



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 06:51 PM BST

PDB ID : 5M8H  
Title : ATP phosphoribosyltransferase (HisZG ATPPRT) from *Psychrobacter arcticus*  
Authors : Alphey, M.S.; Ge, Y.; Naismith, J.H.; da Silva, R.G.  
Deposited on : 2016-10-28  
Resolution : 2.34 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

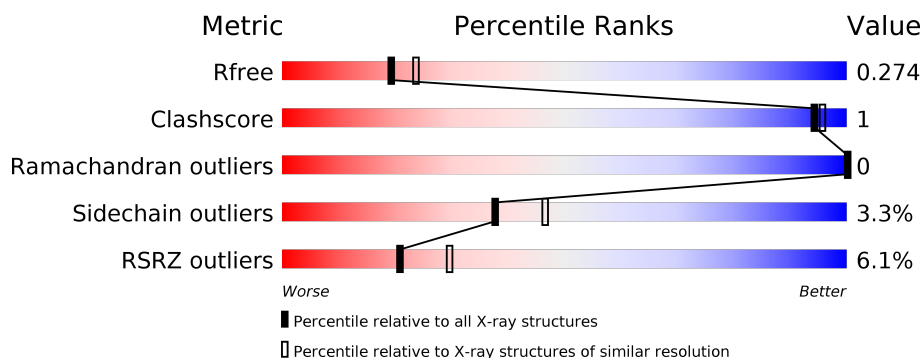
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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  $\geq 3$ , 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	388	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>•</div> </div> </div>
1	B	388	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>•</div> </div> </div>
1	C	388	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>•</div> <div>•</div> </div> </div>
1	D	388	<div> <div>7%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>•</div> <div>•</div> </div> </div>
2	E	232	<div> <div>9%</div> <div> <div></div> <div>86%</div> <div>•</div> <div>10%</div> </div> </div>
2	F	232	<div> <div>7%</div> <div> <div></div> <div>86%</div> <div>•</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	232	
2	H	232	

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
5	MPD	A	406	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18971 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 ATP phosphoribosyltransferase regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2947	1862	516	555	14			
1	B	378	Total	C	N	O	S	0	1	0
			2958	1869	519	556	14			
1	C	377	Total	C	N	O	S	1	1	0
			2955	1870	516	555	14			
1	D	378	Total	C	N	O	S	0	0	0
			2951	1864	517	556	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q4FTX3
B	0	GLY	-	expression tag	UNP Q4FTX3
C	0	GLY	-	expression tag	UNP Q4FTX3
D	0	GLY	-	expression tag	UNP Q4FTX3

- Molecule 2 is a protein called ATP phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	208	Total	C	N	O	S	0	0	0
			1601	1019	281	296	5			
2	F	209	Total	C	N	O	S	0	0	0
			1610	1024	282	299	5			
2	G	207	Total	C	N	O	S	0	0	0
			1593	1015	279	294	5			
2	H	209	Total	C	N	O	S	0	0	0
			1606	1021	281	299	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLY	-	expression tag	UNP Q4FQF7
F	0	GLY	-	expression tag	UNP Q4FQF7
G	0	GLY	-	expression tag	UNP Q4FQF7
H	0	GLY	-	expression tag	UNP Q4FQF7

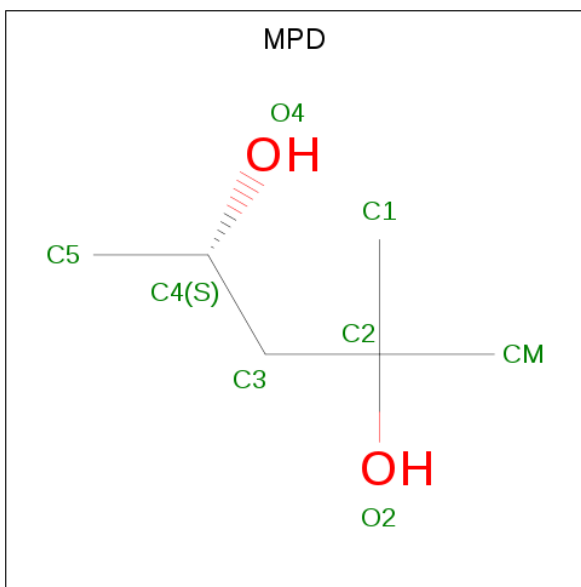
- Molecule 3 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0
4	E	3	Total 3	Cl 3	0	0
4	H	2	Total 2	Cl 2	0	0
4	B	3	Total 3	Cl 3	0	0
4	C	1	Total 1	Cl 1	0	0
4	A	2	Total 2	Cl 2	0	0
4	F	2	Total 2	Cl 2	0	0

