355	ILE
1	E	124	GLU
1	E	144	LYS
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	154	ASN
1	A	171	GLN
1	A	179	HIS
1	A	192	HIS
1	A	209	GLN
1	A	263	ASN
1	A	353	ASN
1	A	359	ASN
1	B	130	GLN
1	B	171	GLN
1	B	192	HIS
1	B	209	GLN
1	B	263	ASN
1	B	353	ASN
1	B	359	ASN
1	C	130	GLN
1	C	154	ASN
1	C	185	ASN
1	C	209	GLN
1	C	263	ASN
1	C	312	ASN
1	C	353	ASN
1	D	130	GLN
1	D	154	ASN
1	D	179	HIS
1	D	209	GLN
1	D	263	ASN
1	D	312	ASN
1	D	353	ASN
1	D	359	ASN
1	E	130	GLN
1	E	154	ASN
1	E	185	ASN
1	E	192	HIS
1	E	209	GLN
1	E	263	ASN
1	E	312	ASN
1	E	353	ASN
1	F	59	HIS
1	F	130	GLN
1	F	154	ASN
1	F	179	HIS

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Mol	Chain	Res	Type
1	F	185	ASN
1	F	192	HIS
1	F	197	ASN
1	F	209	GLN
1	F	263	ASN
1	F	312	ASN
1	F	313	HIS
1	F	353	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	402	-	5,5,5	0.38	0	5,5,5	0.20	0
3	GOL	D	404	-	5,5,5	0.33	0	5,5,5	0.49	0
3	GOL	A	406	-	5,5,5	0.36	0	5,5,5	0.30	0
3	GOL	A	405	-	5,5,5	0.33	0	5,5,5	0.40	0
3	GOL	F	401	-	5,5,5	0.33	0	5,5,5	0.80	0
3	GOL	C	402	-	5,5,5	0.28	0	5,5,5	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	E	405	-	5,5,5	0.26	0	5,5,5	0.36	0
3	GOL	D	405	-	5,5,5	0.23	0	5,5,5	0.47	0
3	GOL	F	402	-	5,5,5	0.37	0	5,5,5	0.37	0
3	GOL	E	401	-	5,5,5	0.28	0	5,5,5	0.50	0
3	GOL	D	406	-	5,5,5	0.31	0	5,5,5	0.49	0
3	GOL	A	404	-	5,5,5	0.31	0	5,5,5	0.24	0
3	GOL	E	403	-	5,5,5	0.44	0	5,5,5	0.44	0
3	GOL	B	405	-	5,5,5	0.32	0	5,5,5	0.30	0
3	GOL	D	403	-	5,5,5	0.35	0	5,5,5	0.72	0
3	GOL	A	403	-	5,5,5	0.44	0	5,5,5	0.42	0
3	GOL	F	403	-	5,5,5	0.48	0	5,5,5	0.87	0
3	GOL	C	403	-	5,5,5	0.40	0	5,5,5	0.40	0
3	GOL	E	404	-	5,5,5	0.42	0	5,5,5	0.48	0
3	GOL	B	404	-	5,5,5	0.30	0	5,5,5	0.47	0
3	GOL	B	403	-	5,5,5	0.18	0	5,5,5	0.69	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	402	-	-	2/4/4/4	-
3	GOL	D	404	-	-	2/4/4/4	-
3	GOL	A	406	-	-	2/4/4/4	-
3	GOL	A	405	-	-	2/4/4/4	-
3	GOL	F	401	-	-	2/4/4/4	-
3	GOL	C	402	-	-	0/4/4/4	-
3	GOL	E	405	-	-	2/4/4/4	-
3	GOL	D	405	-	-	2/4/4/4	-
3	GOL	F	402	-	-	2/4/4/4	-
3	GOL	E	401	-	-	0/4/4/4	-
3	GOL	D	406	-	-	2/4/4/4	-
3	GOL	A	404	-	-	4/4/4/4	-
3	GOL	E	403	-	-	4/4/4/4	-
3	GOL	B	405	-	-	2/4/4/4	-
3	GOL	D	403	-	-	3/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-
