



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2017 – 05:59 PM EST

PDB ID : 5MLD  
Title : Crystal Structure of RosB with bound intermediate AFP (8-demethyl-8-amin oriboflavin-5'-phosphate)  
Authors : Konjik, V.; Bruenle, S.; Demmer, U.; Vanselow, A.; Sandhoff, R.; Mack, M.; Ermler, U.  
Deposited on : unknown  
Resolution : 1.70 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

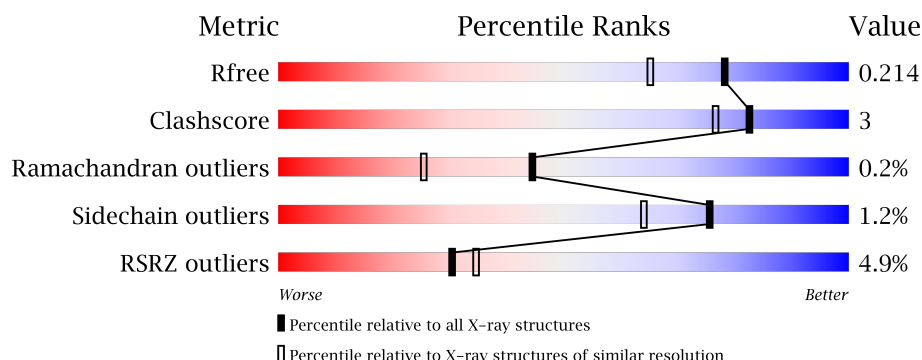
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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. 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	257	<div> <div>6%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	B	257	<div> <div>5%</div> <div>89%</div> <div>7%</div> <div>..</div> </div>
1	C	257	<div> <div>5%</div> <div>93%</div> <div>5%</div> <div>.</div> </div>
1	D	257	<div> <div>3%</div> <div>92%</div> <div>5%</div> <div>.</div> </div>
1	E	257	<div> <div>6%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	257	<div><div>5%</div><div><div></div><div></div><div></div></div><div>89%</div><div>7% ..</div></div>
1	G	257	<div><div>4%</div><div><div></div><div></div><div></div></div><div>91%</div><div>7% •</div></div>
1	H	257	<div><div>4%</div><div><div></div><div></div><div></div></div><div>92%</div><div>6% •</div></div>

## 2 Entry composition

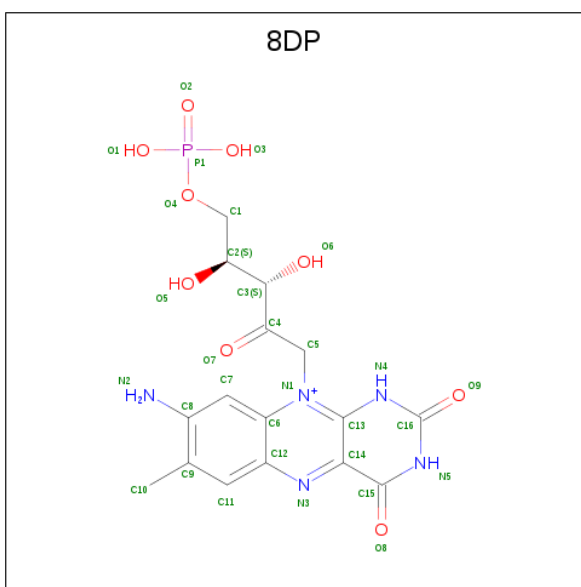
There are 3 unique types of molecules in this entry. The entry contains 18138 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BRAMP domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	8	0
			2054	1292	358	395	9			
1	B	252	Total	C	N	O	S	0	6	0
			2041	1285	355	392	9			
1	C	252	Total	C	N	O	S	0	1	0
			2000	1259	350	383	8			
1	D	252	Total	C	N	O	S	0	0	0
			1995	1256	350	381	8			
1	E	252	Total	C	N	O	S	0	2	0
			2008	1263	352	385	8			
1	F	252	Total	C	N	O	S	0	1	0
			2003	1260	351	384	8			
1	G	252	Total	C	N	O	S	0	1	0
			2000	1259	350	383	8			
1	H	252	Total	C	N	O	S	0	2	0
			2005	1262	351	384	8			

- Molecule 2 is 8-demethyl-8-aminoriboflavin-5'-phosphate (three-letter code: 8DP) (formula: C<sub>16</sub>H<sub>19</sub>N<sub>5</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	16	5	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	16	5	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	16	5	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	16	5	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	16	5	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	16	5	9	1		
2	G	1	Total	C	N	O	P	0	0
			31	16	5	9	1		
2	H	1	Total	C	N	O	P	0	0
			31	16	5	9	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	246	Total	O	0	0
			246	246		
3	B	205	Total	O	0	0
			205	205		
3	C	191	Total	O	0	0
			191	191		
3	D	246	Total	O	0	0
			246	246		

