



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:44 pm BST

PDB ID : 1LNX
Title : Crystal structure of the P.aerophilum SmAP1 heptamer in a new crystal form (C2221)
Authors : Mura, C.; Kozhukhovsky, A.; Eisenberg, D.
Deposited on : 2002-05-04
Resolution : 2.05 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 : 2.11
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) : 2.11

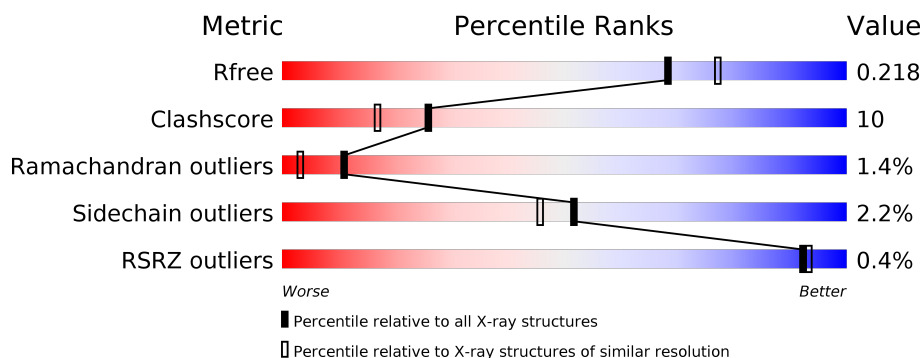
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	81	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>• 9%</div> </div> </div>
1	B	81	<div> <div>74%</div> <div>14%</div> <div>• 10%</div> </div>
1	C	81	<div> <div>77%</div> <div>12%</div> <div>• 10%</div> </div>
1	D	81	<div> <div>79%</div> <div>10%</div> <div>• 10%</div> </div>
1	E	81	<div> <div>80%</div> <div>9%</div> <div>• 10%</div> </div>
1	F	81	<div> <div>%</div> <div>78%</div> <div>11%</div> <div>• 9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	81	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	URI	A	8003	-	-	-	X
2	URI	D	8006	-	-	X	-
2	URI	E	8007	-	-	-	X
2	URI	G	8002	-	-	X	-
3	GOL	A	8209	-	X	-	-
3	GOL	B	8202	-	X	-	-
3	GOL	C	8208	-	X	-	-
3	GOL	D	8207	-	X	-	-
3	GOL	E	8204	-	X	-	-
3	GOL	E	8205	-	X	-	-
3	GOL	E	8210	-	X	-	-
3	GOL	F	8203	-	X	-	-
3	GOL	F	8206	-	X	-	-
3	GOL	G	8201	-	X	-	-
4	ACY	C	8102	-	-	X	-
4	ACY	D	8101	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4519 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.

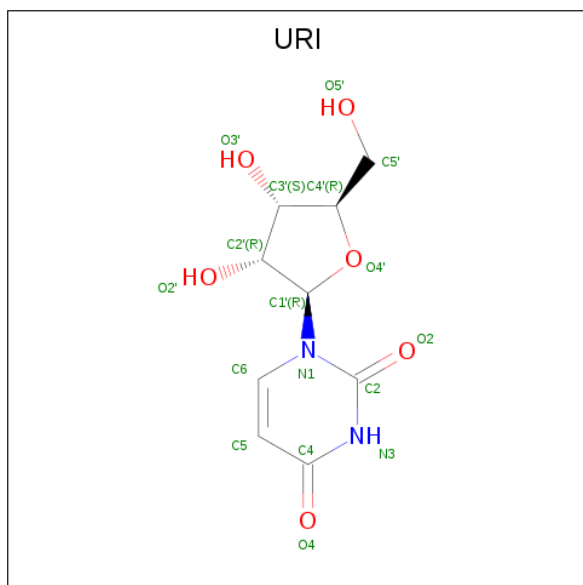
- Molecule 1 is a protein called small nuclear ribonucleoprotein homolog (Sm-like).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	S	0	0	0
			576	363	102	109	2			
1	B	73	Total	C	N	O	S	0	0	0
			571	361	101	107	2			
1	C	73	Total	C	N	O	S	0	0	0
			571	361	101	107	2			
1	D	73	Total	C	N	O	S	0	0	0
			571	361	101	107	2			
1	E	73	Total	C	N	O	S	0	0	0
			571	361	101	107	2			
1	F	74	Total	C	N	O	S	0	0	0
			576	363	102	109	2			
1	G	73	Total	C	N	O	S	0	0	0
			571	361	101	107	2			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	GLY	-	CLONING ARTIFACT	UNP Q8ZYG5
B	81	GLY	-	CLONING ARTIFACT	UNP Q8ZYG5
C	81	GLY	-	CLONING ARTIFACT	UNP Q8ZYG5
D	81	GLY	-	CLONING ARTIFACT	UNP Q8ZYG5
E	81	GLY	-	CLONING ARTIFACT	UNP Q8ZYG5
F	81	GLY	-	CLONING ARTIFACT	UNP Q8ZYG5
G	81	GLY	-	CLONING ARTIFACT	UNP Q8ZYG5

- Molecule 2 is URIDINE (three-letter code: URI) (formula: C₉H₁₂N₂O₆).



