



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:33 PM GMT

PDB ID : 3U2Q  
Title : EF-Tu (Escherichia coli) in complex with NVP-LFF571  
Authors : Palestrant, D.J.  
Deposited on : 2011-10-04  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

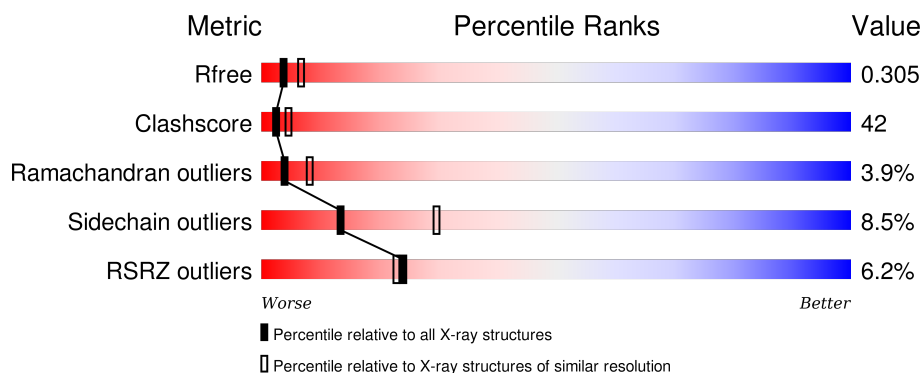
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	394	<div> <div>6%</div> <div>38%</div> <div>53%</div> <div>6% ..</div> </div>
2	B	12	<div> <div>75%</div> <div>25%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MH6	B	11	-	X	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3176 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 Elongation factor Tu 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2966	1874	510	569	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP P0CE47
A	1	ALA	-	EXPRESSION TAG	UNP P0CE47

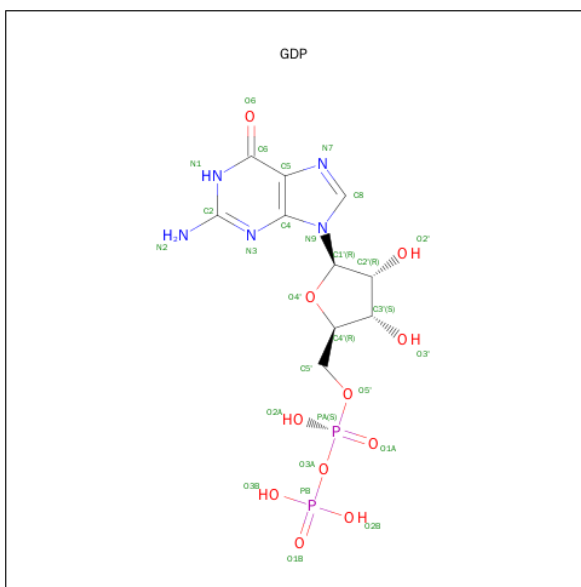
- Molecule 2 is a protein called Thiocillin GE2270 analogue NVP-LFF571.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	S	0	0	0
			92	60	13	13	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	12	7BB	CYS	SEE REMARK 999	UNP Q7M0J8

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</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
			28	10	5	11	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	82	Total	O	0	0
			82	82		
5	B	7	Total	O	0	0
			7	7		

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 ( $\text{RSRZ} > 2$ ). 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.

Chain A:

6% 38% 53% 6%

MET ALA LYS GLU LYS PHE E6 R7 T8 K9 P10 H11 V12 M13 V14 G15 T16 H19 V20 D21 G23 K24 K25 T26 L27 T31 T32 T33 V34 L35 A36 K37 G41 A42 A43 A44 A45 F46 D47 Q48 I49 D50 N51 A52 P53 E54 E55 K56 A57 ARG GLY ILE T61 P62 F63 T64 N65 S65 H66 V67 E68 V69 D70 R74 H75 Y76 A77 H79 D80 C81 P82 D86 H87 W88 K89 N90 T93 G94 T96 A96 G97 N98 D99 G100 L103 V104 V105 A106 T108 P111 M112 P113 Q114 T115 I119 D120 L121 G122 R123 Q124 V125 G126 V127 P128 V132 P133 F134 L134 N135 K136 C137 D138 M139 Y140 D141 D142 E143 A144 L145 L146 E147 V148 V149 G224 M151 E152 V153 E154 E155 L156 L157 Y160 D161 F162 P163 G164 T167 P168 I169 G172 S173 A174 L175 K176 A177 L178 E179 G180 D181 A182 E183 W184 E185 A186 K187 L189 Y198 I199 E201 P202 E284 E285 L286 T206 D207 K208 P209 F210 L211 L212 V217 I220 G222 R223 G224 T225 V226 V227 V231 E232 R233 G234 I235 K236 K237 E240 E243 I244 V245 G246 I247 K248 K252 S253 T256 E259 M260 F261 R262 K263 L264 A270 V276 L277 L278 R279 K282 R283 E284 E285 L286 G289 K290 V291 L292 K293 K294 P295 T296 T297 L298 H301 T302 K303 F304 E305 S306 E307 V308 L311 S312 K313 R318 R319 T320 P321 F322 F323 V326 G327 P328 K329 F330 V331 F332 K333 T334 T335 D336 V337 T338 G339 T340 P344 V347 K351 K357 K358 T361 L362 L363 H364 G368 D369 D370 G371 L372 R373 E378 R381 L382 V383 V387 K390 V391 L392 G393

