



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:15 AM GMT

PDB ID : 1D2E  
Title : CRYSTAL STRUCTURE OF MITOCHONDRIAL EF-TU IN COMPLEX  
WITH GDP  
Authors : Andersen, G.R.; Thirup, S.; Spemulli, L.L.; Nyborg, J.  
Deposited on : 1999-09-23  
Resolution : 1.94 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

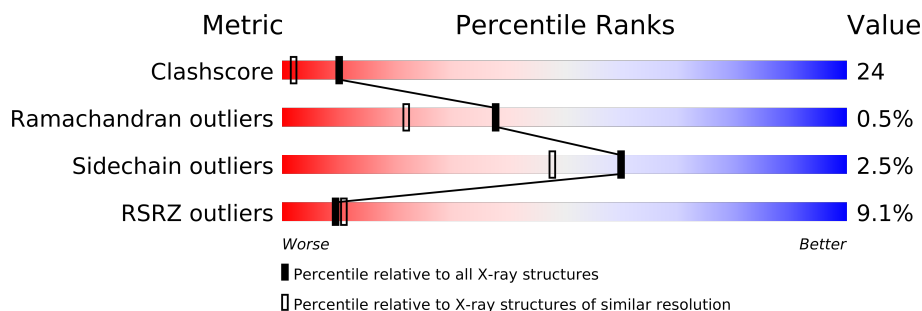
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.94 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))
Clashscore	79885	2281 (1.96-1.92)
Ramachandran outliers	78287	2255 (1.96-1.92)
Sidechain outliers	78261	2255 (1.96-1.92)
RSRZ outliers	66119	2024 (1.96-1.92)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	397	
1	B	397	
1	C	397	
1	D	397	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13597 atoms, of which 0 are hydrogen and 0 are deuterium.

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 (EF-TU).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3070	1938	539	577	16			
1	B	397	Total	C	N	O	S	0	0	0
			3070	1938	539	577	16			
1	C	397	Total	C	N	O	S	0	0	0
			3070	1938	539	577	16			
1	D	397	Total	C	N	O	S	0	0	0
			3070	1938	539	577	16			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- 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		
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is water.

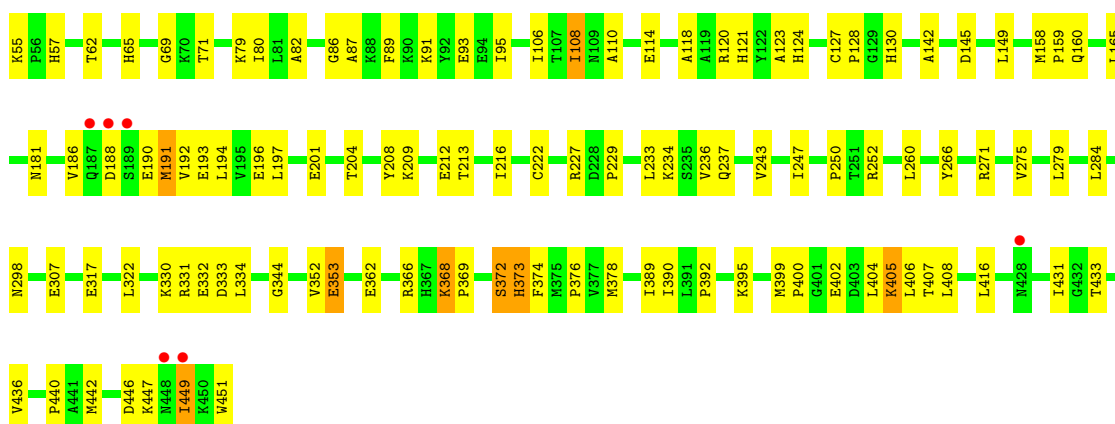
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	387	Total	O	0	0
			387	387		
4	B	274	Total	O	0	0
			274	274		
4	C	295	Total	O	0	0
			295	295		
4	D	245	Total	O	0	0
			245	245		

### 3 Residue-property plots

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

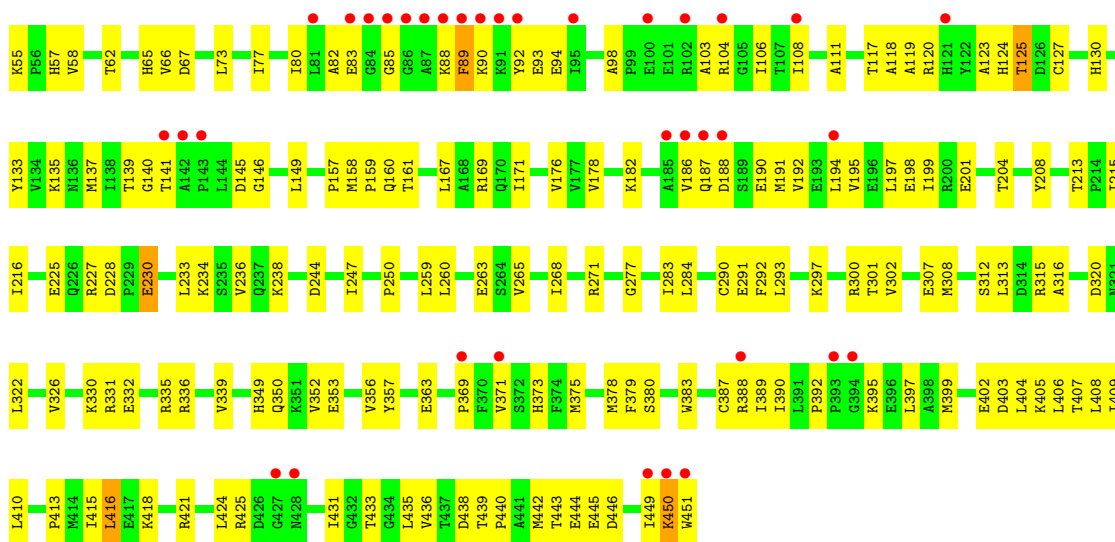
#### • Molecule 1: ELONGATION FACTOR TU (EF-TU)

Chain A:



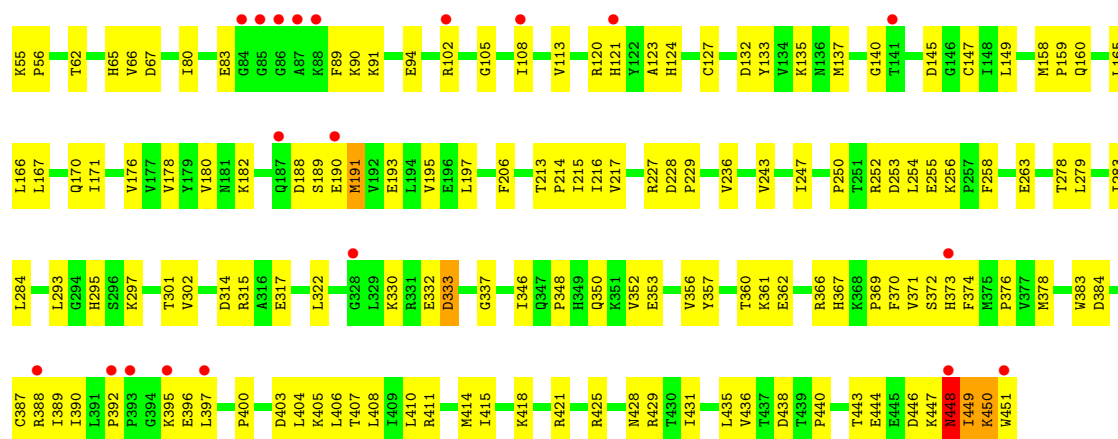
#### • Molecule 1: ELONGATION FACTOR TU (EF-TU)

Chain B:



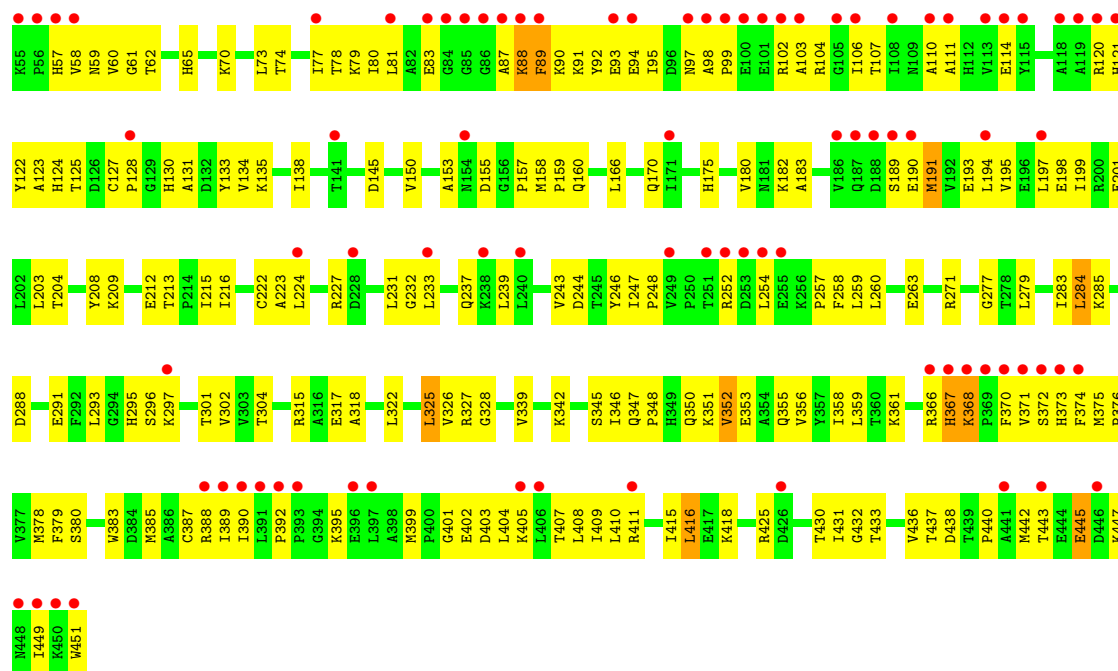
#### • Molecule 1: ELONGATION FACTOR TU (EF-TU)

