



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2018 – 03:45 AM EST

PDB ID : 1EJH  
Title : EIF4E/EIF4G PEPTIDE/7-METHYL-GDP  
Authors : Marcotrigiano, J.; Gingras, A.-C.; Sonenberg, N.; Burley, S.K.  
Deposited on : 2000-03-02  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

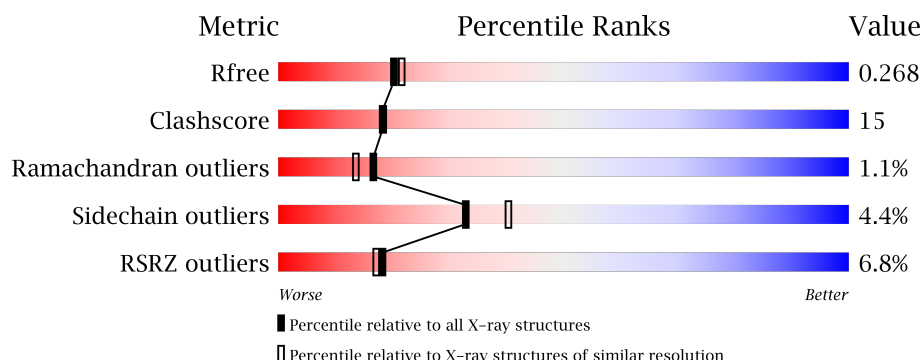
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	190	<div> <div>6%</div> <div>64% 27% 5%</div> </div>
1	B	190	<div> <div>2%</div> <div>67% 25% 5%</div> </div>
1	C	190	<div> <div>4%</div> <div>65% 28% 5%</div> </div>
1	D	190	<div> <div>11%</div> <div>62% 26% 11%</div> </div>
2	E	16	<div> <div>6%</div> <div>81% 6% 13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	16	
2	G	16	
2	H	16	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	M7G	A	1001	-	-	-	X
3	M7G	D	1004	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6481 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.

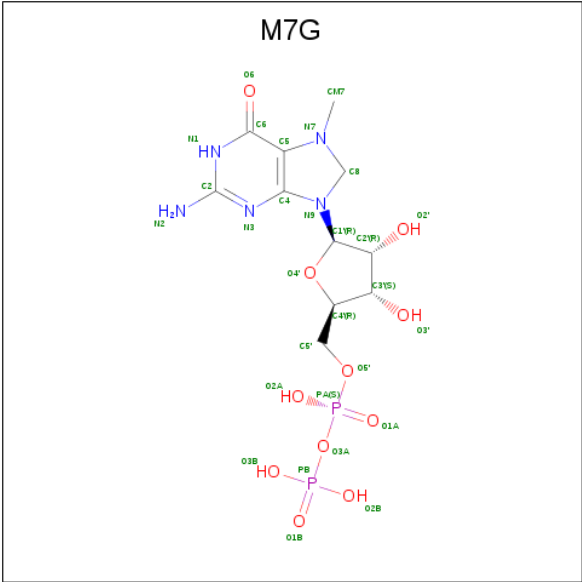
- Molecule 1 is a protein called EUKARYOTIC INITIATION FACTOR 4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1456	933	250	267	6			
1	B	180	Total	C	N	O	S	0	0	0
			1467	938	254	269	6			
1	C	181	Total	C	N	O	S	0	0	0
			1480	947	259	268	6			
1	D	169	Total	C	N	O	S	0	0	0
			1372	879	234	253	6			

- Molecule 2 is a protein called EUKARYOTIC INITIATION FACTOR 4GII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	S	0	0	0
			128	86	20	21	1			
2	F	16	Total	C	N	O	S	0	0	0
			140	94	22	23	1			
2	G	12	Total	C	N	O		0	0	0
			109	72	18	19				
2	H	11	Total	C	N	O		0	0	0
			102	70	15	17				

- Molecule 3 is 7N-METHYL-8-HYDROGUANOSINE-5'-DIPHOSPHATE (three-letter code: M7G) (formula: C<sub>11</sub>H<sub>19</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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

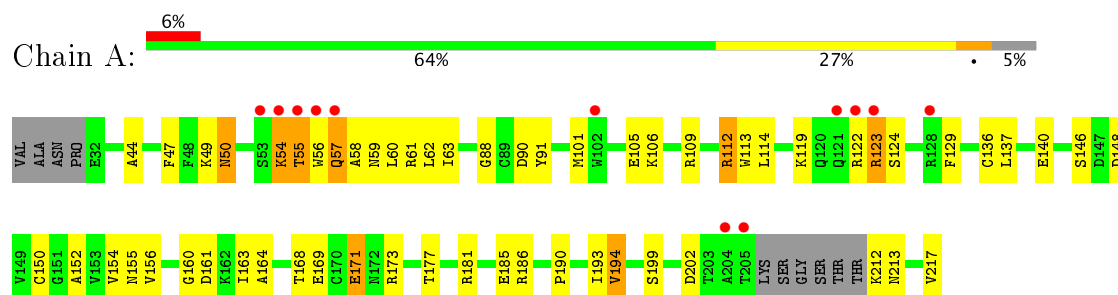
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	38	Total	O	0	0
			38	38		
4	C	19	Total	O	0	0
			19	19		
4	D	10	Total	O	0	0
			10	10		
4	E	5	Total	O	0	0
			5	5		
4	F	4	Total	O	0	0
			4	4		

