



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 10:22 am BST

PDB ID : 3U6K  
Title : Ef-tu (escherichia coli) in complex with nvp-ldk733  
Authors : Palestrant, D.J.  
Deposited on : 2011-10-12  
Resolution : 2.45 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

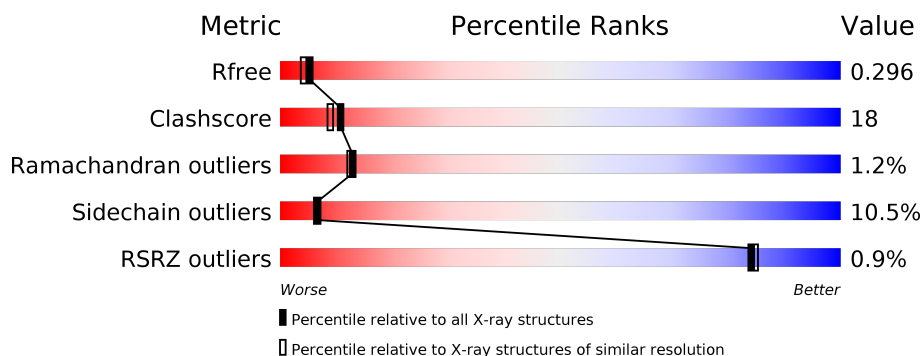
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 respectively. 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 style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <div style="width: 100%; height: 10px; background-color: green;"></div> <span>63%</span> <span>31%</span> <span>• •</span> </div> </div>
1	B	394	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <div style="width: 100%; height: 10px; background-color: green;"></div> <span>58%</span> <span>36%</span> <span>5%</span> <span>•</span> </div> </div>
2	C	12	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>83%</span> <span>17%</span> </div> </div>
2	D	12	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>83%</span> <span>17%</span> </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	MH6	C	11	-	X	-	-
2	BB9	C	9	-	X	-	-
2	MH6	D	11	-	X	-	-
2	BB9	D	9	-	X	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6311 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	386	Total	C	N	O	S	0	0	0
			2969	1877	511	568	13			
1	B	386	Total	C	N	O	S	0	0	0
			2969	1877	511	568	13			

There are 4 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
B	0	MET	-	EXPRESSION TAG	UNP P0CE47
B	1	ALA	-	EXPRESSION TAG	UNP P0CE47

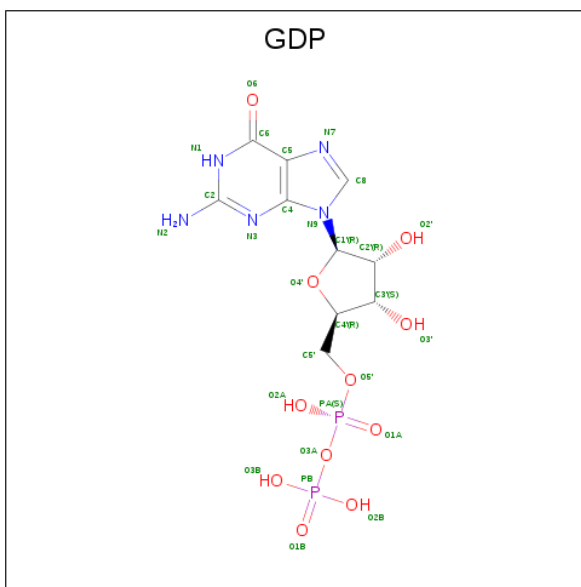
- Molecule 2 is a protein called Thiocillin GE2270 analogue NVP-LDK733.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	S	0	0	0
			85	55	13	11	6			
2	D	12	Total	C	N	O	S	0	0	0
			85	55	13	11	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	12	9BB	CYS	SEE REMARK 999	UNP Q7M0J8
D	12	9BB	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
			28	10	5	11	2	
3	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	69	Total	O	0	0
			69	69		
5	B	72	Total	O	0	0
			72	72		
5	C	1	Total	O	0	0
			1	1		
5	D	3	Total	O	0	0
			3	3		

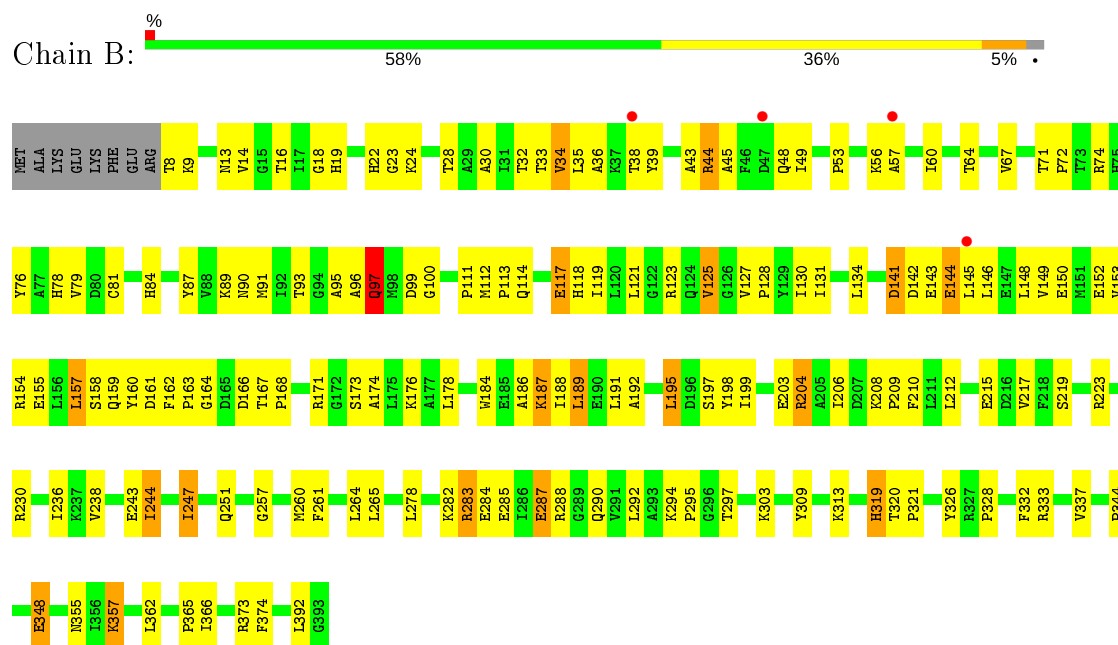
### 3 Residue-property plots [i](#)