Chain B:

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.30 Å 132.47 Å 37.43 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.02 – 2.70 39.02 – 2.69	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.02-2.70) 93.5 (39.02-2.69)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.69 Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.233 , 0.315 0.229 , 0.305	Depositor DCC
$R_{free}$ test set	582 reflections (5.46%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.4	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 69.9	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 11337 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3176	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: GDP, MG, MEN, BB7, 7BB, BB9, BB8, MH6, BB6

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	0.37	0/3020	0.70	0/4089
2	B	2.18	1/10 (10.0%)	2.57	1/9 (11.1%)
All	All	0.39	1/3030 (0.0%)	0.71	1/4098 (0.0%)

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
2	B	1	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	SER	CA-CB	-5.87	1.44	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	SER	CB-CA-C	5.16	119.91	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	SER	CA

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	2966	0	2973	256	0
2	B	92	0	63	1	0
3	A	28	0	12	6	0
4	A	1	0	0	0	0
5	A	82	0	0	11	0
5	B	7	0	0	0	0
All	All	3176	0	3048	257	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 42.

All (257) 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:55:GLU:HG2	1:A:61:THR:HA	1.24	1.11
1:A:52:ALA:HB1	1:A:63:ASN:HB3	1.23	1.10
1:A:119:ILE:HD12	1:A:156:LEU:HD12	1.41	0.99
1:A:44:ARG:HB3	1:A:49:ILE:HD11	1.51	0.93
1:A:202:PRO:HD3	5:A:446:HOH:O	1.69	0.92
1:A:208:LYS:HB2	1:A:233:ARG:HD2	1.50	0.91
1:A:22:HIS:CD2	1:A:106:ALA:H	1.89	0.90
1:A:112:MET:HB3	1:A:113:PRO:HD2	1.55	0.88
1:A:327:ARG:CD	1:A:340:THR:HG22	2.03	0.88
1:A:52:ALA:HB2	1:A:82:PRO:HG2	1.56	0.86
1:A:55:GLU:HG2	1:A:61:THR:CA	2.08	0.84
1:A:318:ARG:HD3	1:A:320:THR:O	1.83	0.79
1:A:55:GLU:CG	1:A:56:LYS:H	1.97	0.77
1:A:52:ALA:CB	1:A:63:ASN:HB3	2.12	0.77
1:A:327:ARG:HD2	1:A:340:THR:HG22	1.64	0.76
1:A:370:ASP:OD1	1:A:390:LYS:HA	1.86	0.74
1:A:303:LYS:HG2	1:A:361:THR:HG22	1.69	0.73
1:A:243:GLU:HG2	1:A:252:LYS:HE3	1.71	0.72
1:A:62:ILE:HG21	1:A:90:ASN:ND2	2.03	0.72
1:A:88:VAL:HG22	1:A:121:LEU:HD11	1.72	0.71
1:A:22:HIS:HD2	1:A:105:VAL:HA	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:TYR:HA	1:A:336:ASP:HA	1.73	0.70
1:A:55:GLU:HG3	1:A:56:LYS:H	1.57	0.69