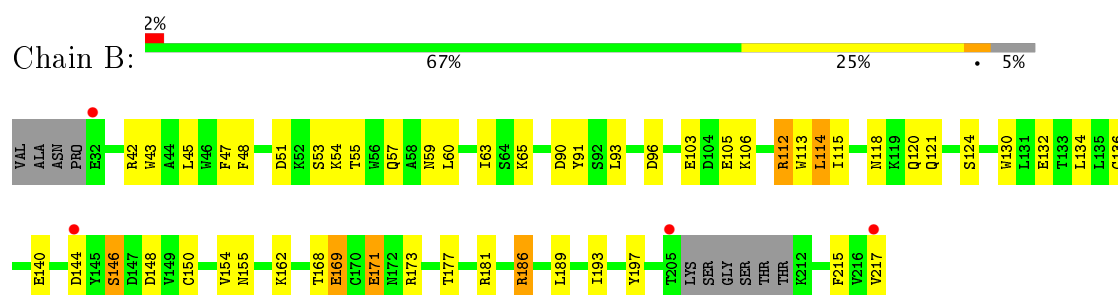
### 3 Residue-property plots [i](#)

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.

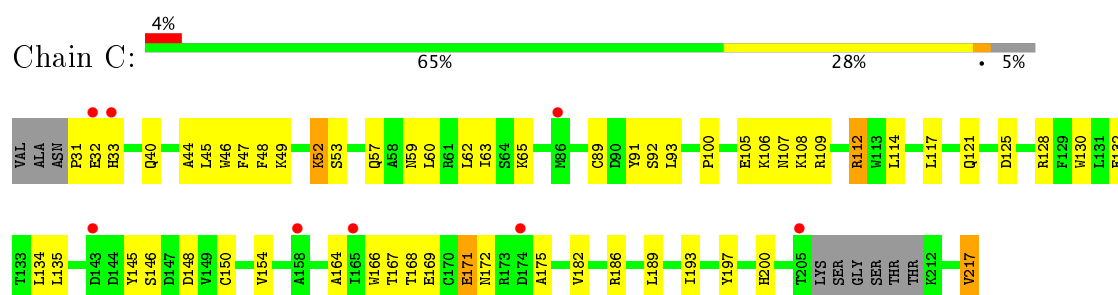
#### • Molecule 1: EUKARYOTIC INITIATION FACTOR 4E



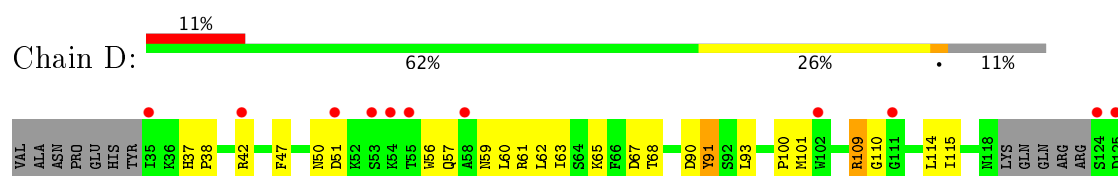
#### • Molecule 1: EUKARYOTIC INITIATION FACTOR 4E

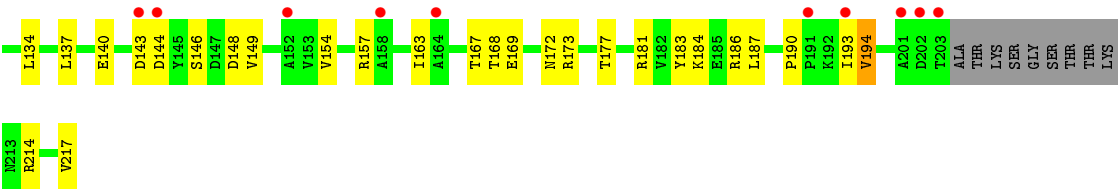


#### • Molecule 1: EUKARYOTIC INITIATION FACTOR 4E

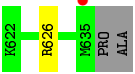
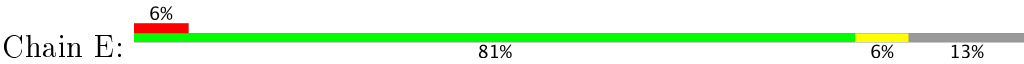


