



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:06 am BST

PDB ID : 3Q5E  
Title : crystal structure of human Atlantin-1 (residues 1-447) bound to GDP, crystal form 2  
Authors : Byrnes, L.J.; Sondermann, H.  
Deposited on : 2010-12-28  
Resolution : 3.01 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

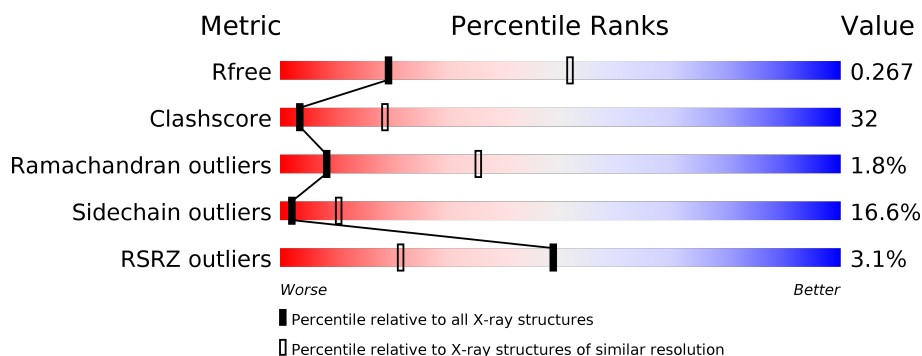
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	447	<div> <div>2%</div> <div> <div></div> <div>41%</div> <div>37%</div> <div>15%</div> <div>8%</div> </div> </div>
1	C	447	<div> <div>4%</div> <div> <div></div> <div>50%</div> <div>34%</div> <div>7%</div> <div>9%</div> </div> </div>
1	E	447	<div> <div>%</div> <div> <div></div> <div>43%</div> <div>34%</div> <div>9%</div> <div>14%</div> </div> </div>
1	G	447	<div> <div>5%</div> <div> <div></div> <div>45%</div> <div>34%</div> <div>7%</div> <div>14%</div> </div> </div>

## 2 Entry composition [i](#)

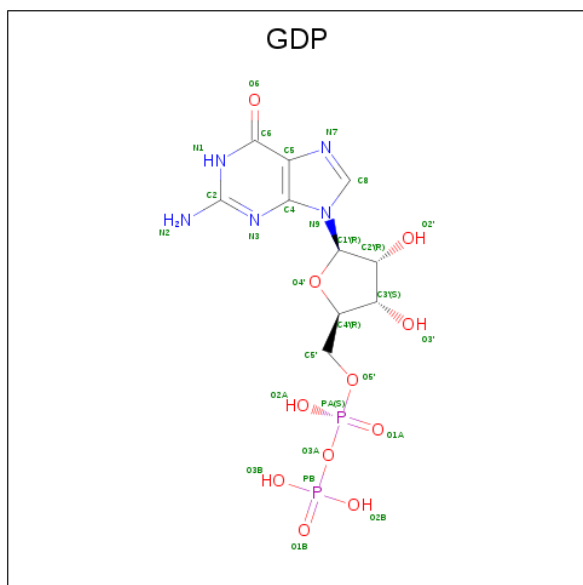
There are 3 unique types of molecules in this entry. The entry contains 12936 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Atlastin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3310	2116	554	627	13			
1	C	409	Total	C	N	O	S	0	0	0
			3293	2106	550	624	13			
1	E	386	Total	C	N	O	S	0	0	0
			3116	2006	514	583	13			
1	G	384	Total	C	N	O	S	0	0	0
			3101	1995	515	578	13			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	G	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

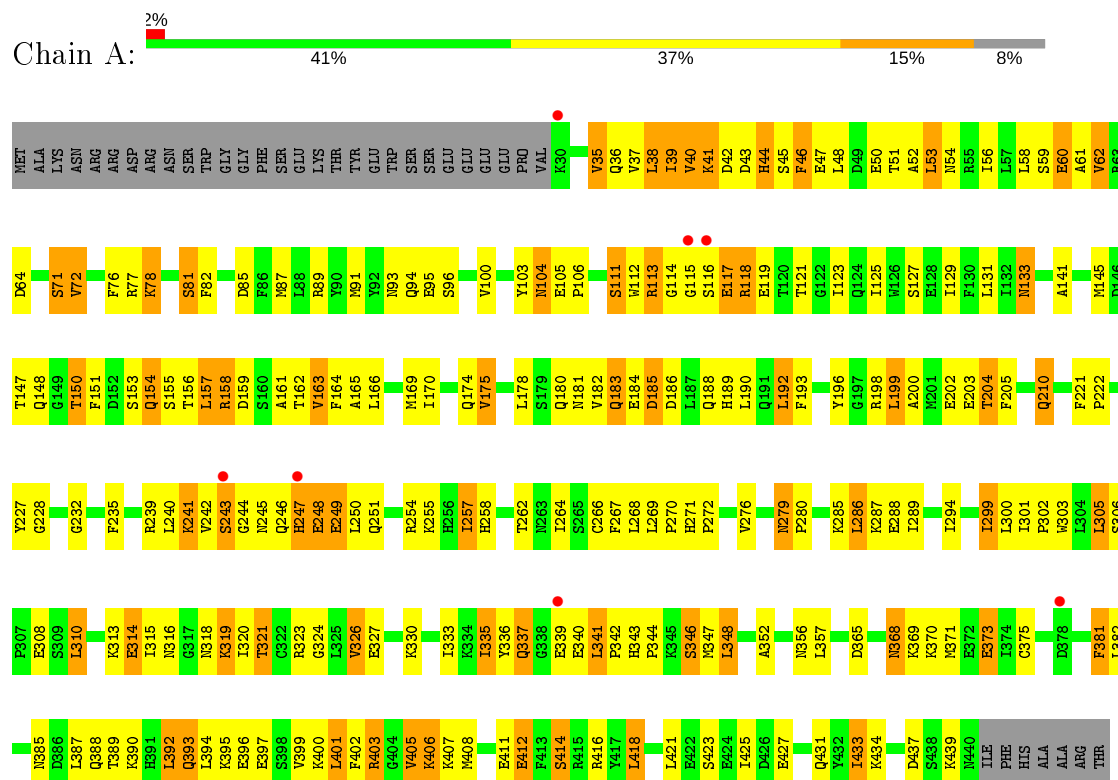
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

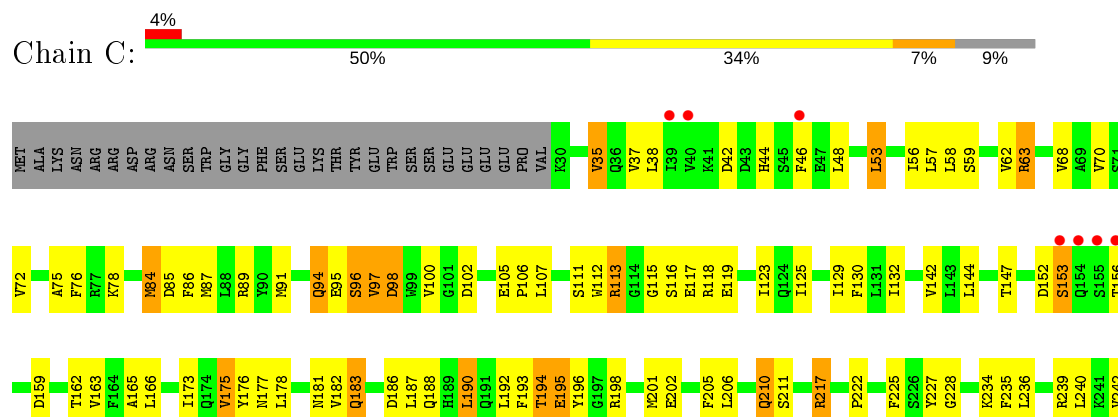
### 3 Residue-property plots

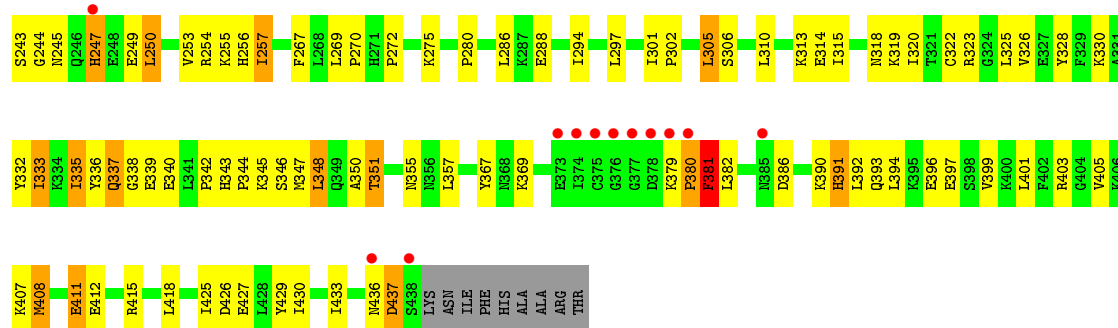
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Atlastin-1

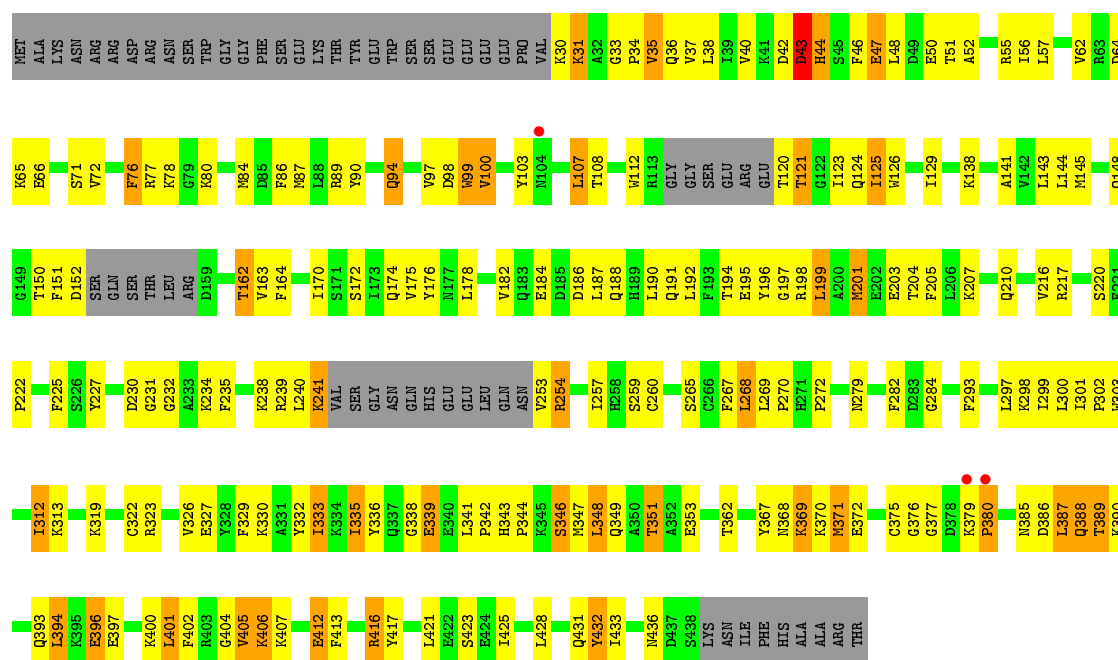
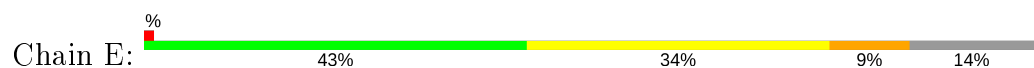


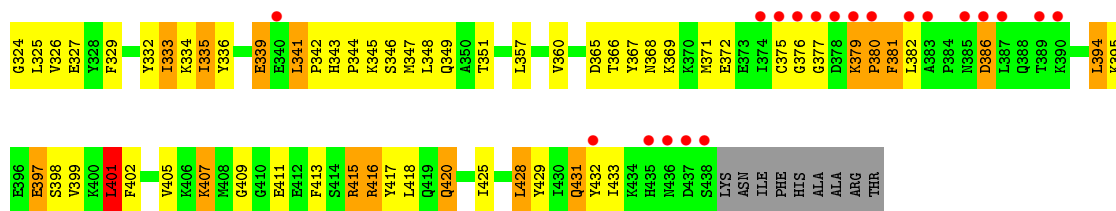
#### • Molecule 1: Atlastin-1





• Molecule 1: Atlastin-1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.39Å 133.55Å 175.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.54 – 3.01 50.04 – 3.01	Depositor EDS
% Data completeness (in resolution range)	94.2 (42.54-3.01) 93.2 (50.04-3.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.70 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.197 , 0.273 0.192 , 0.267	Depositor DCC
$R_{free}$ test set	2000 reflections (4.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.7	Xtriage
Anisotropy	0.735	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 65.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12936	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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

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	0.48	0/3379	0.58	0/4556
1	C	0.46	0/3362	0.58	0/4534
1	E	0.50	2/3181 (0.1%)	0.64	0/4287
1	G	0.46	0/3165	0.61	1/4264 (0.0%)
All	All	0.47	2/13087 (0.0%)	0.60	1/17641 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	339	GLU	CD-OE1	6.04	1.32	1.25
1	E	339	GLU	CD-OE2	5.08	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	401	LEU	CA-CB-CG	5.75	128.52	115.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3310	0	3291	291	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3293	0	3272	180	0
1	E	3116	0	3109	187	0
1	G	3101	0	3102	186	0
2	A	28	0	12	2	0
2	C	28	0	12	3	0
2	E	28	0	12	2	0
2	G	28	0	12	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
All	All	12936	0	12822	826	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 32.

