



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:37 pm GMT

PDB ID : 1XMM  
Title : Structure of human Dcps bound to m7GDP  
Authors : Chen, N.; Song, H.  
Deposited on : 2004-10-04  
Resolution : 2.50 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 : trunk28683  
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) : recalc28949

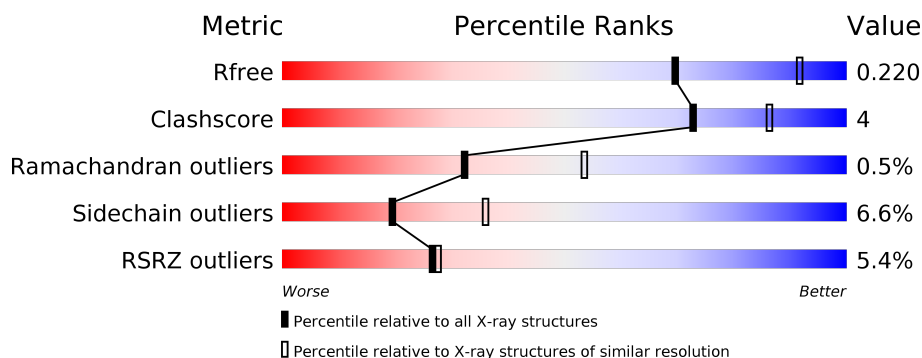
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	342	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>13%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	342	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>11%</div> <div>•</div> <div>16%</div> </div> </div>
1	C	342	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>13%</div> <div>•</div> <div>15%</div> </div> </div>
1	D	342	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>11%</div> <div>•</div> <div>15%</div> </div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	1601	-	-	-	X
2	PO4	B	602	-	-	X	-
3	M7G	A	401	-	-	-	X
3	M7G	D	404	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10108 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 heat shock-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	288	Total	C	N	O	S	0	0	0
			2384	1526	427	428	3			
1	A	287	Total	C	N	O	S	0	0	0
			2377	1523	425	426	3			
1	C	289	Total	C	N	O	S	0	0	0
			2389	1529	427	430	3			
1	D	292	Total	C	N	O	S	0	0	0
			2411	1542	430	436	3			

There are 20 discrepancies between the modelled and reference sequences:

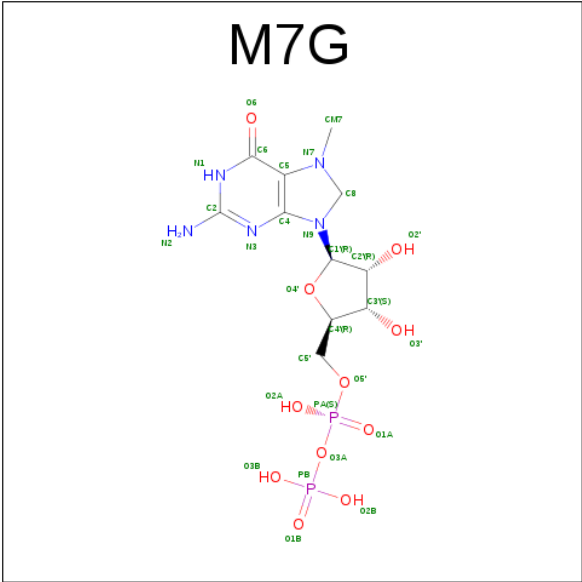
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	CLONING ARTIFACT	GB 30138167
B	-3	PRO	-	CLONING ARTIFACT	GB 30138167
B	-2	LEU	-	CLONING ARTIFACT	GB 30138167
B	-1	GLY	-	CLONING ARTIFACT	GB 30138167
B	0	SER	-	CLONING ARTIFACT	GB 30138167
A	-4	GLY	-	CLONING ARTIFACT	GB 30138167
A	-3	PRO	-	CLONING ARTIFACT	GB 30138167
A	-2	LEU	-	CLONING ARTIFACT	GB 30138167
A	-1	GLY	-	CLONING ARTIFACT	GB 30138167
A	0	SER	-	CLONING ARTIFACT	GB 30138167
C	-4	GLY	-	CLONING ARTIFACT	GB 30138167
C	-3	PRO	-	CLONING ARTIFACT	GB 30138167
C	-2	LEU	-	CLONING ARTIFACT	GB 30138167
C	-1	GLY	-	CLONING ARTIFACT	GB 30138167
C	0	SER	-	CLONING ARTIFACT	GB 30138167
D	-4	GLY	-	CLONING ARTIFACT	GB 30138167
D	-3	PRO	-	CLONING ARTIFACT	GB 30138167
D	-2	LEU	-	CLONING ARTIFACT	GB 30138167
D	-1	GLY	-	CLONING ARTIFACT	GB 30138167
D	0	SER	-	CLONING ARTIFACT	GB 30138167