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	C	1	Total	C	O	0	0
			8	6	2		
5	C	1	Total	C	O	0	0
			8	6	2		
5	D	1	Total	C	O	0	0
			8	6	2		
5	D	1	Total	C	O	0	0
			8	6	2		
5	E	1	Total	C	O	0	0
			8	6	2		
5	G	1	Total	C	O	0	0
			8	6	2		

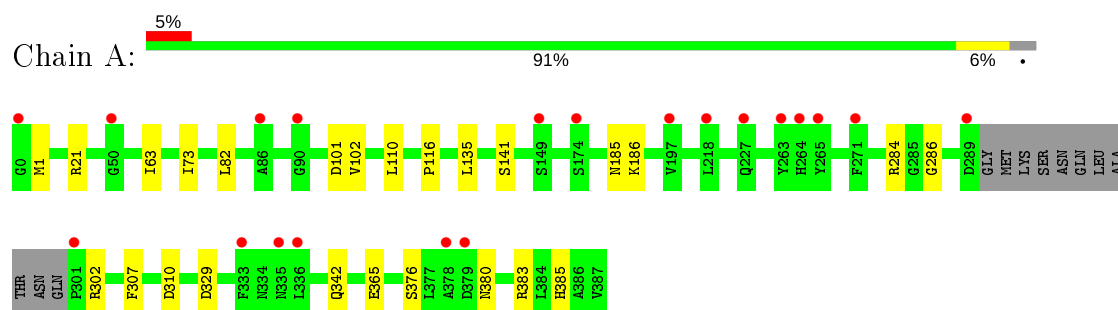
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	96	Total 96	O 96	0	0
6	B	157	Total 157	O 157	0	0
6	C	128	Total 128	O 128	0	0
6	D	117	Total 117	O 117	0	0
6	E	26	Total 26	O 26	0	0
6	F	41	Total 41	O 41	0	0
6	G	41	Total 41	O 41	0	0
6	H	23	Total 23	O 23	0	0

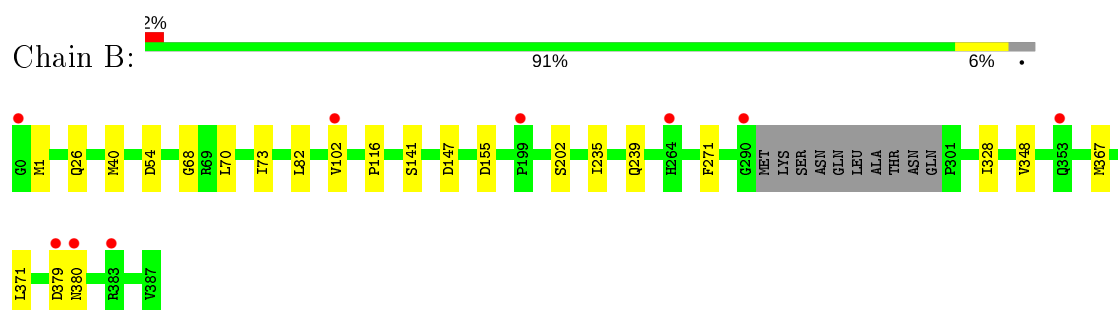
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

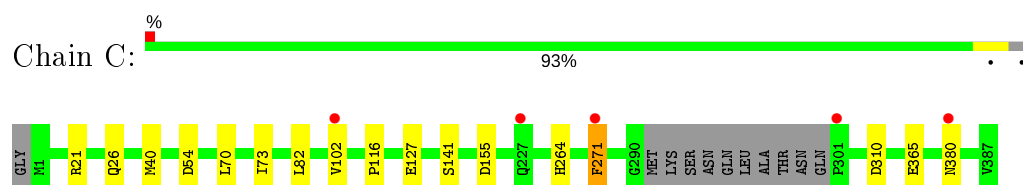
- Molecule 1: ATP phosphoribosyltransferase regulatory subunit