All (826) 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:37:VAL:HG21	1:A:53:LEU:HD23	1.22	1.14
1:A:403:ARG:HG2	1:A:403:ARG:HH11	1.09	1.14
1:C:48:LEU:HB2	1:C:333:ILE:HG13	1.26	1.14
1:A:341:LEU:HG	1:A:342:PRO:HD2	1.31	1.12
1:A:381:PHE:HB2	1:A:439:LYS:HD3	1.32	1.11
1:C:245:ASN:HD21	1:G:397:GLU:HA	1.09	1.11
1:G:379:LYS:HB3	1:G:380:PRO:HD3	1.36	1.05
1:A:154:GLN:O	1:A:158:ARG:HG2	1.61	1.01
1:A:111:SER:HA	1:A:113:ARG:NH1	1.78	0.98
1:E:56:ILE:HD13	1:E:125:ILE:HD11	1.44	0.98
1:C:379:LYS:HB3	1:C:380:PRO:HD3	1.46	0.97
1:A:269:LEU:HD12	1:A:270:PRO:HD2	1.44	0.96
1:A:39:ILE:HG23	1:A:47:GLU:HG3	1.47	0.94
1:E:343:HIS:CD2	1:E:344:PRO:HD2	2.02	0.94
1:A:158:ARG:O	1:A:162:THR:HG23	1.68	0.94
1:G:196:TYR:HB2	1:G:347:MET:CE	1.97	0.94
1:A:200:ALA:O	1:A:204:THR:HG23	1.68	0.93
1:A:316:ASN:O	1:A:406:LYS:HE2	1.72	0.90
1:G:190:LEU:HD23	1:G:257:ILE:HD11	1.52	0.90
1:G:332:TYR:OH	1:G:351:THR:HG22	1.72	0.90
1:E:269:LEU:HD12	1:E:270:PRO:HD2	1.53	0.89
1:A:50:GLU:HG2	1:A:54:ASN:HD21	1.35	0.89

