



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:53 PM GMT

PDB ID : 1M5Q
Title : Crystal structure of a novel Sm-like archaeal protein from *Pyrobaculum aerophilum*
Authors : Mura, C.; Phillips, M.; Kozhukhovskiy, A.; Eisenberg, D.
Deposited on : 2002-07-09
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

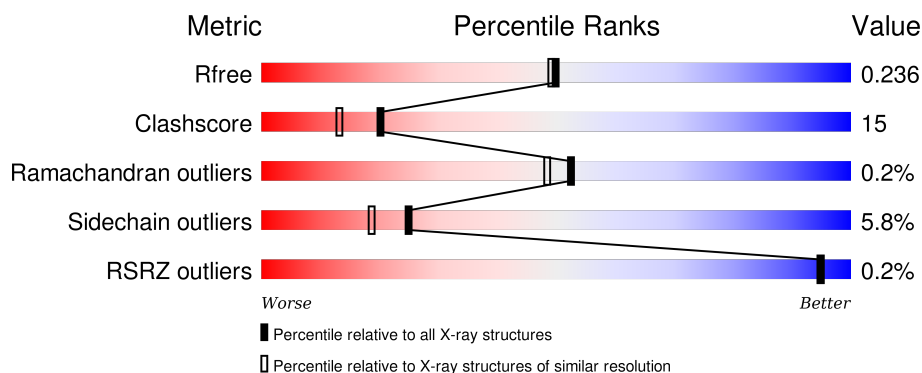
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




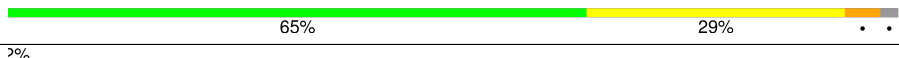

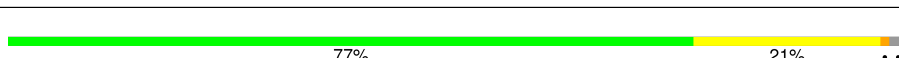


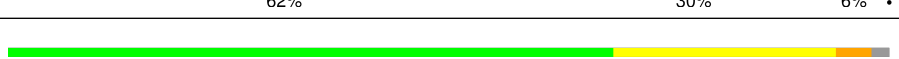

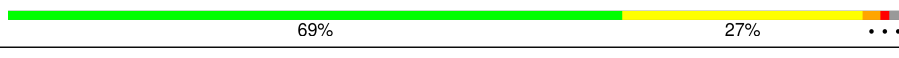

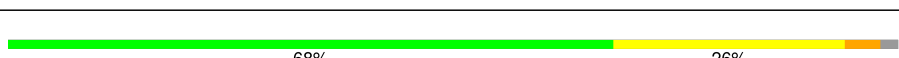


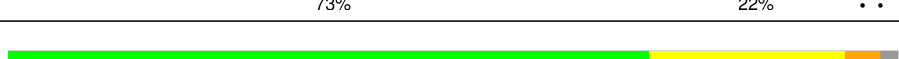
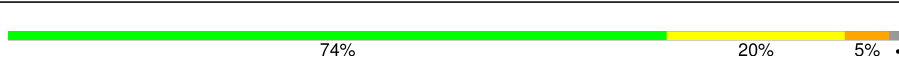

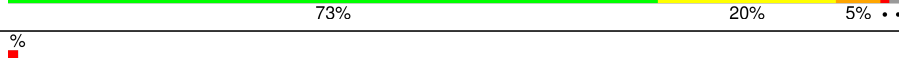


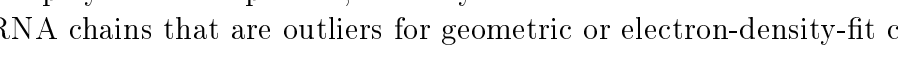



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1	130	
1	2	130	
1	A	130	
1	B	130	
1	C	130	

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Mol	Chain	Length	Quality of chain
1	D	130	
1	E	130	
1	F	130	
1	G	130	
1	H	130	
1	I	130	
1	J	130	
1	K	130	
1	L	130	
1	M	130	
1	N	130	
1	O	130	
1	P	130	
1	Q	130	
1	R	130	
1	S	130	
1	T	130	
1	U	130	
1	V	130	
1	W	130	
1	X	130	
1	Y	130	
1	Z	130	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	A	3004	-	-	-	X
3	NA	B	3001	-	-	-	X
3	NA	R	3005	-	-	-	X
3	NA	S	3002	-	-	-	X
3	NA	V	3003	-	-	-	X
4	GOL	1	4010	-	X	-	X
4	GOL	2	4009	-	X	-	X
4	GOL	A	4012	-	X	-	X
4	GOL	G	4001	-	X	-	X
4	GOL	H	4002	-	X	X	X
4	GOL	H	4011	-	X	-	-
4	GOL	J	4005	-	X	-	-
4	GOL	M	4003	-	X	-	X
4	GOL	R	4007	-	X	-	X
4	GOL	V	4008	-	X	-	X
4	GOL	W	4006	-	X	-	-
4	GOL	X	4004	-	X	-	X
5	ACY	F	5015	-	-	-	X
5	ACY	H	5012	-	-	-	X
5	ACY	I	5004	-	-	-	X
5	ACY	K	5013	-	-	X	-
5	ACY	W	5011	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30641 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	126	Total	C	N	O	Se	0	0	0
			1008	644	177	184	3			
1	B	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	C	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	D	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	E	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	F	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	G	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	H	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	I	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	J	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	K	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	L	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	M	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	N	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	O	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	P	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	R	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	S	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	T	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	U	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	V	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	W	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	X	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	Y	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	Z	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	1	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	2	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
A	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
A	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
B	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
B	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
B	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
C	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
C	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
C	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
D	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
D	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
D	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
E	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
E	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
E	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
F	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
F	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
G	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
G	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
G	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
H	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
H	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
H	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
I	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
I	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
I	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
J	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
J	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
J	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
K	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
K	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
K	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
L	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
L	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
L	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
M	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
M	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
M	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
N	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
N	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
N	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
O	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
O	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
O	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
P	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
P	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
P	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
Q	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
Q	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
Q	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
R	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
R	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
R	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
S	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
S	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
S	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2

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Chain	Residue	Modelled	Actual	Comment	Reference
T	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
T	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
T	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
U	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
U	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
U	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
V	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
V	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
V	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
W	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
W	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
W	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
X	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
X	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
X	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
Y	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
Y	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
Y	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
Z	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
Z	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
Z	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
1	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
1	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
1	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
2	66	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
2	82	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2
2	96	MSE	MET	CLONING ARTIFACT	UNP Q8ZVU2