1:A:208:LYS:CB	1:A:233:ARG:HD2	2.22	0.69
1:A:303:LYS:HG2	1:A:361:THR:CG2	2.21	0.69
1:A:244:ILE:HD12	1:A:244:ILE:N	2.07	0.69
1:A:331:TYR:HD1	1:A:336:ASP:HB3	1.57	0.69
1:A:204:ARG:HD2	5:A:457:HOH:O	1.93	0.69
1:A:55:GLU:HG3	1:A:56:LYS:N	2.08	0.68
1:A:55:GLU:CD	1:A:56:LYS:H	1.97	0.68
1:A:55:GLU:CG	1:A:56:LYS:N	2.58	0.67
1:A:20:VAL:HG23	1:A:114:GLN:HE22	1.60	0.65
1:A:7:ARG:CB	1:A:7:ARG:HH11	2.09	0.65
1:A:25:THR:HA	1:A:80:ASP:OD1	1.97	0.64
1:A:327:ARG:HD3	1:A:340:THR:HG22	1.79	0.64
1:A:243:GLU:CG	1:A:252:LYS:HE3	2.27	0.64
1:A:181:ASP:OD1	1:A:183:GLU:HB3	1.98	0.64
1:A:119:ILE:HD13	1:A:157:LEU:HD23	1.80	0.63
1:A:283:ARG:O	1:A:283:ARG:HD3	1.99	0.63
1:A:44:ARG:HD2	1:A:49:ILE:HG13	1.82	0.62
1:A:302:THR:HG23	1:A:303:LYS:HG3	1.81	0.62
1:A:100:GLY:HA3	1:A:199:ILE:HD12	1.80	0.62
1:A:150:GLU:O	1:A:154:ARG:HG2	2.00	0.62
1:A:201:GLU:HA	5:A:446:HOH:O	1.99	0.61
1:A:20:VAL:HG23	1:A:114:GLN:NE2	2.15	0.61
1:A:252:LYS:HE2	1:A:295:PRO:HB3	1.82	0.61
1:A:259:GLU:OE2	1:A:262:ARG:HA	2.00	0.61
1:A:212:LEU:HB3	1:A:292:LEU:HB2	1.83	0.61
1:A:145:LEU:C	1:A:147:GLU:H	2.03	0.60
1:A:52:ALA:HB2	1:A:82:PRO:CG	2.30	0.60
1:A:55:GLU:OE2	1:A:62:ILE:HB	2.01	0.60
1:A:203:GLU:HG2	1:A:207:ASP:HB2	1.84	0.60
1:A:135:ASN:CG	1:A:136:LYS:H	2.05	0.60
1:A:107:ALA:HB1	1:A:146:LEU:CD2	2.31	0.60
1:A:31:ILE:O	1:A:35:LEU:HB2	2.01	0.60
1:A:112:MET:HB3	1:A:113:PRO:CD	2.30	0.59
1:A:261:PHE:O	1:A:262:ARG:HB2	2.01	0.59
1:A:373:ARG:HD2	1:A:387:VAL:HG23	1.84	0.59
1:A:44:ARG:HD3	1:A:45:ALA:H	1.66	0.59
1:A:99:ASP:O	1:A:128:PRO:HG2	2.02	0.59
1:A:52:ALA:CB	1:A:82:PRO:HG2	2.30	0.59
1:A:150:GLU:HG2	1:A:169:ILE:HG21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:CYS:HB2	1:A:172:GLY:O	2.02	0.59
1:A:111:PRO:HG2	1:A:152:GLU:HB3	1.85	0.59
1:A:308:VAL:HG11	1:A:358:MET:HE1	1.84	0.58
1:A:160:TYR:O	1:A:161:ASP:HB2	2.04	0.58
1:A:226:VAL:HA	1:A:276:VAL:O	2.04	0.58
1:A:142:ASP:OD1	1:A:143:GLU:N	2.37	0.58
1:A:119:ILE:CD1	1:A:156:LEU:HD12	2.24	0.57
1:A:7:ARG:HD2	1:A:7:ARG:N	2.18	0.57
1:A:6:GLU:O	1:A:7:ARG:CB	2.53	0.57
1:A:136:LYS:HA	3:A:501:GDP:O6	2.05	0.57
1:A:107:ALA:HB1	1:A:146:LEU:HD21	1.86	0.57
1:A:198:TYR:O	1:A:200:PRO:HD3	2.04	0.57
1:A:67:VAL:HG23	1:A:78:HIS:HB3	1.87	0.56
1:A:136:LYS:HZ3	1:A:139:MET:HG3	1.69	0.56
1:A:225:THR:HG21	1:A:286:ILE:HD12	1.87	0.56
1:A:244:ILE:HG22	1:A:290:GLN:NE2	2.21	0.56
1:A:6:GLU:O	1:A:7:ARG:HB2	2.06	0.56
1:A:33:THR:HG22	1:A:34:VAL:N	2.20	0.56
1:A:329:GLN:HB3	1:A:336:ASP:HB2	1.87	0.56
1:A:51:ASN:O	1:A:53:PRO:HD3	2.06	0.55