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLU:HB2	1:A:119:GLU:HB3	1.54	0.88
1:E:120:THR:HB	1:E:151:PHE:CE2	2.09	0.88
1:A:241:LYS:HD3	1:A:242:VAL:N	1.88	0.88
1:C:117:GLU:HG2	1:C:119:GLU:HB3	1.56	0.87
1:E:379:LYS:HB2	1:E:380:PRO:HD3	1.56	0.87
1:C:87:MET:HE3	1:C:305:LEU:HD11	1.56	0.86
1:A:105:GLU:HG3	1:A:106:PRO:HD2	1.55	0.86
1:A:46:PHE:HD2	1:A:46:PHE:N	1.73	0.86
1:G:196:TYR:HB2	1:G:347:MET:HE1	1.58	0.85
1:A:400:LYS:HA	1:A:403:ARG:HD2	1.59	0.84
1:A:112:TRP:H	1:A:113:ARG:NH1	1.75	0.84
1:A:403:ARG:NH1	1:A:403:ARG:HG2	1.86	0.82
1:A:321:THR:HG22	1:A:324:GLY:H	1.43	0.82
1:A:389:THR:HA	1:A:392:LEU:HD11	1.60	0.82
1:A:243:SER:HB3	1:E:401:LEU:HD13	1.62	0.82
1:C:183:GLN:O	1:C:186:ASP:HB2	1.79	0.82
1:C:245:ASN:ND2	1:G:397:GLU:HA	1.93	0.82
1:E:40:VAL:HG22	1:E:46:PHE:HD1	1.43	0.82
1:A:72:VAL:HG13	1:A:175:VAL:HG22	1.61	0.82
1:E:40:VAL:HG22	1:E:46:PHE:CD1	2.14	0.81
1:E:86:PHE:CD2	1:E:297:LEU:HD21	2.15	0.81
1:C:247:HIS:CE1	1:C:254:ARG:CZ	2.64	0.80
1:E:402:PHE:CE2	1:E:407:LYS:HE3	2.16	0.80
1:A:46:PHE:CD2	1:A:46:PHE:N	2.47	0.80
1:A:243:SER:N	1:A:247:HIS:NE2	2.30	0.79
1:G:123:ILE:HG12	1:G:147:THR:HG22	1.62	0.79
1:A:316:ASN:CG	1:A:406:LYS:HD2	2.03	0.79
1:E:413:PHE:O	1:E:416:ARG:HG3	1.83	0.78
1:A:316:ASN:CB	1:A:406:LYS:HD2	2.13	0.78
1:C:244:GLY:O	1:C:245:ASN:HB2	1.83	0.78
1:G:210:GLN:NE2	1:G:313:LYS:HA	1.98	0.78
1:A:421:LEU:O	1:A:425:ILE:HG13	1.82	0.78
1:E:327:GLU:HA	1:E:330:LYS:HB2	1.65	0.78
1:C:332:TYR:HE1	1:C:351:THR:HG22	1.48	0.78
1:G:332:TYR:CE1	1:G:351:THR:HG22	2.20	0.77
1:C:335:ILE:HG22	1:C:336:TYR:N	2.00	0.77
1:G:227:TYR:CE1	1:G:270:PRO:HB3	2.19	0.77
1:C:245:ASN:HD21	1:G:397:GLU:CA	1.95	0.77
1:A:111:SER:HA	1:A:113:ARG:HH11	1.49	0.76
1:A:412:GLU:H	1:A:412:GLU:CD	1.87	0.76
1:C:46:PHE:H	1:C:337:GLN:HB2	1.48	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:LYS:HA	1:E:241:LYS:HE2	1.66	0.76
1:C:335:ILE:HD11	1:C:347:MET:HA	1.66	0.75
1:G:394:LEU:O	1:G:397:GLU:HB3	1.87	0.75
1:A:153:SER:C	1:A:157:LEU:HD12	2.07	0.75
1:A:154:GLN:HG3	1:C:105:GLU:OE2	1.87	0.75
1:G:84:MET:HE1	1:G:112:TRP:CZ2	2.22	0.75
1:G:321:THR:HG23	1:G:324:GLY:H	1.49	0.75
1:G:48:LEU:HD12	1:G:49:ASP:N	2.02	0.75
1:C:76:PHE:CE1	1:C:119:GLU:HG3	2.21	0.74
1:A:316:ASN:HB3	1:A:406:LYS:HD2	1.69	0.74
1:A:111:SER:CA	1:A:113:ARG:NH1	2.50	0.74
1:A:368:ASN:HD22	1:A:368:ASN:C	1.90	0.74
1:G:332:TYR:CZ	1:G:351:THR:HG22	2.21	0.74
1:G:254:ARG:HH21	1:G:258:HIS:HE1	1.32	0.74
1:C:269:LEU:HD12	1:C:270:PRO:HD2	1.68	0.74
1:E:371:MET:O	1:E:375:CYS:HB3	1.87	0.74
1:G:254:ARG:HH21	1:G:258:HIS:CE1	2.05	0.74
1:E:232:GLY:HA2	1:E:268:LEU:HD22	1.70	0.74
1:A:41:LYS:HE2	1:A:41:LYS:HA	1.68	0.73
1:A:118:ARG:HG3	1:A:118:ARG:O	1.86	0.73
1:A:111:SER:CA	1:A:113:ARG:HH11	2.01	0.73
1:E:335:ILE:HG22	1:E:336:TYR:CD1	2.24	0.73
1:A:41:LYS:CE	1:A:41:LYS:HA	2.17	0.72
1:E:240:LEU:HB3	1:E:254:ARG:HG2	1.69	0.72
1:G:214:PHE:HD2	1:G:236:LEU:HD21	1.54	0.72
1:A:154:GLN:HA	1:A:157:LEU:HB2	1.71	0.72
1:A:117:GLU:HB2	1:A:119:GLU:CB	2.20	0.72
1:A:241:LYS:HA	1:A:241:LYS:HE3	1.70	0.72
1:A:401:LEU:C	1:A:401:LEU:HD12	2.09	0.72
1:G:123:ILE:HG12	1:G:147:THR:CG2	2.19	0.72
1:E:56:ILE:HD13	1:E:125:ILE:CD1	2.19	0.72
1:C:332:TYR:CE1	1:C:351:THR:HG22	2.25	0.71
1:E:71:SER:HB3	1:E:174:GLN:NE2	2.04	0.71
1:A:240:LEU:O	1:A:254:ARG:HD3	1.90	0.71
1:G:196:TYR:O	1:G:199:LEU:HD12	1.91	0.71
1:A:104:ASN:HD22	1:A:285:LYS:HE2	1.55	0.71
1:A:50:GLU:HG2	1:A:54:ASN:ND2	2.05	0.71
1:C:247:HIS:CE1	1:C:254:ARG:NE	2.58	0.71
1:G:196:TYR:OH	1:G:351:THR:HG21	1.90	0.71
1:G:48:LEU:HD12	1:G:49:ASP:H	1.56	0.71
1:A:269:LEU:HD12	1:A:270:PRO:CD	2.20	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:C	1:A:38:LEU:HD23	2.09	0.70
1:C:343:HIS:HD2	1:C:345:LYS:H	1.38	0.70
1:C:222:PRO:HG3	1:C:227:TYR:CZ	2.26	0.70
1:C:205:PHE:O	1:C:206:LEU:HD23	1.92	0.70
1:A:381:PHE:CB	1:A:439:LYS:HD3	2.17	0.69
1:C:72:VAL:HG13	1:C:175:VAL:HG22	1.74	0.69
1:G:199:LEU:HA	1:G:202:GLU:HG2	1.74	0.69
1:C:188:GLN:HE21	1:C:250:LEU:HG	1.56	0.69
1:G:104:ASN:HD22	1:G:287:LYS:NZ	1.91	0.69
1:G:379:LYS:CB	1:G:380:PRO:HD3	2.17	0.69
1:E:207:LYS:HG2	1:E:259:SER:O	1.92	0.69
1:A:403:ARG:CG	1:A:403:ARG:HH11	1.97	0.69
1:C:117:GLU:CG	1:C:119:GLU:HB3	2.23	0.69
1:A:112:TRP:H	1:A:113:ARG:CZ	2.05	0.69
1:A:106:PRO:HA	1:A:285:LYS:HA	1.74	0.69
1:G:147:THR:HG21	1:G:167:SER:HB2	1.74	0.69
1:E:387:LEU:HD21	1:E:433:ILE:HG22	1.75	0.69
1:C:390:LYS:O	1:C:394:LEU:HD13	1.92	0.69
1:A:154:GLN:NE2	1:A:154:GLN:H	1.90	0.68
1:C:84:MET:HB2	1:C:112:TRP:CD1	2.28	0.68
1:E:343:HIS:CD2	1:E:344:PRO:CD	2.75	0.68
1:G:241:LYS:HE2	1:G:241:LYS:HA	1.73	0.68
1:A:341:LEU:HG	1:A:342:PRO:CD	2.17	0.68
1:C:115:GLY:O	1:C:118:ARG:HD3	1.92	0.68
1:C:343:HIS:CD2	1:C:345:LYS:H	2.11	0.68
1:C:202:GLU:HB2	1:G:205:PHE:CD1	2.29	0.68
1:C:379:LYS:CB	1:C:380:PRO:HD3	2.22	0.68
1:E:94:GLN:H	1:E:94:GLN:HE21	1.40	0.68
1:G:409:GLY:HA3	1:G:413:PHE:HD2	1.59	0.68
1:C:247:HIS:CD2	1:C:250:LEU:HB2	2.29	0.68
1:G:170:ILE:O	1:G:313:LYS:HE2	1.94	0.68
1:A:85:ASP:OD1	1:A:113:ARG:NH1	2.27	0.68
1:E:48:LEU:HD22	1:E:333:ILE:HG13	1.76	0.68
1:G:401:LEU:HD12	1:G:401:LEU:O	1.94	0.68
1:G:254:ARG:C	1:G:254:ARG:HD3	2.13	0.68
1:A:112:TRP:N	1:A:113:ARG:NH1	2.42	0.67
1:A:76:PHE:HE2	1:A:148:GLN:NE2	1.92	0.67
1:E:240:LEU:O	1:E:254:ARG:HG3	1.94	0.67
1:E:412:GLU:HG2	1:G:95:GLU:O	1.95	0.67
1:C:96:SER:O	1:C:97:VAL:HB	1.94	0.66
1:A:267:PHE:CD2	1:A:300:LEU:HD13	2.31	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:TYR:CZ	1:A:270:PRO:HB3	2.30	0.66
1:C:315:ILE:HD13	1:C:328:TYR:CE2	2.30	0.66
1:G:222:PRO:HG3	1:G:227:TYR:CZ	2.30	0.66
1:A:111:SER:HB2	1:A:113:ARG:HH11	1.61	0.66
1:E:270:PRO:HG2	1:E:293:PHE:HA	1.77	0.65
1:A:154:GLN:N	1:A:157:LEU:HD12	2.12	0.65
1:A:244:GLY:C	1:A:246:GLN:H	2.00	0.65
1:C:381:PHE:HD2	1:C:381:PHE:C	1.99	0.65
1:E:376:GLY:HA3	1:E:377:GLY:C	2.16	0.65
1:C:115:GLY:O	1:C:116:SER:HB3	1.94	0.65
1:E:120:THR:C	1:E:151:PHE:HZ	2.00	0.65
1:G:236:LEU:HD22	1:G:266:CYS:HB2	1.78	0.65
1:C:210:GLN:HE22	1:C:314:GLU:H	1.44	0.65
1:C:196:TYR:CB	1:C:347:MET:HE1	2.26	0.65
1:G:301:ILE:HB	1:G:302:PRO:HD3	1.79	0.65
1:E:97:VAL:O	1:E:98:ASP:HB3	1.97	0.65
1:G:200:ALA:HA	1:G:348:LEU:HD12	1.78	0.64
1:A:150:THR:C	1:A:151:PHE:HD1	2.00	0.64
1:A:87:MET:HE3	1:A:305:LEU:HD11	1.79	0.64
1:A:87:MET:O	1:A:91:MET:HG2	1.97	0.64
1:G:170:ILE:HG23	1:G:325:LEU:HD11	1.79	0.64
1:G:269:LEU:HD12	1:G:270:PRO:HD2	1.80	0.64
1:A:316:ASN:O	1:A:406:LYS:CE	2.45	0.64
1:A:315:ILE:HD12	1:A:315:ILE:N	2.12	0.64
1:A:52:ALA:O	1:A:56:ILE:HG13	1.98	0.64
1:G:394:LEU:HA	1:G:397:GLU:HB3	1.80	0.64
1:C:347:MET:O	1:C:351:THR:HG23	1.98	0.63
1:C:222:PRO:HG3	1:C:227:TYR:CE1	2.33	0.63
1:E:225:PHE:CD2	1:E:235:PHE:HB2	2.33	0.63
1:C:381:PHE:CD2	1:C:381:PHE:C	2.72	0.63
1:A:111:SER:CB	1:A:113:ARG:HH11	2.11	0.63
1:A:165:ALA:HA	1:A:193:PHE:HE1	1.64	0.63
1:E:99:TRP:HE3	1:E:99:TRP:O	1.81	0.63
1:A:115:GLY:HA3	1:A:118:ARG:HH11	1.63	0.62
1:A:115:GLY:HA3	1:A:118:ARG:NH1	2.13	0.62
1:A:241:LYS:HD3	1:A:242:VAL:H	1.59	0.62
1:C:343:HIS:CD2	1:C:345:LYS:HB2	2.33	0.62
1:C:336:TYR:O	1:C:337:GLN:HB3	1.99	0.62
1:A:116:SER:O	1:A:118:ARG:HB3	1.99	0.62
1:G:214:PHE:CD2	1:G:236:LEU:HD21	2.34	0.62
1:C:76:PHE:CZ	1:C:119:GLU:HG3	2.33	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:HIS:HD2	1:C:345:LYS:HB2	1.63	0.62
1:C:196:TYR:HB3	1:C:347:MET:HE1	1.80	0.62
1:E:120:THR:C	1:E:151:PHE:CZ	2.73	0.62
1:E:379:LYS:CB	1:E:380:PRO:HD3	2.28	0.62
1:A:356:ASN:OD1	1:A:407:LYS:HG2	1.99	0.62
1:E:239:ARG:HG2	1:E:239:ARG:HH11	1.64	0.62
1:E:176:TYR:CE1	1:E:178:LEU:HD21	2.35	0.61
1:A:56:ILE:HD12	1:A:125:ILE:HD11	1.81	0.61
1:G:210:GLN:HE21	1:G:313:LYS:HA	1.63	0.61
1:G:270:PRO:HG2	1:G:293:PHE:HA	1.82	0.61
1:G:196:TYR:HB2	1:G:347:MET:HE3	1.81	0.61
1:E:387:LEU:HD21	1:E:433:ILE:CG2	2.31	0.61
1:E:72:VAL:HG12	1:E:80:LYS:HG2	1.83	0.61
1:G:314:GLU:OE2	1:G:319:LYS:HE2	2.00	0.61
1:A:313:LYS:HE3	1:A:315:ILE:HD11	1.82	0.61
1:A:183:GLN:O	1:A:186:ASP:HB2	2.00	0.61
1:A:85:ASP:OD2	1:A:113:ARG:CZ	2.48	0.61
1:E:90:TYR:HB2	1:E:99:TRP:CE3	2.36	0.61
1:G:286:LEU:HD22	1:G:294:ILE:HD11	1.82	0.61
1:G:409:GLY:HA3	1:G:413:PHE:CD2	2.35	0.61
1:A:100:VAL:HG13	1:A:286:LEU:HD11	1.81	0.61
1:C:196:TYR:CB	1:C:347:MET:CE	2.78	0.61
1:C:275:LYS:HD3	1:C:288:GLU:HB3	1.83	0.61
1:C:113:ARG:O	1:C:113:ARG:HG2	2.00	0.61
1:E:99:TRP:O	1:E:99:TRP:CE3	2.53	0.61
1:A:205:PHE:HE1	1:E:201:MET:O	1.85	0.60
1:A:38:LEU:HD23	1:A:39:ILE:N	2.16	0.60
1:A:37:VAL:HG21	1:A:53:LEU:CD2	2.15	0.60
1:A:401:LEU:O	1:A:401:LEU:HD12	2.01	0.60
1:G:343:HIS:O	1:G:346:SER:HB3	2.01	0.60
1:G:379:LYS:HB3	1:G:380:PRO:CD	2.21	0.60
1:C:255:LYS:HG2	1:C:256:HIS:CE1	2.36	0.60
1:A:111:SER:CB	1:A:113:ARG:HD2	2.32	0.60
1:E:86:PHE:CD1	1:E:89:ARG:NH1	2.70	0.60
1:A:46:PHE:HE1	1:A:162:THR:HG1	1.47	0.60
1:A:369:LYS:N	1:A:369:LYS:HD2	2.16	0.60
1:E:396:GLU:O	1:E:396:GLU:HG2	2.01	0.60
1:A:327:GLU:OE1	1:A:357:LEU:HD13	2.02	0.60
1:G:196:TYR:O	1:G:197:GLY:C	2.40	0.60
1:G:56:ILE:HG22	1:G:129:ILE:HD11	1.84	0.60
1:A:39:ILE:HG23	1:A:47:GLU:CG	2.26	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:371:MET:HG2	1:G:394:LEU:HD23	1.83	0.59
1:A:113:ARG:CD	1:A:113:ARG:H	2.14	0.59
1:A:53:LEU:HD12	1:A:326:VAL:CG2	2.33	0.59
1:G:200:ALA:HA	1:G:348:LEU:CD1	2.32	0.59
1:G:348:LEU:HD23	1:G:348:LEU:O	2.03	0.59
1:G:402:PHE:O	1:G:407:LYS:HE3	2.02	0.59
1:A:170:ILE:O	1:A:313:LYS:HE2	2.02	0.59
1:E:121:THR:N	1:E:151:PHE:CE2	2.71	0.59
1:E:112:TRP:HZ3	1:E:124:GLN:HB2	1.67	0.59
1:G:232:GLY:O	1:G:266:CYS:HB3	2.03	0.59
1:A:113:ARG:NE	1:A:113:ARG:H	2.01	0.59
1:E:120:THR:HB	1:E:151:PHE:CZ	2.37	0.59
1:E:267:PHE:CE2	1:E:300:LEU:HB2	2.37	0.59
1:G:66:GLU:OE1	1:G:138:LYS:HD2	2.03	0.59
1:A:393:GLN:HG3	1:A:394:LEU:HD12	1.85	0.59
1:A:46:PHE:HE1	1:A:162:THR:CB	2.16	0.59
1:C:379:LYS:HB3	1:C:380:PRO:CD	2.27	0.59
1:A:335:ILE:HG23	1:A:342:PRO:HB3	1.85	0.58
1:E:393:GLN:O	1:E:397:GLU:HG3	2.03	0.58
1:G:67:VAL:HG12	1:G:320:ILE:O	2.03	0.58
1:A:85:ASP:HB3	1:A:89:ARG:NH1	2.18	0.58
1:E:196:TYR:OH	1:E:351:THR:HG21	2.02	0.58
1:G:367:TYR:CD1	1:G:394:LEU:HB3	2.37	0.58
1:G:381:PHE:C	1:G:381:PHE:CD2	2.76	0.58
1:C:210:GLN:HE22	1:C:314:GLU:N	2.00	0.58
1:E:172:SER:HB3	1:E:313:LYS:HB2	1.86	0.58
1:G:197:GLY:HA3	1:G:260:CYS:SG	2.44	0.58
1:E:120:THR:CA	1:E:151:PHE:HZ	2.17	0.58
1:A:396:GLU:HG3	1:A:397:GLU:N	2.17	0.58
1:A:352:ALA:HA	1:A:408:MET:HB2	1.85	0.58
1:C:182:VAL:O	1:C:239:ARG:NH1	2.29	0.58
1:E:269:LEU:CD1	1:E:270:PRO:HD2	2.31	0.58
1:G:209:PHE:HB2	1:G:260:CYS:O	2.04	0.58
1:A:111:SER:HA	1:A:113:ARG:HH12	1.68	0.58
1:E:178:LEU:HD12	1:E:182:VAL:HG22	1.84	0.58
1:A:243:SER:CB	1:E:401:LEU:HD13	2.34	0.57
1:A:227:TYR:CE2	1:A:270:PRO:HB3	2.39	0.57
1:A:41:LYS:NZ	1:A:42:ASP:H	2.03	0.57
1:A:44:HIS:ND1	1:A:339:GLU:HA	2.19	0.57
1:G:365:ASP:O	1:G:369:LYS:HD3	2.04	0.57
1:G:221:PHE:N	1:G:222:PRO:HD3	2.19	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ASP:C	1:E:44:HIS:H	2.08	0.57
1:G:332:TYR:OH	1:G:351:THR:CG2	2.51	0.57
1:A:316:ASN:HB3	1:A:406:LYS:CD	2.35	0.57
1:E:107:LEU:HD11	1:E:282:PHE:HE1	1.68	0.57
1:A:154:GLN:HG2	1:A:155:SER:N	2.18	0.57
1:A:162:THR:HG22	1:A:341:LEU:HD12	1.87	0.57
1:A:165:ALA:HA	1:A:193:PHE:CE1	2.39	0.57
1:A:50:GLU:OE1	1:A:330:LYS:HE2	2.04	0.57
1:E:194:THR:HA	1:E:260:CYS:SG	2.44	0.57
1:A:258:HIS:CD2	1:A:264:ILE:HD12	2.40	0.57
1:C:53:LEU:HD22	1:C:53:LEU:O	2.05	0.57
1:E:80:LYS:HB2	2:E:3850:GDP:O2B	2.04	0.57
1:A:242:VAL:HG23	1:A:247:HIS:NE2	2.20	0.57
1:A:46:PHE:HE1	1:A:162:THR:OG1	1.87	0.57
1:A:62:VAL:HG11	1:A:129:ILE:HD12	1.87	0.57
1:E:121:THR:N	1:E:151:PHE:HE2	2.03	0.57
1:E:48:LEU:HD22	1:E:333:ILE:CG1	2.35	0.57
1:A:45:SER:C	1:A:46:PHE:HD2	2.09	0.56
1:C:367:TYR:HD1	1:C:394:LEU:HB3	1.70	0.56
1:E:72:VAL:HA	1:E:175:VAL:HG13	1.86	0.56
1:E:38:LEU:HD12	1:E:47:GLU:O	2.05	0.56
1:G:104:ASN:HD22	1:G:287:LYS:HZ3	1.50	0.56