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	2	Total Cd 2 2	0	0
2	K	1	Total Cd 1 1	0	0
2	B	1	Total Cd 1 1	0	0
2	W	1	Total Cd 1 1	0	0
2	X	1	Total Cd 1 1	0	0
2	2	1	Total Cd 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	S	1	Total	Cd	0	0
			1	1		
2	J	1	Total	Cd	0	0
			1	1		
2	E	1	Total	Cd	0	0
			1	1		
2	V	1	Total	Cd	0	0
			1	1		
2	A	2	Total	Cd	0	0
			2	2		
2	R	1	Total	Cd	0	0
			1	1		
2	M	1	Total	Cd	0	0
			1	1		
2	1	1	Total	Cd	0	0
			1	1		
2	D	2	Total	Cd	0	0
			2	2		
2	I	1	Total	Cd	0	0
			1	1		
2	Z	1	Total	Cd	0	0
			1	1		
2	U	1	Total	Cd	0	0
			1	1		
2	L	1	Total	Cd	0	0
			1	1		
2	Q	1	Total	Cd	0	0
			1	1		
2	H	2	Total	Cd	0	0
			2	2		
2	O	1	Total	Cd	0	0
			1	1		
2	Y	1	Total	Cd	0	0
			1	1		
2	F	1	Total	Cd	0	0
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

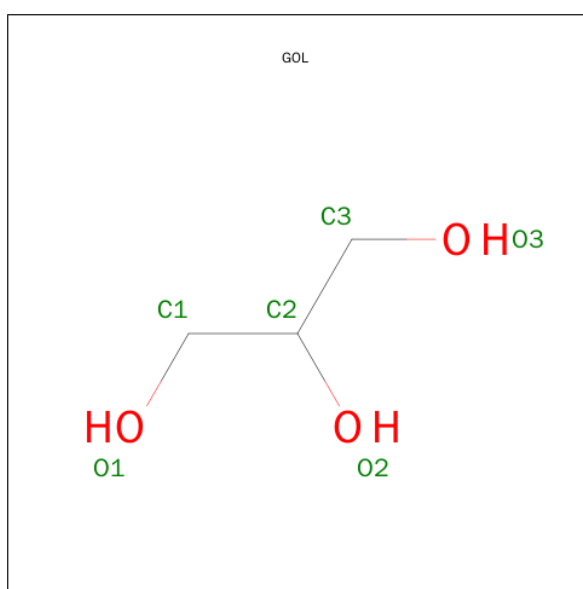
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	S	1	Total 1	Na 1	0	0
3	V	1	Total 1	Na 1	0	0
3	R	1	Total 1	Na 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



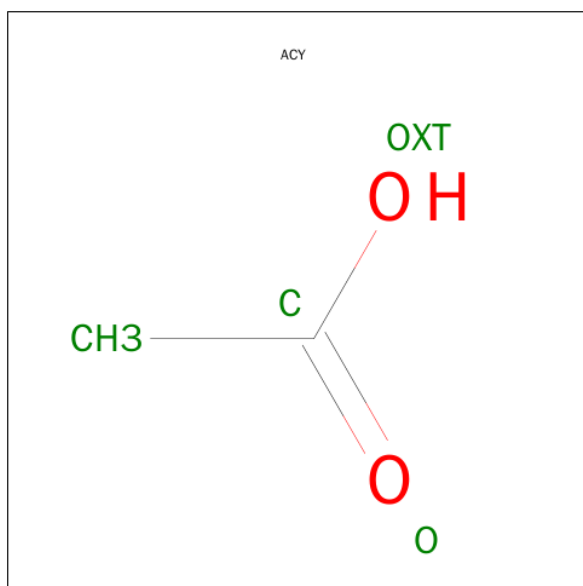
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total 6	C 3	O 3	0	0
4	H	1	Total 6	C 3	O 3	0	0
4	M	1	Total 6	C 3	O 3	0	0
4	X	1	Total 6	C 3	O 3	0	0
4	J	1	Total 6	C 3	O 3	0	0
4	W	1	Total 6	C 3	O 3	0	0
4	R	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	V	1	Total	C	O	0	0
			6	3	3		
4	2	1	Total	C	O	0	0
			6	3	3		
4	1	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	W	1	Total	C	O	0	0
			4	2	2		
5	X	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	2	1	Total	C	O	0	0
			4	2	2		
5	Z	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	V	1	Total C O 4 2 2	0	0
5	Y	1	Total C O 4 2 2	0	0
5	N	1	Total C O 4 2 2	0	0
5	I	1	Total C O 4 2 2	0	0
5	W	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	K	1	Total C O 4 2 2	0	0
5	1	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	1	52	Total O 52 52	0	0
6	2	75	Total O 75 75	0	0
6	A	67	Total O 67 67	0	0
6	B	64	Total O 64 64	0	0
6	C	64	Total O 64 64	0	0
6	D	46	Total O 46 46	0	0
6	E	48	Total O 48 48	0	0
6	F	69	Total O 69 69	0	0
6	G	74	Total O 74 74	0	0
6	H	67	Total O 67 67	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	58	Total 58	O 58	0	0
6	J	47	Total 47	O 47	0	0
6	K	42	Total 42	O 42	0	0
6	L	59	Total 59	O 59	0	0
6	M	98	Total 98	O 98	0	0
6	N	89	Total 89	O 89	0	0
6	O	72	Total 72	O 72	0	0
6	P	63	Total 63	O 63	0	0
6	Q	63	Total 63	O 63	0	0
6	R	52	Total 52	O 52	0	0
6	S	52	Total 52	O 52	0	0
6	T	63	Total 63	O 63	0	0
6	U	69	Total 69	O 69	0	0
6	V	115	Total 115	O 115	0	0
6	W	86	Total 86	O 86	0	0
6	X	93	Total 93	O 93	0	0
6	Y	77	Total 77	O 77	0	0
6	Z	64	Total 64	O 64	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

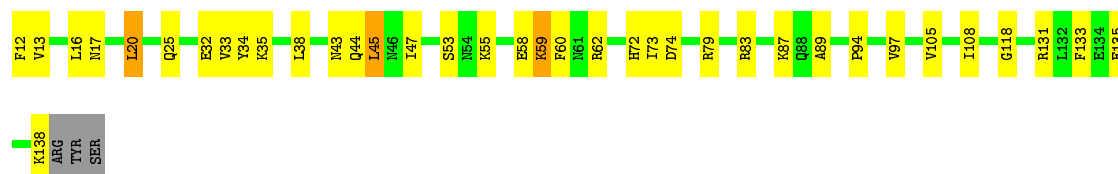
- Molecule 1: small nuclear ribonucleoprotein homolog

Chain A: 



