



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:53 AM GMT

PDB ID : 2BZN  
Title : CRYSTAL STRUCTURE OF HUMAN GUANOSINE MONOPHOSPHATE REDUCTASE 2 GMPR2 IN COMPLEX WITH IMP  
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Deposited on : 2005-08-19  
Resolution : 2.15 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

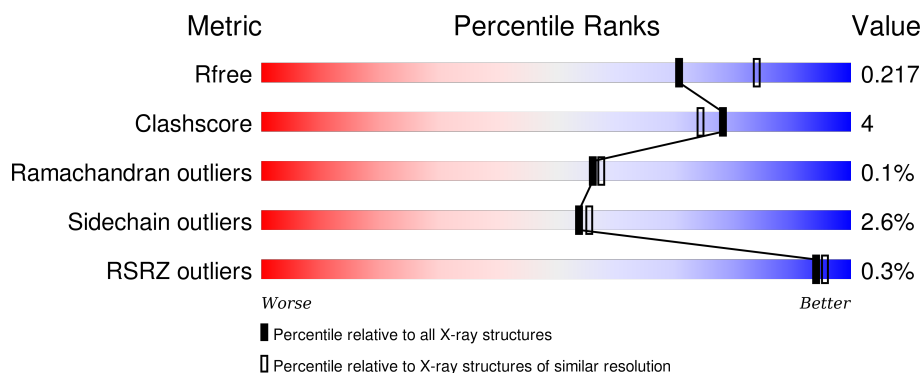
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	351	<div> <div>84%</div> <div>6% • 9%</div> </div>
1	B	351	<div> <div>84%</div> <div>6% • 10%</div> </div>
1	C	351	<div> <div>82%</div> <div>7% • 10%</div> </div>
1	D	351	<div> <div>81%</div> <div>8% • 10%</div> </div>
1	E	351	<div> <div>82%</div> <div>8% • 9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	351	<div><div>%</div><div><div></div><div>86%</div><div>5% • 9%</div></div></div>
1	G	351	<div><div></div><div>82%</div><div>6% • 10%</div></div>
1	H	351	<div><div></div><div>84%</div><div>7% • 9%</div></div>

## 2 Entry composition

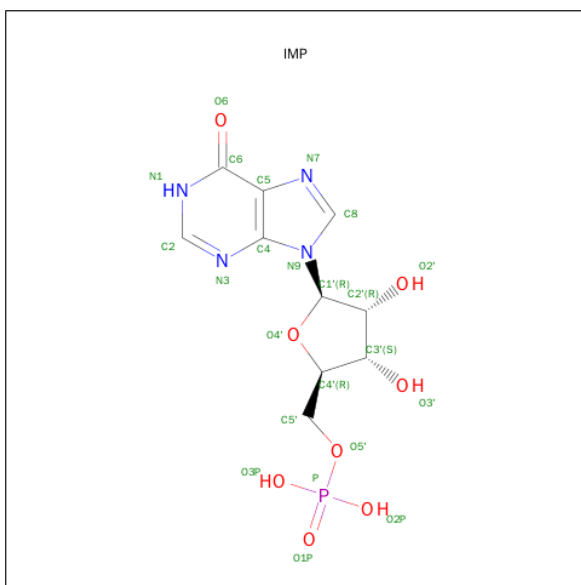
There are 3 unique types of molecules in this entry. The entry contains 21516 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GMP REDUCTASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2437	1538	419	462	18			
1	B	317	Total	C	N	O	S	0	0	0
			2412	1524	412	458	18			
1	C	317	Total	C	N	O	S	0	0	0
			2414	1526	413	457	18			
1	D	316	Total	C	N	O	S	0	1	0
			2416	1526	415	457	18			
1	E	320	Total	C	N	O	S	0	1	0
			2443	1541	420	463	19			
1	F	321	Total	C	N	O	S	0	1	0
			2450	1545	421	465	19			
1	G	317	Total	C	N	O	S	0	0	0
			2412	1524	412	458	18			
1	H	320	Total	C	N	O	S	0	0	0
			2437	1538	419	462	18			

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	219	Total	O	0	0
			219	219		
3	B	211	Total	O	0	0
			211	211		
3	C	267	Total	O	0	0
			267	267		
3	D	226	Total	O	0	0
			226	226		