1:C:105:GLU:HG3	1:C:106:PRO:HD2	1.87	0.56
1:C:335:ILE:HG22	1:C:336:TYR:CD1	2.39	0.56
1:G:286:LEU:HD22	1:G:294:ILE:CD1	2.36	0.56
1:A:400:LYS:HA	1:A:403:ARG:CD	2.34	0.56
1:E:52:ALA:O	1:E:56:ILE:HD12	2.05	0.56
1:G:162:THR:HG23	1:G:341:LEU:HD21	1.86	0.56
1:G:210:GLN:HE22	1:G:313:LYS:HD2	1.69	0.56
1:A:154:GLN:HG3	1:C:105:GLU:CD	2.26	0.56
1:A:247:HIS:ND1	1:A:251:GLN:HG2	2.20	0.56
1:A:335:ILE:CD1	1:A:347:MET:HA	2.35	0.56
1:E:254:ARG:O	1:E:254:ARG:NE	2.38	0.56
1:A:118:ARG:CG	1:A:118:ARG:O	2.52	0.56
1:A:46:PHE:CE1	1:A:162:THR:OG1	2.56	0.56
1:G:336:TYR:CE2	1:G:342:PRO:HG2	2.40	0.56
1:A:279:ASN:C	1:A:279:ASN:HD22	2.08	0.56
1:A:258:HIS:HD2	1:A:264:ILE:HD12	1.70	0.56
1:C:347:MET:O	1:C:350:ALA:HB3	2.06	0.56
1:E:379:LYS:HB2	1:E:380:PRO:CD	2.34	0.56
1:C:411:GLU:N	1:C:411:GLU:CD	2.59	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:SER:OG	1:C:117:GLU:N	2.39	0.56
1:E:46:PHE:CZ	1:E:162:THR:OG1	2.59	0.56
1:A:53:LEU:CD1	1:A:326:VAL:HG23	2.36	0.55
1:G:197:GLY:HA2	1:G:208:PRO:HG3	1.88	0.55
1:A:123:ILE:HG21	1:A:145:MET:HE3	1.88	0.55
1:A:251:GLN:HE22	1:E:400:LYS:CE	2.19	0.55
1:C:315:ILE:HD13	1:C:328:TYR:CZ	2.41	0.55
1:E:204:THR:O	1:E:205:PHE:HB2	2.05	0.55
1:G:415:ARG:HG3	1:G:415:ARG:HH11	1.70	0.55
1:A:111:SER:OG	1:A:113:ARG:HD2	2.07	0.55
1:A:423:SER:O	1:A:427:GLU:HG3	2.07	0.55
1:E:36:GLN:HG2	1:E:124:GLN:HE21	1.71	0.55
1:G:319:LYS:HD2	1:G:319:LYS:N	2.21	0.55
1:A:77:ARG:O	1:A:78:LYS:HD2	2.06	0.55
1:C:335:ILE:HG23	1:C:342:PRO:HB3	1.89	0.55
1:A:337:GLN:HE21	1:A:337:GLN:HA	1.71	0.55
1:G:170:ILE:HD13	1:G:329:PHE:CZ	2.42	0.55
1:E:56:ILE:CD1	1:E:125:ILE:HD11	2.29	0.55
1:E:344:PRO:O	1:E:347:MET:HB2	2.06	0.55
1:G:371:MET:O	1:G:375:CYS:HB3	2.07	0.55
1:A:381:PHE:N	1:A:381:PHE:HD1	2.05	0.55
1:E:71:SER:CB	1:E:174:GLN:HE22	2.20	0.55
1:G:214:PHE:HD2	1:G:236:LEU:CD2	2.19	0.55
1:G:321:THR:CG2	1:G:324:GLY:H	2.18	0.55
1:G:402:PHE:CE2	1:G:407:LYS:HE2	2.42	0.55
1:A:184:GLU:OE1	1:A:250:LEU:HD13	2.07	0.54
1:A:375:CYS:SG	1:A:387:LEU:HD11	2.47	0.54
1:E:301:ILE:HB	1:E:302:PRO:HD3	1.89	0.54
1:A:153:SER:O	1:A:157:LEU:N	2.41	0.54
1:C:313:LYS:HE3	1:C:315:ILE:HD11	1.90	0.54
1:C:411:GLU:H	1:C:411:GLU:CD	2.11	0.54
1:E:227:TYR:CE1	1:E:270:PRO:HB3	2.42	0.54
1:G:191:GLN:HA	1:G:191:GLN:HE21	1.72	0.54
1:E:123:ILE:HG21	1:E:145:MET:HE3	1.89	0.54
1:G:175:VAL:HG12	1:G:213:ILE:HD13	1.90	0.54
1:E:86:PHE:CE1	1:E:89:ARG:NH1	2.76	0.54
1:G:286:LEU:HD23	1:G:289:ILE:HD12	1.89	0.54
1:A:178:LEU:HD13	1:A:182:VAL:HA	1.89	0.54
1:C:382:LEU:HD11	1:C:386:ASP:HB2	1.89	0.54
1:C:176:TYR:CZ	1:C:178:LEU:HD21	2.43	0.54
1:E:335:ILE:HD11	1:E:346:SER:O	2.08	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:GLN:HE21	1:A:337:GLN:CA	2.20	0.54
1:E:97:VAL:O	1:E:98:ASP:CB	2.55	0.54
1:A:247:HIS:CE1	1:A:251:GLN:HG2	2.43	0.54
1:A:41:LYS:HZ3	1:A:42:ASP:H	1.55	0.54
1:G:147:THR:HG21	1:G:167:SER:CB	2.37	0.54
1:G:73:ALA:HB2	1:G:147:THR:OG1	2.07	0.54
1:A:104:ASN:O	1:A:285:LYS:HE2	2.09	0.53
1:E:332:TYR:OH	1:E:351:THR:HB	2.08	0.53
1:A:188:GLN:HE21	1:A:250:LEU:CD2	2.20	0.53
1:C:196:TYR:HB2	1:C:347:MET:CE	2.38	0.53
1:C:335:ILE:CD1	1:C:347:MET:HA	2.35	0.53
1:G:241:LYS:CE	1:G:241:LYS:HA	2.38	0.53
1:C:187:LEU:HB2	1:C:250:LEU:HD22	1.90	0.53
1:C:386:ASP:O	1:C:390:LYS:HB2	2.09	0.53
1:A:368:ASN:C	1:A:368:ASN:ND2	2.59	0.53
1:E:186:ASP:C	1:E:188:GLN:H	2.11	0.53
1:G:190:LEU:HD23	1:G:257:ILE:CD1	2.34	0.53
1:G:429:TYR:O	1:G:433:ILE:HG23	2.09	0.53
1:E:270:PRO:O	1:E:293:PHE:HD1	1.90	0.53
1:A:76:PHE:CE2	1:A:148:GLN:HB3	2.44	0.53
1:A:335:ILE:CG2	1:A:342:PRO:HG3	2.39	0.53
1:E:164:PHE:CE1	1:E:176:TYR:CD2	2.97	0.53
1:E:300:LEU:O	1:E:303:TRP:HB3	2.08	0.53
1:G:313:LYS:HE3	1:G:315:ILE:HD11	1.91	0.53
1:A:381:PHE:N	1:A:381:PHE:CD1	2.76	0.53
1:C:188:GLN:HG2	1:C:250:LEU:HD21	1.91	0.53
1:C:95:GLU:HA	1:C:95:GLU:OE1	2.09	0.53
1:G:222:PRO:HG3	1:G:227:TYR:CE2	2.43	0.53
1:G:376:GLY:HA3	1:G:377:GLY:C	2.29	0.52
1:G:57:LEU:HD23	1:G:129:ILE:HD11	1.89	0.52
1:G:348:LEU:C	1:G:348:LEU:HD23	2.30	0.52
1:A:112:TRP:HB2	1:A:113:ARG:NH2	2.24	0.52
1:A:228:GLY:HA2	1:A:267:PHE:CZ	2.45	0.52
1:E:335:ILE:HD11	1:E:346:SER:C	2.30	0.52
1:E:335:ILE:HG22	1:E:336:TYR:N	2.23	0.52
1:G:332:TYR:HE1	1:G:351:THR:HG22	1.72	0.52
1:C:187:LEU:O	1:C:190:LEU:HB2	2.10	0.52
1:A:62:VAL:HG21	1:A:129:ILE:HG21	1.92	0.52
1:G:194:THR:HB	1:G:256:HIS:HB3	1.90	0.52
1:A:301:ILE:HB	1:A:302:PRO:HD3	1.92	0.52
1:A:38:LEU:CD2	1:A:38:LEU:C	2.77	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:ILE:N	1:C:302:PRO:CD	2.72	0.52
1:E:241:LYS:HA	1:E:241:LYS:CE	2.38	0.52
1:A:82:PHE:O	1:A:85:ASP:HB2	2.10	0.52
1:A:356:ASN:OD1	1:A:407:LYS:CG	2.58	0.52
1:A:48:LEU:HB2	1:A:333:ILE:HG12	1.91	0.52
1:G:33:GLY:O	1:G:127:SER:HB3	2.09	0.52
1:G:367:TYR:CE1	1:G:394:LEU:HB3	2.45	0.52
1:A:315:ILE:HD13	1:A:320:ILE:HG12	1.92	0.51
1:A:393:GLN:HA	1:A:396:GLU:HG2	1.91	0.51
1:G:68:VAL:HG22	1:G:311:ASP:O	2.10	0.51
1:G:382:LEU:HD23	1:G:386:ASP:HB3	1.93	0.51
1:C:401:LEU:O	1:C:401:LEU:HD12	2.10	0.51
1:A:412:GLU:N	1:A:412:GLU:CD	2.60	0.51
1:E:120:THR:CA	1:E:151:PHE:CZ	2.93	0.51
1:C:57:LEU:HD22	1:C:322:CYS:HB3	1.91	0.51
1:A:38:LEU:HD11	1:A:166:LEU:HD13	1.92	0.51
1:C:165:ALA:HA	1:C:193:PHE:CZ	2.46	0.51
1:E:184:GLU:O	1:E:188:GLN:HG2	2.10	0.51
1:G:48:LEU:HB2	1:G:333:ILE:HG13	1.93	0.51
1:A:147:THR:CG2	1:A:163:VAL:HG13	2.41	0.51
1:A:157:LEU:HD23	1:A:189:HIS:NE2	2.26	0.51
1:G:271:HIS:ND1	1:G:272:PRO:HD2	2.26	0.51
1:G:367:TYR:CE2	1:G:425:ILE:HG23	2.46	0.51
1:A:370:LYS:O	1:A:373:GLU:HG3	2.10	0.51
1:A:389:THR:HA	1:A:392:LEU:CD1	2.37	0.51
1:C:343:HIS:HD2	1:C:345:LYS:N	2.04	0.51
1:A:315:ILE:O	1:A:316:ASN:HB2	2.09	0.51
1:A:343:HIS:O	1:A:344:PRO:C	2.47	0.51
1:E:370:LYS:HB3	1:E:394:LEU:HD21	1.93	0.51
1:G:253:VAL:HG23	1:G:253:VAL:O	2.10	0.51
1:G:381:PHE:HD2	1:G:382:LEU:N	2.09	0.51
1:G:407:LYS:HB2	1:G:407:LYS:NZ	2.26	0.51
1:A:71:SER:HB2	1:A:145:MET:HB2	1.93	0.51
1:C:202:GLU:HB2	1:G:205:PHE:CE1	2.46	0.51
1:C:425:ILE:C	1:C:427:GLU:H	2.12	0.51
1:E:94:GLN:N	1:E:94:GLN:HE21	2.07	0.51
1:A:222:PRO:HG3	1:A:227:TYR:CE1	2.46	0.50
1:A:393:GLN:HG3	1:A:394:LEU:N	2.25	0.50
1:A:53:LEU:HD12	1:A:326:VAL:HG22	1.92	0.50
1:C:194:THR:CG2	1:C:257:ILE:HD13	2.41	0.50
1:A:60:GLU:HG3	1:A:61:ALA:N	2.25	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:428:LEU:HD23	1:G:431:GLN:NE2	2.25	0.50
1:A:300:LEU:O	1:A:303:TRP:HB3	2.12	0.50
1:A:41:LYS:HB2	1:A:45:SER:O	2.11	0.50
1:G:257:ILE:HG13	1:G:264:ILE:HD13	1.93	0.50
1:C:56:ILE:HD12	1:C:125:ILE:HD11	1.94	0.50
1:C:228:GLY:HA2	1:C:267:PHE:CE2	2.45	0.50
1:G:163:VAL:HG12	1:G:164:PHE:N	2.25	0.50
1:G:84:MET:HA	1:G:87:MET:HG3	1.93	0.50
1:A:302:PRO:O	1:A:306:SER:N	2.36	0.50
1:C:411:GLU:HG2	1:C:412:GLU:HG2	1.92	0.50
1:E:124:GLN:O	1:E:145:MET:HA	2.11	0.50
1:G:319:LYS:C	1:G:320:ILE:HD12	2.32	0.50
1:C:269:LEU:HD12	1:C:270:PRO:CD	2.41	0.50
1:E:84:MET:HE1	1:E:112:TRP:CZ2	2.47	0.50
1:C:247:HIS:HE1	1:C:254:ARG:NE	2.06	0.50
1:A:117:GLU:HB2	1:A:119:GLU:N	2.27	0.50
1:A:163:VAL:HG12	1:A:164:PHE:N	2.26	0.50
1:A:249:GLU:CD	1:A:249:GLU:H	2.15	0.50
1:C:210:GLN:NE2	1:C:314:GLU:N	2.60	0.50
1:C:367:TYR:CD1	1:C:394:LEU:HB3	2.46	0.50
1:A:85:ASP:CG	1:A:113:ARG:CZ	2.80	0.49
1:A:402:PHE:O	1:A:405:VAL:HG13	2.12	0.49
1:E:326:VAL:CG1	1:E:326:VAL:O	2.59	0.49
1:G:343:HIS:HD2	1:G:345:LYS:H	1.60	0.49
1:A:318:ASN:HD21	1:A:406:LYS:HZ1	1.59	0.49
1:C:195:GLU:HB3	1:C:344:PRO:HG3	1.94	0.49
1:E:71:SER:CB	1:E:174:GLN:NE2	2.74	0.49
1:A:251:GLN:HE22	1:E:400:LYS:HE2	1.76	0.49
1:G:305:LEU:O	1:G:310:LEU:HD11	2.11	0.49
1:C:225:PHE:CE1	1:C:234:LYS:HB2	2.47	0.49
1:C:337:GLN:HG2	1:C:337:GLN:O	2.11	0.49
1:G:372:GLU:HA	1:G:376:GLY:O	2.12	0.49
1:A:243:SER:C	1:A:245:ASN:H	2.15	0.49
1:A:248:GLU:HB2	1:A:249:GLU:OE2	2.13	0.49
1:C:201:MET:HA	1:C:206:LEU:O	2.11	0.49
1:E:66:GLU:OE1	1:E:138:LYS:HD3	2.11	0.49
1:E:388:GLN:O	1:E:388:GLN:HG3	2.12	0.49
1:E:71:SER:HB3	1:E:174:GLN:HE22	1.78	0.49
1:G:170:ILE:HD13	1:G:329:PHE:CE2	2.47	0.49
1:A:407:LYS:HG2	1:A:414:SER:OG	2.12	0.49
1:A:337:GLN:HA	1:A:337:GLN:NE2	2.28	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:TYR:HA	1:A:344:PRO:HB3	1.95	0.49
1:A:111:SER:HB2	1:A:113:ARG:HD2	1.93	0.49
1:A:406:LYS:CB	1:A:406:LYS:HZ2	2.24	0.49
1:G:395:LYS:O	1:G:399:VAL:HG23	2.12	0.49
1:A:113:ARG:O	1:A:114:GLY:C	2.51	0.49
1:E:35:VAL:HG11	1:E:56:ILE:HD11	1.95	0.49
1:G:68:VAL:HG22	1:G:312:ILE:HA	1.94	0.48
1:C:272:PRO:HG3	2:C:3850:GDP:C6	2.48	0.48
1:E:46:PHE:HD2	1:E:336:TYR:O	1.96	0.48
1:G:360:VAL:HG23	1:G:402:PHE:HE1	1.78	0.48
1:A:243:SER:C	1:A:245:ASN:N	2.63	0.48
1:A:71:SER:OG	1:A:174:GLN:NE2	2.42	0.48
1:A:314:GLU:OE2	1:A:319:LYS:NZ	2.47	0.48
1:C:280:PRO:HA	2:C:3850:GDP:O3'	2.13	0.48
1:C:367:TYR:CE2	1:C:425:ILE:HG23	2.47	0.48
1:C:85:ASP:OD1	1:C:111:SER:HA	2.12	0.48
1:G:360:VAL:HG23	1:G:402:PHE:CE1	2.49	0.48
1:A:235:PHE:CZ	1:A:239:ARG:HG3	2.48	0.48
1:A:247:HIS:CE1	1:A:251:GLN:CD	2.87	0.48
1:A:232:GLY:O	1:A:266:CYS:HB3	2.13	0.48
1:A:279:ASN:ND2	1:A:279:ASN:C	2.67	0.48
1:E:190:LEU:HD23	1:E:257:ILE:HD11	1.94	0.48
1:A:255:LYS:HD2	1:E:404:GLY:HA2	1.95	0.48
1:A:103:TYR:HA	1:A:286:LEU:HB3	1.95	0.48
1:C:399:VAL:O	1:C:403:ARG:HG3	2.14	0.48
1:E:72:VAL:HG22	1:E:175:VAL:CG1	2.44	0.48
1:E:84:MET:HB3	1:E:84:MET:HE2	1.60	0.48
1:A:305:LEU:HA	1:A:310:LEU:CD1	2.44	0.48
1:E:197:GLY:O	1:E:201:MET:HB2	2.14	0.48
1:E:368:ASN:HB2	1:E:428:LEU:HD13	1.96	0.48
1:A:289:ILE:HB	1:A:294:ILE:HD11	1.96	0.48
1:E:38:LEU:HD23	1:E:123:ILE:HG13	1.95	0.48
1:G:335:ILE:HG22	1:G:336:TYR:CD1	2.49	0.48
1:A:247:HIS:HB2	1:A:250:LEU:HB2	1.96	0.47
1:A:336:TYR:C	1:A:337:GLN:HE21	2.16	0.47
1:C:193:PHE:C	1:C:195:GLU:H	2.18	0.47
1:E:239:ARG:NH1	1:E:239:ARG:HG2	2.29	0.47
1:G:102:ASP:HB3	1:G:105:GLU:HB2	1.95	0.47
1:A:112:TRP:N	1:A:113:ARG:CZ	2.74	0.47
1:A:117:GLU:HA	1:A:118:ARG:CB	2.45	0.47
1:C:247:HIS:CG	1:C:250:LEU:HB2	2.50	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:VAL:HG11	1:C:56:ILE:HD11	1.96	0.47
1:E:87:MET:HA	1:E:301:ILE:HD13	1.96	0.47
1:A:158:ARG:HG2	1:A:158:ARG:H	1.46	0.47
1:G:394:LEU:CA	1:G:397:GLU:HB3	2.44	0.47
1:G:86:PHE:CD2	1:G:297:LEU:HD21	2.49	0.47
1:A:199:LEU:HD22	1:A:199:LEU:HA	1.73	0.47
1:E:335:ILE:HG23	1:E:342:PRO:HB3	1.96	0.47
1:G:367:TYR:CD2	1:G:367:TYR:O	2.68	0.47
1:G:84:MET:CE	1:G:112:TRP:CZ2	2.95	0.47
1:A:335:ILE:HD11	1:A:346:SER:O	2.14	0.47
1:C:38:LEU:HD23	1:C:123:ILE:HG13	1.95	0.47
1:A:56:ILE:HD13	1:A:127:SER:HA	1.97	0.47
1:A:222:PRO:HG3	1:A:227:TYR:CZ	2.50	0.47
1:A:299:ILE:HG12	1:A:300:LEU:N	2.28	0.47
1:A:46:PHE:CE1	1:A:336:TYR:HB3	2.50	0.47
1:C:239:ARG:NE	1:C:239:ARG:HA	2.29	0.47
1:E:100:VAL:HG21	1:E:298:LYS:HZ3	1.80	0.47
1:E:220:SER:C	1:E:222:PRO:HD3	2.36	0.47
1:C:242:VAL:HG23	1:G:401:LEU:HD13	1.96	0.47
1:C:57:LEU:HD22	1:C:322:CYS:SG	2.55	0.47
1:E:216:VAL:HB	1:E:268:LEU:HD12	1.97	0.47
1:E:348:LEU:HD23	1:E:348:LEU:HA	1.65	0.47
1:E:43:ASP:O	1:E:44:HIS:HB2	2.14	0.47
1:G:62:VAL:HG11	1:G:129:ILE:HD13	1.97	0.47
1:G:86:PHE:CG	1:G:297:LEU:HD21	2.49	0.47
1:A:242:VAL:CG2	1:A:243:SER:N	2.77	0.47
1:E:196:TYR:O	1:E:199:LEU:HD12	2.14	0.47
1:A:316:ASN:ND2	1:A:408:MET:HG2	2.30	0.46
1:C:243:SER:C	1:C:245:ASN:H	2.17	0.46
1:E:120:THR:CB	1:E:151:PHE:CZ	2.97	0.46
1:A:72:VAL:HG13	1:A:175:VAL:CG2	2.39	0.46
1:C:147:THR:HG22	1:C:163:VAL:HG12	1.97	0.46
1:G:371:MET:HB3	1:G:432:TYR:CD1	2.50	0.46
1:G:394:LEU:C	1:G:397:GLU:HB3	2.35	0.46
1:G:48:LEU:HD22	1:G:333:ILE:HG13	1.97	0.46
1:E:33:GLY:HA2	1:E:126:TRP:CH2	2.50	0.46
1:E:240:LEU:HB3	1:E:254:ARG:CG	2.43	0.46
1:E:343:HIS:HD2	1:E:344:PRO:CD	2.27	0.46
1:A:117:GLU:HB2	1:A:119:GLU:CA	2.45	0.46
1:C:210:GLN:HE22	1:C:313:LYS:HA	1.79	0.46
1:E:72:VAL:HG22	1:E:175:VAL:HG11	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:GLU:OE1	1:E:330:LYS:HE3	2.15	0.46
1:A:316:ASN:HB3	1:A:406:LYS:CE	2.45	0.46
1:A:385:ASN:O	1:A:388:GLN:HB3	2.14	0.46