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



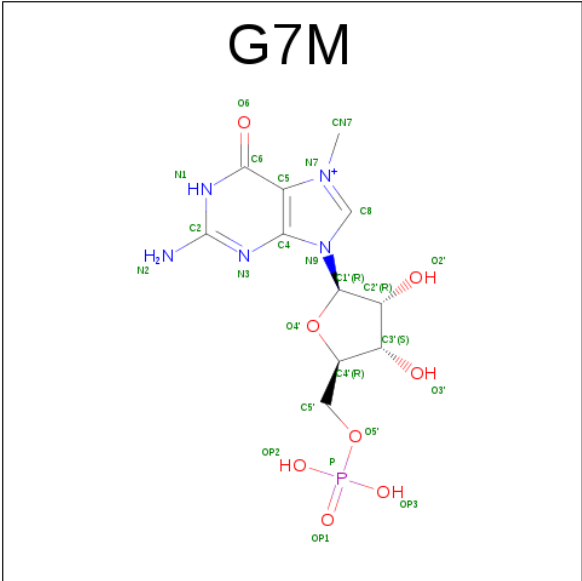
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 7N-METHYL-8-HYDROGUANOSINE-5'-DIPHOSPHATE (three-letter code: M7G) (formula:  $C_{11}H_{19}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 29	C 11	N 5	O 11	P 2	0	0
3	D	1	Total 29	C 11	N 5	O 11	P 2	0	0

- Molecule 4 is N7-METHYL-GUANOSINE-5'-MONOPHOSPHATE (three-letter code: G7M) (formula: C<sub>11</sub>H<sub>17</sub>N<sub>5</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			25	11	5	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			25	11	5	8	1		

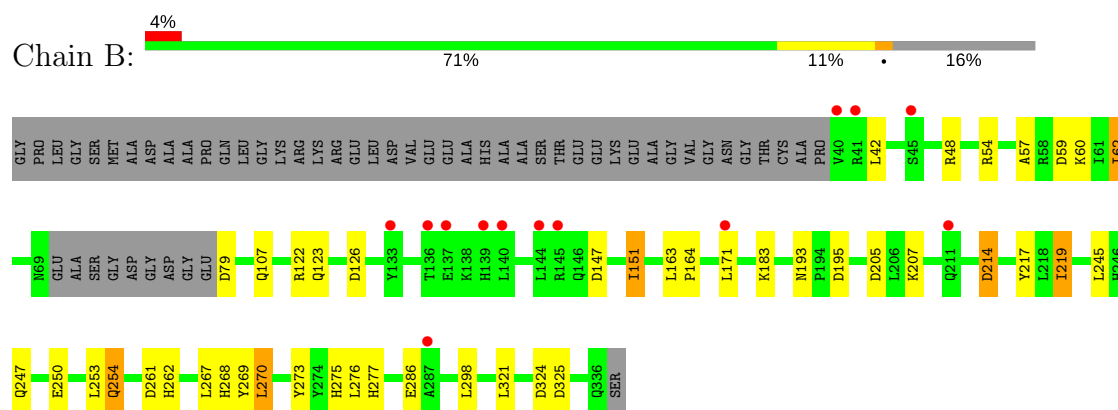
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total	O	0	0
			119	119		
5	B	102	Total	O	0	0
			102	102		
5	C	88	Total	O	0	0
			88	88		
5	D	110	Total	O	0	0
			110	110		