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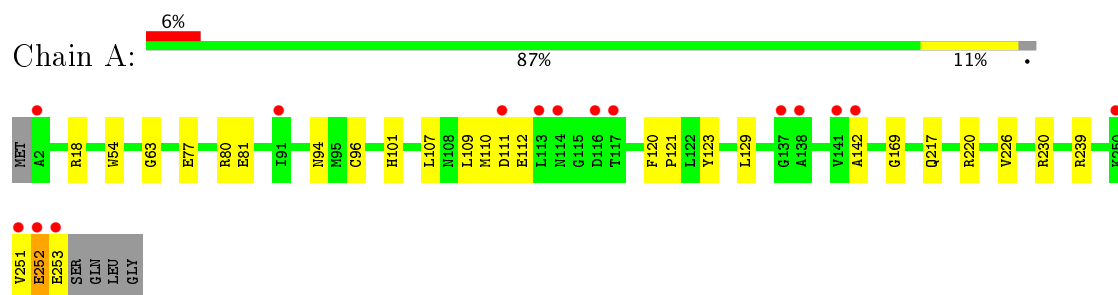
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	217	Total 217	O 217	0	0
3	F	221	Total 221	O 221	0	0
3	G	247	Total 247	O 247	0	0
3	H	211	Total 211	O 211	0	0

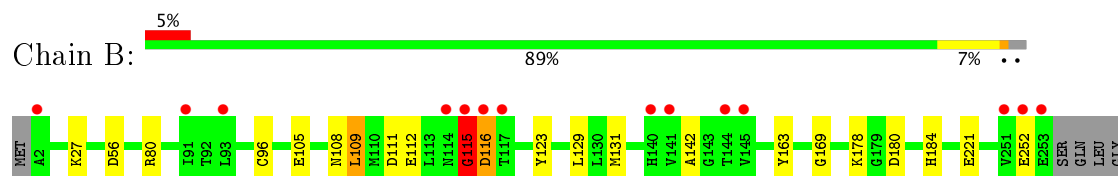
### 3 Residue-property plots [i](#)

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.