Chain C:



• Molecule 1: ELONGATION FACTOR TU (EF-TU)

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.09Å 119.78Å 128.89Å 90.00° 96.97° 90.00°	Depositor
Resolution (Å)	34.70 – 1.94 33.87 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.0 (34.70-1.94) 98.2 (33.87-1.94)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 1.94Å)	Xtriage
Refinement program	CNS 0.3	Depositor
R, $R_{free}$	0.237 , 0.257 0.254 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 128896 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13597	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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

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	0.38	0/3127	0.73	1/4232 (0.0%)
1	B	0.32	0/3127	0.66	0/4232
1	C	0.33	0/3127	0.68	1/4232 (0.0%)
1	D	0.32	0/3127	0.67	0/4232
All	All	0.34	0/12508	0.69	2/16928 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	ALA	N-CA-C	-5.08	97.27	111.00
1	A	353	GLU	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3070	0	3122	106	0
1	B	3070	0	3122	164	0
1	C	3070	0	3122	132	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3070	0	3123	194	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	28	0	12	0	0
3	B	28	0	12	1	0
3	C	28	0	12	1	0
3	D	28	0	12	1	0
4	A	387	0	0	7	0
4	B	274	0	0	8	0
4	C	295	0	0	12	0
4	D	245	0	0	15	0
All	All	13597	0	12537	592	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