#### • Molecule 1: EUKARYOTIC INITIATION FACTOR 4E

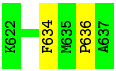
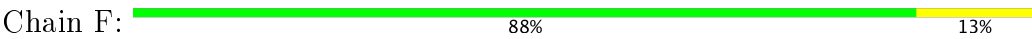




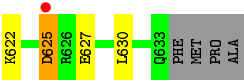
• Molecule 2: EUKARYOTIC INITIATION FACTOR 4GII



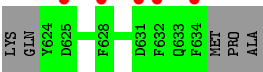
• Molecule 2: EUKARYOTIC INITIATION FACTOR 4GII



• Molecule 2: EUKARYOTIC INITIATION FACTOR 4GII



• Molecule 2: EUKARYOTIC INITIATION FACTOR 4GII



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.60 Å   140.60 Å   39.40 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.87 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.20) 96.3 (19.87-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 2.19 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.218   ,   0.261 0.230   ,   0.268	Depositor DCC
$R_{free}$ test set	4290 reflections (10.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for -h,-k,l 0.025 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6481	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.41	0/1493	0.67	0/2026
1	B	0.40	0/1505	0.64	0/2042
1	C	0.38	0/1519	0.62	0/2059
1	D	0.37	0/1407	0.58	0/1911
2	E	0.59	0/131	0.65	0/173
2	F	0.51	0/144	0.61	0/192
2	G	0.45	0/111	0.47	0/147
2	H	0.49	0/105	0.44	0/140
All	All	0.40	0/6415	0.63	0/8690

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1456	0	1389	53	0
1	B	1467	0	1398	46	0
1	C	1480	0	1424	52	0
1	D	1372	0	1301	50	0
2	E	128	0	118	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	140	0	130	1	0
2	G	109	0	100	3	0
2	H	102	0	88	0	0
3	A	29	0	16	0	0
3	B	29	0	16	0	0
3	C	29	0	16	0	0
3	D	29	0	16	1	0
4	A	35	0	0	0	0
4	B	38	0	0	1	0
4	C	19	0	0	2	0
4	D	10	0	0	0	0
4	E	5	0	0	0	0
4	F	4	0	0	0	0
All	All	6481	0	6012	186	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 15.