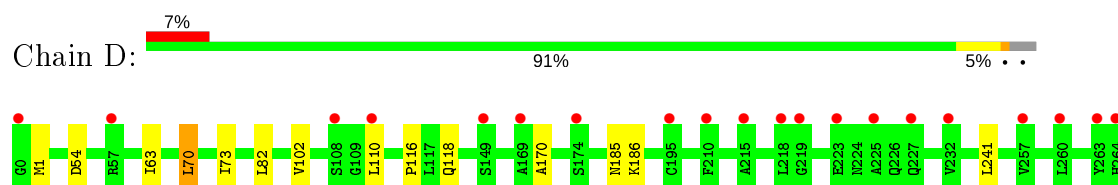
- Molecule 1: ATP phosphoribosyltransferase regulatory subunit



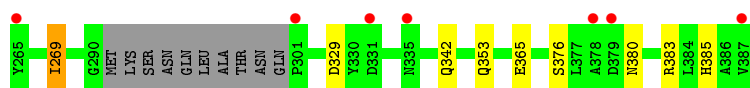
- Molecule 1: ATP phosphoribosyltransferase regulatory subunit



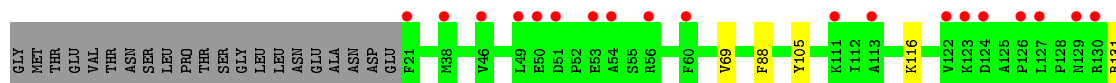
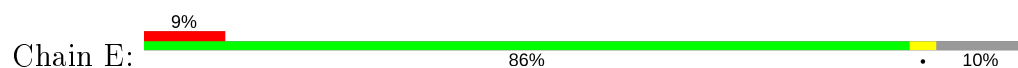
- Molecule 1: ATP phosphoribosyltransferase regulatory subunit



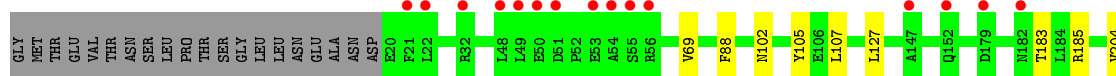
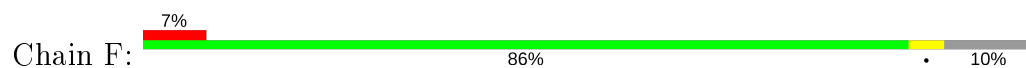




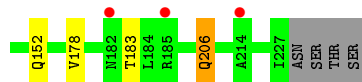
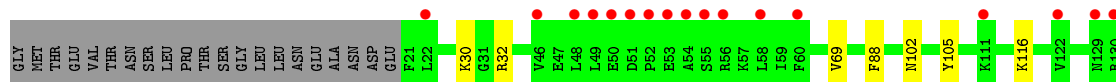
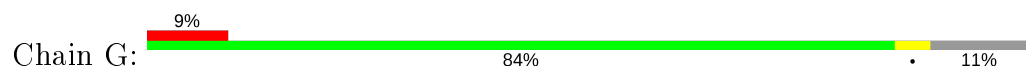
- Molecule 2: ATP phosphoribosyltransferase



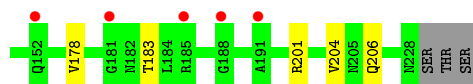
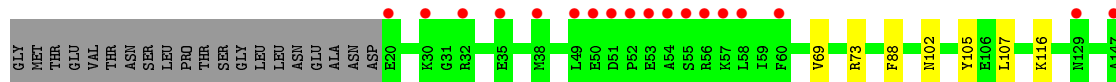
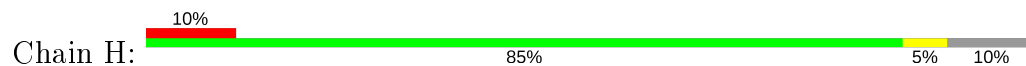
- Molecule 2: ATP phosphoribosyltransferase



- Molecule 2: ATP phosphoribosyltransferase



- Molecule 2: ATP phosphoribosyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.02Å 146.73Å 101.90Å 90.00° 102.40° 90.00°	Depositor
Resolution (Å)	30.63 – 2.34 30.63 – 2.34	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.63-2.34) 97.5 (30.63-2.34)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.227 , 0.269 0.233 , 0.274	Depositor DCC
$R_{free}$ test set	5467 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18971	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.4386e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SR, MPD, CL