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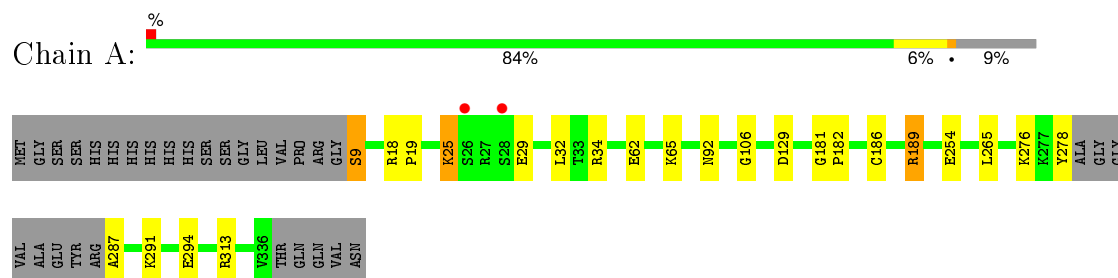
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	283	Total 283	O 283	0	0
3	F	257	Total 257	O 257	0	0
3	G	198	Total 198	O 198	0	0
3	H	250	Total 250	O 250	0	0

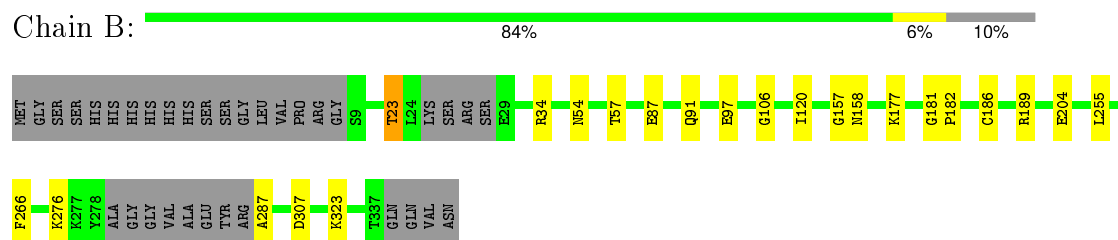
### 3 Residue-property plots [i](#)