3	GOL	F	403	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	403	-	-	1/4/4/4	-
3	GOL	E	404	-	-	2/4/4/4	-
3	GOL	B	404	-	-	1/4/4/4	-
3	GOL	B	403	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (39) torsion outliers are listed below:

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

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

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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%)	0.37	16 (4%) 34 44	22, 30, 50, 93	0
1	B	366/386 (94%)	0.39	19 (5%) 27 37	22, 30, 49, 104	0
1	C	372/386 (96%)	0.11	19 (5%) 28 37	23, 32, 58, 93	0
1	D	367/386 (95%)	0.65	34 (9%) 8 14	23, 32, 56, 111	0
1	E	372/386 (96%)	0.22	18 (4%) 30 40	23, 36, 60, 97	0
1	F	372/386 (96%)	0.18	21 (5%) 24 33	25, 36, 56, 98	0
All	All	2214/2316 (95%)	0.32	127 (5%) 23 32	22, 32, 56, 111	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	38	SER	12.2
1	B	34	ILE	10.8
1	D	34	ILE	9.4
1	E	172	TYR	9.2
1	F	172	TYR	8.9
1	F	73	ALA	8.7
1	A	34	ILE	8.6
1	E	74	HIS	8.0
1	B	33	PHE	7.8
1	D	33	PHE	7.7
1	A	28	SER	7.3
1	B	28	SER	7.3
1	A	33	PHE	7.2
1	F	74	HIS	7.1
1	C	170	ILE	7.0
1	C	172	TYR	6.7
1	C	165	LEU	6.7
1	C	74	HIS	6.7
1	D	39	LYS	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	39	LYS	6.4
1	E	73	ALA	6.0
1	B	32	SER	5.9
1	E	171	GLN	5.9
1	C	73	ALA	5.5
1	F	170	ILE	5.3
1	C	171	GLN	5.3
1	B	31	PRO	5.1
1	D	28	SER	4.7
1	C	174	ASP	4.6
1	B	40	GLU	4.6
1	D	29	HIS	4.5
1	E	170	ILE	4.4
1	A	30	GLY	4.4
1	B	30	GLY	4.4
1	C	173	SER	4.2
1	D	32	SER	4.2
1	E	71	ASN	4.2
1	E	165	LEU	4.2
1	F	174	ASP	4.0
1	A	32	SER	4.0
1	F	173	SER	3.9
1	E	167	GLU	3.9
1	C	166	THR	3.9
1	E	169	LYS	3.8
1	E	173	SER	3.7
1	F	171	GLN	3.7
1	F	169	LYS	3.7
1	D	40	GLU	3.7
1	A	40	GLU	3.6
1	D	65	ASP	3.5
1	D	71	ASN	3.5
1	C	169	LYS	3.5
1	A	29	HIS	3.5
1	A	64[A]	ASP	3.4
1	F	165	LEU	3.4
1	B	29	HIS	3.3
1	A	144	LYS	3.3
1	B	71	ASN	3.3
1	C	167	GLU	3.3
1	D	63	ALA	3.3
1	F	166	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	333	ILE	3.1
1	E	174	ASP	3.1
1	D	125	PHE	3.0
1	D	73	ALA	3.0
1	D	131	ALA	3.0
1	A	31	PRO	3.0
1	D	64[A]	ASP	2.9
1	F	178	TYR	2.9
1	F	64	ASP	2.8
1	D	127	LYS	2.8
1	D	124	GLU	2.8
1	C	64	ASP	2.8
1	D	31	PRO	2.8
1	D	136	LYS	2.8