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	0.54	0/3001	0.75	2/4070 (0.0%)
1	B	0.54	0/3016	0.73	0/4090
1	C	0.55	0/3013	0.76	2/4086 (0.0%)
1	D	0.53	0/3005	0.76	1/4075 (0.0%)
2	E	0.50	0/1625	0.76	0/2203
2	F	0.50	0/1634	0.75	1/2215 (0.0%)
2	G	0.50	0/1617	0.78	0/2192
2	H	0.50	0/1630	0.76	2/2211 (0.1%)
All	All	0.53	0/18541	0.75	8/25142 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	329	ASP	CB-CG-OD1	6.76	124.38	118.30
1	A	329	ASP	CB-CG-OD1	6.70	124.33	118.30
2	H	201	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	A	101	ASP	CB-CG-OD1	5.32	123.08	118.30
2	F	185	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	C	271[A]	PHE	CD1-CE1-CZ	5.05	126.17	120.10
1	C	271[B]	PHE	CD1-CE1-CZ	5.05	126.17	120.10
2	H	201	ARG	NE-CZ-NH2	5.01	122.80	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	2947	0	2936	17	0
1	B	2958	0	2946	11	0
1	C	2955	0	2945	8	0
1	D	2951	0	2939	12	0
2	E	1601	0	1660	2	0
2	F	1610	0	1666	3	0
2	G	1593	0	1654	4	0
2	H	1606	0	1655	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	1	0
4	G	1	0	0	0	0
4	H	2	0	0	0	0
5	A	24	0	42	8	0
5	B	24	0	42	1	0
5	C	16	0	28	1	0
5	D	16	0	28	3	0
5	E	8	0	14	0	0
5	G	8	0	14	0	0
6	A	96	0	0	0	0
6	B	157	0	0	1	0
6	C	128	0	0	1	0
6	D	117	0	0	1	0
6	E	26	0	0	0	0
6	F	41	0	0	0	0
6	G	41	0	0	0	0
6	H	23	0	0	0	0
All	All	18971	0	18569	47	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 (47) 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:B:73:ILE:HD11	1:D:73:ILE:HD11	1.65	0.79
1:B:70:LEU:HD13	1:C:70:LEU:HD13	1.66	0.78
1:A:73:ILE:HD11	1:C:73:ILE:HD11	1.68	0.76
1:A:185:ASN:OD1	2:G:102:ASN:HA	2.00	0.61
1:D:118:GLN:NE2	5:D:405:MPD:H11	2.19	0.58
1:A:284:ARG:HG3	5:A:407:MPD:H51	1.87	0.57
1:A:310:ASP:HB2	5:A:407:MPD:H11	1.90	0.54
1:A:286:GLY:CA	5:A:406:MPD:HM2	2.39	0.53
1:D:63:ILE:HD13	1:D:70:LEU:CD1	2.39	0.52
1:D:118:GLN:HE21	5:D:405:MPD:H11	1.76	0.51
1:A:307:PHE:HD2	5:A:406:MPD:H51	1.76	0.49
2:G:105:TYR:CZ	2:G:206:GLN:HG3	2.47	0.49
2:F:127:LEU:HD11	4:F:301:CL:CL	2.50	0.48
1:A:376:SER:HG	1:A:385:HIS:CE1	2.30	0.48
2:H:105:TYR:CZ	2:H:206:GLN:HG2	2.48	0.48
1:D:376:SER:HG	1:D:385:HIS:CE1	2.30	0.48
1:B:40:MET:HG2	6:B:580:HOH:O	2.14	0.47
1:B:235:ILE:O	1:B:239:GLN:HG3	2.14	0.47
1:B:73:ILE:CD1	1:D:73:ILE:HD11	2.41	0.47
1:A:186:LYS:CB	2:G:105:TYR:CD1	2.98	0.47
1:D:118:GLN:HB2	5:D:405:MPD:HM3	1.99	0.45
1:B:70:LEU:HD22	1:C:70:LEU:HD22	1.98	0.45
1:A:135:LEU:HD13	5:A:406:MPD:C5	2.47	0.44
1:A:286:GLY:HA2	5:A:406:MPD:HM2	1.98	0.44
1:A:73:ILE:HD11	1:C:73:ILE:CD1	2.44	0.44
1:B:147:ASP:OD2	5:B:408:MPD:C5	2.65	0.44
2:F:107:LEU:HD12	2:F:204:VAL:HG21	1.99	0.44
1:A:307:PHE:HB3	5:A:406:MPD:H4	2.00	0.44
1:B:328:ILE:HD11	1:B:348:VAL:HG21	2.00	0.44
1:A:186:LYS:HB2	2:G:105:TYR:CD1	2.52	0.44
1:C:310:ASP:HB2	5:C:406:MPD:H13	1.99	0.44
5:A:406:MPD:HM1	5:A:406:MPD:H52	2.00	0.43
1:B:102:VAL:CG2	1:B:116:PRO:HG2	2.49	0.43
1:B:367:MET:SD	1:B:371:LEU:HD22	2.59	0.43
1:A:102:VAL:CG2	1:A:116:PRO:HG2	2.49	0.43
1:D:241:LEU:HD12	1:D:269:ILE:CD1	2.49	0.43
2:H:107:LEU:HD12	2:H:204:VAL:HG21	2.00	0.43
1:A:21:ARG:HD3	1:C:21:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:VAL:CG2	1:D:116:PRO:HG2	2.49	0.42
1:C:40:MET:HG2	6:C:582:HOH:O	2.19	0.42
1:D:185:ASN:O	2:E:105:TYR:HA	2.19	0.42
1:C:102:VAL:CG2	1:C:116:PRO:HG2	2.50	0.42
1:D:186:LYS:HB2	2:E:105:TYR:CD1	2.55	0.41
1:D:170:ALA:HA	6:D:527:HOH:O	2.21	0.41
1:A:63:ILE:HD13	1:B:68:GLY:HA2	2.03	0.40
1:A:110:LEU:HA	1:A:110:LEU:HD23	1.80	0.40
2:F:105:TYR:CZ	2:F:206:GLN:HG2	2.57	0.40