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

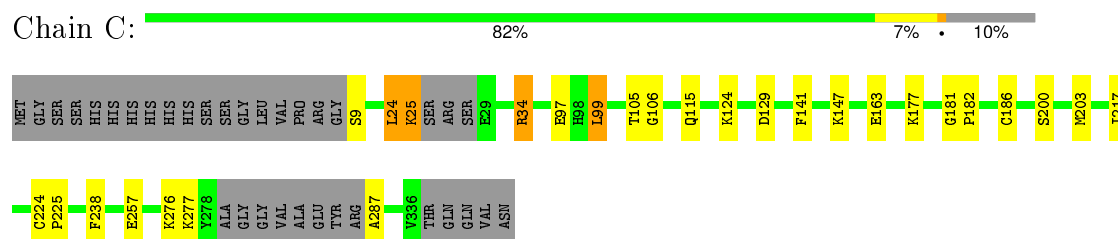
#### • Molecule 1: GMP REDUCTASE 2



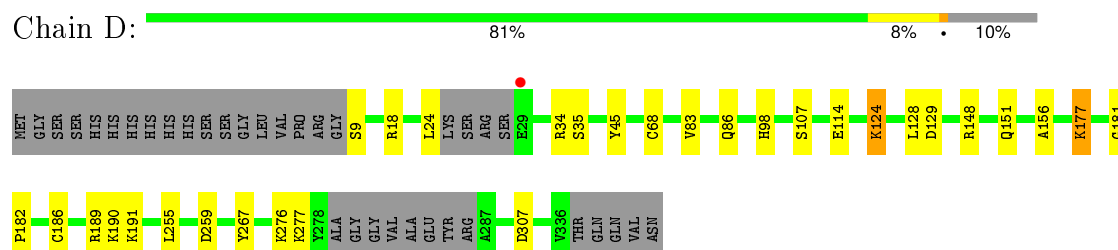
#### • Molecule 1: GMP REDUCTASE 2




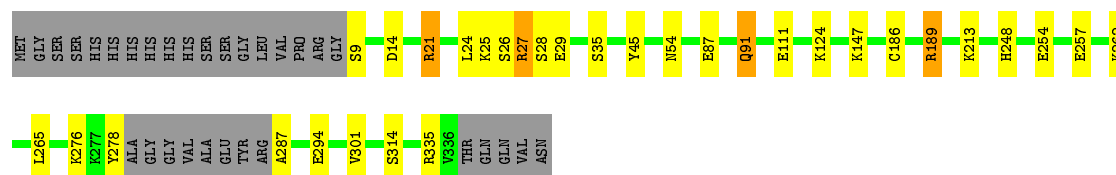
#### • Molecule 1: GMP REDUCTASE 2




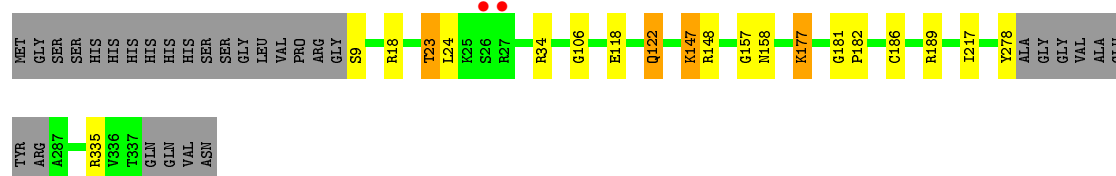
#### • Molecule 1: GMP REDUCTASE 2




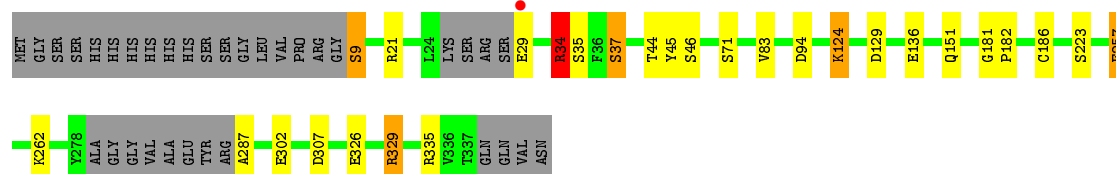
## • Molecule 1: GMP REDUCTASE 2

Chain E:  82% 8% 9%


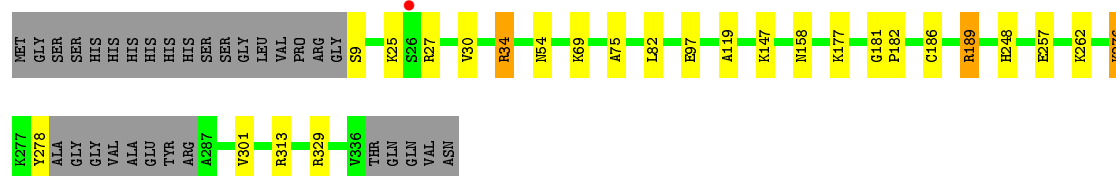
## • Molecule 1: GMP REDUCTASE 2

Chain F:  86% 5% 9%

## • Molecule 1: GMP REDUCTASE 2

Chain G:  82% 6% 10%

## • Molecule 1: GMP REDUCTASE 2

Chain H:  84% 7% 9%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.29Å 141.35Å 164.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.37 – 2.15 51.36 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.1 (51.37-2.15) 99.1 (51.36-2.15)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.158 , 0.210 0.167 , 0.217	Depositor DCC
$R_{free}$ test set	8235 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 164128 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	21516	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 2.46% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.77	0/2480	0.74	1/3333 (0.0%)
1	B	0.74	0/2454	0.73	2/3299 (0.1%)
1	C	0.82	2/2456 (0.1%)	0.80	3/3300 (0.1%)
1	D	0.77	1/2458 (0.0%)	0.76	4/3303 (0.1%)
1	E	0.78	0/2486	0.79	2/3341 (0.1%)
1	F	0.78	0/2493	0.78	2/3351 (0.1%)
1	G	0.76	0/2454	0.75	3/3299 (0.1%)
1	H	0.79	2/2480 (0.1%)	0.80	5/3333 (0.2%)
All	All	0.78	5/19761 (0.0%)	0.77	22/26559 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	68	CYS	CB-SG	-9.23	1.66	1.82
1	C	97	GLU	CG-CD	5.90	1.60	1.51
1	H	276	LYS	CE-NZ	5.38	1.62	1.49
1	H	276	LYS	CD-CE	5.21	1.64	1.51
1	C	163	GLU	CB-CG	5.09	1.61	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	189	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	C	34	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	E	189	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	H	34	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	F	18	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	H	189	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	189	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	G	34	ARG	NE-CZ-NH2	-6.20	117.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	99	LEU	CA-CB-CG	6.16	129.46	115.30
1	D	34	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	F	34	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	D	189	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	D	18	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	34	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	C	34	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	G	223	SER	CB-CA-C	-5.55	99.56	110.10
1	D	189	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	H	34	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	34	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	H	313	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	H	189	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	G	329	ARG	NE-CZ-NH1	5.03	122.82	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	2437	0	2440	16	0
1	B	2412	0	2410	15	0
1	C	2414	0	2416	20	0
1	D	2416	0	2415	22	0
1	E	2443	0	2444	20	0
1	F	2450	0	2451	16	0
1	G	2412	0	2410	16	0
1	H	2437	0	2440	16	0
2	A	23	0	11	2	0
2	B	23	0	11	3	0
2	C	23	0	11	2	0
2	D	23	0	11	2	0
2	E	23	0	11	4	0
2	F	23	0	11	4	0
2	G	23	0	11	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	23	0	11	3	0
3	A	219	0	0	7	0
3	B	211	0	0	3	0
3	C	267	0	0	8	0
3	D	226	0	0	10	0
3	E	283	0	0	6	0
3	F	257	0	0	4	0
3	G	198	0	0	8	0
3	H	250	0	0	4	0
All	All	21516	0	19514	139	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 4.

