



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:28 PM GMT

PDB ID : 2C6Q  
Title : CRYSTAL STRUCTURE OF HUMAN GUANOSINE MONOPHOSPHATE  
REDUCTASE 2 GMPR2 IN COMPLEX WITH IMP AND NADPH  
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Ehle, P.; Ogg, D.; Persson, C.; Sagemark, J.; Schuler, H.; Sundstrom, M.;  
Thorsell, A.; Weigelt, J.; Nordlund, P.  
Deposited on : 2005-11-11  
Resolution : 1.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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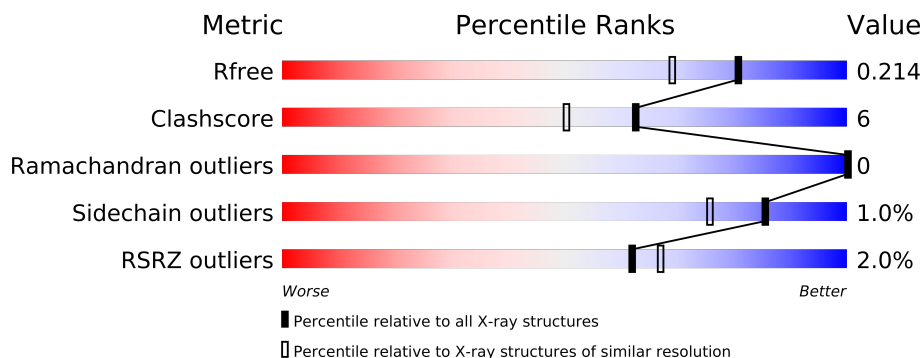
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	351	
1	B	351	
1	C	351	
1	D	351	
1	E	351	
1	F	351	
1	G	351	
1	H	351	

## 2 Entry composition

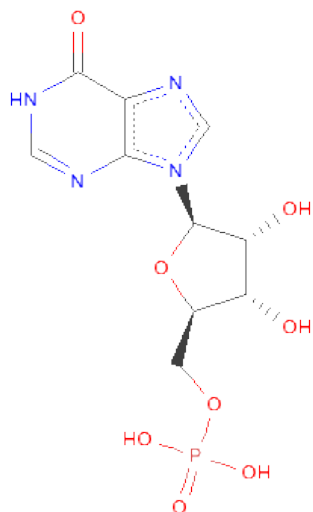
There are 4 unique types of molecules in this entry. The entry contains 23052 atoms, of which 0 are hydrogen and 0 are deuterium.

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 GMP REDUCTASE 2.

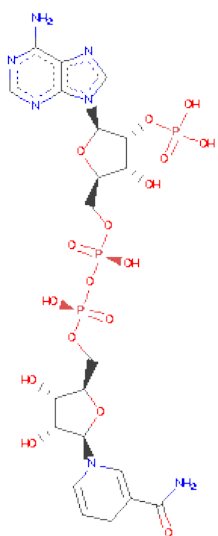
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2494	1573	430	473	18			
1	B	329	Total	C	N	O	S	0	1	0
			2507	1580	432	476	19			
1	C	328	Total	C	N	O	S	0	1	0
			2505	1579	434	474	18			
1	D	328	Total	C	N	O	S	0	0	0
			2494	1573	430	473	18			
1	E	328	Total	C	N	O	S	0	4	0
			2519	1586	434	480	19			
1	F	328	Total	C	N	O	S	0	0	0
			2494	1573	430	473	18			
1	G	321	Total	C	N	O	S	0	0	0
			2444	1542	420	464	18			
1	H	328	Total	C	N	O	S	0	2	0
			2506	1579	432	476	19			

- Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>4</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	G	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	H	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	302	Total	O	0	0
			302	302		
4	B	285	Total	O	0	0
			285	285		
4	C	335	Total	O	0	0
			335	335		
4	D	305	Total	O	0	0
			305	305		
4	E	352	Total	O	0	0
			352	352		

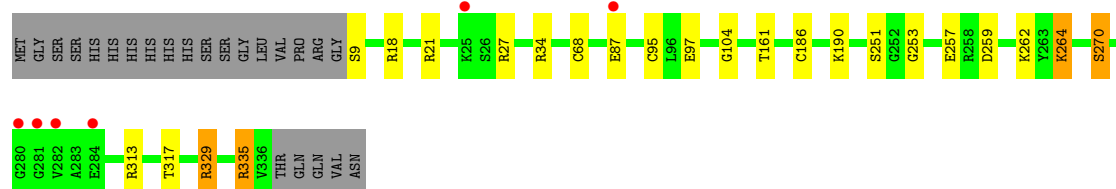
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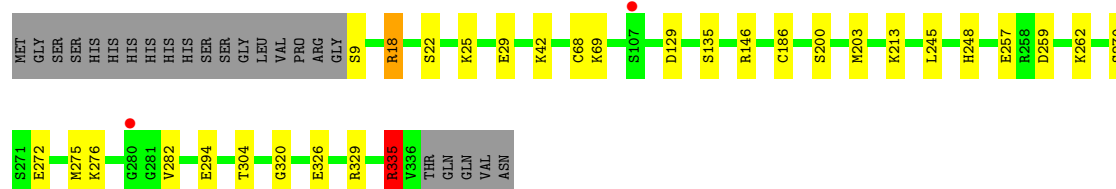
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	346	Total 346	O 346	0	0
4	G	304	Total 304	O 304	0	0
4	H	340	Total 340	O 340	0	0



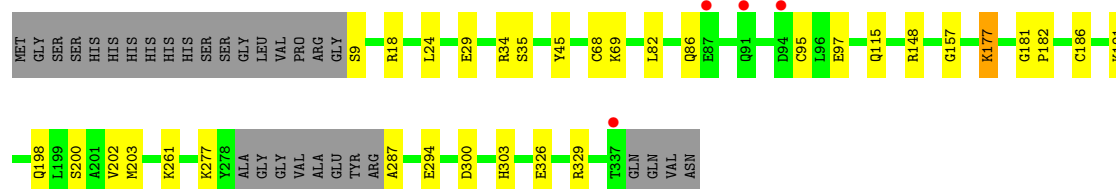
- Molecule 1: GMP REDUCTASE 2

Chain E: 

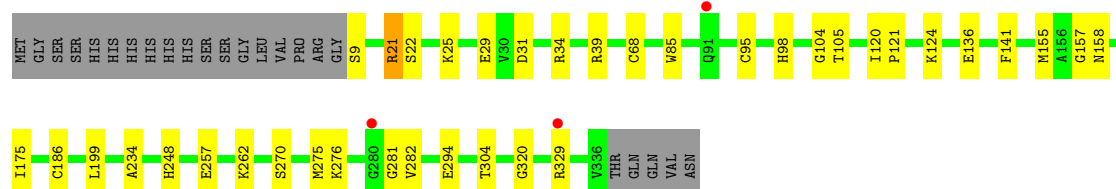
- Molecule 1: GMP REDUCTASE 2

Chain F: 

- Molecule 1: GMP REDUCTASE 2

Chain G: 

- Molecule 1: GMP REDUCTASE 2

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.68Å 141.37Å 164.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.70 10.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (10.00-1.70) 99.9 (10.00-1.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.22 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.163 , 0.206 0.175 , 0.214	Depositor DCC
$R_{free}$ test set	16715 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.48 , 60.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 332307 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	23052	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, IMP