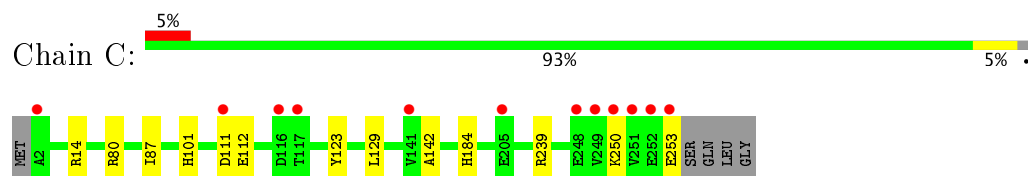
- Molecule 1: BRAMP domain protein



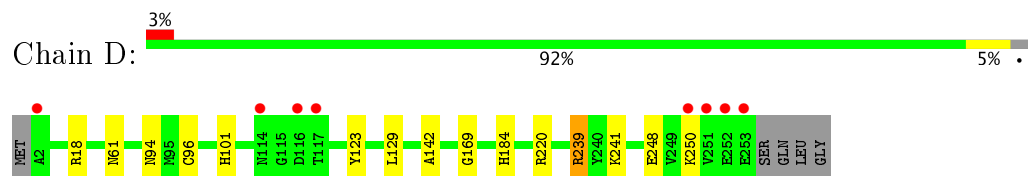
- Molecule 1: BRAMP domain protein



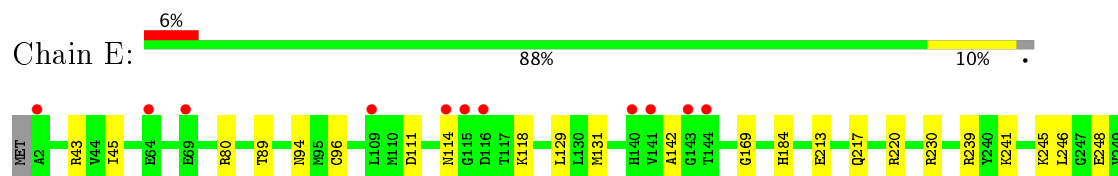
- Molecule 1: BRAMP domain protein

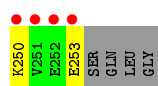


- Molecule 1: BRAMP domain protein

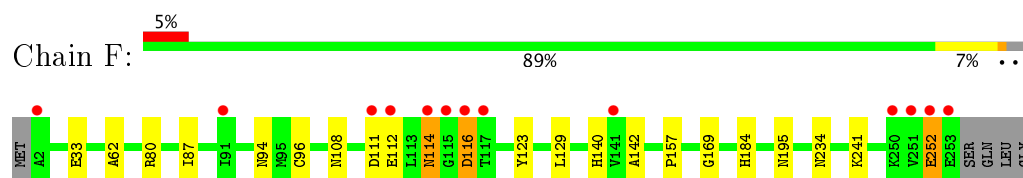


- Molecule 1: BRAMP domain protein

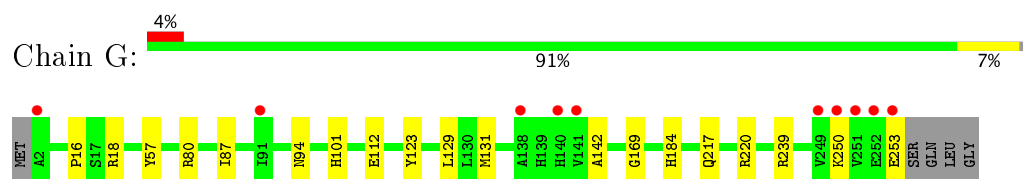




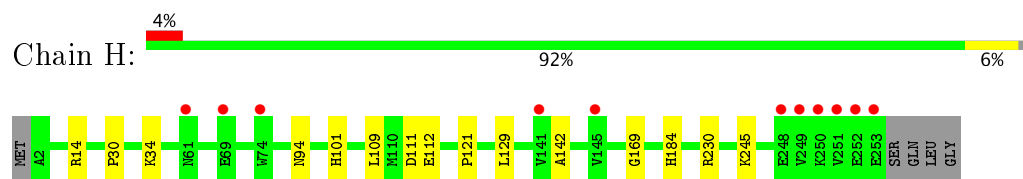
- Molecule 1: BRAMP domain protein



- Molecule 1: BRAMP domain protein



- Molecule 1: BRAMP domain protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.49Å 71.13Å 214.80Å 90.00° 92.08° 90.00°	Depositor
Resolution (Å)	47.54 – 1.70 47.54 – 1.70	Depositor EDS
% Data completeness (in resolution range)	92.9 (47.54-1.70) 92.9 (47.54-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.174 , 0.213 0.174 , 0.214	Depositor DCC
$R_{free}$ test set	10139 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	18138	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 8DP

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	0.39	0/2101	0.59	0/2853
1	B	0.36	0/2085	0.60	1/2831 (0.0%)
1	C	0.36	0/2044	0.56	0/2776
1	D	0.36	0/2036	0.56	0/2765
1	E	0.40	1/2052 (0.0%)	0.56	0/2787
1	F	0.42	2/2044 (0.1%)	0.57	0/2776
1	G	0.36	0/2044	0.56	0/2776
1	H	0.35	0/2052	0.55	0/2787
All	All	0.38	3/16458 (0.0%)	0.57	1/22351 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	252	GLU	CD-OE1	-6.12	1.19	1.25
1	E	241	LYS	CD-CE	-6.04	1.36	1.51
1	F	252	GLU	CD-OE2	-5.45	1.19	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	GLY	C-N-CA	5.16	134.60	121.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2054	0	2019	20	0
1	B	2041	0	2007	18	0
1	C	2000	0	1967	11	0
1	D	1995	0	1963	13	0
1	E	2008	0	1972	17	0
1	F	2003	0	1966	16	0
1	G	2000	0	1967	15	0
1	H	2005	0	1973	11	0
2	A	31	0	0	0	0
2	B	31	0	0	0	0
2	C	31	0	0	0	0
2	D	31	0	0	0	0
2	E	31	0	0	0	0
2	F	31	0	0	0	0
2	G	31	0	0	0	0
2	H	31	0	0	0	0
3	A	246	0	0	1	0
3	B	205	0	0	2	0
3	C	191	0	0	1	0
3	D	246	0	0	2	0
3	E	217	0	0	3	0
3	F	221	0	0	3	0
3	G	247	0	0	0	0
3	H	211	0	0	1	0
All	All	18138	0	15834	92	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 3.