- Molecule 1: small nuclear ribonucleoprotein homolog

Chain B: 



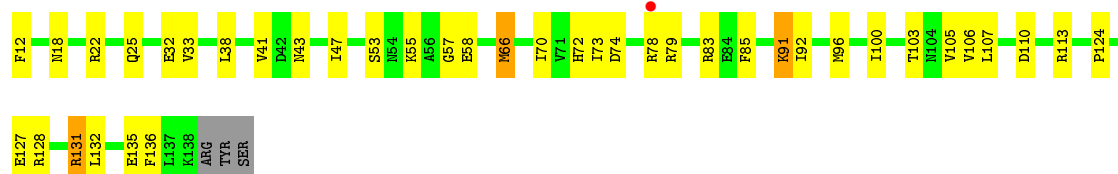
- Molecule 1: small nuclear ribonucleoprotein homolog

Chain C: 



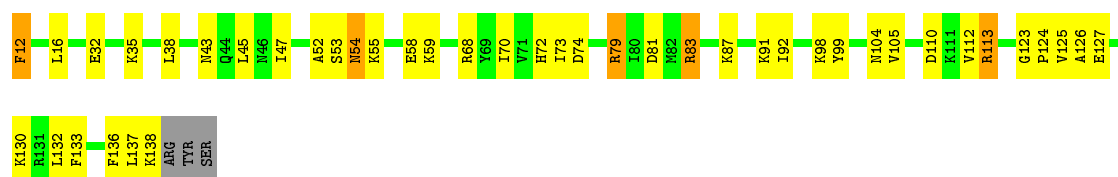
- Molecule 1: small nuclear ribonucleoprotein homolog

Chain D: 

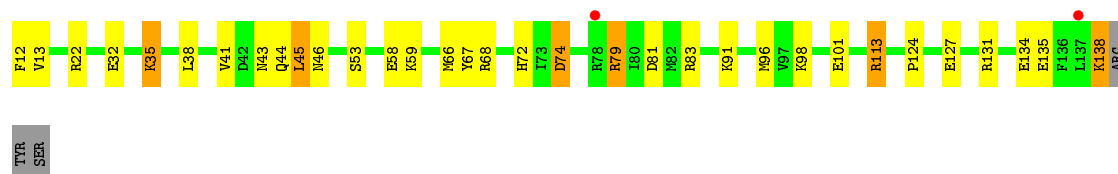


- Molecule 1: small nuclear ribonucleoprotein homolog

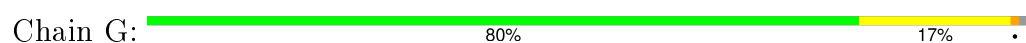
Chain E: 



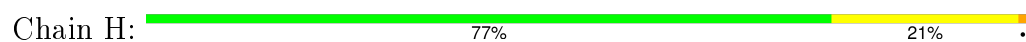
- Molecule 1: small nuclear ribonucleoprotein homolog



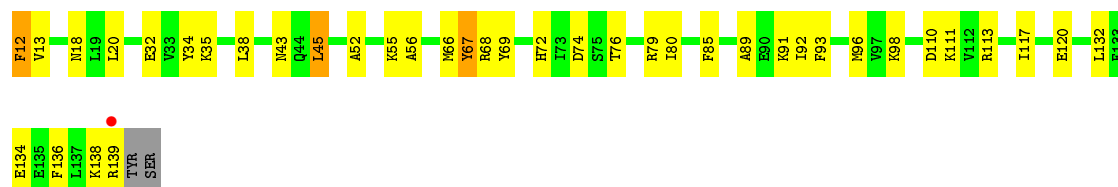
- Molecule 1: small nuclear ribonucleoprotein homolog



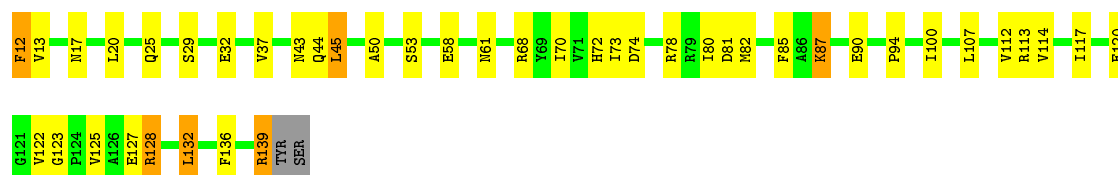
- Molecule 1: small nuclear ribonucleoprotein homolog



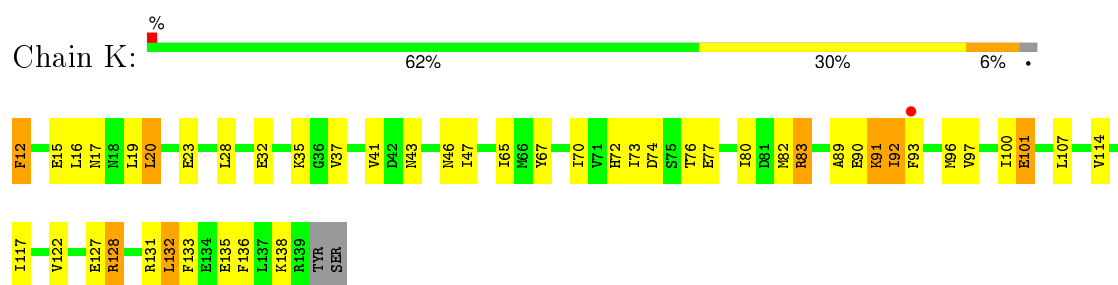
- Molecule 1: small nuclear ribonucleoprotein homolog



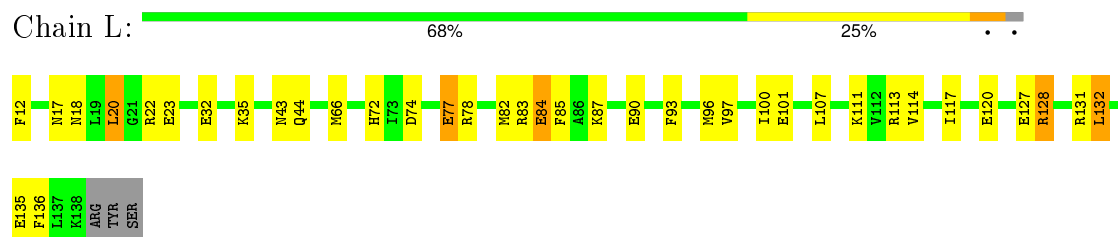
- Molecule 1: small nuclear ribonucleoprotein homolog