All (592) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:368:LYS:HD3	1:A:368:LYS:H	1.08	1.08
1:A:352:VAL:HG11	1:A:416:LEU:HD12	1.30	1.06
1:A:352:VAL:HG11	1:A:416:LEU:CD1	1.92	0.99
1:B:388:ARG:HH12	1:B:450:LYS:HE2	1.30	0.97
1:D:405:LYS:NZ	1:D:437:THR:HG21	1.80	0.96
1:A:449:ILE:H	1:A:449:ILE:HD13	1.35	0.91
1:A:368:LYS:HD3	1:A:368:LYS:N	1.86	0.88
1:B:352:VAL:CG2	1:B:436:VAL:HG13	2.02	0.88
1:A:446:ASP:O	1:A:449:ILE:HG23	1.74	0.87
1:D:405:LYS:HZ1	1:D:437:THR:HG21	1.40	0.86
1:D:416:LEU:HD22	1:D:436:VAL:HG21	1.58	0.86
1:D:443:THR:HG22	1:D:445:GLU:H	1.42	0.84
1:A:332:GLU:HB3	1:C:229:PRO:HG3	1.60	0.84
1:D:81:LEU:HB2	4:D:1380:HOH:O	1.78	0.84
1:A:446:ASP:O	1:A:449:ILE:HD12	1.78	0.83
1:D:91:LYS:HD3	1:D:92:TYR:H	1.42	0.82
1:A:449:ILE:HG12	1:A:451:TRP:HE1	1.41	0.82
1:B:352:VAL:HG21	1:B:436:VAL:HG13	1.59	0.82
1:C:108:ILE:HD11	1:C:135:LYS:HB2	1.59	0.82
1:C:392:PRO:HG3	1:C:405:LYS:O	1.78	0.82
1:D:368:LYS:HD3	1:D:368:LYS:N	1.95	0.81
1:A:392:PRO:HG3	1:A:405:LYS:O	1.81	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:416:LEU:HD22	1:B:436:VAL:HG21	1.62	0.80
1:C:189:SER:O	1:C:193:GLU:HG3	1.82	0.80
1:D:78:THR:HB	1:D:89:PHE:HA	1.63	0.79
1:C:145:ASP:CG	1:C:250:PRO:HG3	2.02	0.79
1:C:361:LYS:HE2	1:C:367:HIS:O	1.82	0.79
1:D:73:LEU:O	1:D:77:ILE:HG13	1.83	0.78
1:A:108:ILE:HD11	1:A:110:ALA:HB2	1.66	0.78
1:A:416:LEU:CD1	1:A:436:VAL:HG21	2.13	0.78
1:D:304:THR:OG1	1:D:325:LEU:HD22	1.83	0.78
1:D:368:LYS:HD3	1:D:368:LYS:H	1.48	0.77
1:C:352:VAL:CG2	1:C:436:VAL:HG13	2.13	0.77
1:B:90:LYS:NZ	1:B:94:GLU:HG2	2.01	0.76
1:D:97:ASN:HB3	4:D:1533:HOH:O	1.86	0.76
1:A:374:PHE:CE2	1:A:376:PRO:HG3	2.20	0.76
1:A:193:GLU:O	1:A:197:LEU:HG	1.86	0.76
1:A:449:ILE:CG1	1:A:451:TRP:HE1	1.96	0.75
1:D:90:LYS:HG2	1:D:94:GLU:HG2	1.68	0.75
1:A:449:ILE:HG12	1:A:451:TRP:NE1	2.00	0.75
1:D:98:ALA:HB2	1:D:111:ALA:HB2	1.65	0.75
1:B:353:GLU:HG3	1:B:440:PRO:HG2	1.67	0.75
1:B:145:ASP:CG	1:B:250:PRO:HG3	2.07	0.75
1:B:98:ALA:HB2	1:B:111:ALA:HB2	1.66	0.75
1:D:375:MET:HE2	1:D:388:ARG:HD3	1.68	0.75
1:A:209:LYS:HB3	1:A:212:GLU:OE2	1.87	0.74
1:D:79:LYS:O	1:D:83:GLU:HG2	1.87	0.74
1:D:153:ALA:HB2	1:D:180:VAL:HG12	1.70	0.74
1:A:266:TYR:HA	1:A:331:ARG:HE	1.52	0.73
1:D:418:LYS:HE2	1:D:438:ASP:HA	1.70	0.73
1:B:228:ASP:HB3	1:B:230:GLU:OE2	1.89	0.72
1:B:58:VAL:HG21	1:B:120:ARG:HH21	1.55	0.72
1:C:243:VAL:HG13	1:C:247:ILE:HD12	1.72	0.71
1:D:392:PRO:HD2	1:D:395:LYS:HD2	1.73	0.70
1:D:405:LYS:NZ	1:D:437:THR:CG2	2.55	0.70
1:D:375:MET:CE	1:D:388:ARG:HD3	2.21	0.70
1:D:353:GLU:HG3	1:D:440:PRO:HG2	1.73	0.70
1:B:58:VAL:HG21	1:B:120:ARG:NH2	2.06	0.70
1:C:387:CYS:HB3	1:C:410:LEU:HD23	1.72	0.69
1:A:416:LEU:HD11	1:A:436:VAL:HG21	1.75	0.69
1:B:388:ARG:NH1	1:B:450:LYS:HE2	2.07	0.69
1:C:443:THR:HG22	1:C:446:ASP:OD2	1.93	0.68
1:C:352:VAL:HG21	1:C:436:VAL:HG13	1.73	0.68
1:D:252:ARG:HH21	1:D:254:LEU:HD11	1.57	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:301:THR:OG1	1:D:327:ARG:HG2	1.93	0.68
1:B:389:ILE:HG12	1:B:408:LEU:CD2	2.23	0.68
1:A:352:VAL:CG1	1:A:416:LEU:HD12	2.15	0.67
1:B:66:VAL:HG13	1:B:160:GLN:OE1	1.95	0.67
1:B:450:LYS:HD3	1:B:450:LYS:H	1.59	0.67
1:B:387:CYS:HB3	1:B:410:LEU:HD23	1.76	0.67
1:B:268:ILE:HG23	1:B:271:ARG:HB2	1.75	0.67
1:D:104:ARG:HH11	1:D:104:ARG:HG2	1.60	0.67
1:C:166:LEU:O	1:C:170:GLN:HG3	1.94	0.66
1:D:209:LYS:O	1:D:213:THR:HG23	1.94	0.66
1:A:145:ASP:CG	1:A:250:PRO:HG3	2.16	0.66
1:D:447:LYS:HB3	4:D:1522:HOH:O	1.95	0.66
1:B:332:GLU:H	1:B:332:GLU:CD	1.99	0.66
1:D:65:HIS:HD2	1:D:160:GLN:H	1.44	0.66
1:B:451:TRP:HB3	4:B:1451:HOH:O	1.96	0.66
1:B:291:GLU:OE2	1:B:293:LEU:HD21	1.95	0.66
1:A:368:LYS:H	1:A:368:LYS:CD	1.97	0.66
1:C:371:VAL:HG12	1:C:397:LEU:HD23	1.78	0.66
1:C:145:ASP:OD1	1:C:250:PRO:HG3	1.95	0.65
1:C:371:VAL:HG12	1:C:397:LEU:CD2	2.27	0.65
1:A:416:LEU:HD13	1:A:436:VAL:HG21	1.78	0.65
1:A:372:SER:O	1:A:373:HIS:HB2	1.97	0.65
1:B:331:ARG:HG3	1:B:331:ARG:HH11	1.61	0.65
1:A:93:GLU:H	1:A:93:GLU:CD	2.00	0.65
1:C:102:ARG:HE	1:C:105:GLY:HA2	1.61	0.65
1:B:90:LYS:HZ1	1:B:94:GLU:HG2	1.60	0.64
1:A:298:ASN:HB2	4:A:1664:HOH:O	1.97	0.64
1:A:449:ILE:H	1:A:449:ILE:CD1	2.08	0.64
1:A:416:LEU:HD11	1:A:436:VAL:CG2	2.27	0.64
1:B:352:VAL:HG23	1:B:438:ASP:O	1.98	0.63
1:A:344:GLY:O	1:D:418:LYS:NZ	2.31	0.63
1:D:252:ARG:NH2	1:D:254:LEU:HD21	2.14	0.63
1:C:102:ARG:HB2	4:C:1543:HOH:O	1.99	0.63
1:D:231:LEU:HD23	4:D:1351:HOH:O	1.98	0.63
1:A:229:PRO:O	1:A:234:LYS:HG2	1.98	0.63
1:C:140:GLY:HA3	1:C:421:ARG:NE	2.13	0.63
1:B:390:ILE:HB	1:B:407:THR:HB	1.81	0.62
1:B:268:ILE:HD13	1:B:271:ARG:HD3	1.81	0.62
1:B:65:HIS:HD2	1:B:160:GLN:H	1.46	0.62
1:D:246:TYR:O	1:D:248:PRO:HD3	2.00	0.62
1:B:268:ILE:CG2	1:B:271:ARG:HB2	2.29	0.62
1:B:409:ILE:HG23	1:B:442:MET:HE1	1.83	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:60:VAL:HG12	1:D:61:GLY:N	2.15	0.61
1:D:366:ARG:NH1	1:D:368:LYS:O	2.33	0.61
1:D:239:LEU:O	1:D:243:VAL:HG23	2.01	0.60
1:D:80:ILE:HD13	1:D:233:LEU:HD12	1.82	0.60
1:C:389:ILE:C	1:C:390:ILE:HD12	2.20	0.60
1:D:322:LEU:C	1:D:322:LEU:HD12	2.22	0.60
1:C:108:ILE:HD12	1:C:132:ASP:HA	1.83	0.60
1:D:431:ILE:HD12	1:D:432:GLY:N	2.16	0.60
1:B:216:ILE:HD12	1:B:216:ILE:N	2.16	0.60
1:D:353:GLU:HG3	1:D:440:PRO:CG	2.31	0.60
1:C:443:THR:HG22	1:C:446:ASP:CG	2.22	0.60
1:D:131:ALA:O	1:D:135:LYS:HG3	2.01	0.60
1:D:352:VAL:HG22	1:D:436:VAL:HG13	1.83	0.60
1:B:308:MET:HE2	1:B:313:LEU:HD12	1.84	0.60
1:D:350:GLN:HG3	1:D:410:LEU:O	2.02	0.59
1:D:405:LYS:HZ2	1:D:437:THR:CB	2.15	0.59
1:C:65:HIS:HE1	4:C:1571:HOH:O	1.85	0.59
1:D:194:LEU:HD23	4:D:1541:HOH:O	2.01	0.59
1:C:425:ARG:HD3	4:C:1546:HOH:O	2.01	0.59
1:A:330:LYS:HG2	1:A:333:ASP:OD1	2.03	0.59
1:C:293:LEU:HB3	1:C:348:PRO:HG3	1.83	0.59
1:C:171:ILE:HG22	1:C:435:LEU:HD22	1.83	0.59
1:B:265:VAL:HB	1:B:331:ARG:HH12	1.68	0.59
1:A:368:LYS:N	1:A:368:LYS:CD	2.63	0.59
1:B:192:VAL:O	1:B:195:VAL:HG12	2.02	0.58
1:C:279:LEU:HD23	1:C:317:GLU:C	2.23	0.58
1:D:433:THR:HG22	4:D:1362:HOH:O	2.03	0.58
1:C:390:ILE:HD12	1:C:390:ILE:N	2.17	0.58
1:A:65:HIS:HD2	1:A:160:GLN:H	1.51	0.58
1:C:449:ILE:HD12	1:C:449:ILE:C	2.23	0.58
1:D:374:PHE:CD2	1:D:376:PRO:HG3	2.39	0.58
1:B:373:HIS:HA	1:B:388:ARG:CG	2.33	0.58
1:C:137:MET:CE	1:C:167:LEU:HD23	2.33	0.58
1:D:385:MET:SD	1:D:411:ARG:HG3	2.44	0.58
1:C:360:THR:HG22	1:C:362:GLU:H	1.67	0.58
1:B:352:VAL:HG23	1:B:436:VAL:HG13	1.82	0.58
1:C:137:MET:HE3	1:C:167:LEU:HD23	1.85	0.57
1:C:278:THR:HG23	4:C:1367:HOH:O	2.04	0.57
1:D:361:LYS:HD3	1:D:367:HIS:CD2	2.38	0.57
1:B:146:GLY:HA3	1:B:247:ILE:HD12	1.85	0.57
1:D:166:LEU:O	1:D:170:GLN:HG3	2.05	0.57