1:A:64:ASP:OD1	1:A:323:ARG:NH2	2.45	0.46
1:C:196:TYR:CB	1:C:347:MET:HE2	2.45	0.46
1:C:247:HIS:CE1	1:C:254:ARG:NH2	2.84	0.46
1:E:225:PHE:CG	1:E:235:PHE:HB2	2.51	0.46
1:A:154:GLN:C	1:A:156:THR:N	2.70	0.46
1:C:91:MET:HB3	1:C:130:PHE:CE2	2.51	0.46
1:C:335:ILE:CG2	1:C:342:PRO:HG3	2.45	0.46
1:C:396:GLU:O	1:C:396:GLU:HG2	2.16	0.46
1:C:96:SER:C	1:C:98:ASP:H	2.18	0.46
1:E:71:SER:O	1:E:175:VAL:HG12	2.15	0.46
1:E:195:GLU:O	1:E:199:LEU:HG	2.15	0.46
1:A:77:ARG:C	1:A:78:LYS:HD2	2.36	0.46
1:E:335:ILE:CD1	1:E:347:MET:HA	2.46	0.46
1:A:348:LEU:HD23	1:A:348:LEU:HA	1.79	0.46
1:C:156:THR:HA	1:C:159:ASP:HB3	1.98	0.46
1:C:196:TYR:HB2	1:C:347:MET:HE1	1.94	0.46
1:G:201:MET:HG3	1:G:206:LEU:O	2.16	0.46
1:C:433:ILE:O	1:C:436:ASN:HB3	2.15	0.45
1:E:421:LEU:O	1:E:425:ILE:HG13	2.15	0.45
1:E:62:VAL:HG22	1:E:322:CYS:SG	2.56	0.45
1:C:335:ILE:HG22	1:C:336:TYR:CG	2.51	0.45
1:C:336:TYR:O	1:C:337:GLN:CB	2.63	0.45
1:E:333:ILE:O	1:E:333:ILE:HG23	2.16	0.45
1:G:56:ILE:HD12	1:G:125:ILE:HD11	1.98	0.45
1:G:190:LEU:HD21	1:G:212:LEU:HD21	1.98	0.45
1:G:425:ILE:HA	1:G:428:LEU:HB2	1.98	0.45
1:A:133:ASN:ND2	1:A:133:ASN:H	2.13	0.45
1:A:39:ILE:HD12	1:A:40:VAL:H	1.82	0.45
1:G:416:ARG:HH11	1:G:416:ARG:HG2	1.82	0.45
1:A:104:ASN:ND2	1:A:285:LYS:HE2	2.28	0.45
1:A:390:LYS:HD3	1:A:390:LYS:HA	1.81	0.45
1:C:210:GLN:NE2	1:C:313:LYS:HA	2.32	0.45
1:E:341:LEU:N	1:E:341:LEU:HD12	2.31	0.45
1:A:54:ASN:O	1:A:58:LEU:HB2	2.16	0.45
1:E:191:GLN:HA	1:E:253:VAL:HG11	1.99	0.45
1:A:271:HIS:ND1	1:A:272:PRO:HD2	2.31	0.45
1:C:227:TYR:CZ	1:C:270:PRO:HB3	2.52	0.45
1:E:170:ILE:HD13	1:E:329:PHE:CZ	2.52	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:PHE:C	1:C:195:GLU:N	2.70	0.45
1:C:193:PHE:O	1:C:195:GLU:N	2.49	0.45
1:C:305:LEU:HA	1:C:310:LEU:HD11	1.99	0.45
1:G:200:ALA:CA	1:G:348:LEU:HD12	2.43	0.45
1:A:243:SER:HA	1:A:247:HIS:CE1	2.52	0.45
1:C:429:TYR:O	1:C:433:ILE:HG23	2.16	0.45
1:C:57:LEU:HD22	1:C:322:CYS:CB	2.46	0.45
1:E:372:GLU:HB3	1:E:432:TYR:OH	2.17	0.45
1:A:161:ALA:HB1	1:A:192:LEU:HD21	1.99	0.44
1:A:183:GLN:O	1:A:186:ASP:N	2.50	0.44
1:A:53:LEU:HD12	1:A:326:VAL:HG23	1.98	0.44
1:C:173:ILE:HG12	1:C:211:SER:OG	2.16	0.44
1:G:34:PRO:HB3	1:G:112:TRP:CE3	2.52	0.44
1:G:217:ARG:HD2	1:G:217:ARG:HA	1.54	0.44
1:A:272:PRO:CG	2:A:3850:GDP:C6	3.00	0.44
1:A:394:LEU:HA	1:A:397:GLU:HG2	1.99	0.44
1:C:94:GLN:HB2	1:C:94:GLN:HE21	1.51	0.44
1:E:386:ASP:HA	1:E:389:THR:OG1	2.18	0.44
1:A:154:GLN:HG3	1:C:105:GLU:OE1	2.17	0.44
1:A:100:VAL:CG1	1:A:286:LEU:HD11	2.48	0.44
1:A:314:GLU:HG2	1:A:314:GLU:O	2.17	0.44
1:G:178:LEU:CD1	1:G:182:VAL:HG13	2.47	0.44
1:A:221:PHE:N	1:A:222:PRO:HD3	2.32	0.44
1:A:85:ASP:HB3	1:A:89:ARG:HH12	1.82	0.44
1:E:186:ASP:C	1:E:188:GLN:N	2.70	0.44
1:G:57:LEU:HB2	1:G:326:VAL:CG2	2.47	0.44
1:C:62:VAL:HG21	1:C:129:ILE:HG21	1.99	0.44
1:E:405:VAL:O	1:E:407:LYS:HG3	2.17	0.44
1:E:76:PHE:CD2	1:E:77:ARG:HG3	2.53	0.44
1:E:231:GLY:HA2	1:E:234:LYS:HG3	2.00	0.44
1:E:66:GLU:HB3	1:E:312:ILE:HG21	2.00	0.44
1:G:112:TRP:CD1	1:G:112:TRP:N	2.86	0.44
1:A:165:ALA:O	1:A:169:MET:HG2	2.18	0.44
1:A:188:GLN:HE21	1:A:250:LEU:HD23	1.83	0.44
1:A:279:ASN:ND2	1:A:280:PRO:N	2.66	0.44
1:C:430:ILE:HA	1:C:433:ILE:HG12	2.00	0.44
1:A:38:LEU:CD1	1:A:166:LEU:HD13	2.47	0.44
1:A:316:ASN:HD21	1:A:408:MET:HG2	1.82	0.44
1:C:117:GLU:HA	1:C:118:ARG:C	2.39	0.44
1:C:379:LYS:CB	1:C:380:PRO:CD	2.94	0.44
1:A:433:ILE:HG22	1:A:437:ASP:OD1	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:GLY:O	1:C:340:GLU:HA	2.18	0.43
1:E:187:LEU:O	1:E:253:VAL:HG21	2.17	0.43
1:G:185:ASP:O	1:G:188:GLN:HB2	2.18	0.43
1:A:154:GLN:HA	1:A:157:LEU:CD1	2.49	0.43
1:A:185:ASP:N	1:A:185:ASP:OD2	2.42	0.43
1:A:181:ASN:OD1	1:A:235:PHE:HZ	2.02	0.43
1:A:46:PHE:HE1	1:A:162:THR:HB	1.83	0.43
1:A:35:VAL:HG11	1:A:56:ILE:HD11	1.99	0.43
1:C:58:LEU:HD22	1:C:323:ARG:HG3	1.98	0.43
1:E:143:LEU:O	1:E:144:LEU:HD23	2.18	0.43
1:A:202:GLU:HA	1:E:205:PHE:CD1	2.53	0.43
1:E:170:ILE:HD13	1:E:329:PHE:CE2	2.53	0.43
1:E:390:LYS:HD3	1:E:390:LYS:HA	1.86	0.43
1:E:40:VAL:HG13	1:E:46:PHE:CD1	2.53	0.43
1:G:341:LEU:HA	1:G:342:PRO:HD3	1.73	0.43
1:G:381:PHE:C	1:G:381:PHE:HD2	2.21	0.43
1:A:318:ASN:HD21	1:A:406:LYS:NZ	2.16	0.43
1:A:316:ASN:C	1:A:406:LYS:HE2	2.34	0.43
1:C:326:VAL:CG1	1:C:330:LYS:HE3	2.48	0.43
1:E:129:ILE:HG21	1:E:141:ALA:HB1	1.99	0.43
1:G:124:GLN:HG3	1:G:146:ASP:HB3	1.99	0.43
1:G:333:ILE:CG2	1:G:334:LYS:N	2.81	0.43
1:A:393:GLN:CG	1:A:394:LEU:HD12	2.47	0.43
1:E:433:ILE:HA	1:E:436:ASN:CB	2.48	0.43
1:G:102:ASP:HB3	1:G:105:GLU:CB	2.48	0.43
1:G:134:LYS:HB3	1:G:134:LYS:HE2	1.76	0.43
1:G:225:PHE:CD2	1:G:235:PHE:HD1	2.37	0.43
1:C:236:LEU:HG	1:C:240:LEU:HD12	2.00	0.43
1:E:210:GLN:NE2	1:E:313:LYS:HA	2.33	0.43
1:G:257:ILE:HG13	1:G:264:ILE:CD1	2.48	0.43
1:G:411:GLU:CD	1:G:411:GLU:H	2.21	0.43
1:A:337:GLN:CA	1:A:337:GLN:NE2	2.81	0.43
1:A:81:SER:O	1:A:113:ARG:NH2	2.52	0.43
1:C:86:PHE:CG	1:C:297:LEU:HD21	2.54	0.43
1:E:343:HIS:O	1:E:344:PRO:C	2.54	0.43
1:A:154:GLN:HA	1:A:157:LEU:HD12	2.01	0.43
1:A:323:ARG:CZ	1:A:323:ARG:HB3	2.48	0.43
1:A:401:LEU:C	1:A:401:LEU:CD1	2.81	0.43
1:E:341:LEU:HB3	1:E:342:PRO:HD2	2.01	0.43
1:E:393:GLN:CG	1:E:394:LEU:N	2.82	0.43
1:E:64:ASP:CG	1:E:323:ARG:HH22	2.22	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ILE:CD1	1:A:315:ILE:N	2.81	0.43
1:C:152:ASP:O	1:C:153:SER:HB2	2.19	0.43
1:C:302:PRO:O	1:C:306:SER:N	2.41	0.43
1:C:59:SER:O	1:C:63:ARG:HB2	2.19	0.43
1:A:154:GLN:O	1:A:157:LEU:N	2.52	0.43
1:A:76:PHE:CE2	1:A:119:GLU:HB2	2.54	0.43
1:C:177:ASN:OD1	1:C:217:ARG:NH1	2.48	0.43
1:C:325:LEU:HA	1:C:325:LEU:HD12	1.78	0.43
1:E:254:ARG:O	1:E:257:ILE:HG22	2.18	0.43
1:E:367:TYR:HD2	1:E:368:ASN:N	2.16	0.43
1:E:42:ASP:C	1:E:44:HIS:N	2.71	0.43
1:E:433:ILE:HA	1:E:436:ASN:HB3	2.00	0.43
1:G:310:LEU:HD12	1:G:310:LEU:H	1.83	0.43
1:E:30:LYS:O	1:E:31:LYS:O	2.36	0.43
1:E:369:LYS:HA	1:E:369:LYS:HD2	1.75	0.43
1:G:70:VAL:HB	1:G:144:LEU:HD23	2.01	0.43
1:G:343:HIS:HD2	1:G:345:LYS:N	2.17	0.43
1:A:241:LYS:CE	1:A:241:LYS:HA	2.40	0.42
1:E:204:THR:O	1:E:205:PHE:CB	2.64	0.42
1:E:222:PRO:HG3	1:E:227:TYR:CZ	2.54	0.42
1:A:62:VAL:HG21	1:A:129:ILE:CG2	2.49	0.42
1:A:183:GLN:HG3	1:A:186:ASP:OD2	2.19	0.42
1:A:393:GLN:O	1:A:396:GLU:HG2	2.20	0.42
1:A:395:LYS:O	1:A:399:VAL:HG23	2.20	0.42
2:C:3850:GDP:H8	2:C:3850:GDP:H2'	1.76	0.42
1:C:42:ASP:C	1:C:44:HIS:H	2.21	0.42
1:E:120:THR:HB	1:E:151:PHE:HE2	1.78	0.42
1:E:257:ILE:HA	1:E:257:ILE:HD12	1.83	0.42
1:G:57:LEU:O	1:G:58:LEU:HD23	2.19	0.42
1:A:35:VAL:O	1:A:35:VAL:HG22	2.19	0.42
1:C:46:PHE:HD2	1:C:337:GLN:HA	1.83	0.42
1:E:34:PRO:HD3	1:E:126:TRP:HZ3	1.83	0.42
1:G:286:LEU:O	1:G:288:GLU:N	2.52	0.42
1:G:307:PRO:HA	1:G:310:LEU:HD13	2.01	0.42
1:A:76:PHE:CE2	1:A:148:GLN:NE2	2.81	0.42
1:A:162:THR:OG1	1:A:163:VAL:N	2.52	0.42
1:C:196:TYR:HE2	1:C:348:LEU:HA	1.84	0.42
1:C:227:TYR:CE2	1:C:270:PRO:HB3	2.53	0.42
1:C:235:PHE:O	1:C:239:ARG:HG2	2.20	0.42
1:C:196:TYR:OH	1:C:351:THR:HG21	2.19	0.42
1:E:89:ARG:NH2	1:E:107:LEU:HB3	2.33	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:PHE:O	1:E:297:LEU:HB2	2.19	0.42
1:E:192:LEU:HD22	1:E:341:LEU:CD2	2.49	0.42
1:E:367:TYR:CD2	1:E:368:ASN:N	2.87	0.42
1:G:272:PRO:HG3	2:G:3850:GDP:C6	2.54	0.42
1:A:129:ILE:CG2	1:A:141:ALA:HB1	2.49	0.42
1:A:242:VAL:HA	1:A:254:ARG:HD2	2.00	0.42
1:A:257:ILE:HA	1:A:257:ILE:HD12	1.78	0.42
1:E:143:LEU:HD12	1:E:144:LEU:N	2.34	0.42
1:G:103:TYR:C	1:G:105:GLU:H	2.23	0.42
1:G:210:GLN:HE22	1:G:313:LYS:CD	2.31	0.42
1:G:83:LEU:O	1:G:87:MET:HG3	2.18	0.42
1:C:181:ASN:OD1	1:C:182:VAL:N	2.52	0.42
1:C:247:HIS:CD2	1:C:250:LEU:HD13	2.55	0.42
1:C:393:GLN:O	1:C:397:GLU:HG3	2.20	0.42
1:E:121:THR:H	1:E:151:PHE:HE2	1.66	0.42
1:G:327:GLU:OE2	1:G:357:LEU:HB3	2.19	0.42
1:A:245:ASN:HD21	1:E:397:GLU:HB3	1.85	0.42
1:C:217:ARG:HH11	1:C:217:ARG:CG	2.33	0.42
1:E:195:GLU:HA	1:E:198:ARG:HB3	2.01	0.42
1:E:204:THR:C	1:E:205:PHE:CD2	2.93	0.42
1:E:217:ARG:HA	1:E:217:ARG:HD2	1.76	0.42
1:E:57:LEU:HD23	1:E:57:LEU:HA	1.79	0.42
1:A:315:ILE:O	1:A:316:ASN:CB	2.68	0.42
1:E:338:GLY:O	1:E:339:GLU:C	2.58	0.42
1:E:35:VAL:HG12	1:E:125:ILE:O	2.20	0.42
1:E:48:LEU:HB2	1:E:333:ILE:HG13	2.01	0.42
1:A:76:PHE:CZ	1:A:119:GLU:HG2	2.55	0.42
1:C:196:TYR:CG	1:C:347:MET:HE2	2.55	0.42
1:G:38:LEU:HB3	1:G:123:ILE:HB	2.02	0.42
1:A:337:GLN:HE21	1:A:337:GLN:N	2.18	0.41
1:A:41:LYS:HB3	1:A:43:ASP:OD1	2.19	0.41
1:C:181:ASN:OD1	1:C:239:ARG:NH1	2.53	0.41
1:C:367:TYR:CZ	1:C:425:ILE:HG23	2.55	0.41
1:C:97:VAL:CG1	1:C:97:VAL:O	2.67	0.41
1:G:187:LEU:N	1:G:187:LEU:HD23	2.35	0.41
1:G:339:GLU:HG3	1:G:339:GLU:H	1.37	0.41
1:A:162:THR:HG22	1:A:341:LEU:CD1	2.48	0.41
1:A:147:THR:HG23	1:A:163:VAL:HG13	2.02	0.41
1:E:375:CYS:O	1:E:375:CYS:SG	2.78	0.41
1:E:272:PRO:HG3	2:E:3850:GDP:C6	2.56	0.41
1:G:228:GLY:HA2	1:G:267:PHE:CZ	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:270:PRO:CG	1:G:293:PHE:HA	2.48	0.41
1:A:133:ASN:ND2	1:A:133:ASN:N	2.67	0.41
1:A:129:ILE:HG21	1:A:141:ALA:HB1	2.01	0.41
1:A:163:VAL:CG1	1:A:164:PHE:N	2.83	0.41
1:A:175:VAL:O	1:A:175:VAL:HG22	2.19	0.41
1:G:335:ILE:HD11	1:G:346:SER:C	2.41	0.41
1:G:335:ILE:HD11	1:G:346:SER:O	2.21	0.41
1:A:330:LYS:O	1:A:333:ILE:HG22	2.21	0.41
1:C:217:ARG:HG3	1:C:217:ARG:NH1	2.34	0.41
1:C:107:LEU:CD2	1:C:286:LEU:HD12	2.51	0.41
1:E:34:PRO:HB3	1:E:112:TRP:CE3	2.54	0.41
1:E:353:GLU:HG2	1:E:417:TYR:OH	2.21	0.41
1:G:344:PRO:HA	1:G:347:MET:HE2	2.03	0.41
1:G:415:ARG:CG	1:G:415:ARG:HH11	2.33	0.41
1:A:319:LYS:C	1:A:320:ILE:HD12	2.41	0.41
1:C:107:LEU:HD21	1:C:286:LEU:HB2	2.02	0.41
1:C:314:GLU:HA	1:C:318:ASN:O	2.21	0.41
1:C:391:HIS:CG	1:C:429:TYR:CD2	3.08	0.41
1:G:196:TYR:HE2	1:G:348:LEU:HA	1.86	0.41
1:E:405:VAL:O	1:E:406:LYS:C	2.59	0.41
1:E:402:PHE:CZ	1:E:407:LYS:HE3	2.55	0.41
1:C:243:SER:OG	1:C:244:GLY:N	2.53	0.41
1:C:243:SER:OG	1:C:245:ASN:OD1	2.39	0.41
1:C:314:GLU:OE2	1:C:319:LYS:HE2	2.20	0.41
1:G:398:SER:HA	1:G:401:LEU:HB3	2.03	0.41
1:A:121:THR:HA	1:A:148:GLN:O	2.21	0.41
1:C:178:LEU:HD12	1:C:182:VAL:HG22	2.03	0.41
1:C:70:VAL:HB	1:C:144:LEU:HD23	2.03	0.41
1:C:228:GLY:HA2	1:C:267:PHE:CZ	2.56	0.41
1:A:158:ARG:C	1:A:162:THR:HG23	2.38	0.41
1:A:242:VAL:HG22	1:A:243:SER:N	2.34	0.41
1:A:365:ASP:O	1:A:369:LYS:HD3	2.21	0.41
1:C:429:TYR:CG	1:C:429:TYR:O	2.74	0.41
1:E:349:GLN:HE22	1:G:102:ASP:CG	2.24	0.41
1:G:417:TYR:HA	1:G:420:GLN:HG2	2.01	0.41
1:C:68:VAL:HB	1:C:142:VAL:HG22	2.03	0.41
1:C:165:ALA:HA	1:C:193:PHE:CE1	2.56	0.41
1:C:176:TYR:CE1	1:C:178:LEU:HD21	2.56	0.41
1:C:94:GLN:OE1	1:C:132:ILE:HD11	2.21	0.41
1:A:117:GLU:HA	1:A:118:ARG:C	2.41	0.40
1:A:154:GLN:CG	1:A:155:SER:N	2.82	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:VAL:HG13	1:A:418:LEU:HD21	2.02	0.40
1:C:339:GLU:HA	1:C:340:GLU:HA	1.92	0.40
1:C:355:ASN:HB3	1:C:408:MET:HG3	2.03	0.40
1:C:418:LEU:O	1:C:418:LEU:HD23	2.20	0.40
1:E:241:LYS:CE	1:E:254:ARG:HD2	2.51	0.40
1:G:269:LEU:CD1	1:G:270:PRO:HD2	2.49	0.40
1:C:225:PHE:HE1	1:C:234:LYS:HB2	1.86	0.40
1:E:76:PHE:HB3	1:E:152:ASP:O	2.21	0.40
1:A:111:SER:HB2	1:A:113:ARG:CD	2.51	0.40
1:A:227:TYR:CD2	1:A:270:PRO:HG3	2.56	0.40
1:C:320:ILE:HD12	1:C:320:ILE:N	2.36	0.40
1:C:411:GLU:O	1:C:415:ARG:HG3	2.21	0.40
1:G:63:ARG:HG2	1:G:64:ASP:OD2	2.20	0.40
1:G:84:MET:HE1	1:G:112:TRP:CH2	2.56	0.40
1:A:247:HIS:HD2	1:A:254:ARG:HH11	1.67	0.40
1:A:81:SER:OG	2:A:3850:GDP:O2B	2.38	0.40
1:G:236:LEU:CD2	1:G:266:CYS:HB2	2.49	0.40
1:G:34:PRO:HD3	1:G:126:TRP:CZ3	2.57	0.40
1:G:84:MET:HB3	1:G:84:MET:HE2	1.86	0.40
1:C:46:PHE:CD2	1:C:46:PHE:N	2.88	0.40
1:E:347:MET:O	1:E:351:THR:HG22	2.22	0.40
1:G:144:LEU:HA	1:G:144:LEU:HD23	1.83	0.40
1:G:178:LEU:HD22	1:G:186:ASP:OD2	2.20	0.40
1:G:196:TYR:CG	1:G:347:MET:HE3	2.56	0.40
1:G:368:ASN:O	1:G:372:GLU:HG2	2.21	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	409/447 (92%)	371 (91%)	36 (9%)	2 (0%)	29 66