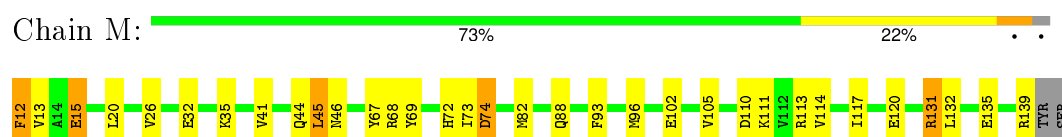
- Molecule 1: small nuclear ribonucleoprotein homolog



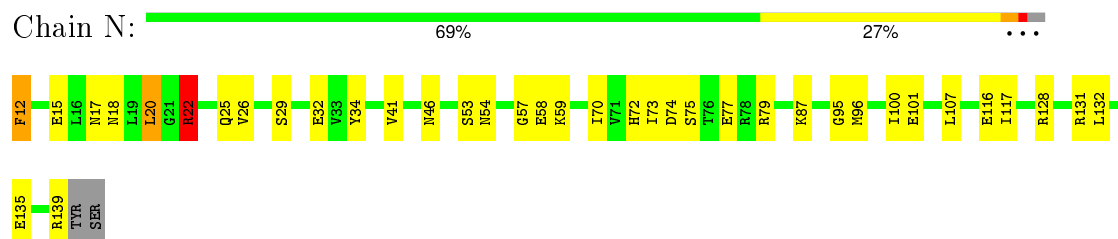
- Molecule 1: small nuclear ribonucleoprotein homolog



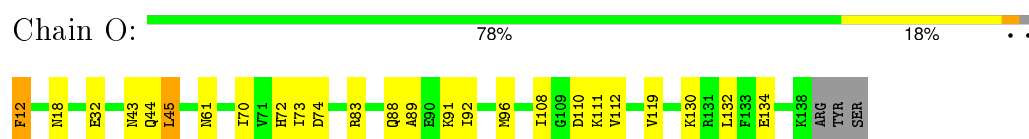
- Molecule 1: small nuclear ribonucleoprotein homolog



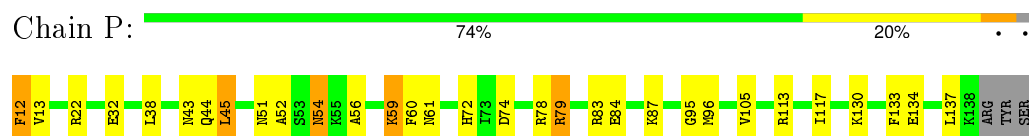
- Molecule 1: small nuclear ribonucleoprotein homolog



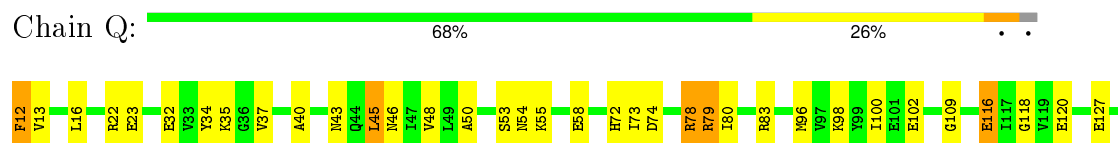
- Molecule 1: small nuclear ribonucleoprotein homolog



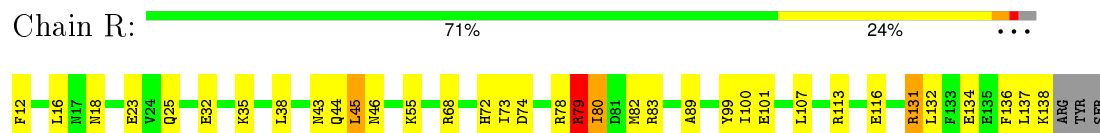
- Molecule 1: small nuclear ribonucleoprotein homolog



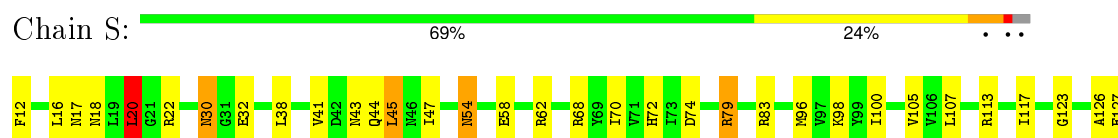
- Molecule 1: small nuclear ribonucleoprotein homolog



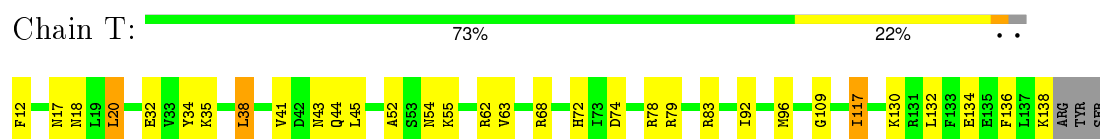
- Molecule 1: small nuclear ribonucleoprotein homolog



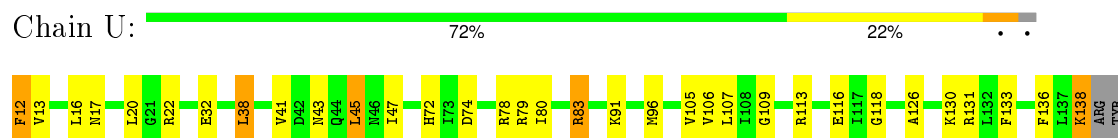
- Molecule 1: small nuclear ribonucleoprotein homolog



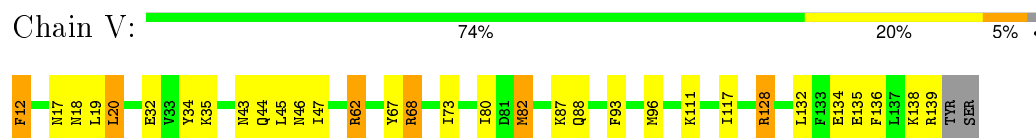
- Molecule 1: small nuclear ribonucleoprotein homolog




- Molecule 1: small nuclear ribonucleoprotein homolog



- Molecule 1: small nuclear ribonucleoprotein homolog



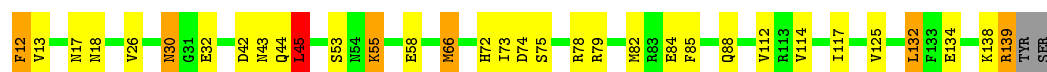
- Molecule 1: small nuclear ribonucleoprotein homolog

Chain W:  84% 14% ..



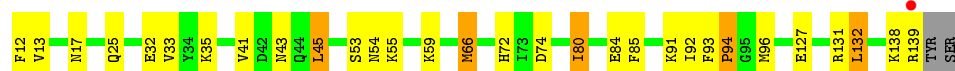
- Molecule 1: small nuclear ribonucleoprotein homolog

Chain X:  73% 20% 5% ..