1:D:89:PHE:CD1	1:D:89:PHE:C	2.78	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:385:MET:SD	1:D:411:ARG:CG	2.92	0.57
1:A:307:GLU:HG2	4:A:1352:HOH:O	2.02	0.57
1:D:315:ARG:HG2	4:D:1394:HOH:O	2.05	0.57
1:C:428:ASN:HA	4:C:1546:HOH:O	2.04	0.57
1:D:368:LYS:N	1:D:368:LYS:CD	2.66	0.57
1:A:197:LEU:O	1:A:201:GLU:HG3	2.04	0.57
1:C:372:SER:O	1:C:373:HIS:HB2	2.04	0.57
1:A:449:ILE:CG1	1:A:451:TRP:NE1	2.61	0.57
1:C:145:ASP:OD2	1:C:250:PRO:HG3	2.04	0.57
1:B:395:LYS:HE2	1:B:404:LEU:HD13	1.86	0.56
1:A:449:ILE:N	1:A:449:ILE:HD13	2.15	0.56
1:D:366:ARG:HD3	1:D:370:PHE:HD2	1.71	0.56
1:B:395:LYS:HE2	1:B:404:LEU:CD1	2.36	0.56
1:B:135:LYS:HE2	1:B:357:TYR:CZ	2.40	0.56
1:B:127:CYS:HB2	1:B:133:TYR:CE1	2.40	0.56
1:A:120:ARG:NH1	1:A:247:ILE:O	2.37	0.56
1:C:62:THR:HG23	1:C:124:HIS:CE1	2.40	0.56
1:D:295:HIS:O	1:D:297:LYS:HG3	2.05	0.56
1:D:197:LEU:O	1:D:201:GLU:HG2	2.05	0.56
1:D:258:PHE:HB2	1:D:279:LEU:HD11	1.88	0.56
1:B:83:GLU:C	1:B:85:GLY:H	2.09	0.56
1:C:188:ASP:HB2	1:C:190:GLU:OE1	2.06	0.56
1:B:93:GLU:H	1:B:93:GLU:CD	2.08	0.56
1:B:335:ARG:NH2	4:B:1309:HOH:O	2.39	0.55
1:B:57:HIS:HB2	4:B:1431:HOH:O	2.05	0.55
1:C:429:ARG:HB2	1:C:429:ARG:HH11	1.71	0.55
1:D:222:CYS:HB3	1:D:227:ARG:O	2.07	0.55
1:B:392:PRO:HG3	1:B:405:LYS:O	2.07	0.55
1:B:65:HIS:CD2	1:B:160:GLN:HB2	2.42	0.55
1:A:216:ILE:N	1:A:216:ILE:HD12	2.22	0.55
1:D:390:ILE:HB	1:D:407:THR:HB	1.86	0.55
1:B:433:THR:HG22	4:B:1357:HOH:O	2.06	0.55
1:B:330:LYS:HB3	1:B:332:GLU:OE2	2.07	0.55
1:C:121:HIS:HB2	4:C:1471:HOH:O	2.07	0.55
1:C:65:HIS:HD2	1:C:160:GLN:H	1.53	0.55
1:D:57:HIS:CE1	1:D:123:ALA:HB2	2.41	0.55
1:D:431:ILE:HD12	1:D:431:ILE:C	2.27	0.55
1:D:79:LYS:HD2	1:D:91:LYS:NZ	2.22	0.55
1:C:102:ARG:NE	1:C:105:GLY:HA2	2.22	0.55
1:D:191:MET:O	1:D:195:VAL:HG23	2.07	0.54
1:D:58:VAL:HB	1:D:122:TYR:CE1	2.41	0.54
1:D:263:GLU:HG3	4:D:1384:HOH:O	2.06	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:438:ASP:C	1:B:440:PRO:HD3	2.28	0.54
1:D:351:LYS:HB2	1:D:442:MET:SD	2.47	0.54
1:A:390:ILE:N	1:A:390:ILE:HD12	2.22	0.54
1:A:209:LYS:O	1:A:213:THR:HG23	2.08	0.54
1:B:353:GLU:HG3	1:B:440:PRO:CG	2.37	0.54
1:B:312:SER:O	1:B:313:LEU:HD23	2.08	0.54
1:C:378:MET:CE	1:C:408:LEU:HD22	2.38	0.54
1:A:404:LEU:N	1:A:404:LEU:HD23	2.22	0.54
1:A:243:VAL:HG13	1:A:247:ILE:HD12	1.88	0.54
1:D:233:LEU:O	1:D:237:GLN:HG3	2.08	0.54
1:C:135:LYS:HE2	1:C:357:TYR:CZ	2.42	0.54
1:B:416:LEU:HD22	1:B:436:VAL:CG2	2.35	0.53
1:D:60:VAL:CG1	1:D:61:GLY:N	2.71	0.53
1:B:139:THR:O	1:B:139:THR:HG22	2.08	0.53
1:C:322:LEU:C	1:C:322:LEU:HD12	2.28	0.53
1:B:106:ILE:HG23	1:B:363:GLU:OE2	2.08	0.53
1:C:353:GLU:OE2	1:C:440:PRO:HG2	2.08	0.53
1:A:352:VAL:HG11	1:A:416:LEU:HD11	1.87	0.53
1:C:252:ARG:HH21	1:C:254:LEU:HD11	1.73	0.53
1:D:104:ARG:NH1	1:D:104:ARG:HG2	2.23	0.53
1:B:140:GLY:HA3	1:B:421:ARG:NE	2.24	0.53
1:B:62:THR:HG23	1:B:124:HIS:CE1	2.44	0.53
1:C:360:THR:CG2	1:C:362:GLU:HG2	2.38	0.53
1:C:360:THR:HG22	1:C:361:LYS:N	2.23	0.53
1:B:450:LYS:HD2	4:B:1457:HOH:O	2.09	0.53
1:A:392:PRO:HD2	1:A:395:LYS:CB	2.39	0.53
1:C:366:ARG:NH1	1:C:370:PHE:HB3	2.23	0.52
1:D:443:THR:CG2	1:D:445:GLU:HB3	2.38	0.52
1:B:120:ARG:HH11	1:B:244:ASP:HA	1.73	0.52
1:D:378:MET:CE	1:D:408:LEU:HD13	2.39	0.52
1:B:65:HIS:CE1	1:B:66:VAL:HG22	2.45	0.52
1:A:65:HIS:CD2	1:A:160:GLN:HB2	2.44	0.52
1:B:178:VAL:HB	1:B:215:ILE:HG12	1.91	0.52
1:A:82:ALA:HA	1:A:87:ALA:O	2.09	0.52
1:D:387:CYS:HB3	1:D:410:LEU:HD23	1.91	0.52
1:B:119:ALA:C	1:B:120:ARG:HG3	2.30	0.52
1:D:257:PRO:CB	1:D:345:SER:HB2	2.39	0.52
1:C:411:ARG:HA	1:C:451:TRP:CZ2	2.45	0.52
1:A:89:PHE:CE2	1:A:91:LYS:HG2	2.45	0.52
1:A:158:MET:HB3	1:A:159:PRO:CD	2.39	0.52
1:D:375:MET:HA	1:D:387:CYS:O	2.09	0.52
1:A:260:LEU:HD13	1:A:260:LEU:C	2.30	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:448:ASN:ND2	1:C:448:ASN:O	2.43	0.52
1:D:62:THR:O	1:D:133:TYR:CE2	2.63	0.52
1:D:243:VAL:HG13	1:D:247:ILE:HD12	1.90	0.52
1:D:404:LEU:HD23	1:D:404:LEU:N	2.25	0.52
1:D:352:VAL:CG2	1:D:436:VAL:HG13	2.40	0.51
1:B:58:VAL:CG2	1:B:120:ARG:HH21	2.22	0.51
1:B:316:ALA:CB	1:B:322:LEU:HD22	2.41	0.51
1:D:213:THR:HG22	4:D:1500:HOH:O	2.11	0.51
1:B:187:GLN:HA	4:B:1458:HOH:O	2.11	0.51
1:B:118:ALA:HB3	4:B:1561:HOH:O	2.09	0.51
1:D:346:ILE:CD1	1:D:415:ILE:HG23	2.41	0.51
1:B:409:ILE:HG23	1:B:442:MET:CE	2.40	0.51
1:B:352:VAL:HG22	1:B:353:GLU:N	2.26	0.51
1:B:389:ILE:HG12	1:B:408:LEU:HD21	1.91	0.51
1:B:449:ILE:HG12	1:B:450:LYS:N	2.26	0.51
1:A:374:PHE:CD2	1:A:376:PRO:HG3	2.45	0.51
1:B:57:HIS:CE1	1:B:123:ALA:HB2	2.45	0.51
1:B:349:HIS:ND1	1:B:439:THR:HG21	2.25	0.51
1:D:271:ARG:HG2	1:D:325:LEU:HD11	1.92	0.51
1:D:98:ALA:HB1	1:D:110:ALA:C	2.31	0.51
1:B:188:ASP:HB3	1:B:190:GLU:OE1	2.11	0.51
1:A:322:LEU:C	1:A:322:LEU:HD12	2.31	0.51
1:B:350:GLN:HG2	1:B:442:MET:HE2	1.93	0.51
1:B:443:THR:CG2	1:B:445:GLU:HG2	2.40	0.51
1:D:65:HIS:HA	1:D:160:GLN:HB2	1.92	0.51
1:B:399:MET:O	1:B:402:GLU:HB3	2.11	0.51
1:B:350:GLN:HG2	1:B:442:MET:CE	2.41	0.51
1:D:284:LEU:HD23	1:D:285:LYS:N	2.26	0.51
1:C:55:LYS:HB2	1:C:56:PRO:CD	2.40	0.50
1:A:332:GLU:CB	1:C:229:PRO:HG3	2.39	0.50
1:D:106:ILE:HD11	1:D:433:THR:OG1	2.11	0.50
1:C:147:CYS:O	1:C:176:VAL:HG13	2.11	0.50
1:C:369:PRO:HG3	1:C:400:PRO:CG	2.42	0.50
1:D:399:MET:HB2	1:D:402:GLU:CD	2.32	0.50
1:D:104:ARG:NH2	1:D:430:THR:OG1	2.44	0.50
1:B:167:LEU:O	1:B:171:ILE:HG23	2.11	0.50
1:D:74:THR:HG22	1:D:95:ILE:HD13	1.92	0.50
1:B:234:LYS:O	1:B:238:LYS:HG3	2.11	0.50
1:B:283:ILE:HD13	1:B:315:ARG:NH2	2.27	0.50
1:A:252:ARG:HD3	4:A:1418:HOH:O	2.12	0.50
1:D:98:ALA:CB	1:D:111:ALA:HB2	2.36	0.50
1:C:451:TRP:HB2	4:C:1523:HOH:O	2.12	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:443:THR:HG23	1:C:446:ASP:H	1.77	0.50
1:B:378:MET:CE	1:B:408:LEU:HD13	2.42	0.50
1:D:283:ILE:HD12	1:D:315:ARG:NH2	2.27	0.50
1:D:389:ILE:HG12	1:D:408:LEU:CD2	2.42	0.50
1:B:58:VAL:HG21	1:B:120:ARG:CZ	2.42	0.50
1:B:265:VAL:HB	1:B:331:ARG:NH1	2.26	0.50
1:C:91:LYS:HD3	1:C:94:GLU:OE2	2.12	0.50
1:D:259:LEU:HD11	1:D:339:VAL:HG11	1.93	0.50
1:D:285:LYS:N	1:D:288:ASP:OD2	2.44	0.49
1:B:443:THR:HG22	1:B:445:GLU:H	1.76	0.49
1:D:216:ILE:HD12	1:D:216:ILE:N	2.26	0.49
1:B:369:PRO:CG	1:B:399:MET:SD	3.00	0.49
1:A:57:HIS:CE1	1:A:123:ALA:HB2	2.47	0.49
1:B:446:ASP:O	1:B:449:ILE:HG22	2.13	0.49
1:B:418:LYS:HA	1:B:436:VAL:HG12	1.95	0.49
1:B:308:MET:CE	1:B:313:LEU:HD12	2.41	0.49
1:A:86:GLY:O	1:A:87:ALA:HB2	2.12	0.49
1:C:450:LYS:HD3	1:C:450:LYS:N	2.28	0.49
1:D:418:LYS:HA	1:D:436:VAL:HG12	1.95	0.49
1:D:285:LYS:NZ	1:D:285:LYS:HB2	2.28	0.49
1:D:62:THR:HG23	1:D:124:HIS:NE2	2.28	0.49
1:C:89:PHE:CZ	1:C:91:LYS:HE3	2.48	0.49
1:D:158:MET:HB3	1:D:159:PRO:CD	2.43	0.49