There are no symmetry-related clashes.

## 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	373/388 (96%)	365 (98%)	8 (2%)	0	100	100
1	B	375/388 (97%)	366 (98%)	9 (2%)	0	100	100
1	C	374/388 (96%)	368 (98%)	6 (2%)	0	100	100
1	D	374/388 (96%)	365 (98%)	9 (2%)	0	100	100
2	E	206/232 (89%)	200 (97%)	6 (3%)	0	100	100
2	F	207/232 (89%)	200 (97%)	7 (3%)	0	100	100
2	G	205/232 (88%)	198 (97%)	7 (3%)	0	100	100
2	H	207/232 (89%)	200 (97%)	7 (3%)	0	100	100
All	All	2321/2480 (94%)	2262 (98%)	59 (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	320/329 (97%)	312 (98%)	8 (2%)	47	58
1	B	321/329 (98%)	311 (97%)	10 (3%)	40	49
1	C	321/329 (98%)	310 (97%)	11 (3%)	37	46
1	D	320/329 (97%)	309 (97%)	11 (3%)	37	46
2	E	174/195 (89%)	167 (96%)	7 (4%)	31	40
2	F	175/195 (90%)	171 (98%)	4 (2%)	50	61
2	G	173/195 (89%)	164 (95%)	9 (5%)	23	28
2	H	174/195 (89%)	167 (96%)	7 (4%)	31	40
All	All	1978/2096 (94%)	1911 (97%)	67 (3%)	38	46

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	82	LEU
1	A	141	SER
1	A	302	ARG
1	A	342	GLN
1	A	365	GLU
1	A	380	ASN
1	A	383	ARG
1	B	1	MET
1	B	26	GLN
1	B	54	ASP
1	B	82	LEU
1	B	141	SER
1	B	155	ASP
1	B	202	SER
1	B	271	PHE
1	B	379	ASP
1	B	380	ASN
1	C	26	GLN

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Mol	Chain	Res	Type
1	C	54	ASP
1	C	82	LEU
1	C	127	GLU
1	C	141	SER
1	C	155	ASP
1	C	264	HIS
1	C	271[A]	PHE
1	C	271[B]	PHE
1	C	365	GLU
1	C	380	ASN
1	D	1	MET
1	D	54	ASP
1	D	70	LEU
1	D	82	LEU
1	D	110	LEU
1	D	269	ILE
1	D	342	GLN
1	D	353	GLN
1	D	365	GLU
1	D	380	ASN
1	D	383	ARG
2	E	69	VAL
2	E	88	PHE
2	E	116	LYS
2	E	131	ARG
2	E	178	VAL
2	E	183	THR
2	E	192	ARG
2	F	69	VAL
2	F	88	PHE
2	F	102	ASN
2	F	183	THR
2	G	30	LYS
2	G	32	ARG
2	G	69	VAL
2	G	88	PHE
2	G	116	LYS
2	G	152	GLN
2	G	178	VAL
2	G	183	THR
2	G	206	GLN
2	H	69	VAL