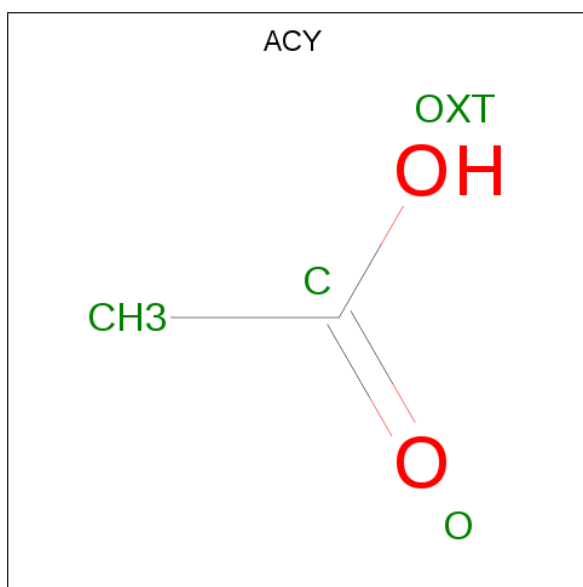
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	9	2	6		
2	B	1	Total	C	N	O	0	0
			17	9	2	6		
2	D	1	Total	C	N	O	0	0
			17	9	2	6		
2	D	1	Total	C	N	O	0	0
			17	9	2	6		
2	E	1	Total	C	N	O	0	0
			17	9	2	6		
2	F	1	Total	C	N	O	0	0
			17	9	2	6		
2	G	1	Total	C	N	O	0	0
			17	9	2	6		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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

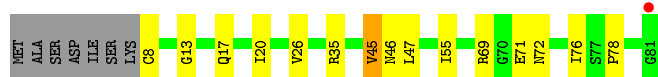
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	37	Total	O	0	0
			37	37		
5	B	43	Total	O	0	0
			43	43		
5	C	48	Total	O	0	0
			48	48		
5	D	60	Total	O	0	0
			60	60		
5	E	47	Total	O	0	0
			47	47		
5	F	49	Total	O	0	0
			49	49		
5	G	41	Total	O	0	0
			41	41		

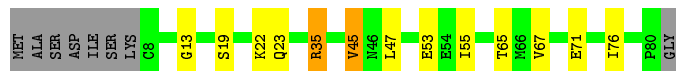
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: small nuclear ribonucleoprotein homolog (Sm-like)



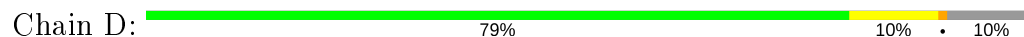
- Molecule 1: small nuclear ribonucleoprotein homolog (Sm-like)



- Molecule 1: small nuclear ribonucleoprotein homolog (Sm-like)



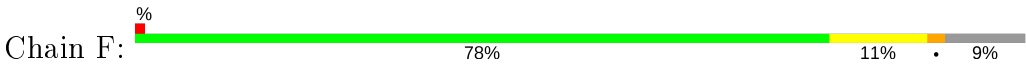
- Molecule 1: small nuclear ribonucleoprotein homolog (Sm-like)



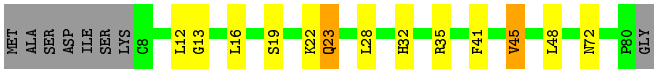
- Molecule 1: small nuclear ribonucleoprotein homolog (Sm-like)



- Molecule 1: small nuclear ribonucleoprotein homolog (Sm-like)



● Molecule 1: small nuclear ribonucleoprotein homolog (Sm-like)



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	91.83Å 113.76Å 126.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.78 – 2.05 71.46 – 2.05	Depositor EDS
% Data completeness (in resolution range)	95.5 (19.78-2.05) 95.6 (71.46-2.05)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.182 , 0.226 0.176 , 0.218	Depositor DCC
R_{free} test set	2039 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4519	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.67% 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, ACY, URI

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	0.58	0/583	0.76	0/785
1	B	0.59	0/578	0.80	0/780
1	C	0.65	0/578	0.79	0/780
1	D	0.64	0/578	0.81	0/780
1	E	0.63	0/578	0.80	0/780
1	F	0.65	0/583	0.82	0/785
1	G	0.64	0/578	0.76	0/780
All	All	0.63	0/4056	0.79	0/5470

There are no bond length outliers.