1:C:188:ASP:OD2	1:C:191:MET:HB2	2.13	0.49
1:D:120:ARG:HD2	1:D:122:TYR:OH	2.12	0.49
1:B:186:VAL:HG12	1:B:188:ASP:H	1.78	0.49
1:C:216:ILE:N	1:C:216:ILE:HD12	2.28	0.49
1:C:127:CYS:HB2	1:C:133:TYR:CE1	2.48	0.49
1:A:192:VAL:HG12	1:A:196:GLU:OE2	2.12	0.48
1:A:204:THR:HA	1:A:208:TYR:O	2.12	0.48
1:B:149:LEU:HD11	1:B:161:THR:HG23	1.94	0.48
1:B:350:GLN:HB2	1:B:413:PRO:HG3	1.95	0.48
1:D:355:GLN:OE1	1:D:405:LYS:HE2	2.14	0.48
1:C:65:HIS:HA	1:C:160:GLN:HB2	1.95	0.48
1:D:346:ILE:HD11	1:D:415:ILE:HG23	1.95	0.48
1:D:223:ALA:HB2	1:D:232:GLY:C	2.33	0.48
1:D:366:ARG:C	1:D:368:LYS:H	2.16	0.48
1:C:418:LYS:HA	1:C:436:VAL:HG12	1.94	0.48
1:B:190:GLU:CD	1:B:190:GLU:H	2.17	0.48
1:B:227:ARG:O	1:B:228:ASP:C	2.51	0.48
1:C:373:HIS:CD2	1:C:388:ARG:NE	2.81	0.48
1:B:443:THR:HB	1:B:446:ASP:OD2	2.12	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:371:VAL:HG23	1:D:373:HIS:H	1.78	0.48
1:C:279:LEU:HD23	1:C:317:GLU:CA	2.42	0.48
1:A:369:PRO:CG	1:A:399:MET:SD	3.01	0.48
1:B:380:SER:HB3	1:B:383:TRP:CZ2	2.49	0.48
1:B:88:LYS:HD3	1:B:89:PHE:N	2.28	0.48
1:C:137:MET:HE3	1:C:167:LEU:HB3	1.96	0.48
1:B:404:LEU:HD11	1:B:406:LEU:HD21	1.95	0.48
1:C:295:HIS:O	1:C:297:LYS:HG3	2.13	0.48
1:B:373:HIS:HA	1:B:388:ARG:HG2	1.94	0.48
1:A:188:ASP:OD2	1:A:190:GLU:HG2	2.14	0.48
1:B:67:ASP:OD1	1:B:67:ASP:O	2.31	0.48
1:A:442:MET:HE3	1:A:446:ASP:HB3	1.96	0.48
1:B:225:GLU:HB2	1:B:227:ARG:HD3	1.96	0.48
1:A:142:ALA:HB2	4:A:1496:HOH:O	2.14	0.48
1:B:418:LYS:HE2	1:B:439:THR:H	1.79	0.47
1:C:350:GLN:HG3	1:C:410:LEU:O	2.14	0.47
1:C:102:ARG:HE	1:C:105:GLY:CA	2.26	0.47
1:B:204:THR:HA	1:B:208:TYR:O	2.14	0.47
1:B:73:LEU:O	1:B:77:ILE:HG13	2.14	0.47
1:D:443:THR:C	1:D:445:GLU:N	2.66	0.47
1:D:283:ILE:HD12	1:D:315:ARG:CZ	2.44	0.47
1:D:79:LYS:HD3	1:D:224:LEU:HD12	1.96	0.47
1:B:145:ASP:OD1	1:B:250:PRO:HG3	2.13	0.47
1:A:279:LEU:HD23	1:A:317:GLU:C	2.35	0.47
1:D:342:LYS:HE3	4:D:1451:HOH:O	2.13	0.47
1:A:62:THR:HG23	1:A:124:HIS:CE1	2.50	0.47
1:D:358:ILE:O	1:D:401:GLY:N	2.38	0.47
1:D:405:LYS:NZ	1:D:437:THR:OG1	2.43	0.47
1:C:252:ARG:NH2	1:C:317:GLU:OE2	2.48	0.47
1:B:190:GLU:O	1:B:194:LEU:HG	2.15	0.47
1:B:89:PHE:C	1:B:89:PHE:CD1	2.88	0.47
1:B:225:GLU:O	1:B:227:ARG:HG3	2.14	0.47
1:C:374:PHE:HE2	1:C:431:ILE:CD1	2.27	0.47
1:B:371:VAL:HG12	1:B:397:LEU:HD23	1.97	0.47
1:B:58:VAL:HG21	1:B:120:ARG:NE	2.30	0.47
1:D:130:HIS:ND1	1:D:160:GLN:HG2	2.30	0.47
1:C:451:TRP:N	1:C:451:TRP:CD1	2.83	0.47
1:C:346:ILE:HD12	1:C:415:ILE:HD12	1.97	0.46
1:C:158:MET:HB3	1:C:159:PRO:CD	2.45	0.46
1:D:405:LYS:HB3	4:D:1478:HOH:O	2.15	0.46
1:D:252:ARG:NH2	1:D:317:GLU:OE2	2.35	0.46
1:D:385:MET:SD	1:D:411:ARG:NE	2.80	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:188:ASP:C	1:C:190:GLU:N	2.69	0.46
1:A:79:LYS:HB2	1:A:89:PHE:CE1	2.51	0.46
1:A:80:ILE:HD12	1:A:236:VAL:HG11	1.96	0.46
1:C:421:ARG:HG2	1:C:421:ARG:HH11	1.79	0.46
1:B:260:LEU:C	1:B:260:LEU:HD13	2.36	0.46
1:B:82:ALA:HA	4:B:1330:HOH:O	2.15	0.46
1:D:366:ARG:HG3	1:D:368:LYS:O	2.16	0.46
1:B:404:LEU:HD23	1:B:404:LEU:N	2.30	0.46
1:C:90:LYS:HD2	1:C:113:VAL:HG12	1.96	0.46
1:A:114:GLU:OE1	1:A:121:HIS:NE2	2.46	0.46
1:D:283:ILE:HG22	4:D:1450:HOH:O	2.16	0.46
1:D:57:HIS:HE1	1:D:123:ALA:HB2	1.81	0.46
1:B:263:GLU:HG2	1:B:277:GLY:HA2	1.97	0.46
1:B:331:ARG:HG3	1:B:331:ARG:NH1	2.28	0.46
1:B:443:THR:HG22	1:B:445:GLU:HG2	1.98	0.46
1:D:252:ARG:NH2	1:D:254:LEU:HD11	2.27	0.46
1:D:195:VAL:O	1:D:199:ILE:HG13	2.15	0.46
1:C:253:ASP:HB3	1:C:256:LYS:HD2	1.97	0.46
1:D:260:LEU:HD11	1:D:277:GLY:HA3	1.98	0.46
1:D:79:LYS:HD2	1:D:91:LYS:HZ3	1.81	0.46
1:D:91:LYS:HD3	1:D:92:TYR:N	2.20	0.46
1:D:366:ARG:HD3	1:D:370:PHE:CD2	2.49	0.46
1:D:373:HIS:HB3	1:D:388:ARG:NH2	2.30	0.46
1:B:225:GLU:OE1	1:B:227:ARG:NH1	2.46	0.46
1:C:376:PRO:HG3	1:C:389:ILE:HD11	1.97	0.46
1:D:190:GLU:O	1:D:194:LEU:HG	2.16	0.46
1:D:134:VAL:O	1:D:138:ILE:HG13	2.16	0.46
1:B:442:MET:SD	1:B:446:ASP:HB3	2.56	0.46
1:C:254:LEU:HD22	1:C:317:GLU:HB2	1.98	0.46
1:A:392:PRO:HD2	1:A:395:LYS:HB2	1.98	0.45
1:B:297:LYS:HE2	1:B:297:LYS:HB3	1.77	0.45
1:B:292:PHE:HZ	1:B:326:VAL:HG11	1.81	0.45
1:D:392:PRO:HG2	1:D:405:LYS:O	2.16	0.45
1:D:366:ARG:O	1:D:368:LYS:N	2.49	0.45
1:D:409:ILE:O	1:D:451:TRP:HH2	1.99	0.45
1:B:158:MET:HB3	1:B:159:PRO:CD	2.46	0.45
1:A:222:CYS:HB3	1:A:227:ARG:O	2.17	0.45
1:B:103:ALA:O	1:B:104:ARG:HB2	2.16	0.45
1:A:108:ILE:CD1	1:A:110:ALA:HB2	2.40	0.45
1:A:188:ASP:OD2	1:A:190:GLU:HB2	2.17	0.45
1:D:157:PRO:HD2	1:D:198:GLU:OE2	2.16	0.45
1:B:356:VAL:O	1:B:403:ASP:HA	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:418:LYS:HE2	1:B:438:ASP:HA	1.98	0.45
1:D:93:GLU:CD	1:D:93:GLU:H	2.20	0.45
1:D:90:LYS:HE2	1:D:94:GLU:HG2	1.98	0.45
1:D:65:HIS:CD2	1:D:160:GLN:HB2	2.51	0.45
1:D:60:VAL:O	1:D:124:HIS:HA	2.16	0.45
1:D:120:ARG:NH1	1:D:247:ILE:O	2.44	0.45
1:C:366:ARG:HH11	1:C:370:PHE:HB3	1.80	0.45
1:C:182:LYS:HG2	3:C:1303:GDP:C6	2.52	0.45
1:D:449:ILE:HG22	4:D:1508:HOH:O	2.15	0.45
1:D:170:GLN:HE22	1:D:405:LYS:HZ1	1.64	0.45
1:D:271:ARG:NH2	4:D:1448:HOH:O	2.49	0.45
1:C:252:ARG:NH2	1:C:254:LEU:HD11	2.30	0.45
1:A:404:LEU:HD11	1:A:406:LEU:HD21	1.99	0.45
1:C:404:LEU:HD11	1:C:406:LEU:HD21	1.99	0.45
1:C:383:TRP:CG	1:C:414:MET:HE2	2.51	0.45
1:D:91:LYS:HG3	1:D:93:GLU:OE1	2.15	0.45
1:B:195:VAL:O	1:B:199:ILE:HG13	2.17	0.45
1:B:388:ARG:NH2	1:B:449:ILE:HG13	2.32	0.45
1:D:356:VAL:O	1:D:403:ASP:HA	2.17	0.45
1:B:55:LYS:NZ	1:B:117:THR:O	2.48	0.45
1:A:106:ILE:HD13	1:A:433:THR:HG21	1.98	0.45
1:D:353:GLU:HB2	1:D:438:ASP:HB2	1.98	0.45
1:C:149:LEU:HD22	1:C:165:LEU:HD21	1.98	0.45
1:D:158:MET:HB3	1:D:159:PRO:HD2	1.99	0.45
1:D:366:ARG:H	1:D:431:ILE:HG22	1.82	0.44
1:D:62:THR:O	1:D:133:TYR:HE2	1.99	0.44
1:B:108:ILE:HD11	1:B:135:LYS:HB3	1.98	0.44
1:A:449:ILE:HG13	1:A:451:TRP:HE1	1.80	0.44
1:D:367:HIS:HA	4:D:1336:HOH:O	2.16	0.44
1:A:190:GLU:O	1:A:194:LEU:HG	2.17	0.44
1:C:283:ILE:HD13	1:C:315:ARG:NH2	2.32	0.44
1:A:431:ILE:HD12	1:A:431:ILE:C	2.38	0.44
1:A:362:GLU:N	1:A:362:GLU:OE1	2.41	0.44
1:D:291:GLU:CD	1:D:293:LEU:HD21	2.37	0.44
1:A:188:ASP:HA	4:A:1477:HOH:O	2.17	0.44
1:B:182:LYS:HG2	3:B:1302:GDP:C6	2.52	0.44
1:C:378:MET:O	1:C:384:ASP:HA	2.17	0.44
1:A:57:HIS:HE1	1:A:123:ALA:HB2	1.83	0.44
1:C:443:THR:CG2	1:C:446:ASP:H	2.30	0.44
1:D:209:LYS:CB	1:D:212:GLU:HG2	2.46	0.44
1:C:102:ARG:HD3	4:C:1508:HOH:O	2.17	0.44
1:C:337:GLY:CA	1:C:383:TRP:HB3	2.48	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:212:GLU:N	1:A:212:GLU:OE2	2.49	0.44
1:D:62:THR:HG23	1:D:124:HIS:CE1	2.52	0.44
1:D:405:LYS:NZ	1:D:437:THR:CB	2.81	0.44
1:A:390:ILE:HB	1:A:407:THR:HB	2.00	0.44