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	0.79	0/2539	0.80	3/3414 (0.1%)
1	B	0.80	0/2552	0.81	1/3432 (0.0%)
1	C	0.87	0/2550	0.87	3/3428 (0.1%)
1	D	0.84	0/2539	0.82	2/3414 (0.1%)
1	E	0.89	1/2564 (0.0%)	0.87	2/3448 (0.1%)
1	F	0.87	1/2539 (0.0%)	0.87	3/3414 (0.1%)
1	G	0.84	0/2487	0.86	5/3343 (0.1%)
1	H	0.89	0/2551	0.84	2/3430 (0.1%)
All	All	0.85	2/20321 (0.0%)	0.84	21/27323 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	270	SER	CB-OG	-6.01	1.34	1.42
1	F	68	CYS	CB-SG	-5.97	1.72	1.81

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	34	ARG	NE-CZ-NH1	8.97	124.79	120.30
1	H	34	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	D	34	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	G	34	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	F	335	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	H	39	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	E	34	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	C	18	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	C	18	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	G	18	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	D	306	ARG	NE-CZ-NH2	-5.82	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	E	18	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	G	18	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	G	34	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	A	313	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	F	146	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	A	34	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	F	18	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	G	300	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	A	18	ARG	NE-CZ-NH1	5.14	122.87	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2494	0	2494	23	0
1	B	2507	0	2505	22	0
1	C	2505	0	2506	27	0
1	D	2494	0	2494	28	0
1	E	2519	0	2512	24	0
1	F	2494	0	2494	29	0
1	G	2444	0	2447	26	0
1	H	2506	0	2502	32	0
2	A	23	0	11	3	0
2	B	23	0	11	6	0
2	C	23	0	11	6	0
2	D	23	0	11	4	0
2	E	23	0	11	3	0
2	F	23	0	11	6	0
2	G	23	0	11	3	0
2	H	23	0	11	2	0
3	A	48	0	26	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	26	6	0
3	C	48	0	26	6	0
3	D	48	0	26	2	0
3	E	48	0	26	3	0
3	F	48	0	26	9	0
3	H	48	0	26	4	0
4	A	302	0	0	10	0
4	B	285	0	0	6	0
4	C	335	0	0	14	0
4	D	305	0	0	5	0
4	E	352	0	0	9	1
4	F	346	0	0	10	1
4	G	304	0	0	10	0
4	H	340	0	0	7	0
All	All	23052	0	20224	222	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (222) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:186:CYS:SG	2:D:1337:IMP:H2	1.31	1.65
1:G:186:CYS:SG	2:G:1338:IMP:H2	1.49	1.52
1:A:186:CYS:SG	2:A:1337:IMP:H2	1.57	1.43
1:F:186:CYS:SG	2:F:1337:IMP:H2	1.68	1.31
1:C:186:CYS:SG	2:C:1337:IMP:H2	1.69	1.31
1:D:186:CYS:HG	2:D:1337:IMP:C2	1.42	1.26
1:E:186:CYS:SG	2:E:1337:IMP:H2	1.76	1.23
1:A:186:CYS:SG	2:A:1337:IMP:C2	2.31	1.18
1:H:186:CYS:SG	2:H:1337:IMP:H2	1.84	1.17
1:G:186:CYS:SG	2:G:1338:IMP:C2	2.34	1.16
1:F:186:CYS:SG	2:F:1337:IMP:C2	2.35	1.14
1:B:186:CYS:SG	2:B:1339:IMP:H2	1.89	1.12
1:E:186:CYS:SG	2:E:1337:IMP:C2	2.41	1.08
1:C:186:CYS:SG	2:C:1337:IMP:C2	2.40	1.07
1:B:186:CYS:SG	2:B:1339:IMP:C2	2.44	1.05
1:H:186:CYS:SG	2:H:1337:IMP:C2	2.44	1.04
3:B:1340:NDP:H52A	4:B:2281:HOH:O	1.58	1.02
1:C:22:SER:HB2	4:C:2015:HOH:O	1.66	0.95
1:E:313:ARG:HD3	4:E:2029:HOH:O	1.68	0.94
1:H:9:SER:N	4:H:2001:HOH:O	1.99	0.94
1:H:276:LYS:HD2	1:H:281:GLY:HA2	1.51	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:68[A]:CYS:HG	1:E:95:CYS:HG	1.10	0.88
3:C:1338:NDP:H52A	4:C:2331:HOH:O	1.73	0.86
1:G:68:CYS:HG	1:G:95:CYS:HG	0.84	0.83
1:A:68:CYS:HG	1:A:95:CYS:HG	0.90	0.83
1:D:9:SER:N	4:D:2001:HOH:O	2.13	0.81
1:A:22:SER:HB3	1:A:320:GLY:HA2	1.65	0.78
1:G:326:GLU:OE1	4:G:2294:HOH:O	2.02	0.77
1:D:68:CYS:HG	1:D:95:CYS:HG	1.29	0.77
1:E:257:GLU:HG2	1:E:262:LYS:HG2	1.64	0.76
1:G:68:CYS:HB2	4:G:2108:HOH:O	1.87	0.75
1:H:21:ARG:HH11	1:H:21:ARG:HG3	1.51	0.75
2:B:1339:IMP:H2	3:B:1340:NDP:H41N	1.68	0.74
1:C:151:GLN:NE2	4:C:2182:HOH:O	2.19	0.74
2:C:1337:IMP:C2	3:C:1338:NDP:H41N	2.18	0.74