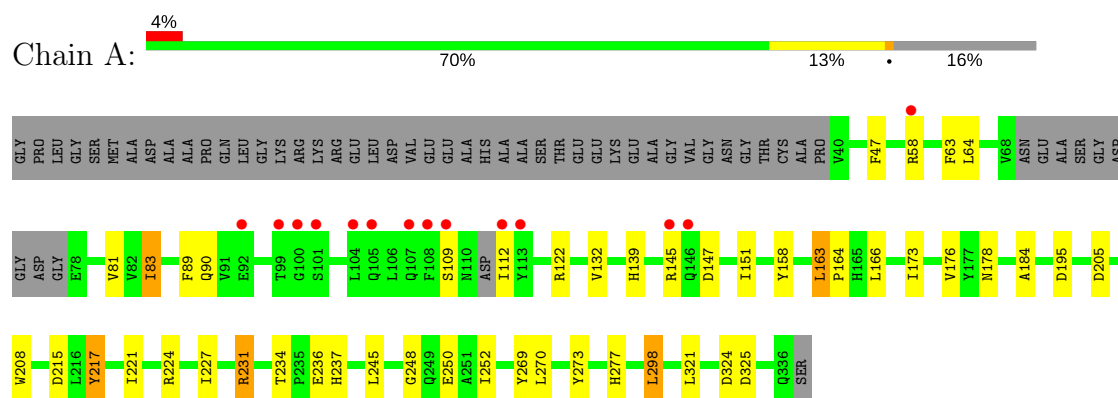
### 3 Residue-property plots [i](#)

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.

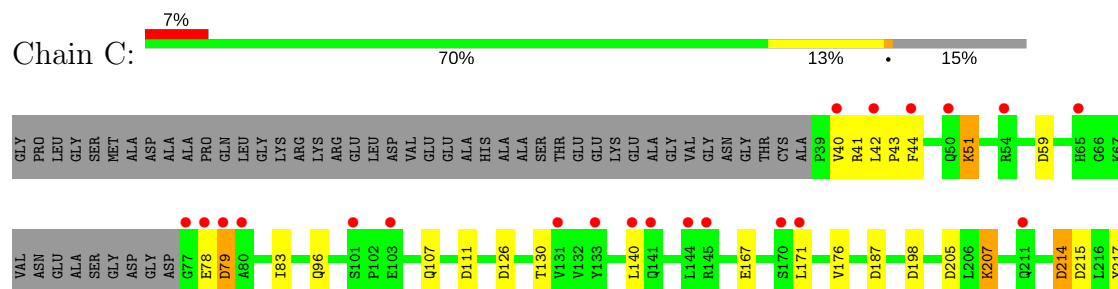
- Molecule 1: heat shock-like protein 1



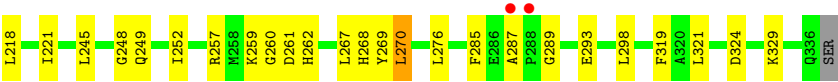
- Molecule 1: heat shock-like protein 1



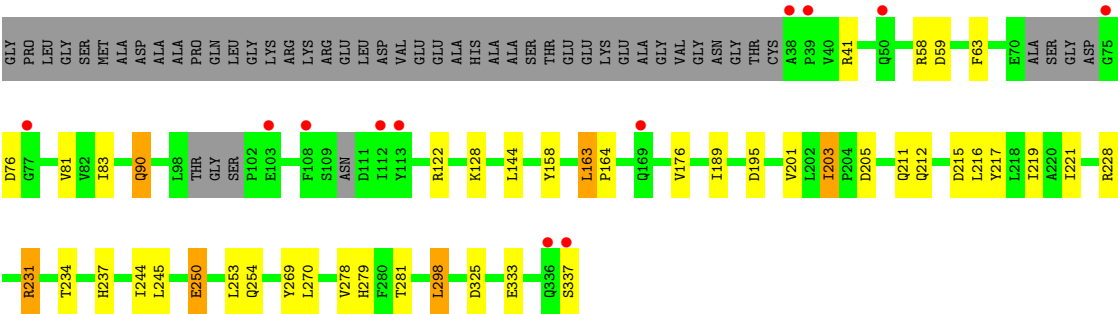
- Molecule 1: heat shock-like protein 1







● Molecule 1: heat shock-like protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.93Å 105.14Å 138.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 32.69 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-2.50) 98.8 (32.69-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.48 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.214 , 0.267 0.223 , 0.220	Depositor DCC
$R_{free}$ test set	2602 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10108	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.57 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.8962e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, PO4, M7G