All (139) 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:E:186:CYS:SG	2:E:1338:IMP:H2	1.59	1.43
1:B:186:CYS:SG	2:B:1338:IMP:H2	1.68	1.33
1:D:186:CYS:SG	2:D:1338:IMP:H2	1.69	1.31
1:C:186:CYS:SG	2:C:1338:IMP:H2	1.80	1.21
1:E:186:CYS:SG	2:E:1338:IMP:C2	2.31	1.18
1:H:186:CYS:SG	2:H:1338:IMP:H2	1.82	1.17
1:F:186:CYS:SG	2:F:1338:IMP:H2	1.87	1.14
1:E:287:ALA:N	3:E:2238:HOH:O	1.85	1.10
1:D:186:CYS:SG	2:D:1338:IMP:C2	2.41	1.07
1:A:186:CYS:SG	2:A:1338:IMP:H2	1.95	1.06
1:B:186:CYS:SG	2:B:1338:IMP:C2	2.46	1.03
1:C:186:CYS:SG	2:C:1338:IMP:C2	2.51	0.97
1:H:186:CYS:SG	2:H:1338:IMP:C2	2.53	0.96
1:F:186:CYS:SG	2:F:1338:IMP:C2	2.53	0.95
1:E:186:CYS:HG	2:E:1338:IMP:H2	1.28	0.93
1:A:186:CYS:SG	2:A:1338:IMP:C2	2.59	0.90
1:E:27:ARG:HD2	1:E:314:SER:OG	1.73	0.88
3:A:2126:HOH:O	1:B:307:ASP:HB3	1.75	0.86
1:E:124:LYS:HD3	3:E:2126:HOH:O	1.74	0.86
1:E:186:CYS:HG	2:E:1338:IMP:C2	1.83	0.86
1:D:9:SER:N	3:D:2003:HOH:O	2.09	0.84
1:G:307:ASP:HB2	3:G:2175:HOH:O	1.78	0.84
1:G:287:ALA:N	3:G:2162:HOH:O	2.17	0.77
1:G:186:CYS:SG	2:G:1338:IMP:H2	2.26	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:SER:N	3:D:2001:HOH:O	2.17	0.76
1:H:257:GLU:OE1	1:H:262:LYS:NZ	2.21	0.71
1:A:287:ALA:N	3:A:2184:HOH:O	2.25	0.70
1:D:307:ASP:HB2	3:D:2205:HOH:O	1.92	0.70
1:A:278:TYR:C	3:A:2183:HOH:O	2.30	0.69
1:H:186:CYS:HG	2:H:1338:IMP:H2	1.55	0.69
1:C:24:LEU:O	1:C:25:LYS:HB3	1.93	0.68
1:A:9:SER:N	3:A:2001:HOH:O	2.27	0.67
1:G:9:SER:N	3:G:2002:HOH:O	2.28	0.66
1:G:186:CYS:SG	2:G:1338:IMP:C2	2.84	0.66
1:F:122:GLN:H	1:F:122:GLN:HE21	1.45	0.65
1:E:21:ARG:NH2	1:G:136:GLU:OE2	2.30	0.65
1:A:65:LYS:HD3	1:A:92:ASN:ND2	2.12	0.64
1:C:257:GLU:HB3	3:C:2204:HOH:O	1.97	0.63
1:B:106:GLY:HA3	3:B:2091:HOH:O	1.98	0.63
1:F:9:SER:N	3:F:2004:HOH:O	2.32	0.63
1:H:9:SER:N	3:H:2001:HOH:O	2.32	0.62
1:B:287:ALA:HB2	3:D:2108:HOH:O	2.04	0.58
1:A:25:LYS:HB2	1:A:29:GLU:HG3	1.85	0.57
1:D:276:LYS:CE	3:D:2186:HOH:O	2.52	0.57
1:F:147:LYS:HE2	3:F:2136:HOH:O	2.05	0.56
2:G:1338:IMP:H2	3:G:2111:HOH:O	2.05	0.56
1:C:106:GLY:HA3	3:C:2107:HOH:O	2.05	0.56
1:H:276:LYS:CE	3:H:2202:HOH:O	2.53	0.56
2:G:1338:IMP:C2	3:G:2111:HOH:O	2.54	0.55
1:G:29:GLU:HA	3:G:2021:HOH:O	2.07	0.55
1:G:94:ASP:O	3:G:2064:HOH:O	2.19	0.54
1:D:276:LYS:HE3	3:D:2186:HOH:O	2.07	0.54
1:F:278:TYR:C	3:F:2207:HOH:O	2.46	0.54
1:B:97:GLU:HG2	3:B:2078:HOH:O	2.06	0.54
1:A:106:GLY:HA3	3:A:2084:HOH:O	2.07	0.53
1:B:23:THR:O	1:B:23:THR:HG23	2.09	0.53
1:C:277:LYS:NZ	3:C:2216:HOH:O	2.41	0.53
1:F:186:CYS:HG	2:F:1338:IMP:H2	1.67	0.53
1:D:24:LEU:C	3:D:2024:HOH:O	2.48	0.51
1:E:276:LYS:HE3	3:E:2232:HOH:O	2.11	0.51
1:H:278:TYR:C	3:H:2204:HOH:O	2.49	0.50
1:G:326:GLU:HG2	1:G:329:ARG:NH2	2.26	0.50
1:F:177:LYS:HG2	1:F:217:ILE:HD12	1.93	0.50
1:E:257:GLU:OE1	1:E:262:LYS:NZ	2.45	0.49
1:F:186:CYS:HG	2:F:1338:IMP:C2	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:257:GLU:CD	1:H:262:LYS:HZ3	2.12	0.49
1:G:34:ARG:O	1:G:46:SER:HA	2.12	0.49
1:C:9:SER:N	3:C:2001:HOH:O	2.46	0.48
1:E:87:GLU:O	1:E:91:GLN:HG2	2.13	0.48
1:D:129:ASP:OD1	1:D:177:LYS:NZ	2.44	0.48
1:G:35:SER:HA	1:G:45:TYR:O	2.14	0.48
1:E:35:SER:HA	1:E:45:TYR:O	2.14	0.47
1:D:267:TYR:OH	1:D:277:LYS:HE3	2.14	0.47
1:E:14:ASP:O	1:E:335:ARG:HD2	2.15	0.47
1:A:65:LYS:HD3	1:A:92:ASN:HD21	1.80	0.47