All (92) 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:115:GLY:HA3	1:B:116:ASP:HB2	1.33	1.06
1:E:250:LYS:NZ	3:E:401:HOH:O	2.19	0.74
1:E:213:GLU:OE2	1:E:217:GLN:NE2	2.22	0.72
1:F:80:ARG:NH2	1:F:112:GLU:OE2	2.24	0.71
1:B:111[A]:ASP:OD2	1:D:241:LYS:NZ	2.26	0.69
1:D:220:ARG:NH2	3:D:401:HOH:O	2.23	0.67
1:A:111[A]:ASP:HB2	1:C:239:ARG:HH11	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110[B]:MET:O	3:A:401:HOH:O	2.14	0.64
1:D:61:ASN:HB3	1:E:248:GLU:HG3	1.80	0.64
1:E:245:LYS:NZ	3:E:403:HOH:O	2.31	0.64
1:B:115:GLY:HA3	1:B:116:ASP:CB	2.20	0.63
1:B:109[A]:LEU:HD12	1:D:239:ARG:NH1	2.15	0.60
1:E:184:HIS:CG	1:F:169:GLY:HA2	2.38	0.59
1:A:112[A]:GLU:HB2	1:A:121:PRO:HG3	1.85	0.58
1:B:115:GLY:CA	1:B:116:ASP:HB2	2.21	0.56
1:C:80:ARG:HH22	1:C:112:GLU:CD	2.08	0.56
1:G:80:ARG:NH2	1:G:112:GLU:OE1	2.28	0.56
1:A:230:ARG:HH12	1:C:253:GLU:HG2	1.71	0.55
1:E:169:GLY:HA2	1:F:184:HIS:CG	2.42	0.54
1:E:239:ARG:NH1	1:F:111:ASP:OD1	2.40	0.53
1:H:30:PRO:O	1:H:34:LYS:HE2	2.09	0.53
1:F:108:ASN:ND2	3:F:403:HOH:O	2.35	0.53
1:A:80:ARG:NH2	1:A:112[A]:GLU:OE1	2.43	0.52
1:H:112:GLU:O	1:H:121:PRO:HD3	2.10	0.52
1:D:18:ARG:HG2	3:D:557:HOH:O	2.09	0.52
1:B:221:GLU:OE1	3:B:401:HOH:O	2.19	0.52
1:D:248:GLU:OE1	1:D:250:LYS:NZ	2.33	0.52
1:C:239:ARG:NH2	3:C:404:HOH:O	2.44	0.51
1:H:34:LYS:NZ	3:H:402:HOH:O	2.31	0.51
1:B:184:HIS:CG	1:D:169:GLY:HA2	2.46	0.51
1:C:80:ARG:NH2	1:C:112:GLU:OE2	2.44	0.51
1:F:33:GLU:OE2	3:F:401:HOH:O	2.19	0.51
1:G:87:ILE:O	1:G:129:LEU:HD12	2.11	0.50
1:G:239:ARG:HD2	1:H:109:LEU:HD13	1.93	0.50
1:A:112[B]:GLU:O	1:A:121:PRO:HD3	2.11	0.50
1:F:80:ARG:HD2	3:F:410:HOH:O	2.11	0.49
1:A:239:ARG:NH1	1:C:111:ASP:HB2	2.27	0.49
1:E:111[B]:ASP:OD1	1:E:111[B]:ASP:N	2.41	0.49
1:G:253:GLU:O	1:H:230:ARG:NH2	2.41	0.49
1:F:94:ASN:OD1	1:F:140:HIS:ND1	2.32	0.48
1:B:105:GLU:O	1:B:109[A]:LEU:HD22	2.14	0.47
1:E:96:CYS:O	1:H:101:HIS:CE1	2.68	0.47
1:A:112[B]:GLU:O	1:A:120:PHE:HA	2.15	0.47
1:G:253:GLU:C	1:H:230:ARG:HH22	2.20	0.45
1:A:169:GLY:HA2	1:C:184:HIS:CG	2.52	0.45
1:B:96:CYS:O	1:C:101:HIS:CE1	2.69	0.45
1:A:226:VAL:HG11	1:A:251:VAL:HG21	1.98	0.45
1:B:111[A]:ASP:HB2	1:D:239:ARG:HE	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:ARG:HG2	1:E:45:ILE:HG22	1.99	0.45
1:E:217:GLN:HG2	1:E:220:ARG:NH2	2.32	0.45
1:F:129:LEU:CD2	1:F:142:ALA:HA	2.47	0.45