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	0.42	0/2432	0.75	4/3298 (0.1%)
1	B	0.41	0/2440	0.76	8/3311 (0.2%)
1	C	0.42	0/2446	0.77	10/3318 (0.3%)
1	D	0.41	0/2466	0.75	4/3342 (0.1%)
All	All	0.41	0/9784	0.76	26/13269 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	324	ASP	CB-CG-OD2	7.27	124.84	118.30
1	C	126	ASP	CB-CG-OD2	7.16	124.74	118.30
1	C	214	ASP	CB-CG-OD2	7.05	124.65	118.30
1	A	215	ASP	CB-CG-OD2	6.83	124.45	118.30
1	A	195	ASP	CB-CG-OD2	6.62	124.26	118.30
1	D	76	ASP	CB-CG-OD2	6.56	124.20	118.30
1	C	59	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	324	ASP	CB-CG-OD2	6.27	123.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	ASP	CB-CG-OD2	6.03	123.72	118.30
1	B	126	ASP	CB-CG-OD2	6.03	123.72	118.30
1	B	324	ASP	CB-CG-OD2	5.91	123.62	118.30
1	D	215	ASP	CB-CG-OD2	5.82	123.54	118.30
1	C	79	ASP	CB-CG-OD2	5.80	123.53	118.30
1	B	214	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	261	ASP	CB-CG-OD2	5.66	123.40	118.30
1	C	111	ASP	CB-CG-OD2	5.53	123.27	118.30
1	C	261	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	325	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	79	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	325	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	195	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	187	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	195	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	215	ASP	CB-CG-OD2	5.07	122.87	118.30
1	C	198	ASP	CB-CG-OD2	5.05	122.84	118.30
1	D	325	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	TYR	Peptide
1	B	269	TYR	Peptide
1	C	269	TYR	Peptide
1	D	269	TYR	Peptide