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: Elongation factor Tu 1



#### • Molecule 1: Elongation factor Tu 1




#### • Molecule 2: Thiocillin GE2270 analogue NVP-LDK733

Chain C:  83% 17%



- Molecule 2: Thiocillin GE2270 analogue NVP-LDK733

Chain D:  83% 17%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.37Å 82.22Å 129.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.04 – 2.45 43.04 – 2.45	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.04-2.45) 94.9 (43.04-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.60 (at 2.45Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.224 , 0.298 0.222 , 0.296	Depositor DCC
$R_{free}$ test set	1590 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.4	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6311	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.10% 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: GDP, MG, MEN, BB7, BB9, BB8, MH6, BB6, 9BB

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	0.51	0/3024	0.65	1/4096 (0.0%)
1	B	0.60	3/3024 (0.1%)	0.62	2/4096 (0.0%)
2	C	2.31	1/10 (10.0%)	2.19	0/9
2	D	2.39	1/10 (10.0%)	2.15	0/9
All	All	0.57	5/6068 (0.1%)	0.64	3/8210 (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
1	A	0	2
2	C	1	0
2	D	1	0
All	All	2	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	230	ARG	C-O	-13.74	0.97	1.23
1	B	230	ARG	CA-C	-7.21	1.34	1.52
1	B	230	ARG	CZ-NH1	-7.18	1.23	1.33
2	C	1	SER	CA-CB	-6.61	1.43	1.52
2	D	1	SER	CA-CB	-6.38	1.43	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ASP	N-CA-C	-5.28	96.75	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	ARG	CD-NE-CZ	5.24	130.94	123.60
1	B	230	ARG	CG-CD-NE	-5.12	101.04	111.80

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	SER	CA
2	D	1	SER	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	VAL	Peptide
1	A	142	ASP	Peptide

## 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	2969	0	2981	103	0
1	B	2969	0	2982	120	0
2	C	85	0	56	1	0
2	D	85	0	56	1	0
3	A	28	0	12	1	0
3	B	28	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	69	0	0	3	0
5	B	72	0	0	5	0
5	C	1	0	0	0	0
5	D	3	0	0	0	0
All	All	6311	0	6099	224	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 18.

All (224) 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:140:VAL:HG11	1:A:146:LEU:HD21	1.44	0.97
1:B:18:GLY:H	1:B:118:HIS:HD2	1.22	0.87
1:B:282:LYS:HD2	1:B:283:ARG:H	1.40	0.87
1:A:93:THR:HG22	1:A:95:ALA:H	1.44	0.82
1:B:131:ILE:HD11	1:B:198:TYR:CD2	2.13	0.82
1:A:18:GLY:H	1:A:118:HIS:HD2	1.28	0.79
1:B:30:ALA:HA	1:B:178:LEU:HD23	1.67	0.77
1:B:294:LYS:O	1:B:297:THR:HG22	1.87	0.75
1:B:178:LEU:O	1:B:178:LEU:HD13	1.86	0.75
1:A:44:ARG:HD3	1:A:67:VAL:HG22	1.70	0.74
1:A:18:GLY:H	1:A:118:HIS:CD2	2.06	0.73
1:B:189:LEU:HD22	1:B:189:LEU:H	1.55	0.71
1:B:71:THR:HB	1:B:72:PRO:HD2	1.72	0.71
1:A:140:VAL:CG1	1:A:146:LEU:HD21	2.19	0.70
1:B:34:VAL:HG21	1:B:188:ILE:HG21	1.73	0.70
1:B:348:GLU:CD	1:B:348:GLU:H	1.96	0.69
1:B:91:MET:O	1:B:125:VAL:HG21	1.93	0.69
1:B:134:LEU:HD11	1:B:149:VAL:HG11	1.75	0.68
1:A:19:HIS:CD2	1:A:20:VAL:H	2.14	0.66
1:A:150:GLU:O	1:A:154:ARG:HG3	1.96	0.66
1:B:155:GLU:HG2	5:B:408:HOH:O	1.95	0.66
1:A:22:HIS:CD2	1:A:106:ALA:H	2.14	0.66
1:A:34:VAL:HG21	1:A:188:ILE:HG21	1.78	0.66
1:B:16:THR:HG23	1:B:78:HIS:CE1	2.30	0.66
1:B:18:GLY:H	1:B:118:HIS:CD2	2.10	0.65
1:A:32:THR:HG23	1:A:44:ARG:H	1.60	0.65
1:A:318:ARG:HH12	1:A:378:GLU:CD	2.00	0.65
1:A:32:THR:CG2	1:A:44:ARG:H	2.09	0.65
1:A:91:MET:O	1:A:125:VAL:HG21	1.96	0.65
1:A:282:LYS:O	1:A:285:GLU:HG2	1.96	0.64
1:B:189:LEU:N	1:B:189:LEU:HD22	2.12	0.64
1:B:158:SER:HA	1:B:162:PHE:O	1.98	0.64
1:A:19:HIS:CD2	1:A:20:VAL:HG12	2.32	0.63
1:A:89:LYS:O	1:A:93:THR:HB	1.99	0.63
1:B:81:CYS:HB2	1:B:87:TYR:CE2	2.34	0.63
1:B:89:LYS:O	1:B:93:THR:HG23	1.99	0.62
1:A:71:THR:HB	1:A:72:PRO:CD	2.29	0.62
1:A:16:THR:HG23	1:A:78:HIS:CE1	2.34	0.62
1:B:30:ALA:CA	1:B:178:LEU:HD23	2.29	0.62
1:A:93:THR:HG22	1:A:95:ALA:N	2.14	0.61
1:B:44:ARG:NH2	1:B:67:VAL:HA	2.15	0.61
1:A:14:VAL:O	1:A:78:HIS:HA	2.01	0.61