1:H:275:MET:HE3	1:H:282:VAL:HG22	1.70	0.74
1:E:329:ARG:HD2	4:E:2329:HOH:O	1.88	0.73
3:F:1338:NDP:H52A	4:F:2343:HOH:O	1.88	0.73
2:F:1337:IMP:C2	3:F:1338:NDP:H41N	2.20	0.72
1:F:335:ARG:HG2	1:F:335:ARG:HH11	1.54	0.72
2:C:1337:IMP:H2	3:C:1338:NDP:H41N	1.72	0.71
1:C:97:GLU:HG2	1:C:98:HIS:CE1	2.26	0.71
1:C:98:HIS:HD2	4:C:2060:HOH:O	1.73	0.70
1:F:186:CYS:HG	2:F:1337:IMP:H2	1.54	0.70
2:F:1337:IMP:H2	3:F:1338:NDP:H41N	1.74	0.69
1:A:23:THR:HG22	1:C:136:GLU:OE1	1.93	0.68
1:G:287:ALA:N	4:G:2262:HOH:O	2.27	0.68
1:E:190:LYS:NZ	4:E:2206:HOH:O	2.24	0.66
1:D:68:CYS:HB2	4:D:2107:HOH:O	1.96	0.66
3:A:1338:NDP:H51A	3:A:1338:NDP:H51N	1.77	0.66
1:H:257:GLU:HG2	1:H:262:LYS:HG2	1.77	0.65
1:G:97:GLU:HG2	4:G:2107:HOH:O	1.96	0.65
1:H:248:HIS:HE1	1:H:304:THR:OG1	1.79	0.65
1:E:259:ASP:OD2	4:E:2264:HOH:O	2.15	0.65
1:G:9:SER:N	4:G:2001:HOH:O	2.29	0.64
2:B:1339:IMP:C2	3:B:1340:NDP:H41N	2.29	0.63
1:H:21:ARG:HH11	1:H:21:ARG:CG	2.11	0.63
1:A:9:SER:N	4:A:2001:HOH:O	2.32	0.62
3:A:1338:NDP:O7N	4:A:2297:HOH:O	2.16	0.62
1:F:335:ARG:CG	1:F:335:ARG:HH11	2.14	0.61
1:D:186:CYS:HG	2:D:1337:IMP:H2	0.78	0.60
1:F:200:SER:HA	1:F:203:MET:HE2	1.84	0.60
1:C:9:SER:N	4:C:2001:HOH:O	2.36	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:270:SER:HB3	3:H:1338:NDP:H2N	1.85	0.59
1:H:104:GLY:HA3	3:H:1338:NDP:O2A	2.03	0.58
1:D:104:GLY:HA3	3:D:1338:NDP:O2A	2.03	0.58
1:E:27:ARG:HA	1:E:317[A]:THR:HG21	1.85	0.58
1:F:69:LYS:NZ	4:F:2071:HOH:O	2.30	0.58
3:H:1338:NDP:H51N	3:H:1338:NDP:H51A	1.86	0.57
1:F:248:HIS:HE1	1:F:304:THR:OG1	1.87	0.57
1:A:98:HIS:HE1	4:A:2098:HOH:O	1.86	0.57
1:E:335:ARG:O	1:G:9:SER:HB2	2.04	0.57
3:B:1340:NDP:C5B	4:B:2281:HOH:O	2.33	0.57
1:B:9:SER:N	4:B:2002:HOH:O	2.38	0.57
1:C:257:GLU:HG2	1:C:262:LYS:HG2	1.86	0.56
2:F:1337:IMP:C2	3:F:1338:NDP:C4N	2.84	0.56
2:C:1337:IMP:C2	3:C:1338:NDP:C4N	2.84	0.56
1:D:248:HIS:HE1	1:D:304:THR:OG1	1.90	0.55
1:B:68[A]:CYS:HG	1:B:95:CYS:HG	1.50	0.55
1:A:329:ARG:HG3	4:A:2284:HOH:O	2.07	0.55
1:B:186:CYS:HG	2:B:1339:IMP:H2	1.68	0.55
1:D:186:CYS:CB	2:D:1337:IMP:C2	2.85	0.54
1:C:98:HIS:CD2	4:C:2060:HOH:O	2.53	0.54
1:F:257:GLU:HG2	1:F:262:LYS:HG2	1.88	0.54
1:D:257:GLU:OE1	1:D:262:LYS:NZ	2.39	0.54
1:D:294:GLU:OE2	1:H:294:GLU:OE2	2.25	0.54
1:D:270:SER:HB3	3:D:1338:NDP:H1D	1.90	0.54
1:H:124:LYS:HD2	4:H:2184:HOH:O	2.06	0.54
1:F:326:GLU:HG2	1:F:329:ARG:NH2	2.23	0.54
1:F:275:MET:HE1	1:F:282:VAL:HG13	1.89	0.53
4:C:2226:HOH:O	1:D:190:LYS:HE2	2.08	0.53
1:C:303:HIS:HD2	4:C:2300:HOH:O	1.90	0.53
1:C:306[A]:ARG:NH1	1:D:284:GLU:OE2	2.42	0.53
1:G:24:LEU:HD23	1:G:29:GLU:CG	2.38	0.53
1:F:25:LYS:HB2	1:F:29:GLU:OE2	2.09	0.53
2:B:1339:IMP:C2	3:B:1340:NDP:C4N	2.87	0.52
1:A:248:HIS:HE1	1:A:304:THR:OG1	1.93	0.52
1:F:272:GLU:HG2	1:F:276:LYS:HE3	1.91	0.52
1:C:97:GLU:CG	1:C:98:HIS:CE1	2.94	0.51
1:A:22:SER:HB3	1:A:320:GLY:CA	2.38	0.51
1:H:22:SER:HB3	1:H:320:GLY:HA2	1.91	0.51
1:B:275:MET:HE3	1:B:282:VAL:HG22	1.94	0.50
1:C:270:SER:HB3	3:C:1338:NDP:H51N	1.92	0.50
1:G:303:HIS:HD2	4:G:2281:HOH:O	1.94	0.50
1:C:294:GLU:OE2	1:F:294:GLU:OE2	2.29	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:253:GLY:O	1:E:264:LYS:HE2	2.12	0.50
1:A:276:LYS:HD2	4:A:2242:HOH:O	2.12	0.50
4:C:2226:HOH:O	1:D:190:LYS:CE	2.60	0.50
1:H:68[A]:CYS:HG	1:H:95:CYS:HG	1.60	0.50
1:C:186:CYS:HG	2:C:1337:IMP:H2	1.67	0.49
1:D:22:SER:CB	1:D:320:GLY:HA2	2.42	0.49
1:B:270:SER:HB2	3:B:1340:NDP:H6N	1.94	0.49
1:F:245:LEU:O	1:F:248:HIS:HD2	1.95	0.49
1:H:98:HIS:HD2	4:H:2080:HOH:O	1.94	0.49
1:D:245:LEU:O	1:D:248:HIS:HD2	1.96	0.49
1:D:22:SER:HB2	1:D:320:GLY:HA2	1.95	0.49
1:A:326:GLU:HG2	1:A:329:ARG:NH1	2.27	0.49
1:A:88:PHE:HE2	1:A:99:LEU:HD11	1.78	0.49
1:F:326:GLU:OE1	4:F:2324:HOH:O	2.20	0.48
1:H:22:SER:HB3	1:H:320:GLY:CA	2.43	0.48
1:E:97:GLU:HG2	4:E:2113:HOH:O	2.13	0.48
1:C:25:LYS:HB2	1:C:29:GLU:OE2	2.13	0.48
1:F:129:ASP:OD2	3:F:1338:NDP:O2D	2.32	0.48
1:A:245:LEU:O	1:A:248:HIS:HD2	1.96	0.48
1:E:21:ARG:HG3	1:E:21:ARG:HH11	1.79	0.48
1:H:25:LYS:N	1:H:29:GLU:OE1	2.41	0.48
3:F:1338:NDP:O2N	4:F:2345:HOH:O	2.20	0.47