There are no bond angle outliers.

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	576	0	587	15	0
1	B	571	0	584	14	0
1	C	571	0	584	10	0
1	D	571	0	584	11	0
1	E	571	0	584	6	0
1	F	576	0	587	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	571	0	584	16	0
2	A	17	0	12	3	0
2	B	17	0	12	3	0
2	D	34	0	24	11	0
2	E	17	0	12	3	0
2	F	17	0	12	3	0
2	G	17	0	12	8	0
3	A	6	0	4	0	0
3	B	6	0	4	0	0
3	C	6	0	4	0	0
3	D	6	0	4	2	0
3	E	18	0	13	3	0
3	F	12	0	8	0	0
3	G	6	0	4	0	0
4	C	4	0	3	2	0
4	D	4	0	3	0	3
5	A	37	0	0	0	0
5	B	43	0	0	0	0
5	C	48	0	0	2	0
5	D	60	0	0	1	1
5	E	47	0	0	2	0
5	F	49	0	0	1	0
5	G	41	0	0	3	0
All	All	4519	0	4225	88	4

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 10.

All (88) 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)
3:D:8207:GOL:O1	3:D:8207:GOL:C1	1.63	1.41
3:E:8210:GOL:O1	3:E:8210:GOL:C1	1.64	1.41
1:E:13:GLY:HA3	2:E:8007:URI:H3'	1.27	1.12
1:D:43:GLN:HB2	2:D:8006:URI:O5'	1.54	1.08
1:A:13:GLY:HA3	2:A:8003:URI:H2'	1.42	1.01
1:B:13:GLY:HA3	2:B:8004:URI:H2'	1.48	0.94
1:D:43:GLN:HA	2:D:8006:URI:H3'	1.50	0.93
1:G:16:LEU:HD12	2:G:8002:URI:H5'1	1.57	0.84
1:G:13:GLY:HA2	2:G:8002:URI:H5'2	1.59	0.83
1:F:19:SER:HA	1:F:22:LYS:HD3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8005:URI:H3'	5:D:8265:HOH:O	1.82	0.78
1:G:13:GLY:HA2	2:G:8002:URI:C5'	2.15	0.77
1:B:13:GLY:CA	2:B:8004:URI:H2'	2.16	0.76
1:E:13:GLY:HA3	2:E:8007:URI:C3'	2.10	0.76
1:B:47:LEU:HD11	1:B:76:ILE:CD1	2.18	0.72
1:A:46:ASN:HB3	2:G:8002:URI:O4	1.88	0.72
1:G:35:ARG:HD3	5:G:8224:HOH:O	1.90	0.70
1:A:76:ILE:HB	1:B:67:VAL:CG2	2.21	0.70
1:D:43:GLN:CA	2:D:8006:URI:H3'	2.20	0.70
1:A:13:GLY:CA	2:A:8003:URI:H2'	2.18	0.70
1:C:29:ARG:HH22	4:C:8102:ACY:H3	1.55	0.69
1:F:43:GLN:HA	2:F:8001:URI:H3'	1.74	0.69
1:D:43:GLN:HB2	2:D:8006:URI:HO5'	1.59	0.66
1:B:47:LEU:HD11	1:B:76:ILE:HD11	1.76	0.66
3:D:8207:GOL:C1	3:D:8207:GOL:HO1	2.07	0.64
1:G:16:LEU:HD12	2:G:8002:URI:C5'	2.27	0.64
1:G:23:GLN:HE22	1:G:35:ARG:HB3	1.62	0.64
1:A:76:ILE:HB	1:B:67:VAL:HG22	1.80	0.64
1:A:13:GLY:HA3	2:A:8003:URI:C2'	2.25	0.63
1:B:35:ARG:HD3	1:B:55:ILE:HD11	1.80	0.62
1:C:26:VAL:HG22	1:C:76:ILE:HD12	1.83	0.61
1:G:45:VAL:O	1:G:45:VAL:HG12	2.00	0.61
1:A:45:VAL:O	1:A:45:VAL:HG12	2.01	0.61
3:E:8210:GOL:C1	3:E:8210:GOL:HO1	2.07	0.61
1:B:13:GLY:HA3	2:B:8004:URI:C2'	2.29	0.60
1:F:12:LEU:HD22	1:G:48:LEU:HB2	1.85	0.59
1:C:23:GLN:NE2	5:C:8255:HOH:O	2.24	0.56