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Mol	Chain	Res	Type
2	H	73	ARG
2	H	88	PHE
2	H	102	ASN
2	H	116	LYS
2	H	178	VAL
2	H	183	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 37 ligands modelled in this entry, 25 are monoatomic - leaving 12 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	$\# Z  > 2$
5	MPD	A	405	-	7,7,7	0.38	0	9,10,10	0.39	0
5	MPD	B	408	-	7,7,7	0.84	0	9,10,10	0.66	0
5	MPD	B	407	-	7,7,7	0.82	0	9,10,10	0.94	0
5	MPD	C	405	-	7,7,7	0.41	0	9,10,10	0.74	0
5	MPD	D	406	-	7,7,7	0.73	0	9,10,10	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MPD	E	304	-	7,7,7	0.92	1 (14%)	9,10,10	1.49	2 (22%)
5	MPD	D	405	-	7,7,7	0.65	0	9,10,10	1.40	1 (11%)
5	MPD	A	407	-	7,7,7	0.72	0	9,10,10	0.72	0
5	MPD	B	406	-	7,7,7	0.64	0	9,10,10	0.95	0
5	MPD	A	406	-	7,7,7	0.20	0	9,10,10	0.57	0
5	MPD	G	302	-	7,7,7	0.79	0	9,10,10	1.71	3 (33%)
5	MPD	C	406	-	7,7,7	0.76	0	9,10,10	0.98	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
5	MPD	A	405	-	-	2/5/5/5	-
5	MPD	B	408	-	-	2/5/5/5	-
5	MPD	B	407	-	-	0/5/5/5	-
5	MPD	C	405	-	-	2/5/5/5	-
5	MPD	D	406	-	-	0/5/5/5	-
5	MPD	E	304	-	-	2/5/5/5	-
5	MPD	D	405	-	-	1/5/5/5	-
5	MPD	A	407	-	-	1/5/5/5	-
5	MPD	B	406	-	-	3/5/5/5	-
5	MPD	A	406	-	-	1/5/5/5	-
5	MPD	G	302	-	-	4/5/5/5	-
5	MPD	C	406	-	-	2/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	304	MPD	O2-C2	-2.11	1.39	1.44

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	302	MPD	CM-C2-C1	-3.15	104.01	110.57
5	E	304	MPD	O2-C2-C1	-2.88	98.85	108.08
5	G	302	MPD	O2-C2-C1	-2.42	100.30	108.08
5	E	304	MPD	CM-C2-C1	2.35	115.48	110.57
5	G	302	MPD	C1-C2-C3	2.35	120.89	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	405	MPD	C1-C2-C3	2.20	120.22	109.96

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	304	MPD	C2-C3-C4-O4
5	E	304	MPD	C2-C3-C4-C5
5	G	302	MPD	C1-C2-C3-C4
5	G	302	MPD	O2-C2-C3-C4
5	B	408	MPD	C1-C2-C3-C4
5	B	408	MPD	O2-C2-C3-C4
5	A	406	MPD	C2-C3-C4-C5
5	B	406	MPD	O2-C2-C3-C4
5	G	302	MPD	C2-C3-C4-C5
5	C	405	MPD	C2-C3-C4-C5
5	A	407	MPD	C2-C3-C4-C5
5	C	406	MPD	C2-C3-C4-C5
5	C	406	MPD	C2-C3-C4-O4
5	G	302	MPD	CM-C2-C3-C4
5	B	406	MPD	C1-C2-C3-C4
5	B	406	MPD	CM-C2-C3-C4
5	D	405	MPD	C2-C3-C4-C5
5	A	405	MPD	C2-C3-C4-C5
5	A	405	MPD	C2-C3-C4-O4
5	C	405	MPD	C2-C3-C4-O4