1:C:34:ARG:NH2	3:C:2032:HOH:O	2.45	0.47
1:D:83:VAL:HA	1:D:86:GLN:HE21	1.78	0.47
1:F:23:THR:CG2	1:F:23:THR:O	2.63	0.47
1:D:181:GLY:N	1:D:182:PRO:CD	2.78	0.47
1:H:276:LYS:HE3	3:H:2202:HOH:O	2.13	0.46
1:E:278:TYR:C	3:E:2235:HOH:O	2.53	0.46
1:G:257:GLU:HG2	1:G:262:LYS:HG2	1.97	0.46
1:B:57:THR:HG1	1:B:266:PHE:HD2	1.63	0.46
1:H:181:GLY:N	1:H:182:PRO:CD	2.79	0.46
1:B:186:CYS:CB	2:B:1338:IMP:C2	2.94	0.45
1:C:225:PRO:HB2	1:D:191:LYS:O	2.16	0.45
1:A:181:GLY:HA3	1:A:189:ARG:HD2	1.98	0.45
1:G:181:GLY:N	1:G:182:PRO:CD	2.79	0.45
1:B:181:GLY:N	1:B:182:PRO:CD	2.79	0.45
1:D:124:LYS:NZ	1:D:151:GLN:O	2.51	0.44
1:A:181:GLY:N	1:A:182:PRO:CD	2.80	0.44
1:E:248:HIS:CD2	1:E:301:VAL:HA	2.52	0.44
1:C:115:GLN:NE2	3:C:2120:HOH:O	2.50	0.44
1:C:224:CYS:SG	1:D:190:LYS:HD2	2.57	0.44
1:F:118:GLU:OE2	1:F:148:ARG:NH2	2.50	0.44
1:C:276:LYS:CE	3:C:2213:HOH:O	2.65	0.44
1:H:54:ASN:HA	1:H:75:ALA:O	2.18	0.43
1:H:25:LYS:HE3	1:H:27:ARG:NH2	2.33	0.43
1:D:124:LYS:HD3	3:D:2111:HOH:O	2.17	0.43
1:A:32:LEU:HD11	1:A:313:ARG:HG3	2.01	0.43
1:A:254:GLU:HB3	1:A:265:LEU:HD12	2.01	0.43
1:D:128:LEU:O	1:D:156:ALA:HA	2.17	0.43
1:C:276:LYS:NZ	3:C:2213:HOH:O	2.43	0.43
1:C:105:THR:HG22	1:C:141:PHE:CD2	2.53	0.43
1:E:26:SER:O	1:E:29:GLU:HB3	2.19	0.43
1:F:157:GLY:HA3	1:F:158:ASN:HA	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:158:ASN:OD1	1:H:177:LYS:NZ	2.47	0.43
1:C:217:ILE:HG12	1:C:238:PHE:HB2	2.01	0.43
1:G:37:SER:HB3	1:G:44:THR:HG22	2.00	0.43
1:C:129:ASP:OD1	1:C:177:LYS:NZ	2.52	0.42
1:G:83:VAL:HG23	3:G:2058:HOH:O	2.19	0.42
1:A:18:ARG:HG2	1:A:19:PRO:O	2.20	0.42
1:C:181:GLY:N	1:C:182:PRO:CD	2.83	0.42
1:G:124:LYS:NZ	1:G:151:GLN:O	2.53	0.42
1:B:157:GLY:HA3	1:B:177:LYS:HB2	2.02	0.42
1:D:114:GLU:OE1	1:D:148[A]:ARG:NE	2.44	0.42
1:H:82:LEU:HD11	1:H:119:ALA:HB3	2.02	0.42
1:C:200:SER:HA	1:C:203:MET:CE	2.50	0.42
1:B:276:LYS:CE	3:B:2175:HOH:O	2.68	0.41
1:B:91:GLN:HB3	1:B:91:GLN:HE21	1.59	0.41
1:C:200:SER:HA	1:C:203:MET:HE2	2.01	0.41
1:B:157:GLY:HA3	1:B:158:ASN:HA	1.94	0.41
3:A:2018:HOH:O	1:C:287:ALA:HB2	2.20	0.41
1:F:181:GLY:HA3	1:F:189:ARG:HD2	2.03	0.41
1:D:98:HIS:HB2	3:D:2093:HOH:O	2.20	0.41
1:H:257:GLU:CD	1:H:262:LYS:NZ	2.71	0.41
1:F:157:GLY:HA3	1:F:177:LYS:HB2	2.02	0.41
1:H:248:HIS:CD2	1:H:301:VAL:HA	2.56	0.41
1:E:254:GLU:HB3	1:E:265:LEU:HD12	2.02	0.41
1:D:259:ASP:OD2	3:D:2177:HOH:O	2.22	0.41
1:E:276:LYS:CE	3:E:2232:HOH:O	2.68	0.40
1:B:23:THR:CG2	1:B:23:THR:O	2.69	0.40
1:D:124:LYS:HA	1:D:124:LYS:HD2	1.96	0.40
1:D:35:SER:HA	1:D:45:TYR:O	2.21	0.40
1:E:9:SER:N	3:E:2004:HOH:O	2.55	0.40
1:F:106:GLY:HA3	3:F:2104:HOH:O	2.21	0.40
1:F:181:GLY:N	1:F:182:PRO:CD	2.84	0.40
1:A:294:GLU:OE1	1:E:294:GLU:OE1	2.39	0.40
1:A:62:GLU:HG3	3:A:2041:HOH:O	2.22	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	316/351 (90%)	309 (98%)	7 (2%)	0	100	100
1	B	311/351 (89%)	304 (98%)	6 (2%)	1 (0%)	46	42
1	C	311/351 (89%)	305 (98%)	6 (2%)	0	100	100
1	D	311/351 (89%)	304 (98%)	7 (2%)	0	100	100
1	E	317/351 (90%)	311 (98%)	5 (2%)	1 (0%)	46	42
1	F	318/351 (91%)	312 (98%)	6 (2%)	0	100	100
1	G	311/351 (89%)	304 (98%)	7 (2%)	0	100	100
1	H	316/351 (90%)	311 (98%)	5 (2%)	0	100	100
All	All	2511/2808 (89%)	2460 (98%)	49 (2%)	2 (0%)	56	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	54	ASN
1	B	54	ASN