1:D:13:GLY:O	1:D:17:GLN:HG3	2.05	0.56
1:F:43:GLN:CB	2:F:8001:URI:H3'	2.36	0.56
1:F:45:VAL:CG1	1:F:76:ILE:HD11	2.36	0.56
1:F:43:GLN:CA	2:F:8001:URI:H3'	2.36	0.56
1:B:19:SER:HA	1:B:22:LYS:HD2	1.88	0.55
1:D:45:VAL:CG1	1:D:76:ILE:HD11	2.39	0.53
1:G:28:LEU:HB2	1:G:32:HIS:HB2	1.91	0.53
1:G:13:GLY:HA2	2:G:8002:URI:O5'	2.09	0.52
1:B:35:ARG:NH2	1:B:53:GLU:OE2	2.37	0.52
1:C:12:LEU:N	1:C:12:LEU:HD12	2.25	0.52
1:A:26:VAL:HG13	1:A:76:ILE:HD13	1.90	0.51
1:G:72:ASN:HB2	5:G:8203:HOH:O	2.10	0.51
1:B:45:VAL:O	1:B:45:VAL:HG12	2.11	0.51
1:F:45:VAL:HG12	1:F:45:VAL:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:ASP:O	1:E:22:LYS:HE3	2.10	0.51
1:A:17:GLN:O	1:A:20:ILE:HD12	2.11	0.50
1:D:43:GLN:CB	2:D:8006:URI:H3'	2.41	0.50
1:C:75:PHE:O	1:C:76:ILE:HD13	2.13	0.49
1:C:55:ILE:N	1:C:55:ILE:HD12	2.29	0.48
1:B:67:VAL:O	1:B:67:VAL:HG23	2.13	0.47
1:G:23:GLN:NE2	1:G:35:ARG:HB3	2.29	0.47
1:G:19:SER:HA	1:G:22:LYS:HD2	1.97	0.47
1:A:72:ASN:HB2	5:G:8202:HOH:O	2.15	0.46
1:A:47:LEU:HD11	1:A:76:ILE:HD11	1.97	0.46
2:D:8005:URI:O2	2:D:8005:URI:H5'2	2.16	0.45
1:F:72:ASN:HB2	5:F:8207:HOH:O	2.17	0.45
1:D:67:VAL:HG11	2:D:8005:URI:H5	1.99	0.45
1:B:71:GLU:O	1:B:71:GLU:HG2	2.16	0.44
1:E:23:GLN:HE21	3:E:8210:GOL:C1	2.29	0.44
1:G:12:LEU:CD2	2:G:8002:URI:O4	2.66	0.44
1:A:35:ARG:HD3	1:A:55:ILE:HD11	1.98	0.44
1:D:79:VAL:HA	1:D:80:PRO:HD3	1.82	0.44
1:A:78:PRO:HD2	1:B:65:THR:O	2.18	0.43
1:A:69:ARG:NH2	1:A:71:GLU:OE1	2.33	0.43
1:F:35:ARG:NH2	1:F:53:GLU:OE2	2.46	0.43
5:C:8217:HOH:O	2:D:8005:URI:H5'1	2.18	0.42
1:G:41:PHE:HE2	2:G:8002:URI:H4'	1.84	0.42
1:G:12:LEU:HD12	1:G:12:LEU:N	2.35	0.42
1:F:55:ILE:N	1:F:55:ILE:HD12	2.35	0.42
1:F:12:LEU:HD23	1:F:12:LEU:H	1.84	0.41
1:E:43:GLN:NE2	5:E:8250:HOH:O	2.53	0.41
1:A:47:LEU:HD11	1:A:76:ILE:CD1	2.49	0.41
1:D:45:VAL:O	1:D:45:VAL:HG12	2.21	0.41
1:C:79:VAL:HA	1:C:80:PRO:HD3	1.95	0.41
2:E:8007:URI:H2'	5:E:8221:HOH:O	2.20	0.41
2:D:8006:URI:O4'	2:D:8006:URI:O2	2.39	0.41
1:C:29:ARG:HH12	4:C:8102:ACY:CH3	2.34	0.40
1:D:43:GLN:HB2	2:D:8006:URI:C5'	2.47	0.40
1:E:35:ARG:HD3	1:E:35:ARG:HH11	1.77	0.40
1:C:26:VAL:HG13	1:C:76:ILE:CD1	2.51	0.40
1:C:45:VAL:O	1:C:45:VAL:HG12	2.22	0.40

All (4) 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)
5:D:8258:HOH:O	5:D:8258:HOH:O[3_656]	1.19	1.01
4:D:8101:ACY:OXT	4:D:8101:ACY:CH3[4_567]	1.36	0.84
4:D:8101:ACY:C	4:D:8101:ACY:CH3[4_567]	1.52	0.68
4:D:8101:ACY:O	4:D:8101:ACY:CH3[4_567]	1.64	0.56