1:B:80:ARG:NH2	1:B:112[A]:GLU:OE2	2.21	0.44
1:G:169:GLY:HA2	1:H:184:HIS:CG	2.53	0.44
1:A:101:HIS:CE1	1:D:96:CYS:O	2.70	0.44
1:B:178:LYS:HD2	1:B:178:LYS:HA	1.83	0.44
1:A:18:ARG:HD3	1:G:18:ARG:HG2	1.99	0.43
1:E:220:ARG:NH1	1:F:234:ASN:OD1	2.47	0.43
1:G:217:GLN:HG2	1:G:220:ARG:HH22	1.83	0.43
1:B:108:ASN:HB3	3:B:569:HOH:O	2.18	0.43
3:E:517:HOH:O	1:F:241:LYS:HE2	2.17	0.43
1:A:96:CYS:O	1:D:101:HIS:CE1	2.72	0.43
1:G:129:LEU:HG	1:G:131:MET:HG3	2.00	0.43
1:G:184:HIS:CG	1:H:169:GLY:HA2	2.53	0.43
1:A:129:LEU:CD2	1:A:142:ALA:HA	2.49	0.43
1:B:169:GLY:HA2	1:D:184:HIS:CG	2.54	0.43
1:G:57:TYR:HE1	1:H:245:LYS:HE3	1.83	0.43
1:E:129:LEU:CD2	1:E:142:ALA:HA	2.48	0.43
1:E:230:ARG:HD2	1:E:246:LEU:O	2.18	0.43
1:F:96:CYS:O	1:G:101:HIS:CE1	2.71	0.43
1:A:217:GLN:HG2	1:A:220:ARG:HH22	1.84	0.42
1:G:217:GLN:HG2	1:G:220:ARG:NH2	2.33	0.42
1:A:107:LEU:C	1:A:109[B]:LEU:H	2.23	0.42
1:C:87:ILE:O	1:C:129:LEU:HD12	2.20	0.42
1:H:129:LEU:CD2	1:H:142:ALA:HA	2.50	0.42
1:F:87:ILE:O	1:F:129:LEU:HD12	2.19	0.42
1:D:129:LEU:CD2	1:D:142:ALA:HA	2.50	0.41
1:A:239:ARG:HH11	1:C:111:ASP:HB2	1.86	0.41
1:A:252:GLU:HB3	1:A:253:GLU:H	1.55	0.41
1:A:77:GLU:HG3	1:A:81:GLU:OE2	2.21	0.41
1:B:252:GLU:OE2	1:D:250:LYS:C	2.59	0.41
1:E:118:LYS:HA	1:E:118:LYS:HD3	1.92	0.41
1:E:80:ARG:HH22	1:E:114:ASN:HD22	1.68	0.41
1:F:62:ALA:HB2	1:G:16:PRO:HD2	2.03	0.41
1:F:114:ASN:O	1:F:116:ASP:N	2.54	0.41
1:G:129:LEU:CD2	1:G:142:ALA:HA	2.51	0.41
1:B:131:MET:O	1:B:163:TYR:HA	2.20	0.41
1:A:54:TRP:CD1	1:A:63:GLY:HA3	2.56	0.40
1:B:129:LEU:CD2	1:B:142:ALA:HA	2.51	0.40
1:B:27:LYS:NZ	1:B:180[B]:ASP:OD1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:LEU:CD2	1:C:142:ALA:HA	2.51	0.40
1:E:89:THR:O	1:E:131:MET:HA	2.21	0.40
1:F:157:PRO:HB2	1:F:195:ASN:HB3	2.04	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	258/257 (100%)	245 (95%)	12 (5%)	1 (0%)	38	20
1	B	256/257 (100%)	246 (96%)	8 (3%)	2 (1%)	22	7
1	C	251/257 (98%)	247 (98%)	4 (2%)	0	100	100
1	D	250/257 (97%)	247 (99%)	3 (1%)	0	100	100
1	E	252/257 (98%)	247 (98%)	5 (2%)	0	100	100
1	F	251/257 (98%)	244 (97%)	5 (2%)	2 (1%)	22	7
1	G	251/257 (98%)	246 (98%)	5 (2%)	0	100	100
1	H	252/257 (98%)	246 (98%)	6 (2%)	0	100	100
All	All	2021/2056 (98%)	1968 (97%)	48 (2%)	5 (0%)	44	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	GLU
1	B	116	ASP
1	B	115	GLY
1	F	116	ASP
1	F	114	ASN