All (186) 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:A:177:THR:HG22	1:A:181:ARG:NH1	1.77	0.99
1:A:54:LYS:HD3	1:A:58:ALA:HB1	1.44	0.97
1:C:52:LYS:H	1:C:52:LYS:HD2	1.28	0.96
1:C:47:PHE:HB2	1:C:63:ILE:HD11	1.48	0.95
1:A:177:THR:HG22	1:A:181:ARG:HH12	1.34	0.92
1:D:109:ARG:HH11	1:D:109:ARG:HB2	1.36	0.89
1:A:136:CYS:SG	1:A:186:ARG:HG2	2.13	0.87
1:D:181:ARG:CZ	1:D:217:VAL:HG13	2.05	0.87
1:B:57:GLN:HB3	1:D:57:GLN:NE2	1.92	0.83
1:A:57:GLN:NE2	1:C:57:GLN:HB3	1.94	0.82
1:B:189:LEU:HD22	1:B:193:ILE:HD11	1.62	0.82
1:A:44:ALA:HB1	1:A:62:LEU:HD11	1.67	0.76
1:C:52:LYS:N	1:C:52:LYS:HD2	2.01	0.74
1:C:106:LYS:O	1:C:168:THR:HG22	1.88	0.74
1:C:112:ARG:HG3	1:C:164:ALA:HB1	1.68	0.74
1:A:177:THR:CG2	1:A:181:ARG:NH1	2.52	0.73
1:A:193:ILE:O	1:A:194:VAL:HG22	1.88	0.73
1:C:47:PHE:HE2	1:C:49:LYS:HG2	1.57	0.69
1:B:106:LYS:O	1:B:168:THR:HG22	1.91	0.69
1:C:52:LYS:CD	1:C:52:LYS:H	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:PRO:HD2	1:A:193:ILE:HD12	1.75	0.69
1:B:186:ARG:HH11	1:B:186:ARG:HB3	1.58	0.69
1:A:123:ARG:O	1:A:124:SER:HB3	1.92	0.69
1:A:212:LYS:HD2	1:A:213:ASN:H	1.56	0.68
1:D:193:ILE:HD12	1:D:194:VAL:N	2.09	0.68
1:A:169:GLU:OE2	1:A:171:GLU:HB2	1.94	0.67
1:A:54:LYS:HD3	1:A:58:ALA:CB	2.21	0.67
1:B:93:LEU:HD22	1:B:134:LEU:HD22	1.76	0.67
1:B:150:CYS:SG	1:B:168:THR:HG23	2.34	0.67
1:B:113:TRP:CH2	1:B:217:VAL:HG23	2.30	0.66
1:D:184:LYS:HE3	1:D:193:ILE:HD11	1.77	0.65
1:B:112:ARG:O	1:B:112:ARG:HG2	1.97	0.65
1:C:150:CYS:SG	1:C:168:THR:HG23	2.36	0.65
1:D:60:LEU:HD21	1:D:100:PRO:HG2	1.77	0.65
1:A:212:LYS:CD	1:A:213:ASN:H	2.10	0.65
1:C:49:LYS:O	1:C:59:ASN:HB3	1.99	0.63
1:B:189:LEU:HD22	1:B:193:ILE:CD1	2.27	0.63
1:A:58:ALA:C	1:A:60:LEU:H	2.02	0.62
1:C:47:PHE:CE2	1:C:49:LYS:HG2	2.35	0.62
1:C:105:GLU:HA	1:C:108:LYS:HE3	1.82	0.62
1:A:112:ARG:HG3	1:A:164:ALA:HB1	1.82	0.61
1:B:47:PHE:HB2	1:B:63:ILE:HD11	1.84	0.60
1:C:186:ARG:HB3	1:C:186:ARG:NH1	2.17	0.60
1:B:54:LYS:HG2	1:D:61:ARG:HE	1.67	0.59
1:C:60:LEU:HD21	1:C:100:PRO:HG2	1.84	0.59
1:A:119:LYS:HD3	1:A:160:GLY:H	1.68	0.59
1:A:44:ALA:HB1	1:A:62:LEU:CD1	2.31	0.58
1:C:62:LEU:HD23	1:D:173:ARG:HB2	1.84	0.58
1:A:55:THR:O	1:A:58:ALA:HB3	2.03	0.58
1:D:169:GLU:HB2	1:D:172:ASN:ND2	2.19	0.58
1:C:65:LYS:CG	1:D:177:THR:HG21	2.34	0.58
1:B:53:SER:O	1:D:61:ARG:HD3	2.04	0.58
1:D:109:ARG:HD2	1:D:169:GLU:OE2	2.05	0.57
1:D:186:ARG:HB3	1:D:186:ARG:NH1	2.20	0.57
1:A:50:ASN:HB2	1:A:88:GLY:O	2.06	0.56
1:A:106:LYS:O	1:A:168:THR:HG22	2.05	0.56
1:C:46:TRP:HB2	1:C:92:SER:HB2	1.87	0.56
1:D:62:LEU:HD21	1:D:65:LYS:HE3	1.87	0.55
1:D:183:TYR:CZ	1:D:187:LEU:HD11	2.41	0.55
1:D:137:LEU:HD22	1:D:149:VAL:HG11	1.89	0.55
1:B:51:ASP:HB3	1:B:59:ASN:OD1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASN:ND2	1:B:120:GLN:H	2.05	0.55
1:D:186:ARG:HB3	1:D:186:ARG:HH11	1.72	0.54
1:B:54:LYS:HG2	1:D:61:ARG:NE	2.22	0.54