1:A:366:ARG:NH2	1:A:368:LYS:HG2	2.33	0.44
1:D:103:ALA:O	1:D:104:ARG:HB3	2.18	0.44
1:B:140:GLY:HA3	1:B:421:ARG:CZ	2.48	0.44
1:D:291:GLU:HG2	1:D:293:LEU:HD21	2.00	0.44
1:C:180:VAL:HB	1:C:217:VAL:HG22	2.00	0.44
1:D:102:ARG:NH1	1:D:102:ARG:HG3	2.32	0.44
1:D:98:ALA:HA	1:D:99:PRO:HD3	1.80	0.44
1:A:353:GLU:HG3	1:A:440:PRO:HG2	1.99	0.44
1:C:263:GLU:HG3	4:C:1514:HOH:O	2.18	0.44
1:D:380:SER:HB3	1:D:383:TRP:CZ2	2.53	0.44
1:D:252:ARG:CZ	1:D:254:LEU:HD21	2.47	0.43
1:D:130:HIS:O	1:D:134:VAL:HG23	2.18	0.43
1:B:349:HIS:CE1	1:B:439:THR:HG21	2.53	0.43
1:D:87:ALA:O	1:D:88:LYS:C	2.56	0.43
1:A:378:MET:CE	1:A:408:LEU:HD22	2.48	0.43
1:B:301:THR:OG1	1:B:302:VAL:N	2.48	0.43
1:B:373:HIS:O	1:B:375:MET:HG3	2.19	0.43
1:B:388:ARG:HH12	1:B:450:LYS:CE	2.15	0.43
1:B:111:ALA:O	1:B:125:THR:HA	2.18	0.43
1:D:153:ALA:HB2	1:D:180:VAL:CG1	2.42	0.43
1:D:203:LEU:HD13	1:D:213:THR:OG1	2.18	0.43
1:D:411:ARG:HA	1:D:451:TRP:CZ2	2.54	0.43
1:D:347:GLN:HA	1:D:348:PRO:HD3	1.82	0.43
1:C:171:ILE:HA	1:C:435:LEU:HD21	1.99	0.43
1:B:188:ASP:O	1:B:191:MET:HB3	2.19	0.43
1:B:157:PRO:HD2	1:B:198:GLU:OE1	2.18	0.43
1:B:431:ILE:HD12	1:B:431:ILE:C	2.39	0.43
1:D:170:GLN:NE2	1:D:405:LYS:HZ1	2.17	0.43
1:D:70:LYS:HA	1:D:150:VAL:HG21	2.00	0.43
1:B:171:ILE:HG22	1:B:435:LEU:HD22	2.00	0.43
1:A:233:LEU:O	1:A:237:GLN:HG3	2.19	0.43
1:C:374:PHE:HE2	1:C:431:ILE:HD11	1.83	0.43
1:B:290:CYS:SG	1:B:301:THR:HG23	2.59	0.43
1:C:55:LYS:HB2	1:C:56:PRO:HD2	1.99	0.43
1:A:130:HIS:ND1	1:A:160:GLN:HG2	2.34	0.43
1:D:114:GLU:HB3	1:D:121:HIS:HE1	1.83	0.43
1:C:356:VAL:O	1:C:403:ASP:HA	2.19	0.43
1:A:106:ILE:CD1	1:A:433:THR:HG21	2.49	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:330:LYS:HB3	1:C:333:ASP:OD1	2.18	0.43
1:C:444:GLU:HA	1:C:447:LYS:HD3	2.01	0.43
1:B:353:GLU:CG	1:B:440:PRO:HG2	2.44	0.42
1:B:216:ILE:CD1	1:B:216:ILE:N	2.81	0.42
1:C:373:HIS:HD2	1:C:388:ARG:NE	2.17	0.42
1:C:396:GLU:O	1:C:397:LEU:HD23	2.18	0.42
1:D:79:LYS:CD	1:D:224:LEU:HD12	2.49	0.42
1:C:360:THR:HG21	1:C:362:GLU:HG2	2.01	0.42
1:D:183:ALA:HB3	1:D:231:LEU:HD22	2.01	0.42
1:B:395:LYS:HE3	1:B:395:LYS:HB3	1.88	0.42
1:C:258:PHE:HB2	1:C:279:LEU:HD11	2.02	0.42
1:D:372:SER:O	1:D:389:ILE:O	2.38	0.42
1:C:176:VAL:O	1:C:213:THR:HG23	2.19	0.42
1:D:107:THR:O	1:D:135:LYS:NZ	2.45	0.42
1:B:335:ARG:HG3	1:B:336:ARG:N	2.34	0.42
1:A:69:GLY:HA3	1:A:181:ASN:ND2	2.35	0.42
1:D:189:SER:O	1:D:193:GLU:HG3	2.20	0.42
1:C:392:PRO:HD2	1:C:395:LYS:HB2	2.02	0.42
1:A:266:TYR:HB2	1:A:331:ARG:HH21	1.84	0.42
1:B:58:VAL:HG21	1:B:120:ARG:HE	1.83	0.42
1:D:209:LYS:HB2	1:D:212:GLU:HG2	2.00	0.42
1:B:133:TYR:HB3	1:B:137:MET:HE1	2.01	0.42
1:A:399:MET:O	1:A:402:GLU:HB3	2.20	0.42
1:C:332:GLU:N	1:C:332:GLU:CD	2.72	0.42
1:D:379:PHE:CE1	1:D:425:ARG:HD3	2.54	0.42
1:D:127:CYS:HB2	1:D:133:TYR:CE1	2.55	0.42
1:C:390:ILE:HB	1:C:407:THR:HB	2.01	0.42
1:C:425:ARG:CD	4:C:1546:HOH:O	2.65	0.42
1:A:389:ILE:C	1:A:390:ILE:HD12	2.39	0.42
1:D:285:LYS:HB2	1:D:288:ASP:OD2	2.20	0.42
1:B:169:ARG:HD2	1:B:169:ARG:HA	1.91	0.42
1:A:372:SER:O	1:A:373:HIS:CB	2.67	0.42
1:C:56:PRO:HB2	1:C:120:ARG:HG2	2.02	0.42
1:B:204:THR:HG23	1:C:255:GLU:HB3	2.01	0.42
1:D:260:LEU:HD13	1:D:260:LEU:C	2.39	0.42
1:C:197:LEU:HD23	4:C:1405:HOH:O	2.20	0.42
1:B:379:PHE:CE1	1:B:425:ARG:HD2	2.54	0.42
1:D:405:LYS:HD3	1:D:405:LYS:HA	1.85	0.42
1:D:90:LYS:CG	1:D:94:GLU:HG2	2.45	0.42
1:D:215:ILE:C	1:D:216:ILE:HD12	2.39	0.42
1:D:301:THR:OG1	1:D:302:VAL:N	2.49	0.42
1:C:191:MET:O	1:C:195:VAL:HG23	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:79:LYS:HE3	1:A:89:PHE:CD1	2.55	0.42
1:B:80:ILE:HD13	1:B:233:LEU:HD12	2.02	0.42
1:A:71:THR:HG23	1:A:95:ILE:HG22	2.02	0.42
1:C:438:ASP:C	1:C:440:PRO:HD3	2.41	0.42
1:C:91:LYS:N	1:C:91:LYS:HD2	2.35	0.42
1:C:404:LEU:HD23	1:C:404:LEU:N	2.35	0.42
1:A:447:LYS:O	1:A:449:ILE:HD13	2.20	0.41
1:B:190:GLU:N	1:B:190:GLU:CD	2.73	0.41
1:A:400:PRO:HD2	4:A:1631:HOH:O	2.20	0.41
1:C:135:LYS:HE2	1:C:357:TYR:CE1	2.55	0.41
1:B:145:ASP:OD2	1:B:250:PRO:HG3	2.21	0.41
1:A:404:LEU:H	1:A:404:LEU:HD23	1.85	0.41
1:C:80:ILE:HD12	1:C:236:VAL:HG11	2.02	0.41
1:A:127:CYS:HA	1:A:128:PRO:HD3	1.89	0.41
1:A:55:LYS:HE2	1:A:118:ALA:O	2.19	0.41
1:B:176:VAL:O	1:B:213:THR:HG23	2.21	0.41
1:D:252:ARG:NH1	1:D:318:ALA:O	2.53	0.41
1:C:411:ARG:HH11	1:C:411:ARG:HG2	1.85	0.41
1:A:408:LEU:HD12	1:A:408:LEU:N	2.34	0.41
1:D:204:THR:HA	1:D:208:TYR:O	2.21	0.41
1:B:339:VAL:HB	1:B:415:ILE:HG13	2.02	0.41
1:B:308:MET:SD	1:B:320:ASP:HB3	2.60	0.41
1:D:352:VAL:HG22	1:D:438:ASP:O	2.20	0.41
1:A:158:MET:HB3	1:A:159:PRO:HD2	2.02	0.41
1:C:158:MET:HB3	1:C:159:PRO:HD2	2.03	0.41
1:D:325:LEU:HD23	1:D:326:VAL:N	2.35	0.41
1:C:166:LEU:HB2	1:C:206:PHE:CE2	2.56	0.41
1:B:135:LYS:HE2	1:B:357:TYR:OH	2.20	0.41
1:B:352:VAL:CG2	1:B:353:GLU:N	2.84	0.41
1:C:227:ARG:O	1:C:228:ASP:C	2.58	0.41
1:D:180:VAL:N	1:D:216:ILE:O	2.51	0.41
1:D:104:ARG:CZ	1:D:430:THR:OG1	2.68	0.41
1:B:291:GLU:OE1	1:B:300:ARG:HD3	2.21	0.41
1:A:93:GLU:CD	1:A:93:GLU:N	2.71	0.41
1:D:122:TYR:OH	1:D:244:ASP:HA	2.20	0.41
1:B:215:ILE:C	1:B:216:ILE:HD12	2.41	0.41
1:D:182:LYS:HG2	3:D:1304:GDP:C6	2.55	0.41
1:A:186:VAL:CG1	1:A:191:MET:HB3	2.51	0.41
1:B:124:HIS:CD2	1:B:124:HIS:C	2.94	0.41
1:C:55:LYS:N	4:C:1510:HOH:O	2.54	0.41
1:A:275:VAL:CG1	1:A:334:LEU:HD13	2.51	0.41
1:B:443:THR:HG22	1:B:444:GLU:N	2.35	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:416:LEU:HD22	1:D:436:VAL:CG2	2.38	0.41
1:D:74:THR:O	1:D:77:ILE:HB	2.20	0.41
1:B:389:ILE:HD11	1:B:424:LEU:HD13	2.03	0.41
1:C:374:PHE:CD2	1:C:376:PRO:HD3	2.56	0.41
1:D:361:LYS:HD3	1:D:367:HIS:NE2	2.35	0.41
1:D:359:LEU:N	1:D:359:LEU:HD12	2.35	0.41
1:C:66:VAL:O	1:C:67:ASP:HB2	2.21	0.41
1:C:421:ARG:NH1	1:C:421:ARG:HG2	2.36	0.41
1:C:213:THR:HA	1:C:214:PRO:HD3	1.95	0.41
1:B:80:ILE:HD12	1:B:236:VAL:HG11	2.03	0.41
1:A:149:LEU:HD22	1:A:165:LEU:HD21	2.01	0.41
1:C:228:ASP:N	1:C:229:PRO:HD3	2.35	0.40
1:B:268:ILE:O	1:B:268:ILE:HG23	2.21	0.40
1:D:175:HIS:CD2	1:D:248:PRO:HD2	2.56	0.40
1:C:188:ASP:O	1:C:191:MET:HB3	2.20	0.40
1:A:271:ARG:HD2	4:A:1684:HOH:O	2.21	0.40
1:B:259:LEU:C	1:B:259:LEU:HD23	2.42	0.40
1:C:301:THR:OG1	1:C:302:VAL:N	2.51	0.40
1:C:178:VAL:HB	1:C:215:ILE:HG12	2.02	0.40
1:D:89:PHE:CE1	1:D:91:LYS:HE2	2.57	0.40
1:B:130:HIS:HB2	1:B:160:GLN:OE1	2.21	0.40
1:D:59:ASN:N	1:D:145:ASP:OD2	2.41	0.40
1:B:197:LEU:O	1:B:201:GLU:HG3	2.22	0.40
1:D:293:LEU:CD1	1:D:346:ILE:HG23	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	395/397 (100%)	381 (96%)	14 (4%)	0	100	100
1	B	395/397 (100%)	376 (95%)	18 (5%)	1 (0%)	50	37
1	C	395/397 (100%)	381 (96%)	12 (3%)	2 (0%)	38	22