### 5.3.2 Protein sidechains [i](#)

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	263/287 (92%)	257 (98%)	6 (2%)	58	62
1	B	260/287 (91%)	254 (98%)	6 (2%)	58	62
1	C	260/287 (91%)	255 (98%)	5 (2%)	65	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	260/287 (91%)	256 (98%)	4 (2%)	72	78
1	E	264/287 (92%)	254 (96%)	10 (4%)	40	37
1	F	265/287 (92%)	259 (98%)	6 (2%)	58	62
1	G	260/287 (91%)	250 (96%)	10 (4%)	40	37
1	H	263/287 (92%)	256 (97%)	7 (3%)	52	53
All	All	2095/2296 (91%)	2041 (97%)	54 (3%)	54	55

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	25	LYS
1	A	129	ASP
1	A	189	ARG
1	A	276	LYS
1	A	291	LYS
1	B	23	THR
1	B	87	GLU
1	B	120	ILE
1	B	204	GLU
1	B	255	LEU
1	B	323	LYS
1	C	24	LEU
1	C	25	LYS
1	C	99	LEU
1	C	124	LYS
1	C	147	LYS
1	D	107	SER
1	D	124	LYS
1	D	177	LYS
1	D	255	LEU
1	E	21	ARG
1	E	24	LEU
1	E	25	LYS
1	E	27	ARG
1	E	28	SER
1	E	91	GLN
1	E	111	GLU
1	E	147	LYS
1	E	189	ARG