1:A:52:ALA:HB1	1:A:63:ASN:CB	2.15	0.55
1:A:332:PHE:O	1:A:334:THR:N	2.39	0.55
1:A:7:ARG:HA	5:A:464:HOH:O	2.06	0.55
1:A:19:HIS:ND1	1:A:20:VAL:N	2.54	0.54
1:A:210:PHE:O	1:A:293:ALA:HA	2.08	0.54
1:A:119:ILE:HD12	1:A:156:LEU:CD1	2.26	0.54
1:A:64:THR:HG22	1:A:65:SER:N	2.23	0.54
1:A:145:LEU:C	1:A:145:LEU:HD13	2.29	0.54
1:A:227:VAL:CG1	1:A:286:ILE:HD13	2.38	0.54
1:A:51:ASN:C	1:A:53:PRO:HD3	2.28	0.53
1:A:331:TYR:HE2	5:A:465:HOH:O	1.90	0.53
1:A:26:THR:HG22	1:A:174:ALA:O	2.07	0.53
1:A:180:GLY:O	1:A:182:ALA:N	2.42	0.53
1:A:195:LEU:O	1:A:199:ILE:HB	2.08	0.53
1:A:344:PRO:HB2	1:A:347:VAL:HG21	1.89	0.53
1:A:308:VAL:HG11	1:A:358:MET:CE	2.38	0.53
1:A:323:PHE:O	1:A:326:TYR:HB2	2.09	0.53
1:A:304:PHE:HE1	1:A:306:SER:HB3	1.74	0.53
1:A:244:ILE:CD1	1:A:244:ILE:N	2.72	0.52
1:A:74:ARG:HD2	1:A:76:TYR:OH	2.09	0.52
1:A:19:HIS:CD2	1:A:113:PRO:HG2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LYS:HE2	1:A:179:GLU:OE1	2.10	0.52
1:A:252:LYS:CE	1:A:295:PRO:HB3	2.38	0.52
1:A:11:HIS:ND1	1:A:75:HIS:HD2	2.08	0.52
1:A:176:LYS:HE2	1:A:176:LYS:HA	1.92	0.52
1:A:162:PHE:O	1:A:164:GLY:N	2.42	0.52
1:A:19:HIS:CD2	1:A:112:MET:HB3	2.44	0.52
1:A:19:HIS:HA	1:A:114:GLN:HB2	1.91	0.52
1:A:252:LYS:HE2	1:A:295:PRO:CG	2.39	0.52
1:A:112:MET:CE	1:A:112:MET:HA	2.40	0.52
1:A:237:LYS:HE3	5:A:467:HOH:O	2.10	0.51
1:A:63:ASN:O	1:A:82:PRO:HD2	2.10	0.51
1:A:20:VAL:CG2	1:A:114:GLN:HE22	2.23	0.51
1:A:304:PHE:CE1	1:A:306:SER:HB3	2.44	0.51
1:A:247:ILE:HD12	1:A:247:ILE:N	2.26	0.51
1:A:259:GLU:HB2	1:A:264:LEU:HD23	1.92	0.51
1:A:55:GLU:CG	1:A:62:ILE:H	2.24	0.51
1:A:90:ASN:OD1	1:A:95:ALA:HB3	2.11	0.51
1:A:154:ARG:NH2	1:A:169:ILE:HG12	2.26	0.51
1:A:135:ASN:OD1	1:A:173:SER:HA	2.10	0.51
1:A:243:GLU:CD	1:A:295:PRO:HA	2.31	0.51
1:A:56:LYS:HG3	1:A:57:ALA:H	1.75	0.51
1:A:87:TYR:HB2	5:A:466:HOH:O	2.10	0.51
1:A:137:CYS:SG	1:A:146:LEU:HD13	2.51	0.51
1:A:332:PHE:HD2	1:A:372:LEU:HD21	1.76	0.51
1:A:157:LEU:HB3	1:A:162:PHE:HB2	1.92	0.50
1:A:145:LEU:C	1:A:147:GLU:N	2.63	0.50
1:A:320:THR:OG1	1:A:321:PRO:HD2	2.12	0.50
1:A:7:ARG:HH11	1:A:7:ARG:HA	1.77	0.50
1:A:231:VAL:HB	1:A:270:ALA:HA	1.94	0.50
1:A:203:GLU:HG2	1:A:207:ASP:CB	2.41	0.50
1:A:21:ASP:HA	3:A:501:GDP:PB	2.52	0.50
1:A:236:ILE:HG23	1:A:236:ILE:O	2.12	0.49
1:A:151:MET:HG2	1:A:151:MET:O	2.11	0.49
1:A:338:THR:O	1:A:363:ILE:HG23	2.12	0.49
1:A:282:LYS:HD2	1:A:285:GLU:OE2	2.12	0.49
1:A:331:TYR:CD1	1:A:336:ASP:HB3	2.41	0.49
1:A:27:LEU:O	1:A:31:ILE:HG13	2.13	0.49
1:A:175:LEU:HD12	3:A:501:GDP:N3	2.28	0.48
1:A:21:ASP:HA	3:A:501:GDP:O3A	2.12	0.48