### 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	219/215 (102%)	217 (99%)	2 (1%)	82	74
1	B	217/215 (101%)	213 (98%)	4 (2%)	64	47
1	C	212/215 (99%)	209 (99%)	3 (1%)	71	58
1	D	211/215 (98%)	208 (99%)	3 (1%)	71	58
1	E	213/215 (99%)	211 (99%)	2 (1%)	82	74
1	F	212/215 (99%)	210 (99%)	2 (1%)	82	74
1	G	212/215 (99%)	209 (99%)	3 (1%)	71	58
1	H	213/215 (99%)	210 (99%)	3 (1%)	71	58
All	All	1709/1720 (99%)	1687 (99%)	22 (1%)	75	60

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	123	TYR
1	B	56	ASP
1	B	109[A]	LEU
1	B	109[B]	LEU
1	B	123	TYR
1	C	14	ARG
1	C	123	TYR
1	C	250	LYS
1	D	94	ASN
1	D	123	TYR
1	D	239	ARG
1	E	94	ASN
1	E	253	GLU
1	F	123	TYR
1	F	252	GLU
1	G	94	ASN
1	G	123	TYR
1	G	250	LYS

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Mol	Chain	Res	Type
1	H	14	ARG
1	H	94	ASN
1	H	111	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	B	94	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](#)

8 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	8DP	A	301	-	30,33,33	1.74	7 (23%)	33,50,50	1.81	7 (21%)
2	8DP	B	301	-	30,33,33	1.73	4 (13%)	33,50,50	2.08	5 (15%)
2	8DP	C	301	-	30,33,33	1.74	6 (20%)	33,50,50	1.49	4 (12%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	8DP	D	301	-	30,33,33	1.73	4 (13%)	33,50,50	1.95	6 (18%)
2	8DP	E	301	-	30,33,33	1.78	6 (20%)	33,50,50	1.81	7 (21%)
2	8DP	F	301	-	30,33,33	1.80	6 (20%)	33,50,50	2.00	5 (15%)
2	8DP	G	301	-	30,33,33	1.66	6 (20%)	33,50,50	1.92	6 (18%)
2	8DP	H	301	-	30,33,33	1.65	5 (16%)	33,50,50	1.60	5 (15%)

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	8DP	A	301	-	-	0/18/18/18	0/3/3/3
2	8DP	B	301	-	-	0/18/18/18	0/3/3/3
2	8DP	C	301	-	-	0/18/18/18	0/3/3/3
2	8DP	D	301	-	-	0/18/18/18	0/3/3/3
2	8DP	E	301	-	-	0/18/18/18	0/3/3/3
2	8DP	F	301	-	-	0/18/18/18	0/3/3/3
2	8DP	G	301	-	-	0/18/18/18	0/3/3/3
2	8DP	H	301	-	-	0/18/18/18	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	8DP	C16-N4	-3.04	1.32	1.38
2	A	301	8DP	C16-N4	-2.99	1.32	1.38
2	H	301	8DP	C16-N4	-2.89	1.32	1.38
2	F	301	8DP	C16-N4	-2.82	1.32	1.38
2	B	301	8DP	C16-N4	-2.80	1.32	1.38
2	G	301	8DP	C16-N4	-2.74	1.32	1.38
2	E	301	8DP	C16-N4	-2.65	1.32	1.38
2	G	301	8DP	C6-N1	-2.58	1.35	1.38
2	C	301	8DP	C16-N4	-2.57	1.33	1.38
2	H	301	8DP	C6-N1	-2.42	1.35	1.38
2	C	301	8DP	C6-N1	-2.33	1.35	1.38
2	F	301	8DP	C6-N1	-2.13	1.36	1.38
2	A	301	8DP	O5-C2	-2.04	1.38	1.43
2	A	301	8DP	C6-N1	-2.02	1.36	1.38
2	A	301	8DP	C13-N4	2.01	1.36	1.33
2	G	301	8DP	O7-C4	2.02	1.25	1.21
2	F	301	8DP	C1-C2	2.02	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	8DP	C8-N2	2.04	1.44	1.37
2	D	301	8DP	C1-C2	2.08	1.54	1.51
2	E	301	8DP	C8-N2	2.08	1.44	1.37
2	E	301	8DP	C14-N3	2.12	1.36	1.33
2	D	301	8DP	C8-N2	2.16	1.45	1.37
2	C	301	8DP	P1-O2	2.16	1.58	1.50
2	H	301	8DP	C8-N2	2.16	1.45	1.37
2	E	301	8DP	C1-C2	2.17	1.55	1.51
2	E	301	8DP	C5-N1	2.17	1.54	1.49
2	B	301	8DP	C1-C2	2.19	1.55	1.51
2	H	301	8DP	C14-N3	2.20	1.36	1.33
2	B	301	8DP	C8-N2	2.21	1.45	1.37
2	F	301	8DP	C14-N3	2.22	1.36	1.33
2	G	301	8DP	C8-N2	2.27	1.45	1.37
2	F	301	8DP	C8-N2	2.29	1.45	1.37
2	A	301	8DP	C14-N3	2.31	1.36	1.33
2	C	301	8DP	C8-N2	2.32	1.45	1.37
2	G	301	8DP	C14-N3	2.92	1.37	1.33
2	C	301	8DP	C14-N3	2.95	1.37	1.33
2	G	301	8DP	O8-C15	5.67	1.38	1.24
2	H	301	8DP	O8-C15	5.85	1.39	1.24
2	A	301	8DP	O8-C15	6.11	1.39	1.24
2	C	301	8DP	O8-C15	6.32	1.40	1.24
2	B	301	8DP	O8-C15	6.70	1.41	1.24
2	D	301	8DP	O8-C15	6.88	1.41	1.24
2	E	301	8DP	O8-C15	6.92	1.42	1.24
2	F	301	8DP	O8-C15	7.03	1.42	1.24