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ALA:HB3	1:B:60:ILE:HB	1.81	0.60
1:A:150:GLU:OE2	1:A:171:ARG:HD2	2.01	0.60
1:B:264:LEU:HD21	5:B:399:HOH:O	2.01	0.60
1:A:168:PRO:HB3	1:A:194:PHE:CD1	2.35	0.60
1:B:99:ASP:O	1:B:128:PRO:HG2	2.02	0.60
1:A:84:HIS:CD2	1:A:118:HIS:HE1	2.18	0.60
1:A:146:LEU:O	1:A:150:GLU:HG3	2.02	0.60
1:A:44:ARG:CZ	1:A:44:ARG:HB2	2.33	0.59
1:A:32:THR:HG21	1:A:44:ARG:HG2	1.84	0.59
1:B:96:ALA:O	1:B:97:GLN:HB2	2.01	0.59
1:B:192:ALA:O	1:B:195:LEU:HB2	2.03	0.59
1:B:148:LEU:O	1:B:152:GLU:HG3	2.04	0.58
1:A:225:THR:HG23	1:A:281:ILE:O	2.04	0.58
1:B:173:SER:OG	1:B:176:LYS:HB2	2.04	0.58
1:A:90:ASN:HD22	1:A:95:ALA:HB3	1.69	0.57
1:B:32:THR:O	1:B:36:ALA:HB2	2.05	0.57
1:A:19:HIS:CD2	1:A:20:VAL:N	2.72	0.57
1:A:34:VAL:CG2	1:A:188:ILE:HG21	2.35	0.57
1:B:64:THR:HG23	1:B:79:VAL:HG23	1.85	0.57
1:A:36:ALA:O	1:A:40:GLY:HA2	2.05	0.57
1:B:8:THR:O	1:B:8:THR:HG23	2.04	0.57
1:B:243:GLU:HG3	1:B:295:PRO:HB3	1.85	0.57
1:A:54:GLU:H	1:A:54:GLU:CD	2.07	0.57
1:B:167:THR:HG22	1:B:168:PRO:O	2.04	0.57
1:A:89:LYS:HD3	1:A:309:TYR:CE2	2.39	0.56
1:A:294:LYS:HG2	1:A:295:PRO:HD2	1.88	0.56
1:B:53:PRO:HD2	1:B:64:THR:O	2.06	0.56
1:B:244:ILE:HD11	1:B:278:LEU:HD13	1.86	0.56
1:B:189:LEU:HA	1:B:192:ALA:HB3	1.88	0.56
1:B:174:ALA:O	1:B:178:LEU:HB2	2.06	0.56
1:A:132:VAL:HB	1:A:169:ILE:HG12	1.89	0.55
1:B:38:THR:HG21	1:B:189:LEU:HD12	1.89	0.55
1:B:160:TYR:O	1:B:161:ASP:HB2	2.06	0.55
1:B:89:LYS:HE2	1:B:309:TYR:CZ	2.42	0.55
1:A:84:HIS:HD2	1:A:118:HIS:HE1	1.54	0.54
1:A:141:ASP:O	1:A:142:ASP:HB2	2.07	0.54
1:A:29:ALA:O	1:A:32:THR:HG22	2.07	0.54
1:A:19:HIS:HA	1:A:114:GLN:HB2	1.90	0.54
1:B:204:ARG:HB2	1:B:206:ILE:HG22	1.90	0.53
1:A:133:PHE:CD1	1:A:191:LEU:HD22	2.44	0.53
1:A:283:ARG:C	1:A:283:ARG:HD3	2.29	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:THR:HB	1:A:72:PRO:HD3	1.90	0.53
1:A:320:THR:HB	1:A:321:PRO:HD2	1.90	0.53
1:B:35:LEU:HD22	1:B:39:TYR:CE2	2.44	0.52
1:A:225:THR:HG21	1:A:283:ARG:N	2.25	0.52
1:A:154:ARG:HD3	1:A:164:GLY:O	2.09	0.52
1:A:209:PRO:HB3	1:A:294:LYS:HE2	1.91	0.52
1:B:189:LEU:HA	1:B:192:ALA:CB	2.40	0.52
1:B:251:GLN:OE1	1:B:285:GLU:HB3	2.10	0.52
1:B:45:ALA:O	1:B:49:ILE:HG12	2.09	0.52
1:B:319:HIS:HE1	5:B:449:HOH:O	1.91	0.52
1:B:119:ILE:HD13	1:B:157:LEU:HD13	1.92	0.51
1:A:89:LYS:HD3	1:A:309:TYR:CZ	2.46	0.51
1:B:163:PRO:HB2	1:B:166:ASP:HB2	1.91	0.51
1:B:303:LYS:HG2	1:B:392:LEU:HB2	1.92	0.51
1:A:210:PHE:CE1	1:A:236:ILE:HB	2.46	0.51
1:B:35:LEU:HD22	1:B:39:TYR:HE2	1.76	0.51
1:A:84:HIS:HD2	1:A:118:HIS:CE1	2.29	0.50
1:A:168:PRO:HB3	1:A:194:PHE:CE1	2.47	0.50
1:B:320:THR:HB	1:B:321:PRO:HD2	1.93	0.50
1:B:34:VAL:HG21	1:B:188:ILE:HG13	1.92	0.50
1:A:370:ASP:OD1	1:A:390:LYS:HA	2.12	0.50
1:B:145:LEU:O	1:B:148:LEU:HB2	2.12	0.50
1:B:14:VAL:HG12	1:B:100:GLY:O	2.12	0.50
1:B:264:LEU:HD22	1:B:264:LEU:N	2.27	0.50
1:A:19:HIS:CE1	1:A:113:PRO:HD2	2.47	0.49
1:B:74:ARG:NH2	1:B:199:ILE:O	2.44	0.49
1:B:294:LYS:O	1:B:297:THR:CG2	2.59	0.49
1:B:28:THR:HG23	1:B:78:HIS:CD2	2.47	0.49
1:A:44:ARG:CZ	1:A:44:ARG:CB	2.85	0.49
1:B:149:VAL:HG12	1:B:153:VAL:HG23	1.95	0.49
1:B:84:HIS:CD2	1:B:118:HIS:HE1	2.31	0.49
1:A:344:PRO:HD2	1:A:356:ILE:HD11	1.94	0.49
1:B:257:GLY:HA3	2:D:12:9BB:O8	2.13	0.49
1:B:282:LYS:CD	1:B:283:ARG:H	2.21	0.49
1:A:21:ASP:OD1	3:A:500:GDP:H5"	2.13	0.49
1:B:141:ASP:N	1:B:141:ASP:OD1	2.44	0.48
1:A:209:PRO:HB3	1:A:294:LYS:CE	2.43	0.48
1:A:215:GLU:OE1	1:A:288:ARG:NH1	2.46	0.48
1:A:377:ARG:NH1	1:A:382:THR:OG1	2.47	0.48
1:B:260:MET:O	1:B:261:PHE:C	2.53	0.47
1:B:130:ILE:O	1:B:131:ILE:HD13	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ASN:ND2	5:B:405:HOH:O	2.41	0.47
1:B:76:TYR:CZ	1:B:195:LEU:HB3	2.49	0.47
1:A:11:HIS:HE1	1:A:13:ASN:OD1	1.98	0.47
1:B:112:MET:HB3	1:B:113:PRO:CD	2.43	0.47
1:B:44:ARG:HE	1:B:67:VAL:HG12	1.80	0.47
1:A:175:LEU:O	1:A:179:GLU:HG3	2.14	0.47
5:A:402:HOH:O	2:C:6:BB7:H31	2.15	0.47
1:B:348:GLU:N	1:B:348:GLU:OE1	2.45	0.47
1:A:34:VAL:HG21	1:A:188:ILE:HG13	1.97	0.47
1:B:19:HIS:ND1	1:B:112:MET:HB3	2.29	0.47
1:B:287:GLU:O	1:B:290:GLN:HG3	2.15	0.47
1:A:251:GLN:HG3	5:A:455:HOH:O	2.14	0.46