1	F	167	GLU	2.8
1	D	69	ALA	2.7
1	D	121	PHE	2.7
1	E	166	THR	2.7
1	B	330	VAL	2.7
1	D	92	GLU	2.7
1	C	37	GLY	2.6
1	D	30	GLY	2.6
1	E	178	TYR	2.6
1	C	168	GLN	2.6
1	C	156	GLU	2.6
1	D	123	GLU	2.5
1	E	120	PRO	2.5
1	E	151	GLU	2.5
1	D	242	VAL	2.5
1	A	151	GLU	2.5
1	F	65	ASP	2.5
1	D	128	ARG	2.4
1	B	45	LYS	2.4
1	D	181[A]	MET	2.4
1	B	151	GLU	2.4
1	D	151	GLU	2.4
1	D	330	VAL	2.4
1	E	64	ASP	2.3
1	A	156	GLU	2.3
1	E	175	LYS	2.3
1	D	245	LEU	2.3
1	A	65	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	151	GLU	2.3
1	F	71	ASN	2.3
1	B	333	ILE	2.3
1	D	76	ALA	2.3
1	D	95	ILE	2.3
1	B	260[A]	LEU	2.3
1	C	164	ILE	2.2
1	B	245	LEU	2.2
1	B	73	ALA	2.2
1	F	158	PHE	2.2
1	E	37	GLY	2.1
1	A	333	ILE	2.1
1	C	163	ALA	2.1
1	C	151	GLU	2.1
1	B	64	ASP	2.1
1	C	144	LYS	2.1
1	A	71	ASN	2.1
1	F	162	ALA	2.1
1	F	164	ILE	2.1
1	F	168	GLN	2.0
1	B	341	ALA	2.0
1	F	163	ALA	2.0
1	D	75	SER	2.0
1	A	123	GLU	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 [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(\AA^2)	Q<0.9
3	GOL	F	403	6/6	0.68	0.23	51,55,58,64	0
3	GOL	B	405	6/6	0.69	0.28	64,66,67,68	0
3	GOL	C	403	6/6	0.78	0.21	41,54,59,59	0
3	GOL	E	402	6/6	0.78	0.19	45,57,60,61	0
3	GOL	E	404	6/6	0.79	0.19	62,65,66,67	0
3	GOL	D	406	6/6	0.83	0.16	51,57,58,59	0
3	GOL	A	405	6/6	0.83	0.26	41,53,57,64	0
3	GOL	B	404	6/6	0.84	0.27	39,50,51,55	0
2	NA	C	401	1/1	0.85	0.28	45,45,45,45	0
3	GOL	A	406	6/6	0.87	0.17	54,57,60,64	0
3	GOL	D	403	6/6	0.87	0.18	41,48,52,56	0
3	GOL	E	401	6/6	0.87	0.18	41,48,51,56	0
3	GOL	E	403	6/6	0.88	0.35	56,61,62,64	0
3	GOL	A	403	6/6	0.88	0.16	35,39,45,49	0
3	GOL	D	405	6/6	0.89	0.23	41,50,53,61	0
3	GOL	F	401	6/6	0.89	0.19	48,61,66,67	0
3	GOL	D	404	6/6	0.90	0.14	33,38,44,47	0
3	GOL	E	405	6/6	0.90	0.28	50,55,57,62	0
3	GOL	C	402	6/6	0.91	0.20	43,49,50,52	0
3	GOL	F	402	6/6	0.92	0.20	52,54,58,60	0
2	NA	D	402	1/1	0.92	0.32	49,49,49,49	0
3	GOL	B	403	6/6	0.93	0.19	33,37,44,46	0
3	GOL	A	404	6/6	0.94	0.29	47,51,53,55	0
2	NA	B	402	1/1	0.97	0.34	41,41,41,41	0
2	NA	A	401	1/1	0.98	0.20	32,32,32,32	0
2	NA	B	401	1/1	0.99	0.08	26,26,26,26	0
2	NA	D	401	1/1	0.99	0.08	25,25,25,25	0
2	NA	A	402	1/1	0.99	0.07	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.