1:A:123:ARG:HH21	1:A:160:TYR:HA	1.79	0.48
1:A:112:MET:HE2	1:A:112:MET:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PRO:HD2	1:A:64:THR:O	2.13	0.48
1:A:173:SER:C	1:A:175:LEU:H	2.17	0.48
1:A:135:ASN:CG	1:A:136:LYS:N	2.67	0.48
1:A:252:LYS:HE2	1:A:295:PRO:CB	2.43	0.48
1:A:148:LEU:O	1:A:151:MET:N	2.46	0.48
1:A:145:LEU:HD13	1:A:146:LEU:N	2.28	0.48
1:A:27:LEU:HD13	1:A:133:PHE:CE2	2.48	0.48
1:A:19:HIS:NE2	1:A:113:PRO:HG2	2.29	0.48
1:A:7:ARG:CA	1:A:7:ARG:HH11	2.27	0.48
1:A:344:PRO:HB2	1:A:347:VAL:CG2	2.44	0.48
1:A:103:LEU:HD11	1:A:115:THR:HG23	1.96	0.48
1:A:284:GLU:HG2	1:A:284:GLU:O	2.14	0.48
1:A:64:THR:HG23	1:A:81:CYS:SG	2.53	0.47
1:A:177:ALA:HB1	1:A:185:GLU:HA	1.96	0.47
1:A:173:SER:OG	1:A:176:LYS:HG2	2.15	0.47
1:A:20:VAL:HG12	1:A:21:ASP:N	2.30	0.47
1:A:19:HIS:CD2	1:A:114:GLN:H	2.32	0.47
1:A:54:GLU:O	1:A:55:GLU:HB2	2.14	0.47
1:A:49:ILE:HG22	1:A:49:ILE:O	2.15	0.47
1:A:243:GLU:C	1:A:244:ILE:HD12	2.34	0.47
1:A:124:GLN:HE21	1:A:307:GLU:HG2	1.80	0.47
1:A:243:GLU:OE1	1:A:295:PRO:HA	2.16	0.46
1:A:259:GLU:OE2	1:A:262:ARG:HD2	2.15	0.46
1:A:16:THR:OG1	1:A:78:HIS:HE1	1.98	0.46
1:A:206:ILE:HG13	1:A:235:ILE:HD11	1.96	0.46
1:A:124:GLN:HE21	1:A:307:GLU:CG	2.29	0.46
1:A:82:PRO:HA	5:A:405:HOH:O	2.14	0.46
1:A:176:LYS:CB	1:A:184:TRP:CD1	2.99	0.46
1:A:210:PHE:CZ	1:A:236:ILE:HB	2.51	0.46
1:A:187:LYS:HA	1:A:187:LYS:HD3	1.60	0.45
1:A:19:HIS:HE2	1:A:113:PRO:HG2	1.80	0.45
1:A:148:LEU:C	1:A:150:GLU:N	2.69	0.45
1:A:24:LYS:HB2	3:A:501:GDP:O2B	2.16	0.45
1:A:100:GLY:HA3	1:A:199:ILE:CD1	2.45	0.45
1:A:332:PHE:CD2	1:A:372:LEU:HD21	2.52	0.45
1:A:12:VAL:HG22	5:A:446:HOH:O	2.17	0.45
1:A:22:HIS:N	3:A:501:GDP:O3B	2.48	0.45
1:A:44:ARG:HD2	1:A:49:ILE:CG1	2.46	0.45
1:A:112:MET:CB	1:A:113:PRO:HD2	2.37	0.45
2:B:2:BB9:N	2:B:10:BB9:N	2.65	0.45
1:A:44:ARG:HG2	1:A:44:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:VAL:CG2	1:A:78:HIS:HB3	2.47	0.45
1:A:256:THR:HG23	1:A:279:ARG:HB2	1.99	0.45
1:A:53:PRO:O	1:A:54:GLU:O	2.35	0.44
1:A:6:GLU:HB3	1:A:7:ARG:H	1.60	0.44
1:A:126:GLY:O	1:A:127:VAL:C	2.55	0.44
1:A:134:LEU:HD22	1:A:150:GLU:HG3	1.99	0.44
1:A:47:ASP:OD1	1:A:48:GLN:HG2	2.17	0.44
1:A:45:ALA:O	1:A:49:ILE:HG13	2.18	0.44
1:A:331:TYR:CE2	5:A:465:HOH:O	2.56	0.44
1:A:211:LEU:HD13	1:A:212:LEU:N	2.32	0.44
1:A:33:THR:O	1:A:36:ALA:N	2.50	0.44
1:A:64:THR:HG22	1:A:65:SER:H	1.80	0.44
1:A:111:PRO:HG2	1:A:152:GLU:CB	2.46	0.44
1:A:311:LEU:HG	1:A:383:VAL:O	2.17	0.44
1:A:149:VAL:O	1:A:153:VAL:HG23	2.18	0.44
1:A:132:VAL:HG23	1:A:167:THR:CG2	2.48	0.44
1:A:246:GLY:O	1:A:248:LYS:N	2.48	0.44