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	407/447 (91%)	344 (84%)	52 (13%)	11 (3%)	5	25
1	E	378/447 (85%)	330 (87%)	41 (11%)	7 (2%)	8	34
1	G	376/447 (84%)	332 (88%)	35 (9%)	9 (2%)	6	28
All	All	1570/1788 (88%)	1377 (88%)	164 (10%)	29 (2%)	8	35

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	75	ALA
1	C	97	VAL
1	E	31	LYS
1	E	150	THR
1	C	63	ARG
1	C	380	PRO
1	C	381	PHE
1	E	284	GLY
1	E	380	PRO
1	G	63	ARG
1	G	197	GLY
1	G	380	PRO
1	A	243	SER
1	C	153	SER
1	C	194	THR
1	C	426	ASP
1	E	76	PHE
1	G	287	LYS
1	G	163	VAL
1	G	196	TYR
1	G	210	GLN
1	A	210	GLN
1	C	210	GLN
1	C	96	SER
1	C	437	ASP
1	E	43	ASP
1	E	238	LYS
1	G	104	ASN
1	G	379	LYS

### 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	364/395 (92%)	274 (75%)	90 (25%)	0	3
1	C	362/395 (92%)	319 (88%)	43 (12%)	5	21
1	E	342/395 (87%)	288 (84%)	54 (16%)	2	12
1	G	340/395 (86%)	293 (86%)	47 (14%)	3	16
All	All	1408/1580 (89%)	1174 (83%)	234 (17%)	2	10