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	395/397 (100%)	361 (91%)	29 (7%)	5 (1%)	18	5
All	All	1580/1588 (100%)	1499 (95%)	73 (5%)	8 (0%)	38	22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	83	GLU
1	D	88	LYS
1	D	367	HIS
1	C	448	ASN
1	D	128	PRO
1	D	328	GLY
1	B	92	TYR
1	D	296	SER

### 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	332/332 (100%)	324 (98%)	8 (2%)	61	50
1	B	332/332 (100%)	324 (98%)	8 (2%)	61	50
1	C	332/332 (100%)	325 (98%)	7 (2%)	66	56
1	D	332/332 (100%)	322 (97%)	10 (3%)	53	38
All	All	1328/1328 (100%)	1295 (98%)	33 (2%)	60	48

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ILE
1	A	191	MET
1	A	284	LEU
1	A	368	LYS
1	A	372	SER
1	A	373	HIS
1	A	405	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	449	ILE
1	B	89	PHE
1	B	125	THR
1	B	141	THR
1	B	230	GLU
1	B	284	LEU
1	B	307	GLU
1	B	416	LEU
1	B	450	LYS
1	C	191	MET
1	C	284	LEU
1	C	314	ASP
1	C	333	ASP
1	C	448	ASN
1	C	449	ILE
1	C	450	LYS
1	D	89	PHE
1	D	125	THR
1	D	155	ASP
1	D	191	MET
1	D	284	LEU
1	D	325	LEU
1	D	352	VAL
1	D	368	LYS
1	D	416	LEU
1	D	445	GLU