1:B:30:ALA:HA	1:B:178:LEU:CD2	2.41	0.46
1:A:331:TYR:HD2	1:A:336:ASP:OD1	1.98	0.46
1:B:9:LYS:HD2	1:B:74:ARG:N	2.30	0.46
1:A:243:GLU:HG3	1:A:295:PRO:HA	1.97	0.46
1:B:144:GLU:O	1:B:148:LEU:HD23	2.15	0.46
1:B:210:PHE:CE1	1:B:236:ILE:HB	2.50	0.46
1:B:171:ARG:O	1:B:187:LYS:HG3	2.16	0.46
1:B:114:GLN:HA	1:B:117:GLU:HB2	1.98	0.45
1:B:176:LYS:HB3	1:B:184:TRP:CD1	2.51	0.45
1:B:208:LYS:HB3	1:B:209:PRO:HD2	1.99	0.45
1:A:342:GLU:O	1:A:342:GLU:HG2	2.17	0.45
1:A:68:GLU:CD	1:A:75:HIS:HE2	2.20	0.45
1:B:178:LEU:C	1:B:178:LEU:HD13	2.37	0.45
1:A:27:LEU:O	1:A:31:ILE:HG13	2.16	0.45
1:A:90:ASN:ND2	1:A:95:ALA:HB3	2.31	0.45
1:A:34:VAL:CB	1:A:188:ILE:HG21	2.47	0.45
1:A:120:LEU:O	1:A:120:LEU:HD12	2.16	0.45
1:A:145:LEU:HD12	1:A:145:LEU:N	2.32	0.45
1:A:125:VAL:HG22	1:A:373:ARG:NH2	2.32	0.45
1:A:184:TRP:C	1:A:186:ALA:N	2.70	0.45
1:B:19:HIS:CE1	1:B:112:MET:HB3	2.52	0.45
1:B:74:ARG:NH1	1:B:199:ILE:O	2.49	0.44
1:B:189:LEU:N	1:B:189:LEU:CD2	2.79	0.44
1:B:344:PRO:HG3	1:B:357:LYS:O	2.16	0.44
1:A:129:TYR:CE2	1:A:200:PRO:HD2	2.53	0.44
1:A:105:VAL:O	1:A:134:LEU:HD13	2.18	0.44
1:A:246:GLY:C	1:A:248:LYS:H	2.21	0.44
1:B:19:HIS:HA	1:B:114:GLN:HB2	1.98	0.44
1:B:187:LYS:HA	1:B:187:LYS:HD2	1.74	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:MET:HB3	1:A:113:PRO:CD	2.48	0.44
1:A:241:GLU:HG3	1:A:253:SER:O	2.17	0.43
1:B:19:HIS:ND1	1:B:112:MET:CB	2.81	0.43
1:B:319:HIS:CE1	5:B:449:HOH:O	2.67	0.43
1:B:247:ILE:N	1:B:365:PRO:O	2.41	0.43
1:B:143:GLU:O	1:B:146:LEU:HB2	2.19	0.43
1:A:81:CYS:HB2	1:A:87:TYR:CE2	2.52	0.43
1:B:76:TYR:OH	1:B:195:LEU:HB3	2.17	0.43
1:B:96:ALA:O	1:B:97:GLN:CB	2.65	0.43
1:A:256:THR:CG2	1:A:279:ARG:HB2	2.49	0.43
1:B:9:LYS:HE2	1:B:71:THR:O	2.19	0.43
1:B:188:ILE:O	1:B:191:LEU:HB3	2.18	0.43
1:A:74:ARG:NH1	1:A:195:LEU:O	2.52	0.43
1:A:149:VAL:HG13	1:A:150:GLU:N	2.33	0.43
1:B:244:ILE:HG22	1:B:290:GLN:NE2	2.34	0.42
1:A:135:ASN:CG	1:A:136:LYS:N	2.72	0.42
1:B:33:THR:HA	1:B:43:ALA:HB2	2.00	0.42
1:B:34:VAL:CG2	1:B:188:ILE:HG21	2.45	0.42
1:A:184:TRP:C	1:A:186:ALA:H	2.22	0.42
1:A:201:GLU:HG3	1:A:201:GLU:O	2.20	0.42
1:B:337:VAL:HG21	1:B:366:ILE:HD11	2.02	0.42
1:B:91:MET:O	1:B:125:VAL:CG2	2.64	0.42
1:A:34:VAL:HB	1:A:188:ILE:HG21	2.02	0.42
1:B:16:THR:HG23	1:B:78:HIS:HE1	1.79	0.42
1:A:134:LEU:HD13	1:A:134:LEU:HA	1.71	0.41
1:B:168:PRO:HD3	1:B:198:TYR:CE1	2.55	0.41
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.75	0.41
1:A:282:LYS:N	1:A:282:LYS:HD2	2.36	0.41
1:A:38:THR:HG22	1:A:39:TYR:N	2.35	0.41
1:A:84:HIS:CD2	1:A:118:HIS:CE1	3.03	0.41
1:A:261:PHE:O	1:A:262:ARG:HB2	2.21	0.41
1:A:71:THR:CB	1:A:72:PRO:CD	2.98	0.41
1:B:34:VAL:HG21	1:B:188:ILE:CG2	2.48	0.41
1:B:87:TYR:O	1:B:91:MET:HG2	2.20	0.41
1:B:238:VAL:HG22	1:B:257:GLY:HA2	2.02	0.41
1:A:135:ASN:CG	1:A:136:LYS:H	2.24	0.41
1:B:23:GLY:O	1:B:24:LYS:C	2.59	0.41
1:B:326:TYR:CE2	1:B:328:PRO:HG3	2.54	0.41
1:A:32:THR:HG21	1:A:44:ARG:CG	2.49	0.41
1:A:378:GLU:HG3	1:A:383:VAL:HG11	2.03	0.41
1:B:123:ARG:HH21	1:B:160:TYR:HD1	1.67	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:MET:O	1:A:115:THR:N	2.51	0.41
1:A:363:ILE:HD11	5:A:462:HOH:O	2.21	0.41
1:B:131:ILE:HD11	1:B:198:TYR:CG	2.53	0.41
1:B:164:GLY:HA2	1:B:167:THR:OG1	2.20	0.41
1:B:212:LEU:C	1:B:212:LEU:HD23	2.41	0.41
1:A:112:MET:HB3	1:A:113:PRO:HD2	2.03	0.40
1:A:140:VAL:HG11	1:A:146:LEU:CD2	2.32	0.40
1:A:46:PHE:O	1:A:47:ASP:C	2.60	0.40
1:B:125:VAL:CG1	1:B:127:VAL:HG23	2.52	0.40
1:B:153:VAL:O	1:B:157:LEU:HD22	2.21	0.40
1:B:215:GLU:O	1:B:288:ARG:HD2	2.21	0.40
1:B:90:ASN:OD1	1:B:95:ALA:HB3	2.21	0.40
1:A:141:ASP:O	1:A:142:ASP:CB	2.66	0.40
1:B:150:GLU:O	1:B:154:ARG:HG3	2.22	0.40
1:B:184:TRP:C	1:B:186:ALA:N	2.73	0.40
1:B:282:LYS:HD2	1:B:283:ARG:N	2.22	0.40
1:B:282:LYS:O	1:B:283:ARG:C	2.59	0.40
1:B:332:PHE:CE1	1:B:374:PHE:HB3	2.57	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	384/394 (98%)	357 (93%)	24 (6%)	3 (1%)	19	22
1	B	384/394 (98%)	354 (92%)	24 (6%)	6 (2%)	9	8
2	C	2/12 (17%)	1 (50%)	1 (50%)	0	100	100
2	D	2/12 (17%)	1 (50%)	1 (50%)	0	100	100
All	All	772/812 (95%)	713 (92%)	50 (6%)	9 (1%)	13	12