1:A:57:GLN:NE2	1:C:57:GLN:CB	2.69	0.54
1:A:150:CYS:SG	1:A:168:THR:HG23	2.48	0.54
1:C:217:VAL:HG13	4:C:1016:HOH:O	2.07	0.54
1:A:129:PHE:HB3	1:A:163:ILE:HD12	1.89	0.54
1:A:194:VAL:HA	1:A:217:VAL:O	2.09	0.53
1:B:54:LYS:HE3	1:D:61:ARG:HH21	1.72	0.53
1:C:40:GLN:HA	2:G:622:LYS:HD2	1.89	0.53
1:C:91:TYR:HB2	1:C:154:VAL:CG1	2.39	0.53
1:A:49:LYS:O	1:A:59:ASN:HB3	2.09	0.52
1:A:58:ALA:C	1:A:60:LEU:N	2.63	0.52
1:B:55:THR:HG21	1:D:60:LEU:HD23	1.91	0.52
1:D:109:ARG:NH1	1:D:109:ARG:HB2	2.17	0.52
1:A:57:GLN:HE21	1:C:57:GLN:HB3	1.71	0.52
1:D:51:ASP:HB3	1:D:59:ASN:OD1	2.09	0.52
1:C:32:GLU:O	1:C:32:GLU:HG2	2.10	0.52
1:B:112:ARG:HD2	4:B:1037:HOH:O	2.11	0.51
1:D:114:LEU:HD23	1:D:115:ILE:N	2.25	0.51
1:D:42:ARG:HB2	1:D:42:ARG:NH1	2.26	0.51
1:A:140:GLU:OE1	1:A:146:SER:HB3	2.10	0.50
1:A:156:VAL:HA	1:A:161:ASP:OD1	2.12	0.50
1:D:181:ARG:NE	1:D:217:VAL:HG13	2.25	0.50
1:D:181:ARG:NH1	1:D:217:VAL:HG13	2.26	0.50
1:D:47:PHE:HB2	1:D:63:ILE:HD11	1.94	0.50
1:B:132:GLU:OE2	1:B:186:ARG:NH1	2.45	0.50
1:A:122:ARG:O	1:A:124:SER:N	2.45	0.50
1:B:55:THR:OG1	1:D:57:GLN:HG2	2.12	0.49
1:B:45:LEU:HG	1:B:63:ILE:HD12	1.93	0.49
1:A:112:ARG:O	1:A:112:ARG:HG2	2.11	0.49
1:A:47:PHE:HB2	1:A:63:ILE:HD11	1.94	0.49
1:C:145:TYR:CD2	1:C:175:ALA:HA	2.47	0.49
1:C:186:ARG:HB3	1:C:186:ARG:HH11	1.76	0.49
1:C:65:LYS:HG3	1:D:177:THR:HG21	1.94	0.49
1:B:42:ARG:HD3	1:B:96:ASP:OD2	2.12	0.49
1:C:189:LEU:HB3	1:C:193:ILE:HD11	1.94	0.48
1:B:189:LEU:HB3	1:B:193:ILE:HD11	1.95	0.48
2:G:625:ASP:OD1	2:G:627:GLU:N	2.47	0.48
1:D:109:ARG:HH11	1:D:109:ARG:CB	2.18	0.47
1:D:67:ASP:OD1	1:D:68:THR:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:PRO:O	1:D:193:ILE:HG13	2.15	0.47
1:A:54:LYS:CD	1:A:58:ALA:HB1	2.30	0.47
1:C:182:VAL:O	1:C:186:ARG:HG2	2.13	0.47
1:C:112:ARG:HG3	1:C:164:ALA:CB	2.43	0.47
1:C:166:TRP:HB3	4:C:1021:HOH:O	2.14	0.47
1:B:154:VAL:HG13	1:B:154:VAL:O	2.15	0.47
1:B:140:GLU:OE1	1:B:146:SER:HB3	2.14	0.47
1:A:91:TYR:HB2	1:A:154:VAL:CG1	2.46	0.46
1:C:169:GLU:HG3	1:C:171:GLU:H	1.80	0.46
1:B:48:PHE:HD1	1:B:60:LEU:HD12	1.79	0.46
1:D:91:TYR:HB2	1:D:154:VAL:CG1	2.45	0.46
1:A:177:THR:CG2	1:A:181:ARG:HH11	2.29	0.45
1:A:56:TRP:C	1:A:58:ALA:H	2.19	0.45
1:D:110:GLY:HA3	1:D:167:THR:O	2.16	0.45
1:A:173:ARG:O	1:A:177:THR:HB	2.17	0.45
1:B:130:TRP:CE3	1:B:154:VAL:HB	2.51	0.45
1:B:136:CYS:SG	1:B:186:ARG:NH1	2.90	0.45
1:B:57:GLN:HB3	1:D:57:GLN:HE21	1.79	0.45
1:A:113:TRP:O	1:A:164:ALA:HA	2.17	0.45
1:C:135:LEU:HD11	2:G:630:LEU:HD21	1.98	0.45
1:C:65:LYS:HB2	1:D:177:THR:HG21	1.98	0.44
1:B:173:ARG:HG2	1:B:215:PHE:CZ	2.52	0.44
1:C:189:LEU:HD13	1:C:193:ILE:HD11	1.99	0.44
1:D:194:VAL:HA	1:D:217:VAL:O	2.17	0.44
1:A:56:TRP:CZ3	1:A:101:MET:HG2	2.52	0.44
1:B:118:ASN:HD21	1:B:120:GLN:CB	2.29	0.44
1:D:101:MET:HA	3:D:1004:M7G:O6	2.18	0.44
1:A:105:GLU:OE2	1:A:109:ARG:NH2	2.45	0.44
1:A:199:SER:HB3	1:A:202:ASP:OD2	2.18	0.44