1:A:108:THR:OG1	1:A:136:LYS:HD3	2.17	0.43
1:A:142:ASP:OD1	1:A:144:GLU:N	2.51	0.43
1:A:27:LEU:HD22	1:A:133:PHE:CD2	2.54	0.43
1:A:208:LYS:HB3	1:A:209:PRO:HD2	1.99	0.43
1:A:283:ARG:C	1:A:283:ARG:HD3	2.39	0.43
1:A:176:LYS:HA	1:A:179:GLU:OE1	2.18	0.43
1:A:24:LYS:HG2	1:A:104:VAL:HB	2.01	0.43
1:A:260:MET:HG2	1:A:261:PHE:CD2	2.54	0.43
1:A:294:LYS:HD2	1:A:297:THR:HG21	2.01	0.43
1:A:7:ARG:HB3	1:A:7:ARG:HH11	1.83	0.43
1:A:154:ARG:HD3	1:A:164:GLY:O	2.18	0.43
1:A:20:VAL:HG23	1:A:114:GLN:OE1	2.18	0.43
1:A:63:ASN:HB2	1:A:86:ASP:OD2	2.19	0.42
1:A:147:GLU:OE2	1:A:147:GLU:HA	2.19	0.42
1:A:36:ALA:HB1	1:A:41:GLY:O	2.20	0.42
1:A:301:HIS:HD2	1:A:393:GLY:HA2	1.84	0.42
1:A:108:THR:CG2	1:A:136:LYS:HD3	2.50	0.42
1:A:144:GLU:O	1:A:147:GLU:HB3	2.20	0.42
1:A:363:ILE:HG13	1:A:364:HIS:CD2	2.54	0.42
1:A:206:ILE:CD1	1:A:235:ILE:HD11	2.49	0.42
1:A:6:GLU:O	1:A:7:ARG:CG	2.67	0.42
1:A:89:LYS:O	1:A:93:THR:HG23	2.20	0.42
1:A:289:GLY:HA2	5:A:445:HOH:O	2.20	0.42
1:A:136:LYS:HG2	1:A:139:MET:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:C	1:A:211:LEU:CD1	2.88	0.41
1:A:321:PRO:HB3	1:A:351:MET:SD	2.60	0.41
1:A:337:VAL:HG12	1:A:338:THR:N	2.35	0.41
1:A:378:GLU:O	1:A:381:ARG:HB3	2.20	0.41
1:A:14:VAL:HG21	1:A:69:TYR:OH	2.20	0.41
1:A:237:LYS:HB2	1:A:240:GLU:CD	2.41	0.41
1:A:148:LEU:O	1:A:150:GLU:N	2.53	0.41
1:A:20:VAL:CG1	1:A:21:ASP:N	2.83	0.41
1:A:32:THR:O	1:A:36:ALA:HB2	2.20	0.41
1:A:69:TYR:OH	1:A:78:HIS:HD2	2.04	0.41
1:A:252:LYS:O	1:A:253:SER:HB2	2.21	0.41
1:A:69:TYR:CE1	1:A:76:TYR:HB2	2.56	0.41
1:A:13:ASN:HB3	1:A:97:GLN:O	2.19	0.41
1:A:62:ILE:HG22	1:A:64:THR:OG1	2.21	0.41
1:A:176:LYS:HB2	1:A:184:TRP:CD1	2.55	0.41
1:A:262:ARG:HA	1:A:262:ARG:HD2	1.67	0.41
1:A:206:ILE:HD11	1:A:235:ILE:HD11	2.02	0.41
1:A:220:ILE:HG22	1:A:223:ARG:HG2	2.02	0.41
1:A:298:ILE:HD11	1:A:368:MET:N	2.35	0.41
1:A:7:ARG:HH11	1:A:7:ARG:CG	2.33	0.41
1:A:261:PHE:O	1:A:262:ARG:CB	2.68	0.41
1:A:313:LYS:HG2	1:A:319:HIS:HA	2.03	0.41
1:A:69:TYR:CD1	1:A:76:TYR:HB2	2.56	0.40
1:A:97:GLN:HE21	1:A:97:GLN:CA	2.35	0.40
1:A:124:GLN:NE2	1:A:307:GLU:HG2	2.37	0.40
1:A:294:LYS:HG2	1:A:297:THR:HG23	2.03	0.40
1:A:323:PHE:CD1	1:A:323:PHE:N	2.88	0.40
1:A:9:LYS:CB	1:A:10:PRO:CD	2.99	0.40
1:A:24:LYS:HE3	1:A:87:TYR:CE1	2.57	0.40
1:A:210:PHE:CE1	1:A:236:ILE:HB	2.56	0.40
1:A:305:GLU:CD	1:A:357:LYS:HE3	2.42	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	381/394 (97%)	331 (87%)	35 (9%)	15 (4%)	4	8
2	B	2/12 (17%)	1 (50%)	1 (50%)	0	100	100
All	All	383/406 (94%)	332 (87%)	36 (9%)	15 (4%)	4	8