## 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	2377	0	2384	24	0
1	B	2384	0	2389	17	0
1	C	2389	0	2391	16	0
1	D	2411	0	2406	23	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	2	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
3	A	29	0	16	1	0
3	D	29	0	16	2	0
4	B	25	0	15	0	0
4	C	25	0	15	0	0
5	A	119	0	0	0	0
5	B	102	0	0	0	0
5	C	88	0	0	1	0
5	D	110	0	0	3	0
All	All	10108	0	9632	76	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 (76) 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:D:254:GLN:HG3	5:D:1607:HOH:O	1.49	1.13
1:D:63:PHE:CD2	1:D:83:ILE:HD12	2.27	0.69
1:A:132:VAL:HG11	1:A:139:HIS:CD2	2.29	0.67
1:A:173:ILE:HG22	1:A:173:ILE:O	1.96	0.64
1:A:205:ASP:OD1	3:A:401:M7G:O2'	2.19	0.60
1:B:270:LEU:CD2	1:B:321:LEU:HD21	2.32	0.59
1:D:158:TYR:CG	1:D:231:ARG:HD3	2.38	0.58
1:D:163:LEU:HB3	1:D:164:PRO:HD3	1.85	0.58
1:A:63:PHE:CD2	1:A:83:ILE:HD12	2.39	0.57
1:B:270:LEU:HD22	1:B:321:LEU:HD21	1.86	0.57
1:C:249:GLN:HE21	1:C:260:GLY:CA	2.17	0.57
1:D:234:THR:H	1:D:237:HIS:HD2	1.50	0.57
1:C:248:GLY:O	1:C:252:ILE:HG12	2.05	0.56
1:B:247:GLN:NE2	1:D:254:GLN:OE1	2.38	0.56
1:A:166:LEU:HD23	1:A:166:LEU:O	2.06	0.55
1:B:275:HIS:O	1:B:277:HIS:HD2	1.90	0.55
1:B:250:GLU:HG3	1:D:253:LEU:HD21	1.88	0.55
1:A:163:LEU:HB3	1:A:164:PRO:HD3	1.89	0.55
1:D:158:TYR:CD1	1:D:231:ARG:HD3	2.43	0.54
1:C:270:LEU:HD22	1:C:321:LEU:HD21	1.89	0.54
1:D:189:ILE:HD12	1:D:201:VAL:CG1	2.37	0.54
1:B:277:HIS:HE1	2:B:602:PO4:O3	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LEU:HB2	1:A:298:LEU:HD13	1.92	0.52
1:D:205:ASP:OD1	3:D:404:M7G:O2'	2.24	0.52
1:A:234:THR:H	1:A:237:HIS:HD2	1.58	0.52
1:C:270:LEU:CD2	1:C:321:LEU:HD21	2.40	0.51
1:A:248:GLY:O	1:A:252:ILE:HG12	2.11	0.51
1:D:245:LEU:HB2	1:D:298:LEU:HD13	1.93	0.50
1:A:176:VAL:HG13	1:A:221:ILE:HG21	1.94	0.50
1:B:205:ASP:OD1	1:B:207:LYS:HG2	2.12	0.50
1:C:249:GLN:HE21	1:C:260:GLY:HA3	1.76	0.50
1:B:163:LEU:HB3	1:B:164:PRO:HD3	1.93	0.49
1:D:203:ILE:HD13	1:D:203:ILE:N	2.27	0.49
1:D:176:VAL:HG13	1:D:221:ILE:HG21	1.95	0.49
1:C:51:LYS:NZ	1:C:140:LEU:HD21	2.28	0.49
1:D:219:ILE:HD12	1:D:279:HIS:HA	1.94	0.48
1:C:218:LEU:HD13	1:C:252:ILE:CD1	2.43	0.48
1:B:254:GLN:NE2	1:D:250:GLU:OE2	2.46	0.48
1:A:64:LEU:O	1:A:81:VAL:HA	2.14	0.47
1:A:277:HIS:N	1:A:277:HIS:HD1	2.12	0.47
1:B:193:ASN:HB2	1:D:254:GLN:NE2	2.29	0.47
1:A:158:TYR:CD1	1:A:231:ARG:HD3	2.50	0.47
1:B:273:TYR:CZ	1:B:277:HIS:CD2	3.02	0.47
2:D:1604:PO4:O1	3:D:404:M7G:O3B	2.32	0.47
1:C:205:ASP:OD2	1:C:207:LYS:HG2	2.14	0.46
1:B:57:ALA:O	1:B:60:LYS:HD3	2.14	0.46
1:A:224:ARG:HD3	1:A:227:ILE:HD11	1.97	0.45
1:B:267:LEU:CD2	1:B:276:LEU:HD11	2.46	0.45
1:C:176:VAL:HG13	1:C:221:ILE:HG21	1.99	0.45
1:D:244:ILE:HG21	1:D:278:VAL:HG21	1.97	0.45
1:D:228:ARG:HD3	5:D:1693:HOH:O	2.17	0.45
1:A:270:LEU:HD22	1:A:321:LEU:HD21	1.98	0.44
1:A:158:TYR:CG	1:A:231:ARG:HD3	2.52	0.44
1:D:90:GLN:HE22	1:D:211:GLN:HB3	1.81	0.44
1:D:254:GLN:CG	5:D:1607:HOH:O	2.30	0.44
1:C:285:PHE:CD1	1:C:287:ALA:HB2	2.53	0.44
1:C:267:LEU:N	1:C:267:LEU:HD12	2.32	0.43
1:A:173:ILE:CG2	1:A:173:ILE:O	2.65	0.43
1:A:270:LEU:CD2	1:A:321:LEU:HD21	2.48	0.43
1:B:151:ILE:HA	1:B:151:ILE:HD13	1.90	0.43
1:C:293:GLU:O	1:C:319:PHE:HA	2.19	0.43
1:D:90:GLN:HE21	1:D:212:GLN:HB3	1.85	0.42
1:B:219:ILE:HD12	1:B:277:HIS:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ILE:HB	1:C:130:THR:HB	2.00	0.42
1:C:44:PHE:HB3	5:C:666:HOH:O	2.18	0.42
1:A:178:ASN:HB3	1:A:184:ALA:HB3	2.02	0.42
1:A:173:ILE:HG22	1:A:176:VAL:HB	2.01	0.41
1:D:216:LEU:O	1:D:281:THR:HA	2.20	0.41
1:A:173:ILE:CG2	1:A:176:VAL:HB	2.50	0.41
1:B:268:HIS:ND1	2:B:602:PO4:O1	2.53	0.41
1:A:208:TRP:HB2	1:A:217:TYR:HB3	2.02	0.41
1:C:51:LYS:HZ2	1:C:140:LEU:HD21	1.86	0.40
1:B:62:ILE:HG12	1:A:89:PHE:CD1	2.57	0.40
1:C:268:HIS:NE2	1:C:289:GLY:O	2.55	0.40
1:A:173:ILE:CD1	1:A:273:TYR:HB3	2.51	0.40
1:D:81:VAL:CG1	1:D:83:ILE:HD11	2.52	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	281/342 (82%)	272 (97%)	8 (3%)	1 (0%)	38	59
1	B	284/342 (83%)	273 (96%)	10 (4%)	1 (0%)	38	59
1	C	285/342 (83%)	269 (94%)	13 (5%)	3 (1%)	17	29
1	D	284/342 (83%)	273 (96%)	10 (4%)	1 (0%)	38	59
All	All	1134/1368 (83%)	1087 (96%)	41 (4%)	6 (0%)	32	53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	43	PRO
1	C	40	VAL