All (234) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	36	GLN
1	A	38	LEU
1	A	39	ILE
1	A	40	VAL
1	A	41	LYS
1	A	44	HIS
1	A	46	PHE
1	A	51	THR
1	A	53	LEU
1	A	59	SER
1	A	60	GLU
1	A	62	VAL
1	A	71	SER
1	A	72	VAL
1	A	78	LYS
1	A	81	SER
1	A	93	ASN
1	A	94	GLN
1	A	95	GLU
1	A	96	SER
1	A	104	ASN
1	A	111	SER
1	A	113	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	117	GLU
1	A	118	ARG
1	A	131	LEU
1	A	133	ASN
1	A	150	THR
1	A	154	GLN
1	A	157	LEU
1	A	158	ARG
1	A	159	ASP
1	A	163	VAL
1	A	175	VAL
1	A	180	GLN
1	A	183	GLN
1	A	185	ASP
1	A	190	LEU
1	A	192	LEU
1	A	198	ARG
1	A	199	LEU
1	A	203	GLU
1	A	204	THR
1	A	210	GLN
1	A	241	LYS
1	A	247	HIS
1	A	248	GLU
1	A	249	GLU
1	A	257	ILE
1	A	262	THR
1	A	268	LEU
1	A	276	VAL
1	A	279	ASN
1	A	286	LEU
1	A	287	LYS
1	A	288	GLU
1	A	299	ILE
1	A	305	LEU
1	A	308	GLU
1	A	310	LEU
1	A	314	GLU
1	A	319	LYS
1	A	321	THR
1	A	326	VAL
1	A	335	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	337	GLN
1	A	340	GLU
1	A	341	LEU
1	A	346	SER
1	A	348	LEU
1	A	368	ASN
1	A	371	MET
1	A	373	GLU
1	A	381	PHE
1	A	382	LEU
1	A	392	LEU
1	A	393	GLN
1	A	401	LEU
1	A	403	ARG
1	A	405	VAL
1	A	406	LYS
1	A	411	GLU
1	A	412	GLU
1	A	414	SER
1	A	416	ARG
1	A	418	LEU
1	A	431	GLN
1	A	433	ILE
1	A	434	LYS
1	C	35	VAL
1	C	37	VAL
1	C	53	LEU
1	C	78	LYS
1	C	84	MET
1	C	89	ARG
1	C	94	GLN
1	C	98	ASP
1	C	100	VAL
1	C	102	ASP
1	C	113	ARG
1	C	162	THR
1	C	166	LEU
1	C	175	VAL
1	C	183	GLN
1	C	190	LEU
1	C	192	LEU
1	C	195	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	198	ARG
1	C	217	ARG
1	C	247	HIS
1	C	249	GLU
1	C	250	LEU
1	C	253	VAL
1	C	257	ILE
1	C	294	ILE
1	C	305	LEU
1	C	333	ILE
1	C	335	ILE
1	C	337	GLN
1	C	346	SER
1	C	348	LEU
1	C	351	THR
1	C	357	LEU
1	C	369	LYS
1	C	381	PHE
1	C	391	HIS
1	C	392	LEU
1	C	405	VAL
1	C	407	LYS
1	C	408	MET
1	C	411	GLU
1	C	437	ASP
1	E	35	VAL
1	E	37	VAL
1	E	43	ASP
1	E	44	HIS
1	E	47	GLU
1	E	51	THR
1	E	55	ARG
1	E	65	LYS
1	E	78	LYS
1	E	94	GLN
1	E	99	TRP
1	E	100	VAL
1	E	103	TYR
1	E	107	LEU
1	E	108	THR
1	E	121	THR
1	E	125	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	148	GLN
1	E	162	THR
1	E	163	VAL
1	E	199	LEU
1	E	201	MET
1	E	203	GLU
1	E	230	ASP
1	E	241	LYS
1	E	254	ARG
1	E	265	SER
1	E	268	LEU
1	E	279	ASN
1	E	299	ILE
1	E	312	ILE
1	E	319	LYS
1	E	333	ILE
1	E	335	ILE
1	E	346	SER
1	E	348	LEU
1	E	351	THR
1	E	362	THR
1	E	369	LYS
1	E	371	MET
1	E	385	ASN
1	E	387	LEU
1	E	388	GLN
1	E	389	THR
1	E	394	LEU
1	E	396	GLU
1	E	401	LEU
1	E	405	VAL
1	E	406	LYS
1	E	412	GLU
1	E	416	ARG
1	E	423	SER
1	E	431	GLN
1	E	432	TYR
1	G	35	VAL
1	G	39	ILE
1	G	43	ASP
1	G	48	LEU
1	G	65	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	96	SER
1	G	97	VAL
1	G	121	THR
1	G	124	GLN
1	G	125	ILE
1	G	127	SER
1	G	147	THR
1	G	148	GLN
1	G	160	SER
1	G	183	GLN
1	G	185	ASP
1	G	191	GLN
1	G	199	LEU
1	G	203	GLU
1	G	210	GLN
1	G	226	SER
1	G	239	ARG
1	G	241	LYS
1	G	254	ARG
1	G	279	ASN
1	G	287	LYS
1	G	299	ILE
1	G	319	LYS
1	G	333	ILE
1	G	335	ILE
1	G	339	GLU
1	G	341	LEU
1	G	349	GLN
1	G	366	THR
1	G	381	PHE
1	G	386	ASP
1	G	394	LEU
1	G	397	GLU
1	G	401	LEU
1	G	405	VAL
1	G	407	LYS
1	G	415	ARG
1	G	416	ARG
1	G	418	LEU
1	G	420	GLN
1	G	428	LEU
1	G	431	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	94	GLN
1	A	104	ASN
1	A	154	GLN
1	A	174	GLN
1	A	188	GLN
1	A	251	GLN
1	A	256	HIS
1	A	258	HIS
1	A	279	ASN
1	A	318	ASN
1	A	337	GLN
1	A	368	ASN
1	A	419	GLN
1	A	431	GLN
1	A	436	ASN
1	C	104	ASN
1	C	124	GLN
1	C	183	GLN
1	C	188	GLN
1	C	191	GLN
1	C	210	GLN
1	C	245	ASN
1	C	247	HIS
1	C	252	ASN
1	C	343	HIS
1	C	368	ASN
1	C	419	GLN
1	E	94	GLN
1	E	124	GLN
1	E	133	ASN
1	E	174	GLN
1	E	189	HIS
1	E	210	GLN
1	E	256	HIS
1	E	318	ASN
1	E	343	HIS
1	E	349	GLN
1	E	419	GLN
1	G	94	GLN
1	G	104	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	124	GLN
1	G	191	GLN
1	G	210	GLN
1	G	258	HIS
1	G	279	ASN
1	G	318	ASN
1	G	343	HIS
1	G	419	GLN
1	G	431	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
2	GDP	A	3850	3	24,30,30	1.20	2 (8%)	31,47,47	2.04	8 (25%)
2	GDP	C	3850	-	24,30,30	1.17	2 (8%)	31,47,47	1.82	8 (25%)
2	GDP	E	3850	-	24,30,30	1.22	2 (8%)	31,47,47	1.91	9 (29%)
2	GDP	G	3850	-	24,30,30	1.15	2 (8%)	31,47,47	1.88	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
2	GDP	A	3850	3	-	1/12/32/32	0/3/3/3
2	GDP	C	3850	-	-	6/12/32/32	0/3/3/3
2	GDP	E	3850	-	-	6/12/32/32	0/3/3/3
2	GDP	G	3850	-	-	3/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3850	GDP	C6-C5	4.26	1.48	1.41
2	G	3850	GDP	C6-C5	4.16	1.48	1.41
2	A	3850	GDP	C6-C5	4.10	1.48	1.41
2	C	3850	GDP	C6-C5	4.09	1.48	1.41
2	A	3850	GDP	C5-C4	2.84	1.48	1.40
2	E	3850	GDP	C5-C4	2.73	1.48	1.40
2	C	3850	GDP	C5-C4	2.58	1.47	1.40
2	G	3850	GDP	C5-C4	2.21	1.46	1.40

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	3850	GDP	C5-C6-N1	-4.64	117.09	123.43
2	A	3850	GDP	C2-N3-C4	4.63	120.65	115.36
2	C	3850	GDP	C2-N3-C4	4.42	120.40	115.36
2	A	3850	GDP	PA-O3A-PB	-4.24	118.27	132.83
2	A	3850	GDP	C5-C6-N1	-4.19	117.71	123.43
2	G	3850	GDP	C2-N3-C4	4.10	120.04	115.36
2	E	3850	GDP	C5-C6-N1	-4.09	117.83	123.43
2	G	3850	GDP	C6-N1-C2	4.05	122.36	115.93
2	E	3850	GDP	C2-N3-C4	3.94	119.85	115.36
2	A	3850	GDP	C6-N1-C2	3.92	122.16	115.93
2	E	3850	GDP	C6-N1-C2	3.92	122.15	115.93
2	C	3850	GDP	C5-C6-N1	-3.63	118.46	123.43
2	C	3850	GDP	PA-O3A-PB	-3.55	120.64	132.83
2	E	3850	GDP	C6-C5-C4	-3.51	117.44	120.80
2	E	3850	GDP	C4-C5-N7	-3.43	105.83	109.40
2	C	3850	GDP	C6-N1-C2	3.21	121.03	115.93
2	C	3850	GDP	C6-C5-C4	-3.10	117.83	120.80
2	G	3850	GDP	C4-C5-N7	-3.04	106.23	109.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3850	GDP	C6-C5-C4	-3.04	117.90	120.80
2	C	3850	GDP	C4-C5-N7	-3.00	106.27	109.40
2	A	3850	GDP	C4-C5-N7	-2.94	106.33	109.40
2	A	3850	GDP	N3-C2-N1	-2.83	123.44	127.22
2	G	3850	GDP	C6-C5-C4	-2.81	118.11	120.80
2	E	3850	GDP	PA-O3A-PB	-2.60	123.90	132.83
2	E	3850	GDP	O3B-PB-O3A	2.56	113.21	104.64
2	G	3850	GDP	N3-C2-N1	-2.50	123.89	127.22
2	A	3850	GDP	C3'-C2'-C1'	2.44	104.65	100.98
2	E	3850	GDP	N3-C2-N1	-2.41	124.01	127.22
2	G	3850	GDP	PA-O3A-PB	-2.37	124.69	132.83
2	C	3850	GDP	N3-C2-N1	-2.30	124.15	127.22
2	C	3850	GDP	O3B-PB-O3A	2.29	112.31	104.64
2	E	3850	GDP	O4'-C1'-C2'	-2.24	103.65	106.93
2	G	3850	GDP	O3B-PB-O3A	2.24	112.16	104.64
2	G	3850	GDP	O4'-C1'-C2'	-2.14	103.80	106.93

There are no chirality outliers.

All (16) torsion outliers are listed below:

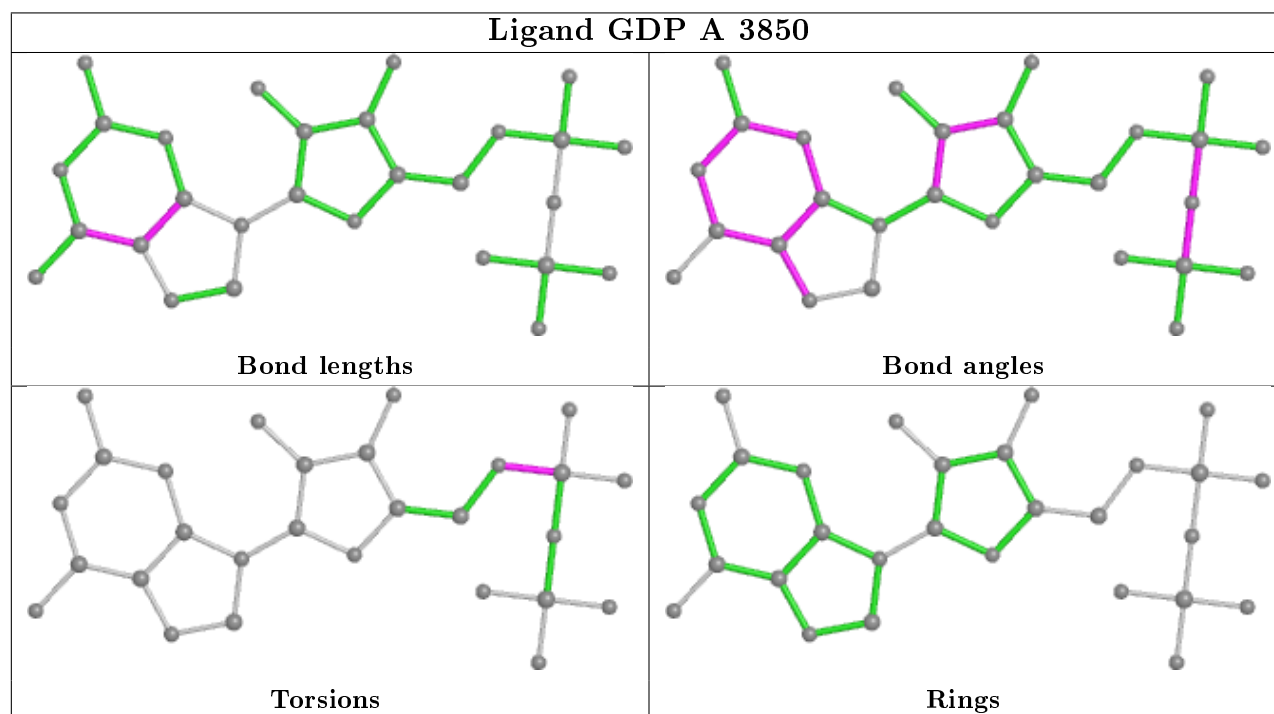
Mol	Chain	Res	Type	Atoms
2	E	3850	GDP	PA-O3A-PB-O3B
2	E	3850	GDP	C5'-O5'-PA-O1A
2	E	3850	GDP	C5'-O5'-PA-O2A
2	G	3850	GDP	C5'-O5'-PA-O1A
2	C	3850	GDP	C5'-O5'-PA-O3A
2	G	3850	GDP	C5'-O5'-PA-O3A
2	C	3850	GDP	C5'-O5'-PA-O1A
2	C	3850	GDP	C5'-O5'-PA-O2A
2	G	3850	GDP	C5'-O5'-PA-O2A
2	C	3850	GDP	PA-O3A-PB-O1B
2	E	3850	GDP	PA-O3A-PB-O2B
2	A	3850	GDP	C5'-O5'-PA-O3A
2	E	3850	GDP	C5'-O5'-PA-O3A
2	C	3850	GDP	PB-O3A-PA-O1A
2	C	3850	GDP	PB-O3A-PA-O2A
2	E	3850	GDP	PB-O3A-PA-O2A