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	72/81 (89%)	70 (97%)	1 (1%)	1 (1%)	11	3
1	B	71/81 (88%)	70 (99%)	0	1 (1%)	11	3
1	C	71/81 (88%)	69 (97%)	1 (1%)	1 (1%)	11	3
1	D	71/81 (88%)	70 (99%)	0	1 (1%)	11	3
1	E	71/81 (88%)	70 (99%)	0	1 (1%)	11	3
1	F	72/81 (89%)	70 (97%)	1 (1%)	1 (1%)	11	3
1	G	71/81 (88%)	70 (99%)	0	1 (1%)	11	3
All	All	499/567 (88%)	489 (98%)	3 (1%)	7 (1%)	11	3

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	45	VAL
1	B	45	VAL
1	E	45	VAL
1	F	45	VAL
1	G	45	VAL
1	A	45	VAL
1	D	45	VAL

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	64/70 (91%)	63 (98%)	1 (2%)	62	59
1	B	64/70 (91%)	62 (97%)	2 (3%)	40	33
1	C	64/70 (91%)	63 (98%)	1 (2%)	62	59
1	D	64/70 (91%)	63 (98%)	1 (2%)	62	59
1	E	64/70 (91%)	62 (97%)	2 (3%)	40	33
1	F	64/70 (91%)	62 (97%)	2 (3%)	40	33
1	G	64/70 (91%)	63 (98%)	1 (2%)	62	59
All	All	448/490 (91%)	438 (98%)	10 (2%)	52	46

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	CYS
1	B	23	GLN
1	B	35	ARG
1	C	8	CYS
1	D	8	CYS
1	E	43	GLN
1	E	71	GLU
1	F	8	CYS
1	F	12	LEU
1	G	23	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	17	GLN
1	B	72	ASN
1	D	72	ASN
1	E	23	GLN
1	E	43	GLN

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Mol	Chain	Res	Type
1	E	59	ASN
1	F	72	ASN
1	G	23	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

19 ligands are modelled in this entry.

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
2	URI	A	8003	-	14,18,18	2.33	2 (14%)	14,26,26	1.69	2 (14%)
4	ACY	D	8101	-	1,3,3	2.73	1 (100%)	0,3,3	0.00	-
3	GOL	A	8209	-	5,5,5	4.67	5 (100%)	5,5,5	5.72	3 (60%)
3	GOL	F	8203	-	5,5,5	4.52	5 (100%)	5,5,5	5.76	3 (60%)
2	URI	G	8002	-	14,18,18	2.40	3 (21%)	14,26,26	1.72	4 (28%)
2	URI	E	8007	-	14,18,18	2.31	2 (14%)	14,26,26	1.69	2 (14%)
3	GOL	B	8202	-	5,5,5	4.41	5 (100%)	5,5,5	5.89	3 (60%)
3	GOL	E	8210	-	5,5,5	4.40	4 (80%)	5,5,5	5.60	3 (60%)
2	URI	D	8005	-	14,18,18	1.99	3 (21%)	14,26,26	1.64	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACY	C	8102	-	1,3,3	1.39	0	0,3,3	0.00	-
2	URI	D	8006	-	14,18,18	1.90	3 (21%)	14,26,26	1.97	4 (28%)
2	URI	F	8001	-	14,18,18	2.16	3 (21%)	14,26,26	1.61	2 (14%)
3	GOL	E	8204	-	5,5,5	4.54	5 (100%)	5,5,5	5.47	3 (60%)
2	URI	B	8004	-	14,18,18	2.42	2 (14%)	14,26,26	1.75	3 (21%)
3	GOL	F	8206	-	5,5,5	4.65	5 (100%)	5,5,5	5.59	3 (60%)
3	GOL	C	8208	-	5,5,5	4.65	5 (100%)	5,5,5	5.68	3 (60%)
3	GOL	D	8207	-	5,5,5	4.60	5 (100%)	5,5,5	5.61	3 (60%)
3	GOL	G	8201	-	5,5,5	4.64	5 (100%)	5,5,5	5.83	3 (60%)
3	GOL	E	8205	-	5,5,5	4.50	5 (100%)	5,5,5	5.78	3 (60%)

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
2	URI	A	8003	-	-	2/4/22/22	0/2/2/2
3	GOL	A	8209	-	-	3/4/4/4	-
3	GOL	F	8203	-	-	3/4/4/4	-
2	URI	G	8002	-	-	1/4/22/22	0/2/2/2
2	URI	E	8007	-	-	1/4/22/22	0/2/2/2
3	GOL	B	8202	-	-	3/4/4/4	-
3	GOL	E	8210	-	-	4/4/4/4	-
2	URI	D	8005	-	-	1/4/22/22	0/2/2/2
2	URI	D	8006	-	-	1/4/22/22	0/2/2/2
2	URI	F	8001	-	-	0/4/22/22	0/2/2/2
3	GOL	E	8204	-	-	3/4/4/4	-
2	URI	B	8004	-	-	2/4/22/22	0/2/2/2
3	GOL	F	8206	-	-	3/4/4/4	-
3	GOL	C	8208	-	-	3/4/4/4	-
3	GOL	D	8207	-	-	3/4/4/4	-
3	GOL	G	8201	-	-	3/4/4/4	-
3	GOL	E	8205	-	-	3/4/4/4	-