- Molecule 1: small nuclear ribonucleoprotein homolog

Chain Y:  75% 19% ..



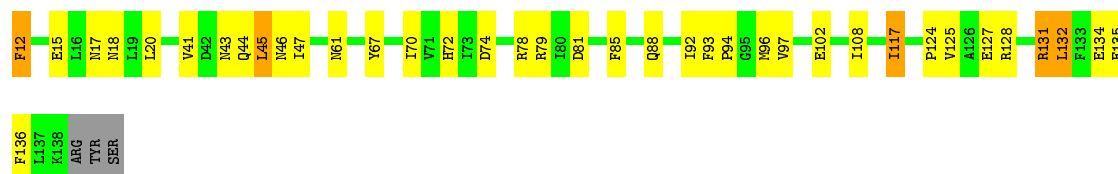
- Molecule 1: small nuclear ribonucleoprotein homolog

Chain Z:  65% 28% 5% ..



- Molecule 1: small nuclear ribonucleoprotein homolog

Chain 1:  68% 25% ..



- Molecule 1: small nuclear ribonucleoprotein homolog

Chain 2:  71% 24% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.32Å 172.43Å 148.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.00 86.21 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.6 (19.97-2.00) 93.4 (86.21-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.191 , 0.236 0.191 , 0.236	Depositor DCC
R_{free} test set	13048 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.8	EDS
Estimated twinning fraction	0.115 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 270896 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	30641	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, CD, 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	1	0.81	0/1028	0.86	2/1377 (0.1%)
1	2	0.90	2/1028 (0.2%)	1.03	3/1377 (0.2%)
1	A	0.87	1/1019 (0.1%)	0.86	1/1366 (0.1%)
1	B	0.87	0/1028	0.86	0/1377
1	C	0.82	0/1028	0.82	2/1377 (0.1%)
1	D	0.78	0/1028	0.84	1/1377 (0.1%)
1	E	0.76	0/1028	0.80	0/1377
1	F	0.83	0/1028	0.85	2/1377 (0.1%)
1	G	0.91	0/1028	0.87	0/1377
1	H	0.84	1/1039 (0.1%)	0.88	0/1391
1	I	0.88	0/1039	0.85	0/1391
1	J	0.76	0/1039	0.84	0/1391
1	K	0.71	0/1039	0.83	1/1391 (0.1%)
1	L	0.78	0/1028	0.81	0/1377
1	M	0.86	0/1039	0.92	1/1391 (0.1%)
1	N	0.86	0/1039	0.90	3/1391 (0.2%)
1	O	0.82	0/1028	0.84	0/1377
1	P	0.87	0/1028	0.83	0/1377
1	Q	0.80	0/1028	0.82	1/1377 (0.1%)
1	R	0.81	0/1028	0.83	1/1377 (0.1%)
1	S	0.82	0/1028	0.84	2/1377 (0.1%)
1	T	0.83	0/1028	0.81	0/1377
1	U	0.83	0/1028	0.86	0/1377
1	V	0.99	1/1039 (0.1%)	1.01	3/1391 (0.2%)
1	W	0.87	0/1039	0.88	0/1391
1	X	0.88	0/1039	0.92	2/1391 (0.1%)
1	Y	0.91	0/1039	0.88	0/1391
1	Z	0.84	1/1039 (0.1%)	0.86	1/1391 (0.1%)
All	All	0.84	6/28896 (0.0%)	0.87	26/38699 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying

if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	1
1	B	0	1
1	C	0	2
1	H	0	1
1	I	0	1
1	V	0	1
1	W	0	1
All	All	0	8

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	82	MSE	SE-CE	-11.70	1.26	1.95
1	Z	15	GLU	CG-CD	7.33	1.62	1.51
1	H	15	GLU	CG-CD	6.14	1.61	1.51
1	2	15	GLU	CG-CD	5.68	1.60	1.51
1	2	69	TYR	CD1-CE1	5.60	1.47	1.39

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	22	ARG	NE-CZ-NH2	-15.74	112.43	120.30
1	V	62	ARG	NE-CZ-NH2	-12.26	114.17	120.30
1	2	22	ARG	NE-CZ-NH1	10.50	125.55	120.30
1	V	62	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	F	41	VAL	CB-CA-C	-7.57	97.02	111.40

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	34	TYR	Sidechain
1	C	34	TYR	Sidechain
1	C	69	TYR	Sidechain
1	H	34	TYR	Sidechain
1	I	34	TYR	Sidechain

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	1	1017	0	1042	36	0
1	2	1017	0	1042	29	0
1	A	1008	0	1029	21	0
1	B	1017	0	1042	33	0
1	C	1017	0	1042	30	0
1	D	1017	0	1042	53	0
1	E	1017	0	1042	46	0
1	F	1017	0	1042	32	0
1	G	1017	0	1042	18	0
1	H	1028	0	1055	26	0
1	I	1028	0	1055	53	0
1	J	1028	0	1055	36	0
1	K	1028	0	1055	50	0
1	L	1017	0	1042	41	0
1	M	1028	0	1055	28	0
1	N	1028	0	1055	38	0
1	O	1017	0	1042	27	0
1	P	1017	0	1042	29	0
1	Q	1017	0	1042	31	0
1	R	1017	0	1042	41	0
1	S	1017	0	1042	41	0
1	T	1017	0	1042	36	0
1	U	1017	0	1042	41	0
1	V	1028	0	1055	28	0
1	W	1028	0	1055	23	0
1	X	1028	0	1055	42	0
1	Y	1028	0	1055	38	0
1	Z	1028	0	1055	43	0
2	1	1	0	0	0	0
2	2	1	0	0	0	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	H	2	0	0	0	0
2	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	O	1	0	0	0	0
2	P	2	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
2	Y	1	0	0	0	0
2	Z	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	V	1	0	0	0	0
4	1	6	0	5	0	0
4	2	6	0	4	0	0
4	A	6	0	4	1	0
4	G	6	0	4	0	0
4	H	12	0	9	5	0
4	J	6	0	4	0	0
4	M	6	0	4	0	0
4	R	6	0	4	0	0
4	V	6	0	4	0	0
4	W	6	0	5	2	0
4	X	6	0	4	2	0
5	1	4	0	3	0	0
5	2	4	0	3	1	0
5	F	4	0	3	0	0
5	H	4	0	3	0	0
5	I	8	0	6	0	0
5	K	4	0	3	4	0
5	M	4	0	3	0	0
5	N	4	0	4	0	0
5	V	4	0	3	0	0
5	W	8	0	6	7	0
5	X	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Y	4	0	3	0	0
5	Z	4	0	3	0	0
6	1	52	0	0	5	0
6	2	75	0	0	1	0
6	A	67	0	0	3	0
6	B	64	0	0	4	0
6	C	64	0	0	5	0
6	D	46	0	0	3	0
6	E	48	0	0	3	0
6	F	69	0	0	4	0
6	G	74	0	0	3	0
6	H	67	0	0	1	0
6	I	58	0	0	6	1
6	J	47	0	0	2	0
6	K	42	0	0	2	0
6	L	59	0	0	5	0
6	M	98	0	0	2	0
6	N	89	0	0	3	0
6	O	72	0	0	1	0
6	P	63	0	0	1	0
6	Q	63	0	0	5	0
6	R	52	0	0	5	0
6	S	52	0	0	3	0
6	T	63	0	0	5	0
6	U	69	0	0	5	0
6	V	115	0	0	5	1
6	W	86	0	0	3	0
6	X	93	0	0	5	0
6	Y	77	0	0	4	0
6	Z	64	0	0	2	0
All	All	30641	0	29403	853	1