1:A:57:GLN:HG3	1:A:101:MET:SD	2.58	0.44
1:B:121:GLN:HA	1:B:124:SER:OG	2.17	0.44
1:A:137:LEU:HD11	1:A:152:ALA:CB	2.48	0.44
1:A:212:LYS:HD2	1:A:213:ASN:N	2.29	0.44
1:A:212:LYS:CG	1:A:213:ASN:N	2.81	0.44
1:C:65:LYS:HB2	1:D:177:THR:CG2	2.48	0.44
1:C:44:ALA:HB1	1:C:62:LEU:HD11	2.00	0.43
1:B:173:ARG:HG2	1:B:215:PHE:HZ	1.83	0.43
1:A:56:TRP:HZ3	1:A:101:MET:HG2	1.83	0.43
1:B:154:VAL:HA	1:B:162:LYS:O	2.19	0.43
1:C:132:GLU:OE2	1:C:186:ARG:NH1	2.41	0.43
1:D:214:ARG:HH11	1:D:214:ARG:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ASP:CG	1:B:155:ASN:HD22	2.22	0.43
1:C:169:GLU:HB3	1:C:172:ASN:ND2	2.34	0.43
2:F:634:PHE:C	2:F:636:PRO:HD3	2.39	0.43
1:A:90:ASP:CG	1:A:155:ASN:HD22	2.22	0.43
1:B:114:LEU:HD23	1:B:115:ILE:N	2.33	0.42
1:B:150:CYS:SG	1:B:168:THR:CG2	3.07	0.42
1:B:169:GLU:OE1	1:B:171:GLU:HB2	2.19	0.42
1:B:103:GLU:OE1	1:B:103:GLU:N	2.44	0.42
1:B:112:ARG:O	1:B:197:TYR:HA	2.19	0.42
1:C:31:PRO:C	1:C:33:HIS:H	2.23	0.42
1:D:154:VAL:HG23	1:D:163:ILE:HG12	2.01	0.42
1:B:118:ASN:OD1	1:B:121:GLN:HG3	2.20	0.42
1:A:61:ARG:HD2	1:C:53:SER:O	2.18	0.42
1:D:93:LEU:HD22	1:D:134:LEU:HD22	2.01	0.42
1:C:117:LEU:HA	1:C:121:GLN:OE1	2.19	0.42
1:D:184:LYS:HE3	1:D:193:ILE:CD1	2.44	0.42
1:C:189:LEU:HB3	1:C:193:ILE:HG12	2.01	0.42
1:C:167:THR:HG1	1:C:197:TYR:HH	1.65	0.42
1:D:140:GLU:OE1	1:D:146:SER:HB3	2.20	0.42
1:C:130:TRP:CZ2	1:C:134:LEU:HD21	2.54	0.42
1:C:93:LEU:HD22	1:C:134:LEU:HD22	2.01	0.42
1:B:177:THR:CG2	1:B:181:ARG:NH1	2.83	0.42
1:C:48:PHE:CE1	1:C:59:ASN:HB2	2.55	0.41
1:C:189:LEU:HB3	1:C:193:ILE:CD1	2.50	0.41
1:D:37:HIS:HA	1:D:38:PRO:HD2	1.87	0.41
1:C:48:PHE:O	1:C:89:CYS:HA	2.20	0.41
1:A:49:LYS:O	1:A:59:ASN:CB	2.68	0.41
1:A:55:THR:O	1:A:58:ALA:CB	2.66	0.41
1:B:171:GLU:OE1	1:B:171:GLU:HA	2.20	0.41
1:C:107:ASN:O	1:C:200:HIS:HD2	2.03	0.41
1:D:214:ARG:HG3	1:D:214:ARG:NH1	2.36	0.41
1:D:42:ARG:HB2	1:D:42:ARG:CZ	2.51	0.41
1:D:56:TRP:CH2	1:D:101:MET:HB3	2.56	0.41
1:A:186:ARG:NH2	2:E:626:ARG:HB2	2.36	0.41
1:B:43:TRP:O	1:B:65:LYS:HA	2.21	0.41
1:B:91:TYR:HB2	1:B:154:VAL:CG1	2.50	0.41
1:B:186:ARG:HH11	1:B:186:ARG:CB	2.31	0.41
1:C:45:LEU:HG	1:C:63:ILE:HD12	2.02	0.41
1:D:114:LEU:C	1:D:114:LEU:HD23	2.40	0.41
1:C:125:ASP:OD1	1:C:128:ARG:NH2	2.48	0.40
1:A:190:PRO:HG2	1:A:193:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:LEU:HB3	1:C:193:ILE:CG1	2.51	0.40
1:D:90:ASP:OD1	1:D:157:ARG:NH1	2.53	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	176/190 (93%)	160 (91%)	11 (6%)	5 (3%)	6	3
1	B	176/190 (93%)	173 (98%)	3 (2%)	0	100	100
1	C	177/190 (93%)	168 (95%)	9 (5%)	0	100	100
1	D	163/190 (86%)	153 (94%)	7 (4%)	3 (2%)	10	6
2	E	12/16 (75%)	12 (100%)	0	0	100	100
2	F	14/16 (88%)	14 (100%)	0	0	100	100
2	G	10/16 (62%)	10 (100%)	0	0	100	100
2	H	9/16 (56%)	7 (78%)	2 (22%)	0	100	100
All	All	737/824 (89%)	697 (95%)	32 (4%)	8 (1%)	17	13