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	8208	GOL	C3-C2	-8.06	1.18	1.51
3	A	8209	GOL	C3-C2	-7.80	1.19	1.51
3	G	8201	GOL	C3-C2	-7.63	1.20	1.51
3	E	8204	GOL	C3-C2	-7.48	1.21	1.51
3	F	8206	GOL	C3-C2	-7.47	1.21	1.51
3	E	8205	GOL	C3-C2	-7.34	1.21	1.51
3	F	8203	GOL	C3-C2	-7.32	1.21	1.51
3	B	8202	GOL	C3-C2	-7.22	1.22	1.51
3	D	8207	GOL	C3-C2	-7.04	1.22	1.51
2	B	8004	URI	C6-N1	6.74	1.44	1.35
3	E	8210	GOL	C3-C2	-6.73	1.24	1.51
2	E	8007	URI	C6-N1	6.34	1.43	1.35
2	A	8003	URI	C6-N1	6.11	1.43	1.35
2	G	8002	URI	C6-N1	6.05	1.43	1.35
2	F	8001	URI	C6-N1	5.83	1.43	1.35
2	G	8002	URI	C4-N3	5.45	1.42	1.33
2	D	8006	URI	C6-N1	5.40	1.42	1.35
3	E	8210	GOL	O1-C1	5.15	1.64	1.42
3	D	8207	GOL	O1-C1	5.02	1.63	1.42
2	A	8003	URI	C4-N3	5.02	1.41	1.33
2	E	8007	URI	C4-N3	4.95	1.41	1.33
2	D	8005	URI	C4-N3	4.88	1.41	1.33
2	B	8004	URI	C4-N3	4.85	1.41	1.33
3	F	8206	GOL	O1-C1	4.75	1.62	1.42
3	G	8201	GOL	O1-C1	4.74	1.62	1.42
3	A	8209	GOL	O1-C1	4.71	1.62	1.42
3	F	8203	GOL	O1-C1	4.58	1.61	1.42
3	E	8204	GOL	O1-C1	4.57	1.61	1.42
3	E	8205	GOL	O1-C1	4.54	1.61	1.42
2	F	8001	URI	C4-N3	4.48	1.40	1.33
3	C	8208	GOL	O1-C1	4.43	1.61	1.42
3	B	8202	GOL	O1-C1	4.37	1.60	1.42
3	E	8210	GOL	O3-C3	4.10	1.59	1.42
2	D	8005	URI	C6-N1	3.93	1.40	1.35
3	D	8207	GOL	O3-C3	3.70	1.58	1.42
3	F	8206	GOL	O2-C2	-3.58	1.32	1.43
3	E	8205	GOL	O3-C3	3.49	1.57	1.42
2	D	8006	URI	C4-N3	3.47	1.39	1.33
3	E	8204	GOL	O3-C3	3.46	1.57	1.42
3	B	8202	GOL	O3-C3	3.38	1.56	1.42
3	F	8203	GOL	O3-C3	3.37	1.56	1.42
3	D	8207	GOL	O2-C2	-3.36	1.33	1.43
3	F	8206	GOL	O3-C3	3.23	1.56	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	8208	GOL	C1-C2	-3.02	1.39	1.51
3	G	8201	GOL	O2-C2	-3.00	1.34	1.43
3	G	8201	GOL	C1-C2	-2.99	1.39	1.51
3	G	8201	GOL	O3-C3	2.99	1.55	1.42
3	A	8209	GOL	O2-C2	-2.97	1.34	1.43
3	A	8209	GOL	O3-C3	2.92	1.54	1.42
3	F	8203	GOL	O2-C2	-2.92	1.34	1.43
3	A	8209	GOL	C1-C2	-2.91	1.39	1.51
2	G	8002	URI	C6-C5	-2.85	1.31	1.38
3	B	8202	GOL	C1-C2	-2.84	1.40	1.51
3	C	8208	GOL	O2-C2	-2.81	1.35	1.43
3	F	8203	GOL	C1-C2	-2.80	1.40	1.51
3	E	8204	GOL	C1-C2	-2.76	1.40	1.51
4	D	8101	ACY	CH3-C	2.73	1.52	1.48
3	E	8205	GOL	O2-C2	-2.72	1.35	1.43
3	E	8205	GOL	C1-C2	-2.70	1.40	1.51
3	E	8204	GOL	O2-C2	-2.60	1.35	1.43
3	F	8206	GOL	C1-C2	-2.60	1.41	1.51
3	B	8202	GOL	O2-C2	-2.58	1.35	1.43
2	D	8005	URI	C6-C5	-2.57	1.32	1.38
3	C	8208	GOL	O3-C3	2.54	1.53	1.42
3	D	8207	GOL	C1-C2	-2.51	1.41	1.51
3	E	8210	GOL	C1-C2	-2.18	1.42	1.51
2	F	8001	URI	C6-C5	-2.14	1.33	1.38
2	D	8006	URI	C6-C5	-2.02	1.33	1.38