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 15.

The worst 5 of 853 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)
4:W:4006:GOL:O1	4:W:4006:GOL:C1	1.63	1.47
1:V:82:MSE:CE	1:V:82:MSE:SE	1.26	1.45
1:V:82:MSE:HE3	1:V:82:MSE:SE	1.83	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:80:ILE:HD11	1:R:116:GLU:HG2	1.25	1.14
1:V:82:MSE:SE	1:V:82:MSE:HE2	1.83	1.10

All (1) 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)
6:I:5051:HOH:O	6:V:5110:HOH:O[1_455]	2.01	0.19

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	1	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	2	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	A	124/130 (95%)	124 (100%)	0	0	100	100
1	B	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	C	125/130 (96%)	122 (98%)	1 (1%)	2 (2%)	12	5
1	D	125/130 (96%)	125 (100%)	0	0	100	100
1	E	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	F	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	G	125/130 (96%)	125 (100%)	0	0	100	100
1	H	126/130 (97%)	125 (99%)	1 (1%)	0	100	100
1	I	126/130 (97%)	126 (100%)	0	0	100	100
1	J	126/130 (97%)	123 (98%)	3 (2%)	0	100	100
1	K	126/130 (97%)	124 (98%)	1 (1%)	1 (1%)	24	15
1	L	125/130 (96%)	125 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	126/130 (97%)	126 (100%)	0	0	100	100
1	N	126/130 (97%)	126 (100%)	0	0	100	100
1	O	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	P	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	Q	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	R	125/130 (96%)	122 (98%)	1 (1%)	2 (2%)	12	5
1	S	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	T	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
1	U	125/130 (96%)	121 (97%)	4 (3%)	0	100	100
1	V	126/130 (97%)	125 (99%)	1 (1%)	0	100	100
1	W	126/130 (97%)	124 (98%)	2 (2%)	0	100	100
1	X	126/130 (97%)	125 (99%)	1 (1%)	0	100	100
1	Y	126/130 (97%)	124 (98%)	1 (1%)	1 (1%)	24	15
1	Z	126/130 (97%)	126 (100%)	0	0	100	100
All	All	3510/3640 (96%)	3476 (99%)	28 (1%)	6 (0%)	52	48

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	79	ARG
1	C	78	ARG
1	R	137	LEU
1	C	79	ARG
1	K	92	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	109/109 (100%)	105 (96%)	4 (4%)	41	38
1	2	109/109 (100%)	103 (94%)	6 (6%)	27	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	108/109 (99%)	102 (94%)	6 (6%)	26	20
1	B	109/109 (100%)	101 (93%)	8 (7%)	17	11
1	C	109/109 (100%)	106 (97%)	3 (3%)	51	50
1	D	109/109 (100%)	102 (94%)	7 (6%)	22	15
1	E	109/109 (100%)	100 (92%)	9 (8%)	14	8
1	F	109/109 (100%)	101 (93%)	8 (7%)	17	11
1	G	109/109 (100%)	106 (97%)	3 (3%)	51	50
1	H	110/109 (101%)	107 (97%)	3 (3%)	52	52
1	I	110/109 (101%)	105 (96%)	5 (4%)	34	29
1	J	110/109 (101%)	100 (91%)	10 (9%)	12	6
1	K	110/109 (101%)	101 (92%)	9 (8%)	14	9
1	L	109/109 (100%)	101 (93%)	8 (7%)	17	11
1	M	110/109 (101%)	102 (93%)	8 (7%)	17	11
1	N	110/109 (101%)	104 (94%)	6 (6%)	27	21
1	O	109/109 (100%)	107 (98%)	2 (2%)	66	69
1	P	109/109 (100%)	101 (93%)	8 (7%)	17	11
1	Q	109/109 (100%)	103 (94%)	6 (6%)	27	21
1	R	109/109 (100%)	102 (94%)	7 (6%)	22	15
1	S	109/109 (100%)	101 (93%)	8 (7%)	17	11
1	T	109/109 (100%)	105 (96%)	4 (4%)	41	38
1	U	109/109 (100%)	104 (95%)	5 (5%)	33	28
1	V	110/109 (101%)	103 (94%)	7 (6%)	22	15
1	W	110/109 (101%)	107 (97%)	3 (3%)	52	52
1	X	110/109 (101%)	101 (92%)	9 (8%)	14	9
1	Y	110/109 (101%)	104 (94%)	6 (6%)	27	21
1	Z	110/109 (101%)	100 (91%)	10 (9%)	12	6
All	All	3062/3052 (100%)	2884 (94%)	178 (6%)	25	19