All (9) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	B	97	GLN
1	A	247	ILE
1	B	34	VAL
1	B	142	ASP
1	A	108	THR
1	B	333	ARG
1	B	247	ILE
1	B	111	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%)	285 (90%)	33 (10%)	7	7
1	B	318/325 (98%)	284 (89%)	34 (11%)	6	6
2	C	1/2 (50%)	1 (100%)	0	100	100
2	D	1/2 (50%)	1 (100%)	0	100	100
All	All	638/654 (98%)	571 (90%)	67 (10%)	7	6

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	44	ARG
1	A	48	GLN
1	A	58	ARG
1	A	90	ASN
1	A	91	MET
1	A	93	THR
1	A	97	GLN
1	A	118	HIS
1	A	134	LEU
1	A	139	MET
1	A	142	ASP
1	A	143	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	157	LEU
1	A	166	ASP
1	A	173	SER
1	A	181	ASP
1	A	190	GLU
1	A	241	GLU
1	A	249	GLU
1	A	252	LYS
1	A	262	ARG
1	A	264	LEU
1	A	283	ARG
1	A	284	GLU
1	A	292	LEU
1	A	313	LYS
1	A	315	GLU
1	A	342	GLU
1	A	357	LYS
1	A	364	HIS
1	A	378	GLU
1	A	381	ARG
1	B	22	HIS
1	B	44	ARG
1	B	48	GLN
1	B	56	LYS
1	B	97	GLN
1	B	117	GLU
1	B	121	LEU
1	B	125	VAL
1	B	141	ASP
1	B	144	GLU
1	B	157	LEU
1	B	159	GLN
1	B	187	LYS
1	B	189	LEU
1	B	195	LEU
1	B	197	SER
1	B	203	GLU
1	B	204	ARG
1	B	217	VAL
1	B	219	SER
1	B	223	ARG
1	B	244	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	265	LEU
1	B	283	ARG
1	B	284	GLU
1	B	287	GLU
1	B	292	LEU
1	B	313	LYS
1	B	319	HIS
1	B	348	GLU
1	B	355	ASN
1	B	357	LYS
1	B	362	LEU
1	B	373	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	22	HIS
1	A	84	HIS
1	A	90	ASN
1	A	114	GLN
1	A	118	HIS
1	A	124	GLN
1	A	159	GLN
1	A	301	HIS
1	B	63	ASN
1	B	84	HIS
1	B	114	GLN
1	B	118	HIS
1	B	159	GLN
1	B	355	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

18 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	BB7	C	6	2	6,8,9	2.15	2 (33%)	3,9,11	1.76	1 (33%)
2	9BB	C	12	2	13,17,17	2.28	3 (23%)	15,22,22	2.13	3 (20%)
2	BB6	C	4	2	4,6,7	2.82	2 (50%)	2,7,9	1.34	0
2	MEN	C	3	2	7,7,9	0.93	0	6,8,11	1.45	1 (16%)
2	BB9	C	9	2	2,4,6	3.45	1 (50%)	3,4,7	2.59	3 (100%)
2	MH6	D	11	2	3,3,6	4.11	3 (100%)	1,3,7	2.25	1 (100%)
2	BB9	D	9	2	2,4,6	3.18	1 (50%)	3,4,7	2.71	3 (100%)
2	BB8	D	8	2	11,11,13	1.75	4 (36%)	12,14,17	1.31	1 (8%)
2	MH6	C	11	2	3,3,6	3.13	2 (66%)	1,3,7	2.47	1 (100%)
2	9BB	D	12	2	13,17,17	2.21	3 (23%)	15,22,22	1.89	4 (26%)
2	BB7	D	6	2	6,8,9	2.11	2 (33%)	3,9,11	1.91	1 (33%)
2	MEN	D	3	2	7,7,9	1.09	1 (14%)	6,8,11	1.45	1 (16%)
2	BB9	C	2	2	3,5,6	3.49	2 (66%)	1,5,7	2.81	1 (100%)
2	BB9	C	10	2	2,4,6	3.90	1 (50%)	3,4,7	4.42	2 (66%)
2	BB6	D	4	2	4,6,7	2.79	2 (50%)	2,7,9	0.98	0
2	BB9	D	2	2	3,5,6	3.70	2 (66%)	1,5,7	2.93	1 (100%)
2	BB9	D	10	2	2,4,6	3.54	1 (50%)	3,4,7	5.22	2 (66%)
2	BB8	C	8	2	11,11,13	1.83	5 (45%)	12,14,17	1.41	1 (8%)