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	54	GLU
1	A	56	LYS
1	A	53	PRO
1	A	55	GLU
1	A	205	ALA
1	A	221	SER
1	A	333	ARG
1	A	33	THR
1	A	181	ASP
1	A	37	LYS
1	A	46	PHE
1	A	163	PRO
1	A	328	PRO
1	A	82	PRO

### 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	318/325 (98%)	291 (92%)	27 (8%)	13	30
2	B	1/2 (50%)	1 (100%)	0	100	100
All	All	319/327 (98%)	292 (92%)	27 (8%)	13	30

All (27) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	6	GLU
1	A	7	ARG
1	A	9	LYS
1	A	16	THR
1	A	22	HIS
1	A	44	ARG
1	A	54	GLU
1	A	66	HIS
1	A	70	ASP
1	A	79	VAL
1	A	137	CYS
1	A	141	ASP
1	A	144	GLU
1	A	155	GLU
1	A	156	LEU
1	A	175	LEU
1	A	211	LEU
1	A	217	VAL
1	A	223	ARG
1	A	262	ARG
1	A	277	LEU
1	A	283	ARG
1	A	284	GLU
1	A	318	ARG
1	A	361	THR
1	A	369	ASP
1	A	391	VAL

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	22	HIS
1	A	63	ASN
1	A	75	HIS
1	A	78	HIS
1	A	97	GLN
1	A	124	GLN
1	A	301	HIS
1	A	329	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues 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	BB9	B	10	2	0,4,6	0.00	-	0,4,7	0.00	-
2	MH6	B	11	2	3,3,6	2.46	3 (100%)	1,3,7	1.31	0
2	7BB	B	12	2	13,24,24	1.70	3 (23%)	16,31,31	1.58	4 (25%)
2	BB9	B	2	2	3,5,6	1.82	1 (33%)	1,5,7	1.71	0
2	MEN	B	3	2	7,7,9	0.97	1 (14%)	6,8,11	1.19	0
2	BB6	B	4	2	4,6,7	3.28	2 (50%)	1,7,9	0.31	0
2	BB7	B	6	2	6,8,9	1.27	1 (16%)	3,9,11	0.95	0
2	BB8	B	8	2	11,11,13	2.19	5 (45%)	13,14,17	0.86	0
2	BB9	B	9	2	0,4,6	0.00	-	0,4,7	0.00	-