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	15	GLU
1	P	59	LYS

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Mol	Chain	Res	Type
1	Z	111	LYS
1	M	45	LEU
1	N	101	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	61	ASN
1	Q	17	ASN
1	Z	25	GLN
1	O	72	HIS
1	P	61	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 33 are monoatomic - leaving 27 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	GOL	1	4010	-	5,5,5	4.80	5 (100%)	5,5,5	5.83	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACY	1	5014	-	1,3,3	2.29	1 (100%)	0,3,3	0.00	-
4	GOL	2	4009	-	5,5,5	4.95	5 (100%)	5,5,5	5.49	3 (60%)
5	ACY	2	5005	-	1,3,3	0.31	0	0,3,3	0.00	-
4	GOL	A	4012	-	5,5,5	4.88	5 (100%)	5,5,5	5.44	3 (60%)
5	ACY	F	5015	-	1,3,3	2.22	1 (100%)	0,3,3	0.00	-
4	GOL	G	4001	-	5,5,5	4.97	5 (100%)	5,5,5	5.58	3 (60%)
4	GOL	H	4002	2	5,5,5	4.64	5 (100%)	5,5,5	5.73	3 (60%)
4	GOL	H	4011	-	5,5,5	4.59	4 (80%)	5,5,5	5.48	3 (60%)
5	ACY	H	5012	-	1,3,3	1.23	0	0,3,3	0.00	-
5	ACY	I	5004	-	1,3,3	1.69	0	0,3,3	0.00	-
5	ACY	I	5010	-	1,3,3	2.14	1 (100%)	0,3,3	0.00	-
4	GOL	J	4005	-	5,5,5	4.85	5 (100%)	5,5,5	5.45	3 (60%)
5	ACY	K	5013	-	1,3,3	1.54	0	0,3,3	0.00	-
4	GOL	M	4003	-	5,5,5	4.72	5 (100%)	5,5,5	5.57	3 (60%)
5	ACY	M	5003	-	1,3,3	0.83	0	0,3,3	0.00	-
5	ACY	N	5009	-	1,3,3	3.97	1 (100%)	0,3,3	0.00	-
4	GOL	R	4007	-	5,5,5	4.82	5 (100%)	5,5,5	5.64	3 (60%)
4	GOL	V	4008	-	5,5,5	5.16	5 (100%)	5,5,5	5.81	3 (60%)
5	ACY	V	5007	-	1,3,3	0.48	0	0,3,3	0.00	-
4	GOL	W	4006	-	5,5,5	4.92	5 (100%)	5,5,5	5.76	3 (60%)
5	ACY	W	5001	-	1,3,3	3.68	1 (100%)	0,3,3	0.00	-
5	ACY	W	5011	-	1,3,3	2.28	1 (100%)	0,3,3	0.00	-
4	GOL	X	4004	-	5,5,5	4.74	5 (100%)	5,5,5	5.87	3 (60%)
5	ACY	X	5002	-	1,3,3	0.06	0	0,3,3	0.00	-
5	ACY	Y	5008	-	1,3,3	2.02	1 (100%)	0,3,3	0.00	-
5	ACY	Z	5006	-	1,3,3	1.23	0	0,3,3	0.00	-

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	GOL	1	4010	-	-	0/4/4/4	0/0/0/0
5	ACY	1	5014	-	-	0/0/0/0	0/0/0/0
4	GOL	2	4009	-	-	0/4/4/4	0/0/0/0
5	ACY	2	5005	-	-	0/0/0/0	0/0/0/0
4	GOL	A	4012	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ACY	F	5015	-	-	0/0/0/0	0/0/0/0
4	GOL	G	4001	-	-	0/4/4/4	0/0/0/0
4	GOL	H	4002	2	-	0/4/4/4	0/0/0/0
4	GOL	H	4011	-	-	0/4/4/4	0/0/0/0
5	ACY	H	5012	-	-	0/0/0/0	0/0/0/0
5	ACY	I	5004	-	-	0/0/0/0	0/0/0/0
5	ACY	I	5010	-	-	0/0/0/0	0/0/0/0
4	GOL	J	4005	-	-	0/4/4/4	0/0/0/0
5	ACY	K	5013	-	-	0/0/0/0	0/0/0/0
4	GOL	M	4003	-	-	0/4/4/4	0/0/0/0
5	ACY	M	5003	-	-	0/0/0/0	0/0/0/0
5	ACY	N	5009	-	-	0/0/0/0	0/0/0/0
4	GOL	R	4007	-	-	0/4/4/4	0/0/0/0
4	GOL	V	4008	-	-	0/4/4/4	0/0/0/0
5	ACY	V	5007	-	-	0/0/0/0	0/0/0/0
4	GOL	W	4006	-	-	0/4/4/4	0/0/0/0
5	ACY	W	5001	-	-	0/0/0/0	0/0/0/0
5	ACY	W	5011	-	-	0/0/0/0	0/0/0/0
4	GOL	X	4004	-	-	0/4/4/4	0/0/0/0
5	ACY	X	5002	-	-	0/0/0/0	0/0/0/0
5	ACY	Y	5008	-	-	0/0/0/0	0/0/0/0
5	ACY	Z	5006	-	-	0/0/0/0	0/0/0/0

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	4009	GOL	C3-C2	-8.97	1.18	1.52
4	V	4008	GOL	C3-C2	-8.72	1.19	1.52
4	W	4006	GOL	C3-C2	-8.51	1.19	1.52
4	R	4007	GOL	C3-C2	-8.47	1.20	1.52
4	1	4010	GOL	C3-C2	-8.33	1.20	1.52

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	4005	GOL	O1-C1-C2	2.71	123.34	110.18
4	1	4010	GOL	O1-C1-C2	2.77	123.64	110.18
4	R	4007	GOL	O1-C1-C2	2.80	123.76	110.18
4	X	4004	GOL	O1-C1-C2	2.81	123.80	110.18
4	H	4002	GOL	O1-C1-C2	2.82	123.84	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	2	5005	ACY	1	0
4	A	4012	GOL	1	0
4	H	4002	GOL	5	0
5	K	5013	ACY	4	0
4	W	4006	GOL	2	0
5	W	5011	ACY	7	0
4	X	4004	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 ⓘ

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	1	124/130 (95%)	-0.20	0 100 100	15, 34, 48, 53	0
1	2	124/130 (95%)	-0.41	0 100 100	16, 29, 51, 56	0
1	A	123/130 (94%)	-0.50	0 100 100	20, 26, 41, 53	0
1	B	124/130 (95%)	-0.52	0 100 100	18, 27, 39, 56	0
1	C	124/130 (95%)	-0.39	1 (0%) 87 88	21, 30, 44, 60	0
1	D	124/130 (95%)	-0.28	1 (0%) 87 88	22, 34, 54, 66	0
1	E	124/130 (95%)	-0.36	0 100 100	19, 33, 50, 64	0
1	F	124/130 (95%)	-0.33	2 (1%) 74 75	19, 30, 47, 61	0
1	G	124/130 (95%)	-0.57	0 100 100	19, 26, 40, 55	0
1	H	125/130 (96%)	-0.52	0 100 100	16, 26, 40, 56	0
1	I	125/130 (96%)	-0.36	1 (0%) 87 88	17, 28, 47, 69	0
1	J	125/130 (96%)	-0.34	0 100 100	18, 34, 55, 71	0
1	K	125/130 (96%)	-0.08	1 (0%) 87 88	20, 39, 63, 72	0
1	L	124/130 (95%)	-0.30	0 100 100	18, 35, 54, 63	0
1	M	125/130 (96%)	-0.53	0 100 100	16, 25, 37, 53	0
1	N	125/130 (96%)	-0.54	0 100 100	16, 24, 37, 54	0
1	O	124/130 (95%)	-0.49	0 100 100	21, 28, 45, 60	0
1	P	124/130 (95%)	-0.43	0 100 100	20, 27, 45, 59	0
1	Q	124/130 (95%)	-0.42	0 100 100	17, 29, 44, 62	0
1	R	124/130 (95%)	-0.42	0 100 100	22, 33, 51, 65	0
1	S	124/130 (95%)	-0.34	0 100 100	21, 31, 50, 63	0
1	T	124/130 (95%)	-0.37	0 100 100	21, 30, 45, 64	0
1	U	124/130 (95%)	-0.52	0 100 100	20, 27, 42, 60	0
1	V	125/130 (96%)	-0.54	0 100 100	15, 23, 33, 56	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	W	125/130 (96%)	-0.47	0 100 100	14, 26, 39, 56	0
1	X	125/130 (96%)	-0.48	0 100 100	14, 26, 40, 63	0
1	Y	125/130 (96%)	-0.41	1 (0%) 87 88	14, 26, 47, 70	0
1	Z	125/130 (96%)	-0.36	1 (0%) 87 88	16, 31, 54, 65	0
All	All	3482/3640 (95%)	-0.41	8 (0%) 95 95	14, 29, 50, 72	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	139	ARG	3.5
1	I	139	ARG	2.8
1	Z	139	ARG	2.8
1	F	137	LEU	2.5
1	F	78	ARG	2.4