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	8202	GOL	O3-C3-C2	10.80	161.96	110.20
3	G	8201	GOL	O3-C3-C2	10.60	161.04	110.20
3	F	8203	GOL	O3-C3-C2	10.52	160.66	110.20
3	E	8205	GOL	O3-C3-C2	10.50	160.56	110.20
3	E	8210	GOL	O3-C3-C2	10.45	160.31	110.20
3	A	8209	GOL	O3-C3-C2	10.40	160.06	110.20
3	C	8208	GOL	O3-C3-C2	10.36	159.87	110.20
3	D	8207	GOL	O3-C3-C2	10.32	159.66	110.20
3	F	8206	GOL	O3-C3-C2	10.18	159.02	110.20
3	E	8204	GOL	O3-C3-C2	10.02	158.24	110.20
3	B	8202	GOL	O2-C2-C3	6.86	139.34	109.12
3	G	8201	GOL	O2-C2-C3	6.81	139.13	109.12
3	E	8205	GOL	O2-C2-C3	6.66	138.46	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	8203	GOL	O2-C2-C3	6.62	138.30	109.12
3	A	8209	GOL	O2-C2-C3	6.62	138.27	109.12
3	C	8208	GOL	O2-C2-C3	6.59	138.15	109.12
3	D	8207	GOL	O2-C2-C3	6.47	137.62	109.12
3	F	8206	GOL	O2-C2-C3	6.44	137.48	109.12
3	E	8204	GOL	O2-C2-C3	6.32	136.98	109.12
3	E	8210	GOL	O2-C2-C3	6.20	136.43	109.12
2	B	8004	URI	C3'-C2'-C1'	4.17	107.26	100.98
2	D	8006	URI	C3'-C2'-C1'	4.09	107.14	100.98
2	E	8007	URI	C3'-C2'-C1'	4.04	107.06	100.98
2	A	8003	URI	C3'-C2'-C1'	3.97	106.95	100.98
2	F	8001	URI	C3'-C2'-C1'	3.95	106.92	100.98
2	G	8002	URI	C3'-C2'-C1'	3.90	106.85	100.98
2	D	8006	URI	O4'-C4'-C5'	-3.81	100.98	109.21
2	D	8005	URI	C3'-C2'-C1'	3.66	106.49	100.98
2	A	8003	URI	C5-C4-N3	-3.39	115.85	123.31
2	E	8007	URI	C5-C4-N3	-3.37	115.89	123.31
3	E	8205	GOL	O1-C1-C2	3.37	126.34	110.20
3	A	8209	GOL	O1-C1-C2	3.31	126.06	110.20
3	F	8206	GOL	O1-C1-C2	3.29	125.99	110.20
3	F	8203	GOL	O1-C1-C2	3.26	125.84	110.20
2	D	8006	URI	C5-C4-N3	-3.17	116.33	123.31
2	B	8004	URI	C5-C4-N3	-3.17	116.33	123.31
3	G	8201	GOL	O1-C1-C2	3.09	125.02	110.20
3	C	8208	GOL	O1-C1-C2	3.08	124.97	110.20
2	F	8001	URI	C5-C4-N3	-3.08	116.54	123.31
2	G	8002	URI	C5-C4-N3	-3.06	116.58	123.31
3	D	8207	GOL	O1-C1-C2	2.99	124.53	110.20
2	D	8005	URI	C5-C4-N3	-2.97	116.78	123.31
3	E	8204	GOL	O1-C1-C2	2.96	124.38	110.20
3	B	8202	GOL	O1-C1-C2	2.93	124.25	110.20
3	E	8210	GOL	O1-C1-C2	2.89	124.08	110.20
2	B	8004	URI	O4'-C4'-C5'	2.25	114.08	109.21
2	D	8006	URI	O5'-C5'-C4'	2.12	118.56	111.29
2	G	8002	URI	C5-C6-N1	2.05	125.27	120.68
2	D	8005	URI	C2'-C3'-C4'	2.05	106.63	102.64
2	G	8002	URI	O4'-C4'-C5'	-2.02	104.84	109.21