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	408	MPD	1	0
5	D	405	MPD	3	0
5	A	407	MPD	2	0
5	A	406	MPD	6	0
5	C	406	MPD	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	377/388 (97%)	0.35	20 (5%) 26 37	21, 42, 75, 107	0
1	B	378/388 (97%)	0.10	9 (2%) 59 68	19, 37, 62, 84	0
1	C	377/388 (97%)	0.11	5 (1%) 77 83	19, 37, 59, 75	0
1	D	378/388 (97%)	0.50	27 (7%) 16 23	25, 43, 81, 106	0
2	E	208/232 (89%)	0.65	22 (10%) 6 10	33, 56, 91, 104	0
2	F	209/232 (90%)	0.43	17 (8%) 12 18	31, 52, 86, 105	0
2	G	207/232 (89%)	0.39	20 (9%) 7 12	29, 47, 78, 102	0
2	H	209/232 (90%)	0.60	23 (11%) 5 9	34, 56, 96, 130	0
All	All	2343/2480 (94%)	0.36	143 (6%) 21 30	19, 44, 81, 130	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	56	ARG	6.0
2	H	52	PRO	5.9
2	H	53	GLU	5.6
2	H	51	ASP	5.6
1	A	335	ASN	5.4
2	G	54	ALA	5.3
2	H	58	LEU	5.1
2	F	54	ALA	5.0
1	D	264	HIS	5.0
2	F	49	LEU	5.0
2	H	54	ALA	5.0
2	G	51	ASP	4.7
1	D	225	ALA	4.7
1	D	110	LEU	4.6
2	E	122	VAL	4.5
2	E	127	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
2	G	56	ARG	4.3
2	F	56	ARG	4.2
2	E	123	LYS	4.2
2	G	52	PRO	4.1
2	F	227	ILE	4.1
1	B	380	ASN	4.0
2	E	21	PHE	4.0
2	H	60	PHE	4.0
2	E	51	ASP	4.0
2	E	129	ASN	3.9
1	C	271[A]	PHE	3.9
2	F	22	LEU	3.9
2	F	32	ARG	3.9
2	H	57	LYS	3.9
1	A	264	HIS	3.9
2	E	56	ARG	3.8
1	D	223	GLU	3.8
2	E	54	ALA	3.8
1	B	0	GLY	3.7
1	A	86	ALA	3.7
1	D	0	GLY	3.7
2	E	130	ARG	3.7
1	D	378	ALA	3.6
1	D	263	TYR	3.6
2	E	124	ASP	3.6
1	D	219	GLY	3.4
1	B	379	ASP	3.4
1	B	199	PRO	3.4
1	D	218	LEU	3.3
2	G	129	ASN	3.3
2	H	188	GLY	3.2
2	G	60	PHE	3.2
2	G	53	GLU	3.2
2	H	185	ARG	3.2
1	A	333	PHE	3.2
1	A	197	VAL	3.2
1	A	174	SER	3.2
2	E	126	PRO	3.2
2	H	30	LYS	3.2
2	H	191	ALA	3.1
1	A	0	GLY	3.1
1	A	149	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	55	SER	3.1
1	A	378	ALA	3.1
1	C	301	PRO	3.1
2	E	49	LEU	3.1
1	D	149	SER	3.0
1	A	263	TYR	3.0
1	D	335	ASN	3.0
1	D	174	SER	2.9
2	H	147	ALA	2.9
2	F	228	ASN	2.9
1	A	265	TYR	2.9
2	H	129	ASN	2.8
1	A	301	PRO	2.8
2	F	48	LEU	2.8
1	D	301	PRO	2.8
1	C	380	ASN	2.8
2	F	21	PHE	2.7
2	G	49	LEU	2.7
2	H	38	MET	2.7
2	H	152	GLN	2.7
2	E	111	LYS	2.7
2	E	53	GLU	2.7
1	A	336	LEU	2.7
1	D	260	LEU	2.7
1	D	108	SER	2.6
2	E	113	ALA	2.6
2	F	50	GLU	2.6
2	G	214	ALA	2.6
1	D	265	TYR	2.6
2	H	55	SER	2.6
1	D	210	PHE	2.6
2	F	53	GLU	2.6
1	D	387	VAL	2.5
2	F	147	ALA	2.5
1	D	227	GLN	2.5
1	D	331	ASP	2.5
2	F	51	ASP	2.5
2	E	227	ILE	2.5
2	G	111	LYS	2.5
1	A	218	LEU	2.5
2	H	49	LEU	2.5