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	NA	A	3004	1/1	0.76	0.25	20.03	65,65,65,65	0
3	NA	B	3001	1/1	0.79	0.55	18.91	76,76,76,76	0
3	NA	R	3005	1/1	0.89	0.47	14.80	82,82,82,82	0
4	GOL	X	4004	6/6	0.90	0.19	12.40	45,48,50,50	0
4	GOL	A	4012	6/6	0.87	0.20	10.48	56,56,57,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NA	V	3003	1/1	0.90	0.32	9.91	67,67,67,67	0
3	NA	S	3002	1/1	0.92	0.25	7.44	59,59,59,59	0
4	GOL	1	4010	6/6	0.90	0.18	6.72	42,44,45,47	0
4	GOL	2	4009	6/6	0.90	0.13	4.70	47,47,48,49	0
4	GOL	V	4008	6/6	0.93	0.18	4.64	47,49,51,53	0
4	GOL	G	4001	6/6	0.95	0.19	4.09	31,42,44,45	0
4	GOL	M	4003	6/6	0.93	0.15	3.96	43,49,50,51	0
5	ACY	I	5004	4/4	0.93	0.17	3.56	36,39,40,40	0
5	ACY	F	5015	4/4	0.89	0.13	2.95	41,44,44,44	0
5	ACY	W	5011	4/4	0.86	0.19	2.84	32,35,37,38	0
4	GOL	R	4007	6/6	0.90	0.15	2.58	49,53,53,54	0
4	GOL	H	4002	6/6	0.80	0.17	2.55	52,54,56,57	0
5	ACY	H	5012	4/4	0.97	0.12	2.32	27,28,28,29	0
4	GOL	J	4005	6/6	0.93	0.11	1.49	46,46,48,49	0
5	ACY	1	5014	4/4	0.97	0.15	1.42	34,35,36,36	0
5	ACY	M	5003	4/4	0.98	0.11	1.35	25,27,27,28	0
4	GOL	W	4006	6/6	0.93	0.11	1.25	34,37,40,46	0
5	ACY	K	5013	4/4	0.95	0.16	0.64	46,47,47,48	0
4	GOL	H	4011	6/6	0.89	0.11	0.62	46,50,51,52	0
5	ACY	Y	5008	4/4	0.98	0.09	0.11	21,24,24,28	0
5	ACY	N	5009	4/4	0.99	0.10	0.08	29,30,30,31	0
5	ACY	X	5002	4/4	0.97	0.09	-0.12	25,27,27,28	0
5	ACY	V	5007	4/4	0.99	0.08	-0.22	23,24,24,27	0
5	ACY	I	5010	4/4	0.98	0.09	-0.24	19,25,25,26	0
5	ACY	Z	5006	4/4	0.98	0.09	-0.28	30,32,32,34	0
5	ACY	2	5005	4/4	0.99	0.09	-1.17	30,31,31,32	0
5	ACY	W	5001	4/4	0.98	0.08	-1.47	23,23,26,27	0
2	CD	D	2003	1/1	1.00	0.07	-	44,44,44,44	0
2	CD	A	2007	1/1	1.00	0.09	-	37,37,37,37	0
2	CD	1	2027	1/1	0.99	0.08	-	42,42,42,42	0
2	CD	X	2024	1/1	0.99	0.07	-	37,37,37,37	0
2	CD	D	2004	1/1	1.00	0.06	-	44,44,44,44	0
2	CD	L	2012	1/1	1.00	0.06	-	39,39,39,39	0
2	CD	Y	2025	1/1	1.00	0.08	-	34,34,34,34	1
2	CD	2	2028	1/1	0.99	0.08	-	36,36,36,36	1
2	CD	R	2018	1/1	1.00	0.06	-	41,41,41,41	0
2	CD	E	2005	1/1	0.99	0.07	-	40,40,40,40	0
2	CD	H	2014	1/1	0.99	0.09	-	40,40,40,40	0
2	CD	Z	2026	1/1	0.99	0.09	-	40,40,40,40	1
2	CD	K	2011	1/1	1.00	0.07	-	44,44,44,44	0
2	CD	O	2021	1/1	1.00	0.08	-	39,39,39,39	0
2	CD	H	2008	1/1	0.99	0.08	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CD	J	2010	1/1	0.99	0.06	-	47,47,47,47	0
2	CD	M	2013	1/1	0.99	0.07	-	36,36,36,36	0
2	CD	W	2023	1/1	1.00	0.07	-	37,37,37,37	0
2	CD	I	2009	1/1	0.99	0.10	-	46,46,46,46	0
2	CD	F	2006	1/1	1.00	0.07	-	37,37,37,37	0
2	CD	P	2016	1/1	1.00	0.08	-	37,37,37,37	1
2	CD	S	2019	1/1	1.00	0.09	-	39,39,39,39	0
2	CD	U	2020	1/1	1.00	0.08	-	41,41,41,41	0
2	CD	Q	2017	1/1	1.00	0.08	-	43,43,43,43	0
2	CD	B	2002	1/1	1.00	0.08	-	38,38,38,38	0
2	CD	A	2001	1/1	1.00	0.07	-	35,35,35,35	0
2	CD	P	2015	1/1	1.00	0.07	-	42,42,42,42	0
2	CD	V	2022	1/1	1.00	0.07	-	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.