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	8DP	C1-C2-C3	-4.60	104.33	111.83
2	G	301	8DP	C1-C2-C3	-4.59	104.36	111.83
2	B	301	8DP	C1-C2-C3	-4.40	104.66	111.83
2	D	301	8DP	C1-C2-C3	-4.37	104.71	111.83
2	A	301	8DP	C1-C2-C3	-4.25	104.91	111.83
2	H	301	8DP	C1-C2-C3	-3.86	105.54	111.83
2	G	301	8DP	C15-C14-C13	-3.68	116.98	119.96
2	D	301	8DP	C14-C15-N5	-3.54	118.45	123.48
2	F	301	8DP	C14-C15-N5	-3.49	118.51	123.48
2	B	301	8DP	C14-C15-N5	-3.41	118.63	123.48
2	E	301	8DP	C14-C15-N5	-3.28	118.82	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	8DP	C1-C2-C3	-3.22	106.59	111.83
2	A	301	8DP	C14-C15-N5	-2.76	119.55	123.48
2	B	301	8DP	C15-C14-C13	-2.75	117.74	119.96
2	H	301	8DP	C15-C14-C13	-2.73	117.75	119.96
2	A	301	8DP	C15-C14-C13	-2.72	117.76	119.96
2	C	301	8DP	C14-C15-N5	-2.62	119.75	123.48
2	E	301	8DP	C1-C2-C3	-2.50	107.76	111.83
2	F	301	8DP	C15-C14-C13	-2.40	118.02	119.96
2	G	301	8DP	C14-C15-N5	-2.24	120.30	123.48
2	E	301	8DP	C15-C14-C13	-2.12	118.25	119.96
2	A	301	8DP	P1-O4-C1	-2.10	112.52	118.30
2	H	301	8DP	C15-C14-N3	2.00	120.88	118.68
2	A	301	8DP	C15-C14-N3	2.15	121.04	118.68
2	D	301	8DP	O7-C4-C5	2.18	124.10	121.36
2	E	301	8DP	C15-C14-N3	2.23	121.13	118.68
2	G	301	8DP	C15-C14-N3	2.26	121.16	118.68
2	D	301	8DP	C14-N3-C12	2.26	119.15	116.76
2	E	301	8DP	C14-N3-C12	2.27	119.16	116.76
2	A	301	8DP	C12-C6-N1	3.36	120.15	117.66
2	H	301	8DP	C15-N5-C16	4.07	118.72	115.16
2	D	301	8DP	C12-C6-N1	4.09	120.69	117.66
2	C	301	8DP	C12-C6-N1	4.24	120.80	117.66
2	H	301	8DP	C12-C6-N1	4.25	120.81	117.66
2	F	301	8DP	C12-C6-N1	4.27	120.83	117.66
2	C	301	8DP	C15-N5-C16	4.50	119.10	115.16
2	E	301	8DP	C12-C6-N1	4.51	121.01	117.66
2	B	301	8DP	C12-C6-N1	4.68	121.13	117.66
2	G	301	8DP	C12-C6-N1	5.17	121.50	117.66
2	G	301	8DP	C15-N5-C16	5.84	120.27	115.16
2	A	301	8DP	C15-N5-C16	6.43	120.78	115.16
2	D	301	8DP	C15-N5-C16	6.52	120.86	115.16
2	E	301	8DP	C15-N5-C16	6.55	120.89	115.16
2	F	301	8DP	C15-N5-C16	6.99	121.27	115.16
2	B	301	8DP	C15-N5-C16	7.65	121.85	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	252/257 (98%)	0.25	15 (5%) 23 25	15, 22, 42, 95	0
1	B	252/257 (98%)	0.17	14 (5%) 25 28	18, 25, 40, 88	0
1	C	252/257 (98%)	0.18	12 (4%) 31 36	17, 28, 45, 93	0
1	D	252/257 (98%)	0.05	8 (3%) 48 54	17, 25, 39, 94	0
1	E	252/257 (98%)	0.14	15 (5%) 23 25	19, 26, 40, 82	0
1	F	252/257 (98%)	0.09	13 (5%) 28 31	18, 26, 43, 79	0