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	BB9	B	10	2	-	0/0/2/6	0/0/0/0
2	MH6	B	11	2	-	0/0/0/6	0/0/0/0
2	7BB	B	12	2	-	0/7/35/35	0/1/1/1
2	BB9	B	2	2	-	0/0/4/6	0/0/0/0
2	MEN	B	3	2	-	0/6/6/10	0/0/0/0
2	BB6	B	4	2	-	0/0/6/8	0/0/0/0
2	BB7	B	6	2	-	0/1/9/11	0/0/0/0
2	BB8	B	8	2	-	0/8/8/12	0/1/1/1
2	BB9	B	9	2	-	0/0/2/6	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	11	MH6	CB-CA	-2.80	1.45	1.49
2	B	11	MH6	C-CA	-2.25	1.46	1.49
2	B	4	BB6	CA-N	2.01	1.41	1.36
2	B	8	BB8	CZ-CE1	2.05	1.43	1.38
2	B	12	7BB	C53-C54	2.09	1.56	1.51
2	B	3	MEN	CB-CG	2.19	1.55	1.51
2	B	8	BB8	CE2-CZ	2.19	1.43	1.38
2	B	8	BB8	CB-CA	2.27	1.56	1.54
2	B	11	MH6	CA-N	2.28	1.35	1.27
2	B	6	BB7	C-CA	2.36	1.48	1.45
2	B	12	7BB	C52-C57	2.59	1.60	1.53
2	B	2	BB9	CA-N	2.92	1.42	1.34
2	B	8	BB8	CD1-CG	3.57	1.44	1.39
2	B	12	7BB	C49-N13	3.60	1.53	1.47
2	B	8	BB8	CD2-CG	3.88	1.45	1.39
2	B	4	BB6	C-CA	6.16	1.54	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	12	7BB	C55-C56-C57	2.25	115.02	110.42
2	B	12	7BB	O9-C54-C53	2.35	116.15	109.09
2	B	12	7BB	N-CA-N13	3.25	121.52	117.77
2	B	12	7BB	C53-C52-C57	3.67	117.92	110.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	10	BB9	1	0
2	B	2	BB9	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	GDP	A	501	4	23,30,30	2.24	4 (17%)	30,47,47	3.17	7 (23%)

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	GDP	A	501	4	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	GDP	C5-C4	-2.42	1.35	1.40
3	A	501	GDP	C6-N1	2.59	1.37	1.33
3	A	501	GDP	C6-C5	4.21	1.49	1.41
3	A	501	GDP	C4-N3	8.44	1.48	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	GDP	C1'-N9-C4	-10.81	110.64	126.94
3	A	501	GDP	C2'-C1'-N9	-7.19	103.31	114.29
3	A	501	GDP	N3-C2-N1	-5.26	119.43	127.44
3	A	501	GDP	C5-C6-N1	-4.66	117.21	123.59
3	A	501	GDP	O3A-PA-O5'	2.19	108.74	102.94
3	A	501	GDP	O4'-C1'-N9	4.38	117.27	108.10
3	A	501	GDP	C6-N1-C2	6.24	124.61	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GDP	6	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	385/394 (97%)	0.38	24 (6%) 24 23	11, 41, 85, 103	0
2	B	3/12 (25%)	0.44	0 100 100	27, 27, 34, 42	0
All	All	388/406 (95%)	0.39	24 (6%) 24 23	11, 41, 85, 103	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	ALA	5.2
1	A	136	LYS	4.8
1	A	107	ALA	4.5
1	A	41	GLY	3.9
1	A	146	LEU	3.9
1	A	56	LYS	3.9
1	A	148	LEU	3.9
1	A	49	ILE	3.6
1	A	57	ALA	3.3
1	A	55	GLU	3.2
1	A	137	CYS	3.1
1	A	105	VAL	3.0
1	A	52	ALA	2.9
1	A	144	GLU	2.7
1	A	155	GLU	2.6
1	A	134	LEU	2.5
1	A	147	GLU	2.4
1	A	108	THR	2.3
1	A	175	LEU	2.3
1	A	174	ALA	2.3
1	A	43	ALA	2.2
1	A	106	ALA	2.1
1	A	64	THR	2.1
1	A	151	MET	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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	MH6	B	11	4/7	0.97	0.15	-	27,27,31,34	0
2	BB9	B	9	5/7	0.97	0.17	-	28,28,29,31	0
2	BB9	B	2	6/7	0.98	0.15	-	29,30,30,32	0
2	BB8	B	8	11/13	0.97	0.17	-	20,24,28,28	0
2	BB9	B	10	5/7	0.97	0.14	-	26,26,26,27	0
2	MEN	B	3	8/10	0.97	0.16	-	21,26,30,31	0
2	BB7	B	6	9/10	0.92	0.25	-	34,41,48,50	0
2	BB6	B	4	7/8	0.96	0.14	-	31,34,37,40	0
2	7BB	B	12	24/24	0.92	0.24	-	35,54,73,75	0

## 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
4	MG	A	503	1/1	0.94	0.19	0.55	42,42,42,42	0
3	GDP	A	501	28/28	0.91	0.24	-0.08	88,92,93,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.