1:E:87:GLU:HB3	4:E:2105:HOH:O	2.14	0.47
1:F:42:LYS:NZ	4:F:2050:HOH:O	2.42	0.47
1:E:335:ARG:O	1:G:9:SER:CB	2.62	0.47
1:C:124:LYS:CE	4:C:2162:HOH:O	2.62	0.47
1:H:21:ARG:NH1	1:H:21:ARG:CG	2.78	0.47
1:B:275:MET:HE1	1:B:282:VAL:HG13	1.96	0.47
3:F:1338:NDP:H2A	3:F:1338:NDP:O1N	2.15	0.47
1:C:155:MET:HA	1:C:175:ILE:O	2.15	0.46
1:C:200:SER:HA	1:C:203:MET:CE	2.45	0.46
1:F:22:SER:HB3	1:F:320:GLY:CA	2.45	0.46
1:A:196:TYR:CD1	1:B:334:ILE:HD13	2.49	0.46
1:G:277:LYS:HD3	4:G:2259:HOH:O	2.16	0.46
1:F:69:LYS:HD3	4:F:2072:HOH:O	2.15	0.46
1:F:213:LYS:NZ	4:F:2218:HOH:O	2.42	0.46
1:B:22:SER:HB3	1:B:320:GLY:HA2	1.97	0.46
1:G:82:LEU:O	1:G:86:GLN:HG3	2.16	0.46
1:G:35:SER:HA	1:G:45:TYR:O	2.16	0.46
1:D:68:CYS:CB	1:D:95:CYS:HG	2.28	0.46
1:B:10:LEU:HD21	1:B:335:ARG:CZ	2.45	0.46
1:A:306:ARG:HD3	1:C:284:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:190:LYS:HD3	4:D:2170:HOH:O	2.14	0.46
1:A:190:LYS:HD3	4:A:2174:HOH:O	2.15	0.46
1:B:97:GLU:HG2	4:B:2094:HOH:O	2.16	0.45
1:E:270:SER:HB3	3:E:1338:NDP:H1D	1.97	0.45
1:D:316:CYS:HB3	1:D:321:ALA:O	2.17	0.45
3:E:1338:NDP:H51A	3:E:1338:NDP:H51N	1.99	0.45
1:G:200:SER:HA	1:G:203:MET:CE	2.47	0.45
1:D:261:LYS:HE2	1:G:261:LYS:NZ	2.31	0.45
1:H:98:HIS:HE1	4:H:2064:HOH:O	2.00	0.45
1:C:259:ASP:HB2	4:C:2252:HOH:O	2.16	0.45
1:D:262:LYS:NZ	4:D:2227:HOH:O	2.45	0.45
1:B:112:GLN:NE2	4:B:2111:HOH:O	2.50	0.45
1:E:68[A]:CYS:CB	1:E:95:CYS:HG	2.28	0.45
1:H:248:HIS:CE1	1:H:304:THR:OG1	2.66	0.44
1:H:22:SER:CB	1:H:320:GLY:HA2	2.47	0.44
1:F:22:SER:HB3	1:F:320:GLY:HA2	1.99	0.44
1:E:259:ASP:HB2	4:E:2269:HOH:O	2.16	0.44
1:H:270:SER:HB3	3:H:1338:NDP:C2N	2.46	0.44
1:A:98:HIS:HD2	4:A:2065:HOH:O	2.00	0.44
1:B:10:LEU:HD21	1:B:335:ARG:NE	2.32	0.44
1:B:157:GLY:HA3	1:B:158:ASN:HA	1.88	0.44
1:F:9:SER:N	4:F:2004:HOH:O	2.51	0.44
1:B:277:LYS:NZ	4:B:2228:HOH:O	2.50	0.44
1:D:34:ARG:HG3	1:D:49:PRO:HG3	1.99	0.44
1:D:25:LYS:HD2	4:D:2026:HOH:O	2.17	0.44
1:G:186:CYS:CB	2:G:1338:IMP:C2	2.96	0.43
1:B:294:GLU:OE2	1:G:294:GLU:OE2	2.36	0.43
1:B:22:SER:CB	1:B:320:GLY:HA2	2.48	0.43
3:C:1338:NDP:C5B	4:C:2331:HOH:O	2.48	0.43
1:D:275:MET:HE3	1:D:282:VAL:HG22	2.01	0.43
1:G:329:ARG:HD3	4:G:2293:HOH:O	2.18	0.43
1:A:303:HIS:HB3	4:A:2270:HOH:O	2.18	0.43
1:G:198:GLN:O	1:G:202:VAL:HG23	2.18	0.43
1:F:259:ASP:HB2	4:F:2263:HOH:O	2.18	0.43
1:H:329:ARG:HG2	4:H:2318:HOH:O	2.19	0.43
1:F:335:ARG:NH1	1:F:335:ARG:CG	2.75	0.43
1:C:109:ASP:O	1:C:112:GLN:HG2	2.18	0.43
1:G:181:GLY:N	1:G:182:PRO:CD	2.82	0.43
1:F:248:HIS:CE1	1:F:304:THR:OG1	2.69	0.43
1:A:313:ARG:NE	4:A:2279:HOH:O	2.37	0.43
1:F:275:MET:HE3	1:F:282:VAL:HG22	2.00	0.43
1:E:190:LYS:HG2	4:E:2202:HOH:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:1337:IMP:C2	4:A:2297:HOH:O	2.67	0.42
1:A:270:SER:HB2	3:A:1338:NDP:H2N	2.02	0.42
1:C:107:SER:HB2	4:C:2133:HOH:O	2.19	0.42
1:D:129:ASP:OD1	1:D:177:LYS:NZ	2.44	0.42
1:G:191:LYS:NZ	4:G:2194:HOH:O	2.47	0.42
1:B:68[B]:CYS:SG	1:B:95:CYS:HB3	2.60	0.42
1:G:69:LYS:HD3	4:G:2074:HOH:O	2.19	0.42
1:H:157:GLY:HA3	1:H:158:ASN:HA	1.90	0.42
1:G:157:GLY:HA3	1:G:177:LYS:HB2	2.01	0.42
1:H:121:PRO:O	1:H:124:LYS:HE3	2.18	0.41
1:A:18:ARG:HB2	1:A:334:ILE:HD11	2.02	0.41
1:E:9:SER:N	4:E:2002:HOH:O	2.53	0.41
1:E:104:GLY:HA3	3:E:1338:NDP:O2A	2.19	0.41
1:G:200:SER:HA	1:G:203:MET:HE3	2.01	0.41
3:F:1338:NDP:H5N	4:F:2340:HOH:O	2.20	0.41
1:H:199:LEU:HD11	1:H:234:ALA:HB2	2.02	0.41
1:E:186:CYS:HG	2:E:1337:IMP:H2	1.73	0.41
1:H:276:LYS:HG3	4:H:2275:HOH:O	2.21	0.41
1:E:251:SER:O	1:E:264:LYS:NZ	2.49	0.41
1:H:85:TRP:HB3	1:H:120:ILE:CD1	2.51	0.41
1:D:251:SER:HB2	1:D:264:LYS:HE2	2.03	0.41
3:F:1338:NDP:H6N	3:F:1338:NDP:H51N	2.03	0.41
1:F:22:SER:CB	1:F:320:GLY:HA2	2.50	0.41
1:C:110:PHE:CE1	1:C:145:VAL:HG22	2.56	0.41
1:H:155:MET:HA	1:H:175:ILE:O	2.21	0.41
1:B:155:MET:HA	1:B:175:ILE:O	2.21	0.41
1:B:22:SER:HB3	1:B:320:GLY:CA	2.51	0.40
1:A:191:LYS:NZ	1:B:307:ASP:OD1	2.43	0.40
1:C:88:PHE:HE2	1:C:99:LEU:HD11	1.85	0.40
1:E:161:THR:HG21	1:F:18:ARG:CZ	2.51	0.40
1:C:303:HIS:HE1	4:C:2290:HOH:O	2.03	0.40
1:H:31:ASP:OD1	4:H:2033:HOH:O	2.22	0.40
1:H:105:THR:HG22	1:H:141:PHE:CD2	2.55	0.40