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Mol	Chain	Res	Type
1	E	213	LYS
1	F	23	THR
1	F	24	LEU
1	F	122	GLN
1	F	147	LYS
1	F	177	LYS
1	F	335	ARG
1	G	9	SER
1	G	21	ARG
1	G	34	ARG
1	G	37	SER
1	G	71	SER
1	G	124	LYS
1	G	129	ASP
1	G	257	GLU
1	G	302	GLU
1	G	335	ARG
1	H	30	VAL
1	H	34	ARG
1	H	69	LYS
1	H	97	GLU
1	H	147	LYS
1	H	189	ARG
1	H	329	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	303	HIS
1	B	86	GLN
1	B	91	GLN
1	B	92	ASN
1	B	112	GLN
1	C	112	GLN
1	C	115	GLN
1	C	151	GLN
1	D	86	GLN
1	D	112	GLN
1	D	303	HIS
1	E	86	GLN
1	E	92	ASN

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Mol	Chain	Res	Type
1	F	92	ASN
1	F	112	GLN
1	F	122	GLN
1	F	151	GLN
1	G	86	GLN
1	G	112	GLN
1	H	112	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

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	IMP	A	1338	-	20,25,25	1.29	2 (10%)	22,38,38	2.95	7 (31%)
2	IMP	B	1338	-	20,25,25	1.47	2 (10%)	22,38,38	2.84	5 (22%)
2	IMP	C	1338	-	20,25,25	1.44	2 (10%)	22,38,38	2.30	6 (27%)
2	IMP	D	1338	-	20,25,25	1.38	2 (10%)	22,38,38	3.04	6 (27%)
2	IMP	E	1338	-	20,25,25	1.49	2 (10%)	22,38,38	2.58	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	IMP	F	1338	-	20,25,25	1.22	2 (10%)	22,38,38	2.55	5 (22%)
2	IMP	G	1338	-	20,25,25	1.44	3 (15%)	22,38,38	2.52	7 (31%)
2	IMP	H	1338	-	20,25,25	1.37	4 (20%)	22,38,38	2.41	4 (18%)

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	1338	-	-	0/6/26/26	0/3/3/3
2	IMP	B	1338	-	-	0/6/26/26	0/3/3/3
2	IMP	C	1338	-	-	0/6/26/26	0/3/3/3
2	IMP	D	1338	-	-	0/6/26/26	0/3/3/3
2	IMP	E	1338	-	-	0/6/26/26	0/3/3/3
2	IMP	F	1338	-	-	0/6/26/26	0/3/3/3
2	IMP	G	1338	-	-	0/6/26/26	0/3/3/3
2	IMP	H	1338	-	-	0/6/26/26	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1338	IMP	O4'-C4'	-2.32	1.39	1.45
2	G	1338	IMP	C6-N1	2.11	1.37	1.33
2	H	1338	IMP	C6-N1	2.38	1.37	1.33
2	D	1338	IMP	C2-N1	2.42	1.38	1.33
2	F	1338	IMP	C2-N1	2.85	1.39	1.33
2	H	1338	IMP	C2-N1	2.88	1.39	1.33
2	G	1338	IMP	C2-N1	2.95	1.39	1.33
2	A	1338	IMP	C2-N1	3.02	1.39	1.33
2	H	1338	IMP	C2-N3	3.21	1.37	1.32
2	E	1338	IMP	C2-N1	3.45	1.40	1.33
2	C	1338	IMP	C2-N1	3.67	1.40	1.33
2	F	1338	IMP	C2-N3	3.70	1.38	1.32
2	B	1338	IMP	C2-N1	3.78	1.41	1.33
2	A	1338	IMP	C2-N3	3.83	1.39	1.32
2	B	1338	IMP	C2-N3	3.94	1.39	1.32
2	C	1338	IMP	C2-N3	4.23	1.39	1.32
2	D	1338	IMP	C2-N3	4.24	1.39	1.32
2	G	1338	IMP	C2-N3	4.46	1.40	1.32
2	E	1338	IMP	C2-N3	4.81	1.40	1.32