1	G	252/257 (98%)	0.21	10 (3%) 39 44	16, 22, 40, 99	0
1	H	252/257 (98%)	0.16	11 (4%) 35 40	16, 29, 43, 102	0
All	All	2016/2056 (98%)	0.16	98 (4%) 30 35	15, 25, 42, 102	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	253	GLU	9.1
1	B	253	GLU	8.9
1	G	253	GLU	8.1
1	F	253	GLU	7.6
1	A	252	GLU	7.6
1	D	253	GLU	7.5
1	C	253	GLU	7.4
1	H	253	GLU	7.2
1	A	251	VAL	7.1
1	C	251	VAL	6.3
1	G	252	GLU	6.2
1	E	252	GLU	6.2
1	E	2	ALA	6.1
1	A	253	GLU	5.8
1	C	252	GLU	5.6
1	F	115	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
1	G	251	VAL	5.1
1	H	252	GLU	5.0
1	C	250	LYS	4.7
1	H	251	VAL	4.6
1	B	252	GLU	4.5
1	D	251	VAL	4.4
1	G	250	LYS	4.4
1	C	117	THR	4.4
1	A	117	THR	4.3
1	H	249	VAL	4.3
1	C	249	VAL	4.2
1	C	2	ALA	4.2
1	D	2	ALA	4.2
1	E	115	GLY	4.0
1	B	115	GLY	4.0
1	F	252	GLU	3.9
1	B	116	ASP	3.9
1	D	252	GLU	3.7
1	H	250	LYS	3.6
1	A	116	ASP	3.6
1	B	114	ASN	3.6
1	F	117	THR	3.6
1	B	2	ALA	3.5
1	D	116	ASP	3.5
1	A	250	LYS	3.4
1	F	111	ASP	3.4
1	F	116	ASP	3.4
1	G	141	VAL	3.3
1	A	111[A]	ASP	3.3
1	C	116	ASP	3.2
1	E	251	VAL	3.2
1	B	117	THR	3.2
1	E	114	ASN	3.2
1	A	141	VAL	3.2
1	E	116	ASP	3.1
1	A	2	ALA	3.1
1	H	248	GLU	3.0
1	A	114	ASN	3.0
1	C	248	GLU	3.0
1	H	74	TRP	3.0
1	D	250	LYS	2.9
1	B	145	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	249	VAL	2.7
1	C	205	GLU	2.6
1	G	91	ILE	2.5
1	E	144	THR	2.5
1	A	91	ILE	2.5
1	A	113[A]	LEU	2.5
1	F	251	VAL	2.4
1	E	109	LEU	2.4
1	F	112	GLU	2.4
1	F	2	ALA	2.4
1	G	2	ALA	2.4
1	E	143	GLY	2.4
1	H	141	VAL	2.4
1	B	93	LEU	2.4
1	E	250	LYS	2.4
1	F	114	ASN	2.4
1	B	140	HIS	2.4
1	E	140	HIS	2.4
1	C	111	ASP	2.3
1	E	141	VAL	2.3
1	F	141	VAL	2.3
1	B	91	ILE	2.3
1	F	250	LYS	2.3
1	E	69	GLU	2.3
1	C	141	VAL	2.2
1	B	144	THR	2.2
1	H	145	VAL	2.2
1	H	69	GLU	2.1
1	D	114	ASN	2.1
1	D	117	THR	2.1
1	H	61	ASN	2.1
1	B	141	VAL	2.1
1	E	64	GLU	2.1
1	F	91	ILE	2.1
1	A	138	ALA	2.1
1	A	142	ALA	2.1
1	B	251	VAL	2.1
1	G	140	HIS	2.1
1	G	138	ALA	2.0
1	A	137	GLY	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 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	8DP	B	301	31/31	0.96	0.12	0.03	20,23,30,33	0
2	8DP	E	301	31/31	0.96	0.11	-0.05	19,24,32,33	0
2	8DP	H	301	31/31	0.97	0.09	-0.41	16,21,28,34	0
2	8DP	F	301	31/31	0.97	0.09	-0.42	18,22,29,33	0
2	8DP	C	301	31/31	0.97	0.09	-0.43	16,19,25,32	0
2	8DP	A	301	31/31	0.97	0.10	-0.45	14,17,29,32	0
2	8DP	G	301	31/31	0.97	0.10	-0.75	14,18,24,31	0
2	8DP	D	301	31/31	0.97	0.08	-0.76	16,21,27,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.