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	BB7	C	6	2	-	1/1/9/11	-
2	9BB	C	12	2	-	0/6/24/24	0/1/1/1
2	BB6	C	4	2	-	0/0/6/8	-
2	MEN	C	3	2	-	1/6/6/10	-
2	BB9	C	9	2	-	0/0/2/6	-
2	BB9	D	9	2	-	0/0/2/6	-
2	BB8	D	8	2	-	3/8/8/12	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9BB	D	12	2	-	2/6/24/24	0/1/1/1
2	BB7	D	6	2	-	1/1/9/11	-
2	BB8	C	8	2	-	5/8/8/12	0/1/1/1
2	BB9	C	2	2	-	0/0/4/6	-
2	BB9	C	10	2	-	0/0/2/6	-
2	BB6	D	4	2	-	0/0/6/8	-
2	BB9	D	2	2	-	0/0/4/6	-
2	BB9	D	10	2	-	0/0/2/6	-
2	MEN	D	3	2	-	1/6/6/10	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	12	9BB	CA-N	5.97	1.47	1.34
2	D	11	MH6	CB-CA	-5.59	1.41	1.49
2	C	10	BB9	CA-N	5.29	1.46	1.33
2	D	12	9BB	CA-N	5.25	1.45	1.34
2	D	4	BB6	CA-N	4.92	1.48	1.36
2	D	2	BB9	CA-N	4.91	1.47	1.35
2	D	10	BB9	CA-N	4.74	1.45	1.33
2	C	11	MH6	CB-CA	-4.59	1.42	1.49
2	C	9	BB9	CA-N	4.55	1.44	1.33
2	C	2	BB9	CA-N	4.50	1.46	1.35
2	C	4	BB6	CA-N	4.34	1.47	1.36
2	D	9	BB9	CA-N	4.27	1.44	1.33
2	D	6	BB7	CA-N	4.25	1.47	1.36
2	D	12	9BB	CA-N13	4.20	1.49	1.40
2	C	6	BB7	CA-N	4.15	1.46	1.36
2	C	12	9BB	CA-N13	4.08	1.49	1.40
2	C	2	BB9	C-CA	3.86	1.51	1.45
2	D	2	BB9	C-CA	3.84	1.51	1.45
2	C	4	BB6	C-CA	3.50	1.50	1.45
2	D	11	MH6	C-CA	-3.33	1.44	1.49
2	C	8	BB8	CD1-CG	3.27	1.44	1.39
2	D	8	BB8	CD1-CG	3.02	1.43	1.39
2	C	6	BB7	C-CA	2.88	1.49	1.45
2	D	11	MH6	CA-N	2.88	1.35	1.27
2	D	6	BB7	C-CA	2.86	1.49	1.45
2	D	4	BB6	C-CA	2.63	1.49	1.45
2	C	8	BB8	CE2-CD2	2.58	1.44	1.38
2	D	8	BB8	CD2-CG	2.49	1.43	1.39
2	D	12	9BB	O11-C49	-2.48	1.40	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	11	MH6	CA-N	2.48	1.33	1.27
2	D	8	BB8	CE2-CD2	2.42	1.44	1.38
2	C	12	9BB	O11-C49	-2.19	1.41	1.46
2	D	8	BB8	CE2-CZ	2.16	1.43	1.38
2	D	3	MEN	CB-CA	2.14	1.57	1.53
2	C	8	BB8	CD2-CG	2.11	1.42	1.39
2	C	8	BB8	CE2-CZ	2.08	1.43	1.38
2	C	8	BB8	CE1-CD1	2.02	1.43	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	10	BB9	C-CA-N	8.44	125.96	116.53
2	C	10	BB9	C-CA-N	6.91	124.25	116.53
2	C	12	9BB	C49-O11-C48	6.67	126.03	116.48
2	D	12	9BB	O11-C48-N13	4.80	115.34	108.02
2	C	8	BB8	C-CA-CB	-4.07	105.75	112.00
2	D	8	BB8	C-CA-CB	-3.73	106.27	112.00
2	D	10	BB9	CB-CA-N	-3.23	112.16	122.50
2	D	6	BB7	O-C-CA	-3.14	119.68	125.54
2	C	10	BB9	CB-CA-N	-3.14	112.46	122.50
2	D	2	BB9	O-C-CA	-2.93	121.66	125.39
2	D	9	BB9	C-CA-CB	2.87	126.62	121.39
2	C	2	BB9	O-C-CA	-2.81	121.82	125.39
2	D	12	9BB	C49-O11-C48	2.80	120.49	116.48
2	D	3	MEN	CB-CG-ND2	-2.80	111.72	115.48
2	C	3	MEN	CB-CG-ND2	-2.74	111.80	115.48
2	C	9	BB9	C-CA-CB	2.67	126.25	121.39
2	C	6	BB7	O-C-CA	-2.67	120.56	125.54
2	D	9	BB9	CB-CA-N	-2.67	113.97	122.50
2	D	9	BB9	C-CA-N	2.57	119.40	116.53
2	C	9	BB9	C-CA-N	2.56	119.39	116.53
2	C	9	BB9	CB-CA-N	-2.55	114.36	122.50
2	C	12	9BB	C53-C54-C49	2.51	114.69	110.82
2	C	11	MH6	CB-CA-C	2.47	122.85	117.63
2	D	12	9BB	O11-C48-O8	-2.45	120.83	124.53
2	D	12	9BB	C53-C54-C49	-2.35	107.20	110.82
2	D	11	MH6	CB-CA-C	2.25	122.37	117.63
2	C	12	9BB	C51-C50-C49	2.11	114.06	110.82

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	12	9BB	O8-C48-O11-C49
2	D	12	9BB	N13-C48-O11-C49
2	D	6	BB7	CB-CB1-OB2-CB3
2	D	8	BB8	C-CA-CB-CG
2	C	8	BB8	C-CA-CB-CG
2	C	8	BB8	OB-CB-CG-CD1
2	C	8	BB8	OB-CB-CG-CD2
2	C	6	BB7	CB-CB1-OB2-CB3
2	C	8	BB8	CA-CB-CG-CD1
2	C	8	BB8	CA-CB-CG-CD2
2	D	8	BB8	OB-CB-CG-CD2
2	D	8	BB8	OB-CB-CG-CD1
2	C	3	MEN	CA-CB-CG-OD1
2	D	3	MEN	CA-CB-CG-OD1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	6	BB7	1	0
2	D	12	9BB	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	B	500	4	24,30,30	2.20	4 (16%)	31,47,47	2.82	9 (29%)
3	GDP	A	500	4	24,30,30	2.38	4 (16%)	31,47,47	2.74	9 (29%)