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1338	IMP	N3-C2-N1	-12.49	119.33	128.89
2	B	1338	IMP	N3-C2-N1	-11.71	119.93	128.89
2	A	1338	IMP	N3-C2-N1	-11.44	120.14	128.89
2	E	1338	IMP	N3-C2-N1	-10.51	120.85	128.89
2	F	1338	IMP	N3-C2-N1	-9.67	121.49	128.89
2	H	1338	IMP	N3-C2-N1	-9.65	121.50	128.89
2	G	1338	IMP	N3-C2-N1	-9.25	121.81	128.89
2	C	1338	IMP	N3-C2-N1	-8.00	122.77	128.89
2	A	1338	IMP	C4-C5-N7	-4.35	105.47	109.48
2	C	1338	IMP	C4-C5-N7	-3.94	105.86	109.48
2	G	1338	IMP	C4'-O4'-C1'	-3.55	105.81	109.72
2	F	1338	IMP	C4'-O4'-C1'	-3.41	105.98	109.72
2	H	1338	IMP	C4-C5-N7	-3.09	106.63	109.48
2	F	1338	IMP	C4-C5-N7	-3.06	106.66	109.48
2	E	1338	IMP	C4-C5-N7	-3.01	106.71	109.48
2	H	1338	IMP	C1'-N9-C4	-2.94	122.50	126.94
2	A	1338	IMP	C2'-C1'-N9	-2.93	109.82	114.29
2	G	1338	IMP	C4-C5-N7	-2.90	106.81	109.48
2	C	1338	IMP	C1'-N9-C4	-2.85	122.63	126.94
2	D	1338	IMP	C4-C5-N7	-2.76	106.94	109.48
2	A	1338	IMP	C1'-N9-C4	-2.64	122.96	126.94
2	D	1338	IMP	C2'-C1'-N9	-2.52	110.45	114.29
2	B	1338	IMP	C1'-N9-C4	-2.48	123.20	126.94
2	C	1338	IMP	C4'-O4'-C1'	-2.43	107.05	109.72
2	C	1338	IMP	C2'-C1'-N9	-2.36	110.69	114.29
2	B	1338	IMP	C4-C5-N7	-2.33	107.34	109.48
2	G	1338	IMP	C1'-N9-C4	-2.13	123.72	126.94
2	D	1338	IMP	C4'-O4'-C1'	-2.07	107.44	109.72
2	G	1338	IMP	C2'-C1'-N9	-2.04	111.17	114.29
2	A	1338	IMP	C2'-C3'-C4'	-2.02	98.47	102.61
2	B	1338	IMP	O4'-C1'-N9	2.15	112.59	108.10
2	A	1338	IMP	O4'-C1'-N9	2.25	112.81	108.10
2	H	1338	IMP	C2-N1-C6	2.37	119.63	116.04
2	G	1338	IMP	O5'-P-O1P	2.54	113.60	107.14
2	F	1338	IMP	O5'-P-O1P	2.56	113.65	107.14
2	D	1338	IMP	O4'-C1'-N9	2.59	113.53	108.10
2	F	1338	IMP	C2-N1-C6	2.68	120.09	116.04
2	D	1338	IMP	C2-N1-C6	2.80	120.27	116.04
2	E	1338	IMP	C2-N1-C6	2.95	120.50	116.04
2	C	1338	IMP	C2-N1-C6	3.00	120.59	116.04
2	G	1338	IMP	C2-N1-C6	3.21	120.91	116.04
2	A	1338	IMP	C2-N1-C6	3.57	121.45	116.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1338	IMP	C2-N1-C6	3.75	121.73	116.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1338	IMP	2	0
2	B	1338	IMP	3	0
2	C	1338	IMP	2	0
2	D	1338	IMP	2	0
2	E	1338	IMP	4	0
2	F	1338	IMP	4	0
2	G	1338	IMP	4	0
2	H	1338	IMP	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	320/351 (91%)	-0.32	2 (0%) 90 92	17, 27, 43, 65	0
1	B	317/351 (90%)	-0.31	0 100 100	19, 29, 44, 51	0
1	C	317/351 (90%)	-0.37	0 100 100	16, 23, 36, 54	0
1	D	316/351 (90%)	-0.31	1 (0%) 94 95	18, 27, 41, 50	0
1	E	320/351 (91%)	-0.27	0 100 100	15, 22, 38, 51	0
1	F	321/351 (91%)	-0.30	2 (0%) 90 92	15, 25, 39, 65	0
1	G	317/351 (90%)	-0.22	1 (0%) 94 95	17, 30, 49, 59	0
1	H	320/351 (91%)	-0.34	1 (0%) 94 95	17, 25, 41, 46	0
All	All	2548/2808 (90%)	-0.30	7 (0%) 94 95	15, 26, 42, 65	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	27	ARG	5.3
1	F	26	SER	5.1
1	A	28	SER	3.0
1	A	26	SER	2.2
1	D	29	GLU	2.2
1	H	26	SER	2.1
1	G	29	GLU	2.1

### 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

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(Å <sup>2</sup> )	Q<0.9
2	IMP	E	1338	23/23	0.98	0.10	0.19	12,16,23,24	0
2	IMP	F	1338	23/23	0.98	0.09	0.18	12,19,27,28	0
2	IMP	C	1338	23/23	0.99	0.10	-0.10	15,18,24,28	0
2	IMP	A	1338	23/23	0.99	0.09	-0.42	13,19,26,28	0
2	IMP	G	1338	23/23	0.99	0.09	-0.54	15,20,28,31	0
2	IMP	B	1338	23/23	0.98	0.09	-0.60	15,23,26,28	0
2	IMP	D	1338	23/23	0.99	0.08	-0.95	13,20,28,29	0
2	IMP	H	1338	23/23	0.99	0.09	-0.96	12,19,23,26	0

## 6.5 Other polymers

There are no such residues in this entry.