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Mol	Chain	Res	Type
1	D	122	ARG
1	B	270	LEU
1	C	270	LEU
1	A	47	PHE

### 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	261/298 (88%)	246 (94%)	15 (6%)	24	44
1	B	262/298 (88%)	242 (92%)	20 (8%)	15	29
1	C	262/298 (88%)	243 (93%)	19 (7%)	16	31
1	D	264/298 (89%)	249 (94%)	15 (6%)	24	44
All	All	1049/1192 (88%)	980 (93%)	69 (7%)	19	36

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	42	LEU
1	B	48	ARG
1	B	54	ARG
1	B	62	ILE
1	B	107	GLN
1	B	122	ARG
1	B	123	GLN
1	B	147	ASP
1	B	151	ILE
1	B	171	LEU
1	B	183	LYS
1	B	214	ASP
1	B	217	TYR
1	B	219	ILE
1	B	245	LEU
1	B	253	LEU
1	B	254	GLN

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Mol	Chain	Res	Type
1	B	262	HIS
1	B	286	GLU
1	B	298	LEU
1	A	58	ARG
1	A	83	ILE
1	A	90	GLN
1	A	109	SER
1	A	112	ILE
1	A	122	ARG
1	A	145	ARG
1	A	147	ASP
1	A	151	ILE
1	A	163	LEU
1	A	217	TYR
1	A	231	ARG
1	A	236	GLU
1	A	250	GLU
1	A	298	LEU
1	C	41	ARG
1	C	42	LEU
1	C	51	LYS
1	C	78	GLU
1	C	79	ASP
1	C	96	GLN
1	C	107	GLN
1	C	167	GLU
1	C	171	LEU
1	C	207	LYS
1	C	214	ASP
1	C	217	TYR
1	C	245	LEU
1	C	257	ARG
1	C	259	LYS
1	C	262	HIS
1	C	276	LEU
1	C	298	LEU
1	C	329	LYS
1	D	41	ARG
1	D	58	ARG
1	D	59	ASP
1	D	90	GLN
1	D	128	LYS