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	Distance(Å)	Clash(Å)
4:E:2329:HOH:O	4:F:2148:HOH:O[4_445]	2.17	0.03

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	326/351 (93%)	320 (98%)	6 (2%)	0	100	100
1	B	328/351 (93%)	321 (98%)	7 (2%)	0	100	100
1	C	327/351 (93%)	324 (99%)	3 (1%)	0	100	100
1	D	326/351 (93%)	321 (98%)	5 (2%)	0	100	100
1	E	330/351 (94%)	325 (98%)	5 (2%)	0	100	100
1	F	326/351 (93%)	320 (98%)	6 (2%)	0	100	100
1	G	317/351 (90%)	311 (98%)	6 (2%)	0	100	100
1	H	328/351 (93%)	323 (98%)	5 (2%)	0	100	100
All	All	2608/2808 (93%)	2565 (98%)	43 (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	267/287 (93%)	264 (99%)	3 (1%)	84	72
1	B	269/287 (94%)	266 (99%)	3 (1%)	84	72
1	C	268/287 (93%)	265 (99%)	3 (1%)	84	72
1	D	267/287 (93%)	266 (100%)	1 (0%)	95	92
1	E	271/287 (94%)	268 (99%)	3 (1%)	84	72
1	F	267/287 (93%)	264 (99%)	3 (1%)	84	72
1	G	264/287 (92%)	261 (99%)	3 (1%)	84	72
1	H	269/287 (94%)	267 (99%)	2 (1%)	91	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2142/2296 (93%)	2121 (99%)	21 (1%)	85	76

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	25	LYS
1	A	111	GLU
1	B	97	GLU
1	B	264	LYS
1	B	336	VAL
1	C	108	SER
1	C	124	LYS
1	C	177	LYS
1	D	190	LYS
1	E	264	LYS
1	E	329	ARG
1	E	335	ARG
1	F	135	SER
1	F	270	SER
1	F	335	ARG
1	G	115	GLN
1	G	148	ARG
1	G	177	LYS
1	H	21	ARG
1	H	136	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	98	HIS
1	A	248	HIS
1	C	43	GLN
1	C	98	HIS
1	C	115	GLN
1	C	303	HIS
1	D	248	HIS
1	E	137	HIS
1	E	303	HIS
1	F	43	GLN

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Mol	Chain	Res	Type
1	F	248	HIS
1	G	43	GLN
1	G	112	GLN
1	G	137	HIS
1	G	303	HIS
1	H	43	GLN
1	H	98	HIS
1	H	248	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

15 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	IMP	A	1337	-	25,25,25	1.40	3 (12%)	35,38,38	3.02	10 (28%)
3	NDP	A	1338	-	52,52,52	1.61	8 (15%)	80,80,80	2.01	11 (13%)
2	IMP	B	1339	-	25,25,25	1.32	5 (20%)	35,38,38	3.00	10 (28%)
3	NDP	B	1340	-	52,52,52	1.50	5 (9%)	80,80,80	1.74	10 (12%)
2	IMP	C	1337	-	25,25,25	1.42	3 (12%)	35,38,38	2.95	11 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NDP	C	1338	-	52,52,52	1.43	7 (13%)	80,80,80	1.68	10 (12%)
2	IMP	D	1337	1	25,25,25	1.59	6 (24%)	35,38,38	3.14	9 (25%)
3	NDP	D	1338	-	52,52,52	1.69	9 (17%)	80,80,80	1.89	11 (13%)
2	IMP	E	1337	-	25,25,25	1.58	5 (20%)	35,38,38	3.06	11 (31%)
3	NDP	E	1338	-	52,52,52	1.66	8 (15%)	80,80,80	1.80	16 (20%)
2	IMP	F	1337	-	25,25,25	1.48	5 (20%)	35,38,38	3.02	12 (34%)
3	NDP	F	1338	-	52,52,52	1.59	8 (15%)	80,80,80	1.68	11 (13%)
2	IMP	G	1338	-	25,25,25	1.58	4 (16%)	35,38,38	2.94	10 (28%)
2	IMP	H	1337	-	25,25,25	1.45	4 (16%)	35,38,38	3.00	8 (22%)
3	NDP	H	1338	-	52,52,52	1.54	9 (17%)	80,80,80	1.79	16 (20%)

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	IMP	A	1337	-	-	0/10/26/26	0/1/3/3
3	NDP	A	1338	-	-	0/35/77/77	0/3/5/5
2	IMP	B	1339	-	-	0/10/26/26	0/1/3/3
3	NDP	B	1340	-	-	0/35/77/77	0/3/5/5
2	IMP	C	1337	-	-	0/10/26/26	0/1/3/3
3	NDP	C	1338	-	-	0/35/77/77	0/3/5/5
2	IMP	D	1337	1	-	0/10/26/26	0/1/3/3
3	NDP	D	1338	-	-	0/35/77/77	0/3/5/5
2	IMP	E	1337	-	-	0/10/26/26	0/1/3/3
3	NDP	E	1338	-	-	0/35/77/77	0/3/5/5
2	IMP	F	1337	-	-	0/10/26/26	0/1/3/3
3	NDP	F	1338	-	-	0/35/77/77	0/3/5/5
2	IMP	G	1338	-	-	0/10/26/26	0/1/3/3
2	IMP	H	1337	-	-	0/10/26/26	0/1/3/3
3	NDP	H	1338	-	-	0/35/77/77	0/3/5/5