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	8003	URI	C2'-C1'-N1-C6
2	A	8003	URI	O4'-C1'-N1-C6
3	A	8209	GOL	O1-C1-C2-C3
3	A	8209	GOL	C1-C2-C3-O3
3	F	8203	GOL	O1-C1-C2-C3
2	G	8002	URI	C2'-C1'-N1-C6
2	E	8007	URI	O4'-C1'-N1-C6
3	E	8210	GOL	O1-C1-C2-C3
3	E	8210	GOL	C1-C2-C3-O3
2	D	8005	URI	C2'-C1'-N1-C6
2	D	8006	URI	C2'-C1'-N1-C6
2	B	8004	URI	C2'-C1'-N1-C6
2	B	8004	URI	O4'-C1'-N1-C6
3	C	8208	GOL	O1-C1-C2-C3
3	C	8208	GOL	C1-C2-C3-O3
3	G	8201	GOL	O1-C1-C2-O2
3	G	8201	GOL	C1-C2-C3-O3
3	E	8205	GOL	C1-C2-C3-O3
3	F	8203	GOL	C1-C2-C3-O3
3	F	8206	GOL	C1-C2-C3-O3
3	B	8202	GOL	C1-C2-C3-O3
3	E	8204	GOL	C1-C2-C3-O3
3	D	8207	GOL	C1-C2-C3-O3
3	E	8205	GOL	O1-C1-C2-C3
3	F	8206	GOL	O1-C1-C2-O2
3	B	8202	GOL	O1-C1-C2-O2
3	E	8204	GOL	O1-C1-C2-O2
3	D	8207	GOL	O1-C1-C2-O2
3	E	8210	GOL	O2-C2-C3-O3
3	A	8209	GOL	O2-C2-C3-O3
3	F	8203	GOL	O2-C2-C3-O3
3	F	8206	GOL	O2-C2-C3-O3
3	B	8202	GOL	O2-C2-C3-O3
3	E	8204	GOL	O2-C2-C3-O3
3	C	8208	GOL	O2-C2-C3-O3
3	D	8207	GOL	O2-C2-C3-O3
3	G	8201	GOL	O2-C2-C3-O3
3	E	8205	GOL	O2-C2-C3-O3
3	E	8210	GOL	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	8003	URI	3	0
4	D	8101	ACY	0	3
2	G	8002	URI	8	0
2	E	8007	URI	3	0
3	E	8210	GOL	3	0
2	D	8005	URI	4	0
4	C	8102	ACY	2	0
2	D	8006	URI	7	0
2	F	8001	URI	3	0
2	B	8004	URI	3	0
3	D	8207	GOL	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	74/81 (91%)	-0.47	1 (1%) 75 78	20, 28, 39, 59	0
1	B	73/81 (90%)	-0.60	0 100 100	18, 26, 35, 39	0
1	C	73/81 (90%)	-0.62	0 100 100	16, 23, 32, 44	0
1	D	73/81 (90%)	-0.68	0 100 100	15, 22, 31, 35	0
1	E	73/81 (90%)	-0.60	0 100 100	17, 22, 33, 45	0
1	F	74/81 (91%)	-0.57	1 (1%) 75 78	17, 24, 34, 57	0
1	G	73/81 (90%)	-0.49	0 100 100	18, 25, 37, 51	0
All	All	513/567 (90%)	-0.58	2 (0%) 92 93	15, 24, 37, 59	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	81	GLY	3.9
1	A	81	GLY	3.5

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 carbohydrates 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	E	8205	6/6	0.56	0.22	73,75,75,75	0
2	URI	A	8003	17/17	0.61	0.45	85,89,94,96	8
3	GOL	E	8204	6/6	0.65	0.28	37,48,51,52	0
2	URI	E	8007	17/17	0.68	0.41	67,73,77,77	9
2	URI	B	8004	17/17	0.69	0.39	68,77,82,83	8
3	GOL	E	8210	6/6	0.73	0.24	41,46,47,49	0
3	GOL	A	8209	6/6	0.75	0.23	65,69,71,71	0
2	URI	F	8001	17/17	0.78	0.39	56,64,72,72	10
3	GOL	D	8207	6/6	0.80	0.18	34,44,45,48	0
3	GOL	F	8203	6/6	0.80	0.15	68,69,69,69	0
3	GOL	B	8202	6/6	0.82	0.17	37,49,51,52	0
2	URI	D	8005	17/17	0.83	0.48	63,69,74,75	12
2	URI	D	8006	17/17	0.84	0.42	66,71,76,77	11
2	URI	G	8002	17/17	0.84	0.45	96,98,101,102	10
3	GOL	C	8208	6/6	0.86	0.21	41,49,52,53	0
3	GOL	F	8206	6/6	0.89	0.17	42,46,48,51	0
3	GOL	G	8201	6/6	0.90	0.24	52,54,56,57	0
4	ACY	D	8101	4/4	0.91	0.12	82,82,82,82	2
4	ACY	C	8102	4/4	0.95	0.42	74,75,75,75	0

6.5 Other polymers

There are no such residues in this entry.