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	THR
1	A	194	VAL
1	A	54	LYS
1	A	123	ARG
1	D	194	VAL
1	A	57	GLN
1	D	144	ASP
1	D	143	ASP

### 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	153/169 (90%)	147 (96%)	6 (4%)	37	46
1	B	155/169 (92%)	146 (94%)	9 (6%)	23	27
1	C	157/169 (93%)	149 (95%)	8 (5%)	28	33
1	D	146/169 (86%)	141 (97%)	5 (3%)	42	53
2	E	13/15 (87%)	13 (100%)	0	100	100
2	F	14/15 (93%)	14 (100%)	0	100	100
2	G	11/15 (73%)	10 (91%)	1 (9%)	11	11
2	H	10/15 (67%)	10 (100%)	0	100	100
All	All	659/736 (90%)	630 (96%)	29 (4%)	33	40

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	112	ARG
1	A	114	LEU
1	A	148	ASP
1	A	171	GLU
1	A	185	GLU
1	B	105	GLU
1	B	112	ARG
1	B	114	LEU
1	B	144	ASP
1	B	146	SER
1	B	148	ASP
1	B	169	GLU
1	B	171	GLU
1	B	186	ARG
1	C	52	LYS
1	C	109	ARG
1	C	112	ARG
1	C	114	LEU

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Mol	Chain	Res	Type
1	C	146	SER
1	C	148	ASP
1	C	171	GLU
1	C	217	VAL
1	D	50	ASN
1	D	91	TYR
1	D	109	ARG
1	D	148	ASP
1	D	168	THR
2	G	625	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	57	GLN
1	B	78	HIS
1	B	118	ASN
1	C	50	ASN
1	D	50	ASN
1	D	57	GLN
1	D	78	HIS