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1338	NDP	O7N-C7N	7.22	1.43	1.24
3	A	1338	NDP	O7N-C7N	7.08	1.43	1.24
3	B	1340	NDP	O7N-C7N	6.85	1.42	1.24
3	E	1338	NDP	O7N-C7N	6.57	1.41	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1338	NDP	O7N-C7N	6.45	1.41	1.24
3	F	1338	NDP	O7N-C7N	6.42	1.41	1.24
3	C	1338	NDP	O7N-C7N	5.69	1.39	1.24
2	E	1337	IMP	C2-N3	4.50	1.39	1.31
2	G	1338	IMP	C2-N3	4.27	1.39	1.31
3	B	1340	NDP	C2A-N3A	4.14	1.40	1.32
2	F	1337	IMP	C4-N9	-4.14	1.31	1.37
3	A	1338	NDP	C6N-C5N	3.99	1.41	1.33
2	C	1337	IMP	C2-N3	3.95	1.38	1.31
2	A	1337	IMP	C2-N3	3.94	1.38	1.31
3	E	1338	NDP	C2A-N1A	3.82	1.41	1.33
3	E	1338	NDP	C2A-N3A	3.65	1.39	1.32
2	D	1337	IMP	C2-N3	3.64	1.38	1.31
3	F	1338	NDP	C2N-C3N	3.63	1.41	1.34
3	C	1338	NDP	C2A-N3A	3.60	1.39	1.32
3	D	1338	NDP	C6N-C5N	3.52	1.40	1.33
3	H	1338	NDP	C6N-C5N	3.51	1.40	1.33
3	D	1338	NDP	C2N-C3N	3.49	1.41	1.34
3	A	1338	NDP	C2A-N3A	3.46	1.39	1.32
3	E	1338	NDP	C6N-C5N	3.38	1.40	1.33
3	D	1338	NDP	C2A-N3A	3.37	1.38	1.32
2	G	1338	IMP	C8-N9	3.37	1.41	1.36
2	H	1337	IMP	C2-N3	3.35	1.37	1.31
2	H	1337	IMP	C6-N1	-3.29	1.31	1.37
2	B	1339	IMP	C2-N3	3.14	1.37	1.31
2	D	1337	IMP	O4'-C4'	-3.12	1.37	1.45
2	D	1337	IMP	C4-N9	-3.11	1.33	1.37
3	E	1338	NDP	PA-O3	3.08	1.65	1.59
3	B	1340	NDP	C2A-N1A	3.04	1.39	1.33
3	E	1338	NDP	C2N-C3N	3.03	1.40	1.34
2	G	1338	IMP	C4-N9	-3.03	1.33	1.37
3	F	1338	NDP	PA-O3	3.00	1.65	1.59
3	E	1338	NDP	PN-O3	2.99	1.65	1.59
3	F	1338	NDP	C2A-N1A	2.97	1.39	1.33
3	H	1338	NDP	PA-O3	2.97	1.65	1.59
3	H	1338	NDP	C2A-N3A	2.87	1.37	1.32
3	F	1338	NDP	C2A-N3A	2.84	1.37	1.32
2	F	1337	IMP	C2-N3	2.83	1.36	1.31
3	A	1338	NDP	C2N-C3N	2.80	1.40	1.34
2	F	1337	IMP	C6-N1	-2.76	1.32	1.37
3	C	1338	NDP	C2A-N1A	2.72	1.39	1.33
3	F	1338	NDP	C6N-C5N	2.69	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1337	IMP	C6-N1	-2.67	1.32	1.37
3	D	1338	NDP	PA-O3	2.66	1.64	1.59
3	C	1338	NDP	C6N-C5N	2.65	1.38	1.33
3	C	1338	NDP	C2N-C3N	2.63	1.39	1.34
2	C	1337	IMP	C6-N1	-2.63	1.32	1.37
3	B	1340	NDP	C2N-C3N	2.58	1.39	1.34
2	A	1337	IMP	C4-N9	-2.56	1.34	1.37
3	A	1338	NDP	C2A-N1A	2.56	1.39	1.33
2	A	1337	IMP	C6-N1	-2.55	1.33	1.37
3	B	1340	NDP	C6N-C5N	2.53	1.38	1.33
3	C	1338	NDP	PA-O3	2.51	1.64	1.59
3	H	1338	NDP	C2A-N1A	2.50	1.38	1.33
3	H	1338	NDP	C2N-C3N	2.44	1.39	1.34
3	D	1338	NDP	C2A-N1A	2.43	1.38	1.33
2	F	1337	IMP	C8-N9	2.43	1.40	1.36
3	A	1338	NDP	C7N-C3N	2.41	1.52	1.47
2	B	1339	IMP	C8-N9	2.41	1.40	1.36
3	D	1338	NDP	C1D-N1N	2.39	1.51	1.46
3	H	1338	NDP	PN-O3	2.38	1.64	1.59
2	D	1337	IMP	O6-C6	2.36	1.29	1.24
2	E	1337	IMP	C4-N3	-2.35	1.32	1.35
3	F	1338	NDP	O5D-C5D	-2.34	1.35	1.44
3	H	1338	NDP	C7N-C3N	2.27	1.52	1.47
2	E	1337	IMP	O4'-C4'	-2.21	1.39	1.45
2	H	1337	IMP	C8-N9	2.19	1.39	1.36
3	D	1338	NDP	PN-O3	2.18	1.63	1.59
2	F	1337	IMP	C2-N1	2.18	1.41	1.35
3	C	1338	NDP	C4N-C3N	2.17	1.54	1.50
3	H	1338	NDP	P2B-O2X	-2.14	1.46	1.54
2	B	1339	IMP	C4-N9	-2.14	1.34	1.37
2	C	1337	IMP	C4-N9	-2.13	1.34	1.37
2	H	1337	IMP	O4'-C4'	-2.11	1.40	1.45
2	D	1337	IMP	C8-N9	2.11	1.39	1.36
2	D	1337	IMP	C6-N1	-2.11	1.33	1.37
3	E	1338	NDP	O5B-C5B	-2.09	1.36	1.44
2	E	1337	IMP	C4-N9	-2.06	1.34	1.37
2	G	1338	IMP	C1'-N9	-2.05	1.42	1.48
3	D	1338	NDP	O4B-C1B	2.04	1.44	1.41
3	A	1338	NDP	PN-O3	2.03	1.63	1.59
3	A	1338	NDP	C1D-N1N	2.03	1.50	1.46
3	F	1338	NDP	PA-O1A	-2.02	1.43	1.51
2	B	1339	IMP	C2'-C1'	-2.01	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1339	IMP	C6-C5	-2.01	1.38	1.41