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Mol	Chain	Res	Type
1	D	144	LEU
1	D	163	LEU
1	D	203	ILE
1	D	217	TYR
1	D	231	ARG
1	D	250	GLU
1	D	270	LEU
1	D	298	LEU
1	D	333	GLU
1	D	337	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	50	GLN
1	B	193	ASN
1	B	211	GLN
1	B	247	GLN
1	B	277	HIS
1	A	96	GLN
1	A	146	GLN
1	A	169	GLN
1	A	210	GLN
1	A	237	HIS
1	A	254	GLN
1	C	107	GLN
1	C	211	GLN
1	C	246	HIS
1	C	249	GLN
1	C	262	HIS
1	C	336	GLN
1	D	50	GLN
1	D	69	ASN
1	D	90	GLN
1	D	96	GLN
1	D	123	GLN
1	D	210	GLN
1	D	237	HIS
1	D	249	GLN
1	D	254	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	PO4	A	1601	-	4,4,4	0.88	0	6,6,6	0.41	0
3	M7G	A	401	-	27,31,31	1.79	3 (11%)	29,49,49	1.87	6 (20%)
4	G7M	B	1502	-	23,27,27	1.68	3 (13%)	26,42,42	2.34	7 (26%)
2	PO4	B	602	-	4,4,4	0.83	0	6,6,6	0.64	0
4	G7M	C	503	-	23,27,27	1.76	4 (17%)	26,42,42	2.22	7 (26%)
2	PO4	C	603	-	4,4,4	0.84	0	6,6,6	0.56	0
2	PO4	D	1604	-	4,4,4	0.76	0	6,6,6	0.54	0
3	M7G	D	404	-	27,31,31	1.76	4 (14%)	29,49,49	1.84	7 (24%)

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	PO4	A	1601	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	M7G	A	401	-	-	0/16/44/44	0/3/3/3
4	G7M	B	1502	-	-	0/6/26/26	0/3/3/3
2	PO4	B	602	-	-	0/0/0/0	0/0/0/0
4	G7M	C	503	-	-	0/6/26/26	0/3/3/3
2	PO4	C	603	-	-	0/0/0/0	0/0/0/0
2	PO4	D	1604	-	-	0/0/0/0	0/0/0/0
3	M7G	D	404	-	-	0/16/44/44	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	404	M7G	PA-O1A	2.01	1.58	1.50
4	C	503	G7M	C8-N7	2.20	1.37	1.33
3	A	401	M7G	PB-O1B	2.28	1.58	1.50
3	D	404	M7G	PB-O1B	2.48	1.59	1.50
4	B	1502	G7M	P-OP1	2.58	1.59	1.50
4	C	503	G7M	P-OP1	2.73	1.60	1.50
4	B	1502	G7M	C6-C5	3.82	1.48	1.41
4	C	503	G7M	C6-C5	4.26	1.49	1.41
3	D	404	M7G	C6-C5	5.14	1.47	1.41
4	B	1502	G7M	C4-N3	5.14	1.44	1.35
4	C	503	G7M	C4-N3	5.24	1.44	1.35
3	A	401	M7G	C6-C5	5.58	1.47	1.41
3	D	404	M7G	PB-O3A	5.95	1.69	1.60
3	A	401	M7G	PB-O3A	5.96	1.69	1.60