1	C	227	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	264	HIS	2.5
2	F	152	GLN	2.5
1	D	379	ASP	2.4
2	E	50	GLU	2.4
2	E	214	ALA	2.4
1	A	379	ASP	2.4
1	D	257	VAL	2.4
1	A	289	ASP	2.4
2	F	182	ASN	2.3
2	G	182	ASN	2.3
2	G	22	LEU	2.3
1	C	102	VAL	2.3
1	D	232	VAL	2.3
2	G	50	GLU	2.3
2	H	20	GLU	2.3
2	G	48	LEU	2.3
2	G	55	SER	2.3
2	E	46	VAL	2.3
2	H	35	GLU	2.2
2	H	50	GLU	2.2
1	D	169	ALA	2.2
2	G	185	ARG	2.2
2	H	32	ARG	2.2
1	A	271	PHE	2.2
2	E	60	PHE	2.2
1	D	57	ARG	2.2
2	E	38	MET	2.2
2	F	179	ASP	2.2
2	G	46	VAL	2.1
1	B	290	GLY	2.1
2	H	181	GLY	2.1
1	B	102	VAL	2.1
1	D	215	ALA	2.1
2	G	122	VAL	2.1
1	D	195	CYS	2.1
1	A	90	GLY	2.1
2	G	130	ARG	2.0
2	G	58	LEU	2.0
1	A	50	GLY	2.0
2	E	183	THR	2.0
1	B	383	ARG	2.0
1	A	227	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	353	GLN	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	CL	B	405	1/1	0.64	0.24	64,64,64,64	0
5	MPD	D	405	8/8	0.72	0.34	40,43,45,46	0
5	MPD	B	406	8/8	0.77	0.37	36,50,56,57	0
5	MPD	G	302	8/8	0.79	0.28	32,43,51,53	0
5	MPD	A	405	8/8	0.79	0.20	60,66,72,72	0
5	MPD	B	407	8/8	0.79	0.19	38,40,42,43	0
5	MPD	C	405	8/8	0.81	0.20	70,72,74,75	0
4	CL	E	302	1/1	0.85	0.16	72,72,72,72	0
5	MPD	B	408	8/8	0.86	0.34	39,41,44,45	0
5	MPD	E	304	8/8	0.86	0.24	44,49,56,56	0
3	SR	D	403	1/1	0.86	0.07	88,88,88,88	1
5	MPD	D	406	8/8	0.88	0.32	41,44,44,45	0
4	CL	E	301	1/1	0.88	0.08	67,67,67,67	0
5	MPD	A	407	8/8	0.88	0.23	35,36,41,44	0
4	CL	E	303	1/1	0.89	0.07	61,61,61,61	0
4	CL	A	404	1/1	0.89	0.22	66,66,66,66	0
5	MPD	A	406	8/8	0.92	0.26	53,56,59,63	0
4	CL	F	302	1/1	0.93	0.14	52,52,52,52	0
3	SR	D	401	1/1	0.93	0.05	58,58,58,58	1
5	MPD	C	406	8/8	0.93	0.22	26,36,41,45	0
3	SR	A	401	1/1	0.94	0.16	45,45,45,45	1
4	CL	G	301	1/1	0.95	0.06	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SR	A	402	1/1	0.95	0.04	71,71,71,71	1
4	CL	H	302	1/1	0.95	0.05	60,60,60,60	0
4	CL	B	403	1/1	0.96	0.05	48,48,48,48	0
4	CL	A	403	1/1	0.97	0.09	47,47,47,47	0
3	SR	D	402	1/1	0.97	0.21	49,49,49,49	1
3	SR	B	401	1/1	0.97	0.04	64,64,64,64	0
4	CL	F	301	1/1	0.97	0.11	54,54,54,54	0
4	CL	B	404	1/1	0.98	0.05	57,57,57,57	0
4	CL	C	404	1/1	0.98	0.07	44,44,44,44	0
3	SR	C	402	1/1	0.98	0.05	66,66,66,66	0
4	CL	H	301	1/1	0.99	0.17	50,50,50,50	0
4	CL	D	404	1/1	0.99	0.22	54,54,54,54	0
3	SR	C	403	1/1	0.99	0.09	59,59,59,59	0
3	SR	C	401	1/1	0.99	0.03	66,66,66,66	0
3	SR	B	402	1/1	0.99	0.10	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.