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1337	IMP	C6-C5-N7	-16.13	131.97	134.14
2	H	1337	IMP	C6-C5-N7	-15.44	132.06	134.14
2	E	1337	IMP	C6-C5-N7	-15.35	132.07	134.14
2	B	1339	IMP	C6-C5-N7	-15.25	132.09	134.14
2	A	1337	IMP	C6-C5-N7	-14.99	132.12	134.14
2	C	1337	IMP	C6-C5-N7	-14.33	132.21	134.14
2	G	1338	IMP	C6-C5-N7	-14.17	132.23	134.14
2	F	1337	IMP	C6-C5-N7	-14.04	132.25	134.14
3	A	1338	NDP	N3A-C2A-N1A	-9.70	120.60	128.71
3	D	1338	NDP	N3A-C2A-N1A	-9.56	120.72	128.71
3	A	1338	NDP	C1D-N1N-C2N	-9.26	105.25	121.02
3	B	1340	NDP	N3A-C2A-N1A	-8.58	121.53	128.71
3	C	1338	NDP	N3A-C2A-N1A	-8.39	121.70	128.71
3	H	1338	NDP	N3A-C2A-N1A	-7.64	122.33	128.71
3	F	1338	NDP	N3A-C2A-N1A	-7.34	122.57	128.71
3	E	1338	NDP	N3A-C2A-N1A	-6.54	123.24	128.71
3	H	1338	NDP	C1D-N1N-C2N	-6.31	110.27	121.02
3	E	1338	NDP	C1D-N1N-C2N	-6.20	110.45	121.02
3	D	1338	NDP	C1D-N1N-C2N	-6.08	110.67	121.02
3	B	1340	NDP	C1D-N1N-C2N	-5.96	110.86	121.02
3	C	1338	NDP	C1D-N1N-C2N	-5.13	112.28	121.02
2	F	1337	IMP	C1'-N9-C4	-4.88	118.20	126.64
3	F	1338	NDP	C3N-C2N-N1N	-4.78	116.26	123.05
3	D	1338	NDP	N3A-C4A-N9A	4.75	134.01	125.43
3	D	1338	NDP	C1D-N1N-C6N	4.68	131.16	120.79
3	E	1338	NDP	O4B-C1B-N9A	-4.65	104.11	108.44
3	C	1338	NDP	N3A-C4A-N9A	4.35	133.28	125.43
3	E	1338	NDP	N3A-C4A-N9A	4.30	133.20	125.43
3	C	1338	NDP	C3N-C2N-N1N	-4.20	117.08	123.05
3	C	1338	NDP	C6N-N1N-C2N	4.20	124.93	119.44
3	F	1338	NDP	N3A-C4A-N9A	4.18	132.97	125.43
3	A	1338	NDP	N3A-C4A-N9A	4.03	132.71	125.43
3	B	1340	NDP	C3N-C2N-N1N	-4.03	117.34	123.05
3	H	1338	NDP	N3A-C4A-N9A	3.94	132.55	125.43
3	A	1338	NDP	O4D-C1D-N1N	3.91	116.32	108.05
2	D	1337	IMP	C1'-N9-C4	-3.89	119.91	126.64
3	A	1338	NDP	C1D-N1N-C6N	3.84	129.29	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1338	IMP	C4'-O4'-C1'	-3.65	105.78	109.75
3	F	1338	NDP	C6N-N1N-C2N	3.65	124.21	119.44
2	F	1337	IMP	N3-C4-N9	3.63	131.99	125.43
2	E	1337	IMP	N3-C4-N9	3.61	131.94	125.43
2	A	1337	IMP	N3-C4-N9	3.60	131.94	125.43
2	D	1337	IMP	N3-C4-N9	3.59	131.92	125.43
2	H	1337	IMP	N3-C4-N9	3.59	131.91	125.43
2	B	1339	IMP	N3-C4-N9	3.59	131.91	125.43
2	C	1337	IMP	N3-C4-N9	3.58	131.90	125.43
2	F	1337	IMP	C8-N9-C1'	3.57	133.42	126.38
2	G	1338	IMP	N3-C4-N9	3.57	131.87	125.43
3	E	1338	NDP	O4B-C4B-C5B	-3.56	96.64	109.36
2	C	1337	IMP	C1'-N9-C4	-3.52	120.56	126.64
3	E	1338	NDP	C1D-N1N-C6N	3.47	128.48	120.79
2	G	1338	IMP	O4'-C1'-N9	3.28	111.49	108.44
3	H	1338	NDP	O4B-C4B-C5B	-3.24	97.79	109.36
3	F	1338	NDP	O2A-PA-O3	3.14	120.02	105.14
2	A	1337	IMP	C1'-N9-C4	-3.12	121.25	126.64
3	B	1340	NDP	O7N-C7N-C3N	-3.08	114.72	120.51
3	B	1340	NDP	N3A-C4A-N9A	3.08	131.00	125.43
3	E	1338	NDP	O2A-PA-O5B	-3.05	93.15	108.51
2	C	1337	IMP	O3P-P-O1P	3.04	120.38	110.44
2	F	1337	IMP	C4'-O4'-C1'	-3.00	106.49	109.75
3	B	1340	NDP	C6N-N1N-C2N	2.99	123.35	119.44
2	G	1338	IMP	C1'-N9-C4	-2.97	121.51	126.64
3	E	1338	NDP	C6A-C5A-C4A	2.91	122.59	117.25
2	D	1337	IMP	C8-N9-C1'	2.86	132.01	126.38
3	F	1338	NDP	O7N-C7N-C3N	-2.85	115.16	120.51
2	E	1337	IMP	C2-N3-C4	2.85	120.17	113.48
3	B	1340	NDP	C4A-C5A-N7A	-2.84	107.09	109.52
2	G	1338	IMP	C2-N3-C4	2.83	120.13	113.48
2	D	1337	IMP	C2-N3-C4	2.81	120.08	113.48
2	C	1337	IMP	C2-N3-C4	2.80	120.07	113.48
2	A	1337	IMP	C2-N3-C4	2.80	120.06	113.48
2	H	1337	IMP	C2-N3-C4	2.79	120.05	113.48
3	F	1338	NDP	O4B-C1B-N9A	2.79	111.03	108.44
3	D	1338	NDP	O2X-P2B-O1X	2.78	119.54	110.44
2	F	1337	IMP	C2-N3-C4	2.78	120.02	113.48
2	B	1339	IMP	C2-N3-C4	2.77	119.99	113.48
3	A	1338	NDP	O4B-C4B-C3B	2.74	110.72	105.17
3	F	1338	NDP	C4N-C3N-C2N	2.71	124.98	121.68
3	H	1338	NDP	O4B-C4B-C3B	2.69	110.62	105.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1338	NDP	C5A-C4A-N3A	-2.68	119.87	125.70
2	G	1338	IMP	C5-C4-N3	-2.66	119.90	125.70
3	D	1338	NDP	PN-O3-PA	-2.64	123.95	131.68
3	H	1338	NDP	O2D-C2D-C1D	2.64	119.02	110.04
3	H	1338	NDP	C4B-O4B-C1B	-2.64	106.89	109.75
2	F	1337	IMP	C5-C4-N3	-2.63	119.96	125.70
2	H	1337	IMP	C5-C4-N3	-2.63	119.97	125.70
2	C	1337	IMP	C5-C4-N3	-2.63	119.98	125.70
2	C	1337	IMP	C8-N9-C1'	2.63	131.56	126.38
3	B	1340	NDP	O2A-PA-O3	2.62	117.58	105.14
2	A	1337	IMP	C5-C4-N3	-2.62	120.00	125.70
2	E	1337	IMP	C5-C4-N3	-2.61	120.02	125.70
2	B	1339	IMP	C5-C4-N3	-2.60	120.03	125.70
2	D	1337	IMP	C5-C4-N3	-2.57	120.10	125.70
3	F	1338	NDP	C5A-C4A-N3A	-2.53	120.19	125.70
3	H	1338	NDP	PN-O3-PA	-2.51	124.33	131.68
3	B	1340	NDP	C4N-C3N-C2N	2.46	124.68	121.68
3	H	1338	NDP	O4D-C1D-N1N	2.46	113.26	108.05
2	E	1337	IMP	C3'-C2'-C1'	2.46	104.75	100.91
3	H	1338	NDP	O4D-C4D-C3D	2.45	110.14	105.17
2	H	1337	IMP	N1-C2-N3	-2.45	119.98	125.75
3	D	1338	NDP	C8A-N9A-C4A	2.45	108.77	106.90
2	H	1337	IMP	O2P-P-O5'	-2.43	99.93	106.65
3	D	1338	NDP	O2D-C2D-C1D	2.43	118.30	110.04
3	A	1338	NDP	O2A-PA-O5B	-2.42	96.29	108.51
2	D	1337	IMP	N1-C2-N3	-2.41	120.07	125.75
2	G	1338	IMP	N1-C2-N3	-2.41	120.07	125.75
2	E	1337	IMP	N1-C2-N3	-2.41	120.08	125.75
3	A	1338	NDP	O3X-P2B-O2B	2.41	114.02	107.09