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

Mol	Chain	Res	Type
1	A	65	HIS
1	A	175	HIS
1	A	347	GLN
1	A	367	HIS
1	A	448	ASN
1	B	65	HIS
1	B	97	ASN
1	B	170	GLN
1	B	355	GLN
1	C	65	HIS
1	C	347	GLN
1	C	349	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	373	HIS
1	C	428	ASN
1	C	448	ASN
1	D	65	HIS
1	D	170	GLN
1	D	175	HIS
1	D	367	HIS
1	D	412	GLN
1	D	448	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	1301	2	30,30,30	1.11	3 (10%)	44,47,47	3.25	4 (9%)
3	GDP	B	1302	2	30,30,30	1.09	2 (6%)	44,47,47	2.91	3 (6%)
3	GDP	C	1303	2	30,30,30	1.12	3 (10%)	44,47,47	2.76	4 (9%)
3	GDP	D	1304	2	30,30,30	1.13	3 (10%)	44,47,47	2.61	6 (13%)

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	1301	2	-	0/16/32/32	0/1/3/3
3	GDP	B	1302	2	-	0/16/32/32	0/1/3/3
3	GDP	C	1303	2	-	0/16/32/32	0/1/3/3
3	GDP	D	1304	2	-	0/16/32/32	0/1/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1303	GDP	C4-N9	-2.42	1.34	1.37
3	C	1303	GDP	PB-O2B	-2.38	1.46	1.54
3	B	1302	GDP	PB-O2B	-2.32	1.46	1.54
3	D	1304	GDP	PA-O3A	2.27	1.64	1.59
3	A	1301	GDP	PB-O3B	-2.18	1.46	1.54
3	A	1301	GDP	C8-N9	2.16	1.39	1.36
3	D	1304	GDP	PB-O2B	-2.11	1.47	1.54
3	C	1303	GDP	C8-N9	2.10	1.39	1.36
3	D	1304	GDP	C8-N9	2.06	1.39	1.36
3	A	1301	GDP	PB-O2B	-2.03	1.47	1.54
3	B	1302	GDP	C8-N9	2.02	1.39	1.36

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1301	GDP	C6-C5-N7	-20.13	131.43	134.14
3	B	1302	GDP	C6-C5-N7	-17.83	131.74	134.14
3	C	1303	GDP	C6-C5-N7	-16.59	131.91	134.14
3	D	1304	GDP	C6-C5-N7	-15.49	132.05	134.14
3	C	1303	GDP	C6-N1-C2	3.24	125.19	119.51
3	B	1302	GDP	C6-N1-C2	3.21	125.13	119.51
3	A	1301	GDP	C6-N1-C2	3.13	124.98	119.51
3	D	1304	GDP	C6-N1-C2	3.06	124.86	119.51
3	C	1303	GDP	O4'-C1'-N9	2.50	110.76	108.44
3	D	1304	GDP	C8-N9-C1'	2.42	131.15	126.38
3	C	1303	GDP	O3'-C3'-C4'	-2.33	104.22	111.08
3	D	1304	GDP	O3'-C3'-C4'	-2.28	104.36	111.08
3	B	1302	GDP	O3'-C3'-C4'	-2.24	104.48	111.08
3	D	1304	GDP	C8-N9-C4	-2.21	105.21	106.90
3	D	1304	GDP	C3'-C2'-C1'	2.19	104.33	100.91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1301	GDP	O3'-C3'-C4'	-2.18	104.64	111.08
3	A	1301	GDP	C8-N9-C4	-2.06	105.32	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	397/397 (100%)	0.40	6 (1%) 70 77	19, 35, 58, 69	0
1	B	397/397 (100%)	0.72	35 (8%) 10 12	33, 47, 66, 71	0
1	C	397/397 (100%)	0.58	20 (5%) 28 32	28, 44, 63, 71	0
1	D	397/397 (100%)	1.25	85 (21%) 1 1	27, 53, 67, 71	0
All	All	1588/1588 (100%)	0.74	146 (9%) 9 11	19, 45, 65, 71	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	85	GLY	10.4
1	B	87	ALA	8.2
1	C	86	GLY	8.0
1	B	141	THR	7.0
1	D	86	GLY	6.7
1	D	373	HIS	6.7
1	B	86	GLY	6.3
1	B	89	PHE	6.1
1	D	389	ILE	6.0
1	B	142	ALA	5.9
1	D	99	PRO	5.7
1	A	187	GLN	5.5
1	B	188	ASP	5.4
1	D	397	LEU	5.4
1	B	451	TRP	5.2
1	B	84	GLY	5.2
1	C	393	PRO	5.0
1	D	392	PRO	4.7
1	D	393	PRO	4.7
1	D	371	VAL	4.7
1	B	88	LYS	4.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	370	PHE	4.5
1	D	374	PHE	4.4
1	D	367	HIS	4.4
1	D	451	TRP	4.4
1	D	89	PHE	4.3
1	D	94	GLU	4.3
1	D	118	ALA	4.2
1	D	98	ALA	4.0
1	D	88	LYS	4.0
1	D	87	ALA	4.0
1	D	119	ALA	3.9
1	D	85	GLY	3.9
1	D	450	LYS	3.9
1	D	81	LEU	3.9
1	D	186	VAL	3.8
1	B	187	GLN	3.8
1	B	85	GLY	3.8
1	B	393	PRO	3.8
1	C	84	GLY	3.8
1	D	187	GLN	3.8
1	D	97	ASN	3.7
1	B	394	GLY	3.7
1	D	391	LEU	3.6
1	B	95	ILE	3.5
1	D	233	LEU	3.5
1	C	448	ASN	3.4
1	D	441	ALA	3.4
1	D	188	ASP	3.4
1	C	87	ALA	3.4
1	D	103	ALA	3.4
1	D	448	ASN	3.3
1	D	249	VAL	3.3
1	D	372	SER	3.3
1	D	194	LEU	3.2
1	D	55	LYS	3.1
1	B	427	GLY	3.1
1	D	390	ILE	3.1
1	D	190	GLU	3.0
1	B	92	TYR	3.0
1	D	369	PRO	3.0
1	C	451	TRP	3.0
1	C	88	LYS	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	84	GLY	3.0
1	D	253	ASP	2.9
1	D	128	PRO	2.9
1	B	449	ILE	2.9
1	C	141	THR	2.9
1	C	328	GLY	2.9
1	B	102	ARG	2.9
1	D	252	ARG	2.9
1	D	406	LEU	2.9
1	B	90	LYS	2.9
1	A	188	ASP	2.9
1	B	91	LYS	2.8
1	B	450	LYS	2.8
1	D	57	HIS	2.8
1	D	101	GLU	2.8
1	D	77	ILE	2.7
1	D	254	LEU	2.7
1	D	396	GLU	2.7
1	B	194	LEU	2.7
1	A	449	ILE	2.7
1	D	251	THR	2.7
1	A	448	ASN	2.7
1	D	93	GLU	2.7
1	D	238	LYS	2.6
1	B	185	ALA	2.6
1	C	397	LEU	2.6
1	D	100	GLU	2.6
1	D	106	ILE	2.6
1	D	443	THR	2.6
1	D	388	ARG	2.6
1	D	114	GLU	2.6
1	C	187	GLN	2.5
1	C	388	ARG	2.5
1	D	255	GLU	2.5
1	B	428	ASN	2.5
1	D	449	ILE	2.5
1	B	100	GLU	2.5
1	D	368	LYS	2.5
1	A	189	SER	2.5
1	D	56	PRO	2.5
1	D	121	HIS	2.5
1	B	121	HIS	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	105	GLY	2.4
1	D	228	ASP	2.4
1	C	395	LYS	2.4
1	B	143	PRO	2.4
1	D	102	ARG	2.4
1	B	108	ILE	2.4
1	D	113	VAL	2.4
1	B	83	GLU	2.3
1	D	224	LEU	2.3
1	D	240	LEU	2.3
1	C	102	ARG	2.3
1	D	446	ASP	2.3
1	C	373	HIS	2.3
1	D	411	ARG	2.3
1	B	371	VAL	2.3
1	B	104	ARG	2.3
1	D	111	ALA	2.3
1	A	428	ASN	2.2
1	D	405	LYS	2.3
1	D	58	VAL	2.2
1	D	110	ALA	2.2
1	D	83	GLU	2.2
1	D	189	SER	2.2
1	C	190	GLU	2.2
1	D	120	ARG	2.2
1	D	366	ARG	2.2
1	D	297	LYS	2.2
1	C	392	PRO	2.2
1	D	141	THR	2.1
1	D	197	LEU	2.1
1	C	121	HIS	2.1
1	D	171	ILE	2.1
1	B	186	VAL	2.1
1	B	369	PRO	2.1
1	B	388	ARG	2.1
1	D	115	TYR	2.1
1	C	108	ILE	2.0
1	D	108	ILE	2.0
1	D	154	ASN	2.0
1	B	81	LEU	2.0
1	D	426	ASP	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GDP	A	1301	28/28	0.13	0.98	18,29,31,32	0
2	MG	B	502	1/1	0.11	-0.04	49,49,49,49	0
3	GDP	C	1303	28/28	0.11	-0.06	31,34,37,39	0
2	MG	D	504	1/1	0.14	-0.81	52,52,52,52	0
3	GDP	B	1302	28/28	0.09	-0.88	44,51,53,55	0
3	GDP	D	1304	28/28	0.12	-1.09	50,54,58,58	0
2	MG	A	501	1/1	0.07	-1.31	26,26,26,26	0
2	MG	C	503	1/1	0.07	-2.42	35,35,35,35	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.