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1502	G7M	C6-C5-C4	-7.20	113.69	120.84
4	C	503	G7M	C6-C5-C4	-6.76	114.12	120.84
3	D	404	M7G	C5-C6-N1	-4.81	115.83	123.37
3	A	401	M7G	C5-C6-N1	-4.23	116.74	123.37
4	B	1502	G7M	N3-C2-N1	-4.09	121.48	127.46
4	C	503	G7M	N3-C2-N1	-3.68	122.09	127.46
4	B	1502	G7M	C5-C6-N1	-2.95	119.28	123.48
4	C	503	G7M	C5-C6-N1	-2.74	119.58	123.48
3	A	401	M7G	C5-C4-N3	-2.55	122.22	126.47
3	A	401	M7G	C4-N9-C1'	-2.36	120.86	126.58
3	D	404	M7G	C5-C4-N3	-2.15	122.88	126.47
3	D	404	M7G	C4-N9-C1'	-2.08	121.53	126.58
3	D	404	M7G	N3-C4-N9	2.19	129.77	126.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	G7M	N2-C2-N1	2.20	120.76	117.24
3	D	404	M7G	N2-C2-N1	2.25	120.84	117.24
4	B	1502	G7M	N2-C2-N1	2.29	120.90	117.24
4	C	503	G7M	C2'-C3'-C4'	2.29	107.07	102.62
4	B	1502	G7M	C2-N3-C4	2.33	117.88	115.16
4	B	1502	G7M	C2'-C3'-C4'	2.39	107.28	102.62
4	C	503	G7M	C2-N3-C4	2.50	118.08	115.16
3	D	404	M7G	C2'-C3'-C4'	2.61	107.71	102.62
3	A	401	M7G	C2'-C3'-C4'	2.71	107.90	102.62
3	A	401	M7G	N3-C4-N9	2.99	130.79	126.98
3	A	401	M7G	C6-N1-C2	5.02	123.28	116.06
3	D	404	M7G	C6-N1-C2	5.07	123.35	116.06
4	C	503	G7M	C6-N1-C2	5.44	123.89	116.06
4	B	1502	G7M	C6-N1-C2	5.92	124.58	116.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	M7G	1	0
2	B	602	PO4	2	0
2	D	1604	PO4	1	0
3	D	404	M7G	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	287/342 (83%)	0.03	14 (4%) 30 32	6, 14, 44, 49	0
1	B	288/342 (84%)	0.05	13 (4%) 34 36	8, 18, 40, 46	0
1	C	289/342 (84%)	0.17	23 (7%) 13 13	6, 20, 43, 49	0
1	D	292/342 (85%)	0.10	12 (4%) 38 40	6, 16, 41, 57	0
All	All	1156/1368 (84%)	0.09	62 (5%) 26 27	6, 17, 42, 57	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	337	SER	7.4
1	D	38	ALA	6.7
1	D	113	TYR	6.1
1	A	108	PHE	5.9
1	A	113	TYR	5.8
1	B	139	HIS	5.4
1	D	39	PRO	5.1
1	A	112	ILE	4.7
1	C	42	LEU	4.6
1	C	170	SER	4.5
1	D	336	GLN	4.4
1	B	211	GLN	4.1
1	A	104	LEU	3.9
1	A	101	SER	3.8
1	C	77	GLY	3.7
1	B	136	THR	3.7
1	B	45	SER	3.6
1	C	101	SER	3.6
1	D	75	GLY	3.5
1	B	41	ARG	3.5
1	B	171	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	78	GLU	3.3
1	C	145	ARG	3.3
1	C	140	LEU	3.2
1	D	108	PHE	3.1
1	D	112	ILE	3.1
1	C	171	LEU	3.1
1	C	133	TYR	3.1
1	B	144	LEU	3.1
1	C	287	ALA	2.9
1	C	211	GLN	2.9
1	C	141	GLN	2.9
1	A	105	GLN	2.8
1	C	50	GLN	2.7
1	C	103	GLU	2.6
1	B	140	LEU	2.6
1	C	65	HIS	2.4
1	B	145	ARG	2.4
1	A	145	ARG	2.4
1	C	40	VAL	2.3
1	A	146	GLN	2.3
1	C	44	PHE	2.3
1	C	288	PRO	2.3
1	C	80	ALA	2.2
1	D	103	GLU	2.2
1	D	50	GLN	2.2
1	B	287	ALA	2.2
1	A	99	THR	2.2
1	C	79	ASP	2.2
1	C	54	ARG	2.2
1	A	109	SER	2.2
1	B	40	VAL	2.1
1	C	144	LEU	2.1
1	B	137	GLU	2.1
1	B	133	TYR	2.1
1	A	92	GLU	2.1
1	A	100	GLY	2.1
1	C	131	VAL	2.1
1	D	77	GLY	2.1
1	A	107	GLN	2.0
1	A	58	ARG	2.0
1	D	169	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no 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(Å <sup>2</sup> )	Q<0.9
2	PO4	A	1601	5/5	0.94	0.18	5.64	56,56,57,57	0
3	M7G	A	401	29/29	0.90	0.23	3.61	29,34,46,48	0
3	M7G	D	404	29/29	0.88	0.24	3.03	32,37,48,49	0
4	G7M	C	503	25/25	0.80	0.23	1.15	61,65,73,73	0
4	G7M	B	1502	25/25	0.83	0.22	1.01	59,61,68,68	0
2	PO4	D	1604	5/5	0.96	0.17	0.90	57,57,58,58	0
2	PO4	C	603	5/5	0.96	0.17	0.87	50,50,52,53	0
2	PO4	B	602	5/5	0.96	0.14	0.32	34,35,36,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.