3	E	1338	NDP	C8A-N9A-C4A	2.40	108.73	106.90
3	A	1338	NDP	C5A-C4A-N3A	-2.40	120.47	125.70
3	H	1338	NDP	C2D-C1D-N1N	-2.40	107.09	113.21
2	F	1337	IMP	N1-C2-N3	-2.40	120.11	125.75
3	F	1338	NDP	C1D-N1N-C2N	-2.40	116.94	121.02
2	B	1339	IMP	N1-C2-N3	-2.39	120.13	125.75
2	B	1339	IMP	C1'-N9-C4	-2.38	122.52	126.64
2	C	1337	IMP	N1-C2-N3	-2.38	120.16	125.75
2	A	1337	IMP	N1-C2-N3	-2.37	120.17	125.75
3	E	1338	NDP	N7A-C8A-N9A	-2.37	107.66	114.36
3	D	1338	NDP	C5A-C4A-N3A	-2.36	120.55	125.70
3	C	1338	NDP	O3-PA-O5B	-2.37	92.83	103.41
2	A	1337	IMP	C8-N9-C1'	2.36	131.04	126.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1338	NDP	C5D-C4D-C3D	-2.35	105.79	115.21
2	H	1337	IMP	C5-C6-N1	2.35	119.94	113.81
3	H	1338	NDP	C8A-N9A-C4A	2.34	108.69	106.90
3	C	1338	NDP	C4B-O4B-C1B	-2.34	107.21	109.75
3	E	1338	NDP	N6A-C6A-N1A	2.34	123.95	119.36
2	B	1339	IMP	C5-C6-N1	2.33	119.89	113.81
3	B	1340	NDP	C6A-C5A-C4A	2.33	121.52	117.25
2	E	1337	IMP	O2'-C2'-C1'	-2.33	104.19	111.23
2	F	1337	IMP	C5-C6-N1	2.31	119.84	113.81
2	A	1337	IMP	C5-C6-N1	2.30	119.83	113.81
2	E	1337	IMP	O3'-C3'-C4'	2.30	117.87	111.08
2	E	1337	IMP	C5-C6-N1	2.30	119.81	113.81
2	F	1337	IMP	N7-C8-N9	-2.29	107.89	114.36
2	G	1338	IMP	C5-C6-N1	2.29	119.79	113.81
2	C	1337	IMP	C5-C6-N1	2.29	119.78	113.81
3	H	1338	NDP	O2A-PA-O5B	-2.28	97.04	108.51
2	D	1337	IMP	C5-C6-N1	2.27	119.74	113.81
2	B	1339	IMP	N7-C8-N9	-2.24	108.02	114.36
2	A	1337	IMP	N7-C8-N9	-2.24	108.03	114.36
2	C	1337	IMP	N7-C8-N9	-2.24	108.03	114.36
2	E	1337	IMP	N7-C8-N9	-2.23	108.04	114.36
2	H	1337	IMP	N7-C8-N9	-2.23	108.05	114.36
3	E	1338	NDP	O4B-C4B-C3B	2.22	109.67	105.17
2	C	1337	IMP	O2P-P-O5'	-2.22	100.52	106.65
2	D	1337	IMP	N7-C8-N9	-2.22	108.08	114.36
2	G	1338	IMP	N7-C8-N9	-2.22	108.08	114.36
3	E	1338	NDP	C3N-C7N-N7N	2.22	121.75	117.48
3	D	1338	NDP	O2B-P2B-O1X	-2.21	100.61	106.79
3	E	1338	NDP	O7N-C7N-C3N	-2.20	116.38	120.51
2	B	1339	IMP	O2P-P-O1P	2.17	117.55	110.44
3	C	1338	NDP	O2A-PA-O3	2.14	115.28	105.14
3	F	1338	NDP	O3-PA-O5B	-2.13	93.87	103.41
3	E	1338	NDP	C5A-C4A-N3A	-2.13	121.06	125.70
3	D	1338	NDP	N7A-C8A-N9A	-2.13	108.34	114.36
3	A	1338	NDP	O4B-C4B-C5B	-2.13	101.77	109.36
2	F	1337	IMP	O4'-C1'-N9	-2.12	106.47	108.44
2	E	1337	IMP	O4'-C1'-N9	2.09	110.38	108.44
3	C	1338	NDP	O4B-C1B-C2B	-2.08	105.00	106.95
3	H	1338	NDP	O2N-PN-O1N	2.06	123.70	112.21
2	F	1337	IMP	O2'-C2'-C1'	-2.05	105.01	111.23
3	E	1338	NDP	C8A-N7A-C5A	2.05	109.92	103.58
3	H	1338	NDP	C6A-C5A-C4A	2.04	121.00	117.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1337	IMP	C3'-C2'-C1'	2.04	104.10	100.91
2	B	1339	IMP	O3'-C3'-C4'	2.03	117.07	111.08
3	H	1338	NDP	N7A-C8A-N9A	-2.01	108.68	114.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	328/351 (93%)	0.07	7 (2%) 60 66	19, 25, 35, 45	0
1	B	329/351 (93%)	0.07	11 (3%) 44 49	19, 25, 35, 46	0
1	C	328/351 (93%)	0.11	7 (2%) 60 66	19, 24, 37, 50	0
1	D	328/351 (93%)	0.09	13 (3%) 36 41	18, 25, 35, 44	0
1	E	328/351 (93%)	0.19	6 (1%) 65 71	20, 25, 36, 45	0
1	F	328/351 (93%)	0.07	2 (0%) 86 91	19, 25, 35, 42	0
1	G	321/351 (91%)	0.14	4 (1%) 75 82	19, 25, 34, 47	0
1	H	328/351 (93%)	0.07	3 (0%) 81 86	20, 25, 34, 45	0
All	All	2618/2808 (93%)	0.10	53 (2%) 62 67	18, 25, 35, 50	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	280	GLY	6.8
1	A	280	GLY	6.6
1	B	280	GLY	5.4
1	E	280	GLY	5.2
1	D	280	GLY	4.7
1	C	279	ALA	4.3
1	C	107	SER	3.4
1	D	282	VAL	3.2
1	D	118	GLU	3.1
1	E	25	LYS	3.1
1	C	282	VAL	3.0
1	B	329	ARG	2.9
1	H	329	ARG	2.8
1	D	107	SER	2.7
1	F	107	SER	2.7
1	D	279	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	90	GLY	2.6
1	F	280	GLY	2.6
1	D	91	GLN	2.6
1	A	279	ALA	2.6
1	G	94	ASP	2.6
1	G	337	THR	2.6
1	D	94	ASP	2.5
1	G	87	GLU	2.5
1	G	91	GLN	2.5
1	B	282	VAL	2.4
1	D	147	LYS	2.4
1	C	284	GLU	2.4
1	E	281	GLY	2.4
1	B	140	GLU	2.4
1	A	107	SER	2.4
1	B	337	THR	2.4
1	A	87	GLU	2.3
1	D	276	LYS	2.3
1	H	280	GLY	2.3
1	D	83	VAL	2.3
1	A	111	GLU	2.3
1	B	284	GLU	2.3
1	E	87	GLU	2.3
1	H	91	GLN	2.3
1	E	282	VAL	2.3
1	B	93	PRO	2.3
1	B	94	ASP	2.2
1	B	118	GLU	2.2
1	B	279	ALA	2.2
1	D	115	GLN	2.2
1	E	284	GLU	2.2
1	C	106	GLY	2.1
1	D	281	GLY	2.1
1	D	87	GLU	2.1
1	A	91	GLN	2.1
1	A	282	VAL	2.0
1	C	276	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NDP	A	1338	48/48	0.14	1.21	24,38,50,52	0
3	NDP	B	1340	48/48	0.12	1.16	20,38,61,68	0
3	NDP	D	1338	48/48	0.15	1.15	22,40,54,58	0
3	NDP	E	1338	48/48	0.14	1.14	26,35,45,47	0
3	NDP	H	1338	48/48	0.12	0.99	23,34,43,45	0
3	NDP	C	1338	48/48	0.14	0.98	27,39,57,62	0
3	NDP	F	1338	48/48	0.11	0.52	23,33,50,57	0
2	IMP	F	1337	23/23	0.10	0.47	20,23,28,32	0
2	IMP	H	1337	23/23	0.10	0.16	21,23,27,29	0
2	IMP	A	1337	23/23	0.09	0.09	22,24,27,31	0
2	IMP	B	1339	23/23	0.08	-0.12	19,23,26,30	0
2	IMP	E	1337	23/23	0.10	-0.13	19,23,26,32	0
2	IMP	D	1337	23/23	0.08	-0.23	19,23,26,29	0
2	IMP	C	1337	23/23	0.09	-0.26	19,23,29,33	0
2	IMP	G	1338	23/23	0.09	-0.31	19,24,27,31	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.