### 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 ⓘ

4 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$
3	M7G	A	1001	-	27,31,31	3.05	7 (25%)	29,49,49	2.26	7 (24%)
3	M7G	B	1002	-	27,31,31	3.04	7 (25%)	29,49,49	2.35	8 (27%)
3	M7G	C	1003	-	27,31,31	3.05	7 (25%)	29,49,49	2.31	5 (17%)
3	M7G	D	1004	-	27,31,31	3.07	7 (25%)	29,49,49	2.29	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
3	M7G	A	1001	-	-	0/16/44/44	0/3/3/3
3	M7G	B	1002	-	-	0/16/44/44	0/3/3/3
3	M7G	C	1003	-	-	0/16/44/44	0/3/3/3
3	M7G	D	1004	-	-	0/16/44/44	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1003	M7G	C6-C5	-11.06	1.28	1.41
3	B	1002	M7G	C6-C5	-10.72	1.28	1.41
3	A	1001	M7G	C6-C5	-10.28	1.29	1.41
3	D	1004	M7G	C6-C5	-10.23	1.29	1.41
3	B	1002	M7G	C8-N9	-6.65	1.35	1.45
3	A	1001	M7G	C8-N9	-6.58	1.35	1.45
3	D	1004	M7G	C8-N9	-6.50	1.36	1.45
3	C	1003	M7G	C8-N9	-6.37	1.36	1.45
3	A	1001	M7G	C8-N7	-2.80	1.31	1.43
3	C	1003	M7G	C8-N7	-2.73	1.31	1.43
3	D	1004	M7G	C8-N7	-2.70	1.31	1.43
3	B	1002	M7G	C8-N7	-2.64	1.31	1.43
3	C	1003	M7G	C5-C4	2.04	1.44	1.39
3	B	1002	M7G	C5-C4	2.09	1.44	1.39
3	A	1001	M7G	C5-C4	2.09	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1004	M7G	C5-C4	2.26	1.45	1.39
3	B	1002	M7G	O2'-C2'	2.50	1.48	1.43
3	C	1003	M7G	O2'-C2'	2.66	1.49	1.43
3	D	1004	M7G	O2'-C2'	2.84	1.49	1.43
3	A	1001	M7G	O2'-C2'	2.95	1.49	1.43
3	C	1003	M7G	C4-N3	4.62	1.40	1.34
3	B	1002	M7G	C6-N1	4.87	1.41	1.33
3	B	1002	M7G	C4-N3	5.03	1.40	1.34
3	C	1003	M7G	C6-N1	5.03	1.42	1.33
3	A	1001	M7G	C6-N1	5.48	1.43	1.33
3	A	1001	M7G	C4-N3	5.50	1.41	1.34
3	D	1004	M7G	C6-N1	5.50	1.43	1.33
3	D	1004	M7G	C4-N3	5.55	1.41	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1004	M7G	C5-C6-N1	-7.06	112.30	123.37
3	C	1003	M7G	C5-C6-N1	-7.00	112.39	123.37
3	B	1002	M7G	C5-C6-N1	-6.93	112.50	123.37
3	A	1001	M7G	C5-C6-N1	-6.88	112.58	123.37
3	C	1003	M7G	C4-N9-C1'	-4.68	115.26	126.58
3	B	1002	M7G	C4-N9-C1'	-4.42	115.89	126.58
3	A	1001	M7G	C4-N9-C1'	-4.25	116.28	126.58
3	D	1004	M7G	C4-N9-C1'	-4.15	116.54	126.58
3	B	1002	M7G	N1-C2-N3	-2.45	121.48	125.45
3	B	1002	M7G	O4'-C4'-C3'	-2.35	100.49	105.17
3	C	1003	M7G	N1-C2-N3	-2.29	121.74	125.45
3	A	1001	M7G	N1-C2-N3	-2.26	121.79	125.45
3	D	1004	M7G	N1-C2-N3	-2.20	121.87	125.45
3	B	1002	M7G	C5-C4-N3	-2.06	123.03	126.47
3	A	1001	M7G	C5-C4-N3	-2.05	123.05	126.47
3	D	1004	M7G	C5-C4-N3	-2.03	123.07	126.47
3	A	1001	M7G	O5'-C5'-C4'	2.17	116.69	109.00
3	D	1004	M7G	O5'-C5'-C4'	2.29	117.13	109.00
3	B	1002	M7G	O5'-C5'-C4'	2.35	117.33	109.00
3	D	1004	M7G	C5-C4-N9	2.87	110.48	106.31
3	A	1001	M7G	C5-C4-N9	2.87	110.48	106.31
3	B	1002	M7G	C5-C4-N9	3.01	110.69	106.31
3	C	1003	M7G	C5-C4-N9	3.08	110.79	106.31
3	A	1001	M7G	C6-N1-C2	6.72	125.72	116.06
3	C	1003	M7G	C6-N1-C2	6.85	125.91	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1004	M7G	C6-N1-C2	6.95	126.06	116.06
3	B	1002	M7G	C6-N1-C2	7.10	126.27	116.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1004	M7G	1	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	180/190 (94%)	0.26	12 (6%) 19 17	12, 26, 58, 69	0
1	B	180/190 (94%)	0.05	4 (2%) 62 60	12, 27, 42, 49	0
1	C	181/190 (95%)	0.29	8 (4%) 35 33	16, 32, 48, 66	0
1	D	169/190 (88%)	0.74	21 (12%) 4 4	27, 41, 58, 67	0
2	E	14/16 (87%)	0.09	1 (7%) 17 16	19, 27, 42, 46	0
2	F	16/16 (100%)	-0.36	0 100 100	16, 24, 34, 34	0
2	G	12/16 (75%)	0.64	1 (8%) 12 11	39, 45, 54, 54	0
2	H	11/16 (68%)	1.69	5 (45%) 0 0	51, 54, 59, 59	0
All	All	763/824 (92%)	0.33	52 (6%) 18 17	12, 31, 54, 69	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	203	THR	6.2
1	A	55	THR	5.1
1	C	205	THR	4.9
1	D	54	LYS	4.7
1	C	158	ALA	4.5
1	A	205	THR	4.3
1	D	55	THR	4.3
1	D	144	ASP	4.2
1	D	53	SER	4.2
1	C	33	HIS	4.1
1	D	201	ALA	4.1
1	D	158	ALA	3.9
2	H	632	PHE	3.9
1	A	123	ARG	3.6
1	A	57	GLN	3.6
2	H	634	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	121	GLN	3.6
1	D	124	SER	3.5
1	A	53	SER	3.4
1	A	56	TRP	3.3
2	H	631	ASP	3.2
1	C	143	ASP	3.2
1	A	204	ALA	3.1
1	C	174	ASP	3.0
2	H	625	ASP	3.0
1	D	143	ASP	3.0
1	A	54	LYS	3.0
1	D	193	ILE	3.0
1	C	86	MET	2.9
1	C	32	GLU	2.9
1	D	111	GLY	2.7
1	A	102	TRP	2.6
1	D	202	ASP	2.6
1	D	125	ASP	2.5
1	D	58	ALA	2.5
1	D	191	PRO	2.4
1	D	35	ILE	2.4
1	A	122	ARG	2.3
1	D	42	ARG	2.3
2	E	635	MET	2.3
1	D	152	ALA	2.3
1	D	164	ALA	2.3
1	D	102	TRP	2.3
1	B	205	THR	2.2
1	C	165	ILE	2.2
1	B	217	VAL	2.2
1	B	144	ASP	2.2
2	H	628	PHE	2.2
1	D	51	ASP	2.2
1	B	32	GLU	2.1
2	G	625	ASP	2.1
1	A	128	ARG	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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	M7G	D	1004	29/29	0.87	0.33	4.13	46,50,59,59	0
3	M7G	A	1001	29/29	0.82	0.36	3.30	45,49,61,62	0
3	M7G	C	1003	29/29	0.95	0.10	-0.99	24,29,35,37	0
3	M7G	B	1002	29/29	0.95	0.10	-1.32	22,31,34,35	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.