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	B	500	4	-	4/12/32/32	0/3/3/3
3	GDP	A	500	4	-	6/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	GDP	C4-N3	8.58	1.49	1.35
3	B	500	GDP	C4-N3	8.25	1.48	1.35
3	A	500	GDP	C6-C5	5.39	1.50	1.41
3	B	500	GDP	C6-C5	4.40	1.48	1.41
3	A	500	GDP	C6-N1	2.85	1.38	1.33
3	B	500	GDP	C6-N1	2.61	1.37	1.33
3	A	500	GDP	C5-C4	-2.36	1.34	1.40
3	B	500	GDP	C5-C4	-2.26	1.34	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	GDP	C1'-N9-C4	-9.83	109.37	126.64
3	A	500	GDP	C1'-N9-C4	-9.61	109.75	126.64
3	B	500	GDP	N3-C2-N1	-6.07	119.12	127.22
3	A	500	GDP	N3-C2-N1	-6.00	119.22	127.22
3	B	500	GDP	C6-N1-C2	5.79	125.12	115.93
3	A	500	GDP	C6-N1-C2	5.76	125.08	115.93
3	A	500	GDP	C5-C6-N1	-4.92	116.71	123.43
3	B	500	GDP	C5-C6-N1	-4.80	116.87	123.43
3	A	500	GDP	C2-N3-C4	3.10	118.90	115.36
3	B	500	GDP	C2-N3-C4	2.85	118.61	115.36
3	A	500	GDP	C6-C5-C4	-2.54	118.37	120.80
3	A	500	GDP	O3B-PB-O3A	2.48	112.95	104.64
3	B	500	GDP	O3B-PB-O3A	2.42	112.76	104.64
3	B	500	GDP	O4'-C1'-C2'	2.42	110.46	106.93
3	B	500	GDP	C6-C5-C4	-2.39	118.52	120.80
3	B	500	GDP	C3'-C2'-C1'	2.38	104.56	100.98
3	A	500	GDP	N2-C2-N1	2.16	120.62	117.25
3	A	500	GDP	O4'-C1'-C2'	2.10	109.99	106.93

There are no chirality outliers.



All (10) torsion outliers are listed below:

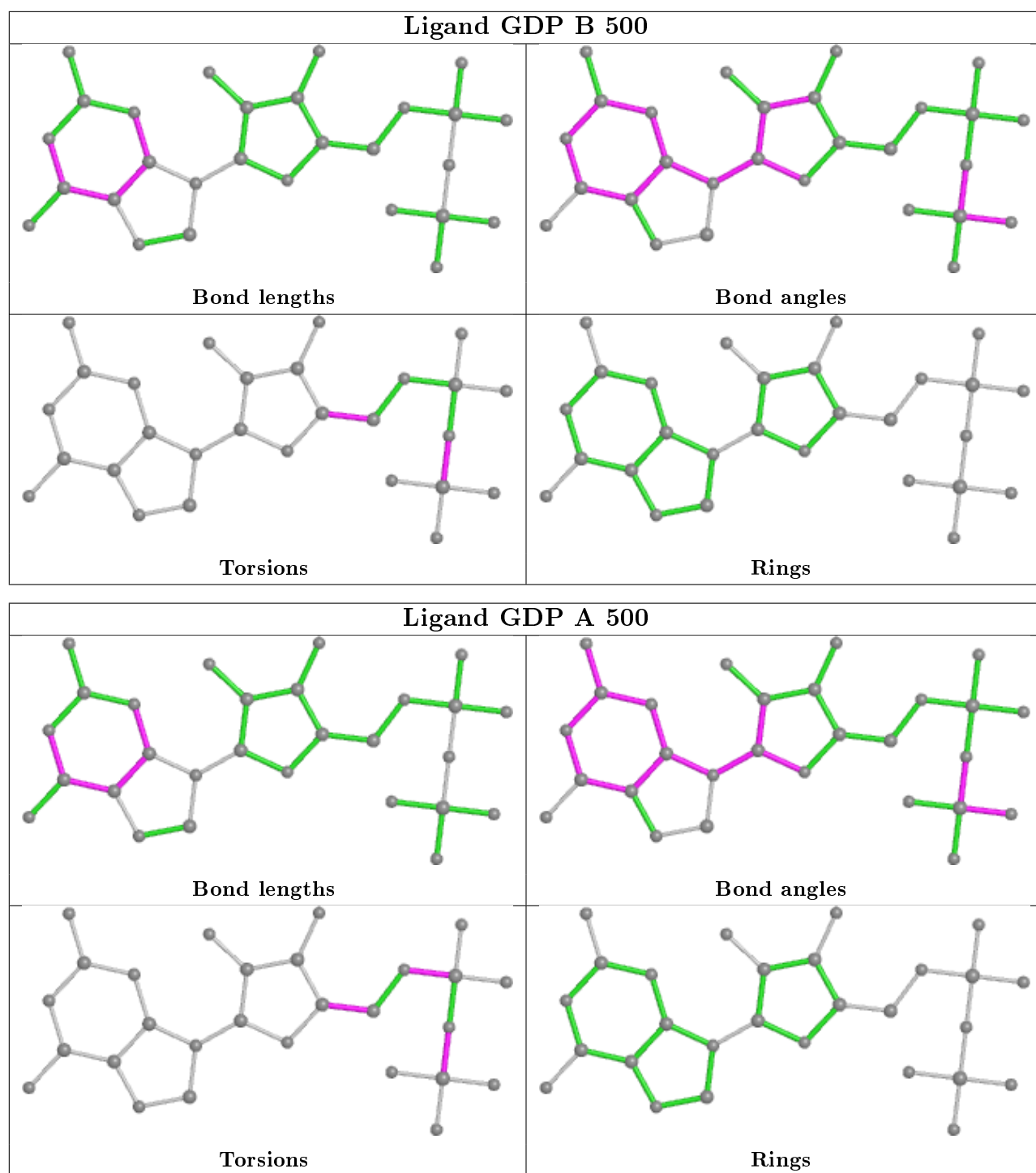
Mol	Chain	Res	Type	Atoms
3	B	500	GDP	PA-O3A-PB-O3B
3	A	500	GDP	PA-O3A-PB-O3B
3	A	500	GDP	C5'-O5'-PA-O3A
3	A	500	GDP	C5'-O5'-PA-O2A
3	A	500	GDP	C5'-O5'-PA-O1A
3	B	500	GDP	PA-O3A-PB-O1B
3	B	500	GDP	PA-O3A-PB-O2B
3	A	500	GDP	PA-O3A-PB-O2B
3	B	500	GDP	C3'-C4'-C5'-O5'
3	A	500	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	386/394 (97%)	0.05	3 (0%) 86 86	21, 48, 80, 101	0
1	B	386/394 (97%)	0.06	4 (1%) 82 83	26, 48, 81, 99	0
2	C	3/12 (25%)	0.11	0 100 100	33, 33, 38, 54	0
2	D	3/12 (25%)	0.00	0 100 100	33, 33, 40, 52	0
All	All	778/812 (95%)	0.06	7 (0%) 84 85	21, 48, 80, 101	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	TYR	3.8
1	B	47	ASP	2.9
1	A	148	LEU	2.6
1	B	145	LEU	2.5
1	A	42	ALA	2.1
1	B	57	ALA	2.1
1	B	38	THR	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	9BB	C	12	17/17	0.91	0.21	38,63,79,80	0
2	BB7	D	6	9/10	0.91	0.18	50,54,66,66	0
2	9BB	D	12	17/17	0.93	0.22	37,65,79,81	0
2	BB8	D	8	11/13	0.93	0.19	35,37,40,42	0
2	MH6	D	11	4/7	0.95	0.11	33,34,36,37	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BB6	C	4	7/8	0.95	0.16	40,43,49,51	0
2	BB9	D	2	6/7	0.95	0.13	32,33,35,36	0
2	BB9	C	2	6/7	0.96	0.17	35,36,38,41	0
2	BB7	C	6	9/10	0.96	0.20	49,55,62,63	0
2	BB8	C	8	11/13	0.96	0.15	27,30,32,33	0
2	MEN	C	3	8/10	0.97	0.17	30,34,38,40	0
2	BB6	D	4	7/8	0.97	0.13	33,34,40,41	0
2	MEN	D	3	8/10	0.97	0.11	25,30,35,35	0
2	MH6	C	11	4/7	0.97	0.11	32,33,35,40	0
2	BB9	D	10	5/7	0.98	0.14	28,28,29,29	0
2	BB9	C	9	5/7	0.98	0.13	23,25,27,27	0
2	BB9	D	9	5/7	0.99	0.14	30,32,34,37	0
2	BB9	C	10	5/7	0.99	0.14	25,26,28,29	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

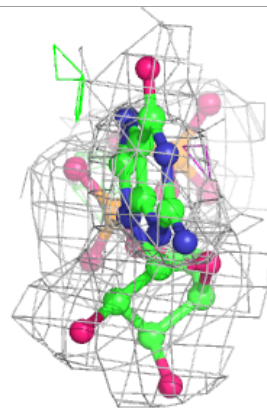
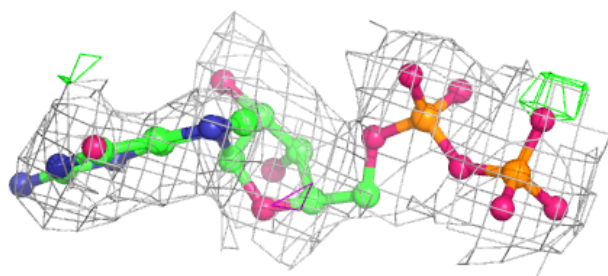
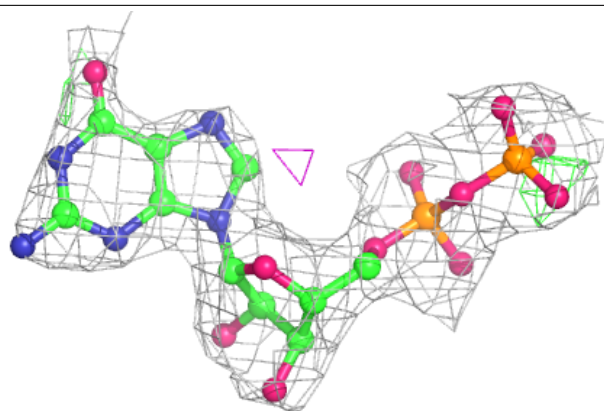
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GDP	A	500	28/28	0.93	0.17	51,75,81,81	0
3	GDP	B	500	28/28	0.96	0.14	39,60,63,64	0
4	MG	A	394	1/1	0.96	0.14	41,41,41,41	0
4	MG	B	394	1/1	0.97	0.11	46,46,46,46	0

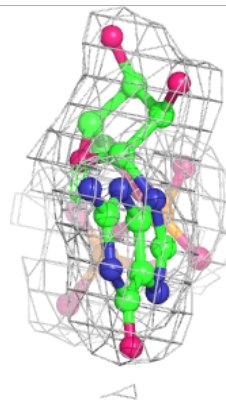
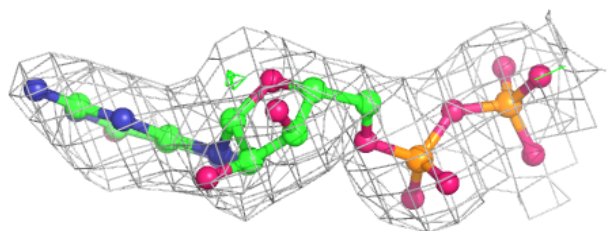
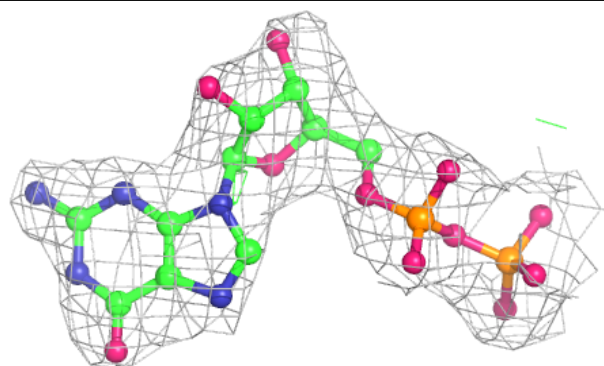
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around GDP A 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around GDP B 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.