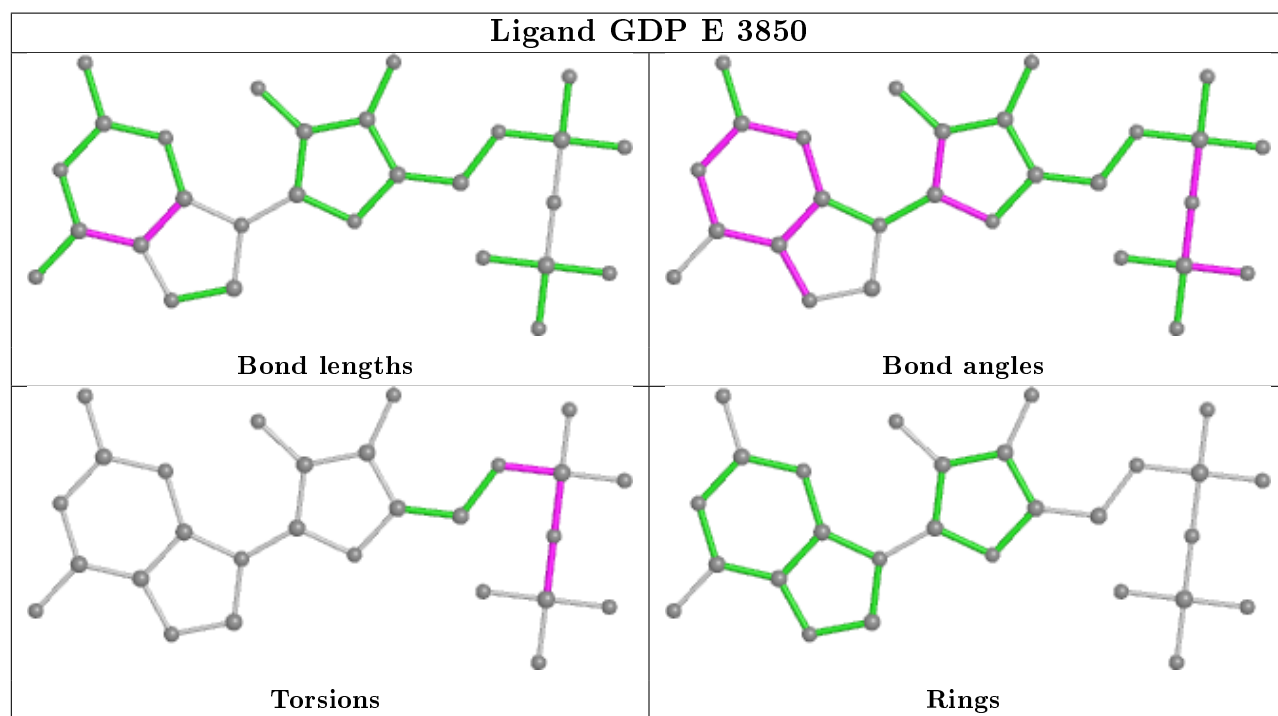
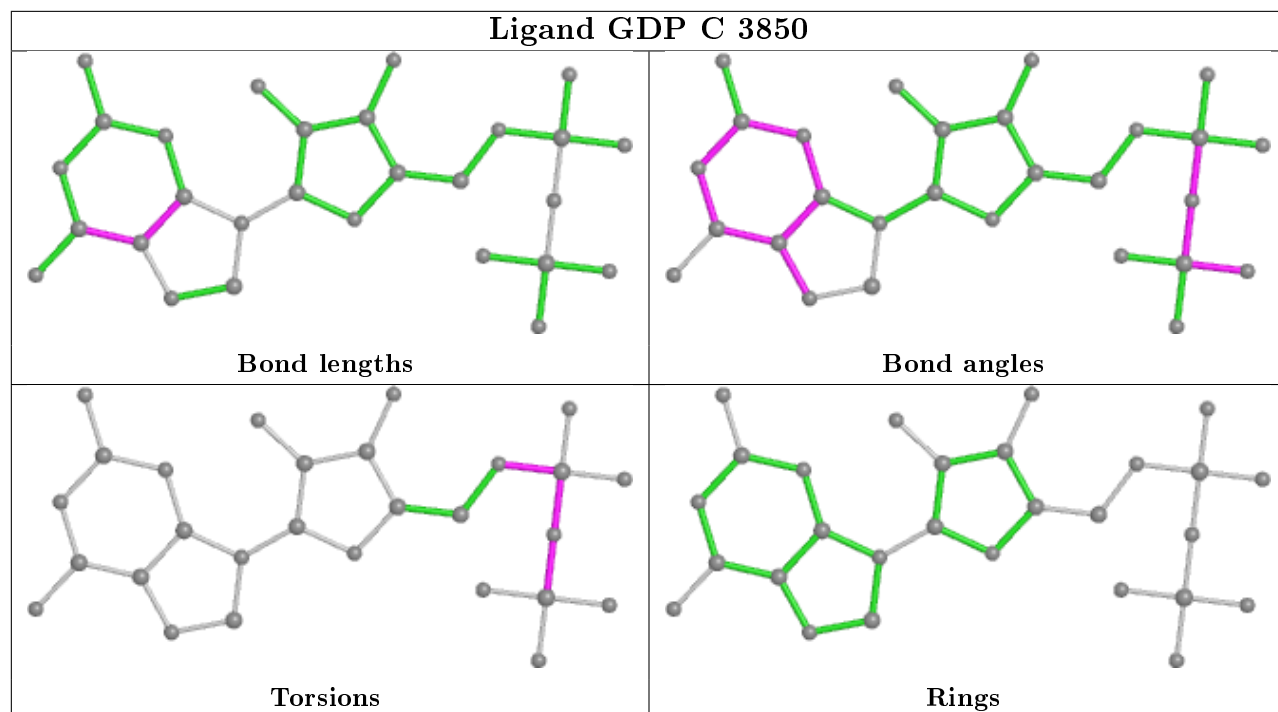
There are no ring outliers.

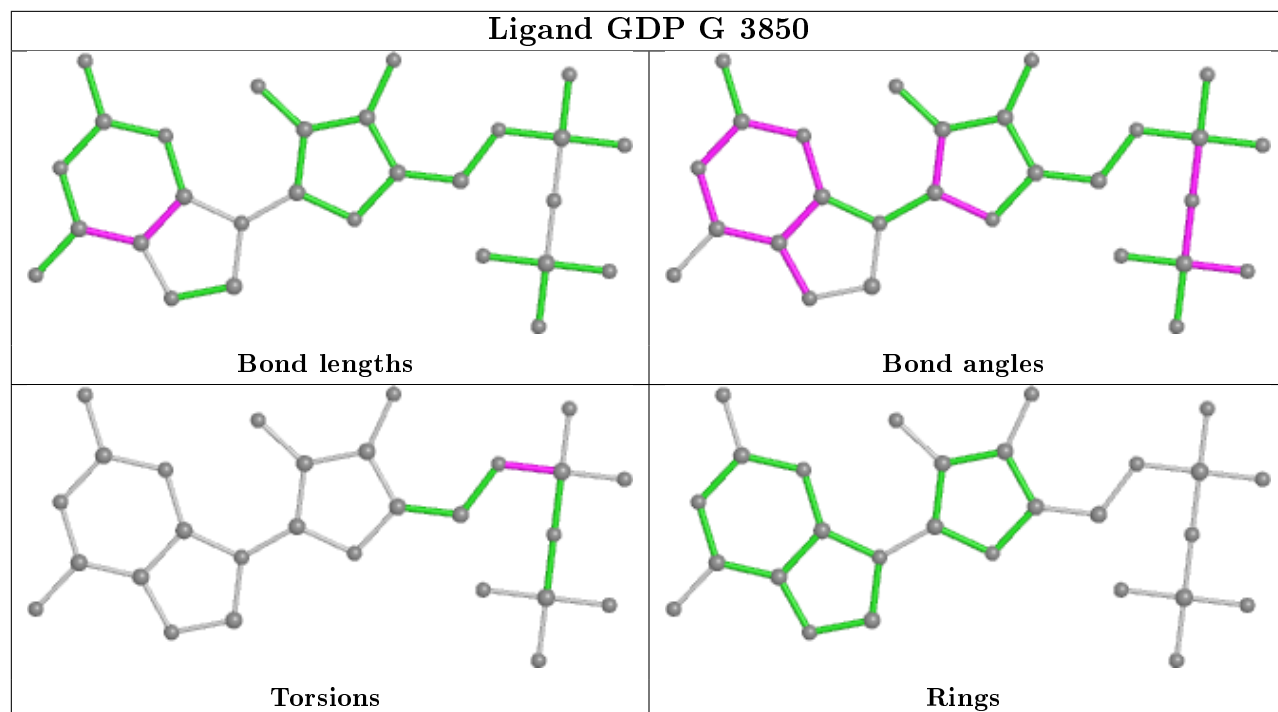
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3850	GDP	2	0
2	C	3850	GDP	3	0
2	E	3850	GDP	2	0
2	G	3850	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 ⓘ

### 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	411/447 (91%)	-0.32	7 (1%) 70 41	19, 70, 145, 214	0
1	C	409/447 (91%)	-0.14	19 (4%) 32 12	28, 70, 169, 234	0
1	E	386/447 (86%)	-0.31	3 (0%) 86 65	18, 52, 119, 178	0
1	G	384/447 (85%)	-0.12	21 (5%) 25 8	24, 63, 190, 291	0
All	All	1590/1788 (88%)	-0.22	50 (3%) 49 21	18, 63, 155, 291	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	380	PRO	13.1
1	G	379	LYS	10.2
1	C	154	GLN	6.5
1	G	374	ILE	5.8
1	C	374	ILE	5.8
1	G	436	ASN	5.8
1	G	386	ASP	4.8
1	G	438	SER	4.7
1	C	153	SER	4.4
1	C	156	THR	4.0
1	G	378	ASP	4.0
1	C	155	SER	3.8
1	G	376	GLY	3.8
1	G	377	GLY	3.6
1	A	116	SER	3.6
1	C	379	LYS	3.3
1	C	375	CYS	3.2
1	A	115	GLY	3.1
1	G	382	LEU	3.1
1	A	378	ASP	3.0
1	C	46	PHE	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	379	LYS	3.0
1	C	39	ILE	2.9
1	C	380	PRO	2.8
1	C	40	VAL	2.8
1	C	436	ASN	2.8
1	C	377	GLY	2.7
1	G	385	ASN	2.6
1	G	435	HIS	2.6
1	G	387	LEU	2.6
1	E	104	ASN	2.6
1	G	437	ASP	2.5
1	A	247	HIS	2.5
1	G	375	CYS	2.5
1	C	385	ASN	2.5
1	C	247	HIS	2.4
1	G	383	ALA	2.4
1	G	389	THR	2.3
1	A	30	LYS	2.3
1	A	339	GLU	2.3
1	C	373	GLU	2.3
1	G	30	LYS	2.3
1	G	390	LYS	2.2
1	G	432	TYR	2.2
1	C	378	ASP	2.2
1	G	340	GLU	2.2
1	C	376	GLY	2.1
1	A	243	SER	2.1
1	C	438	SER	2.0
1	E	380	PRO	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

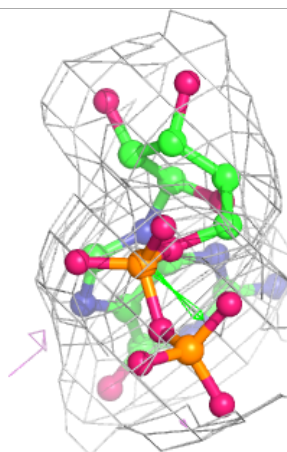
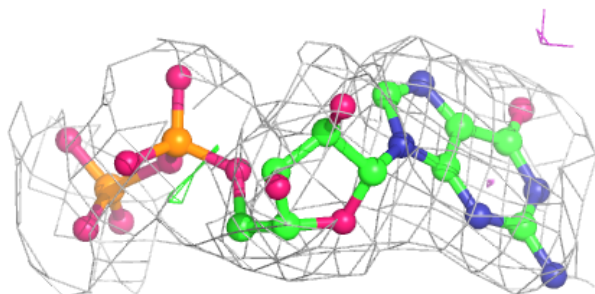
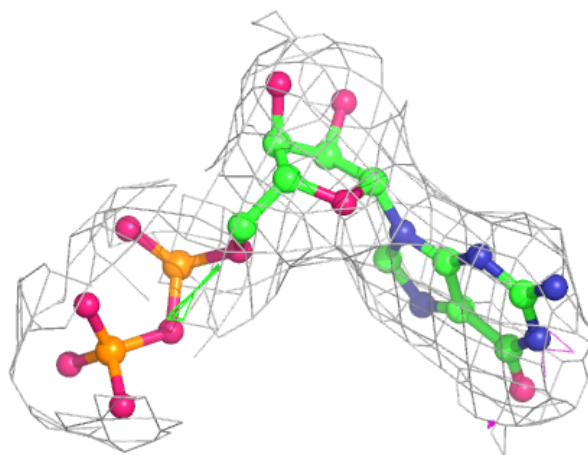
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	MG	G	448	1/1	0.72	0.38	70,70,70,70	0
3	MG	C	448	1/1	0.83	0.14	71,71,71,71	0
3	MG	E	448	1/1	0.88	0.20	68,68,68,68	0
2	GDP	A	3850	28/28	0.97	0.14	32,46,73,88	0
2	GDP	C	3850	28/28	0.98	0.15	29,45,63,69	0
2	GDP	E	3850	28/28	0.98	0.15	22,34,48,57	0
2	GDP	G	3850	28/28	0.98	0.14	22,41,58,69	0
3	MG	A	448	1/1	0.98	0.42	72,72,72,72	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 3850:**

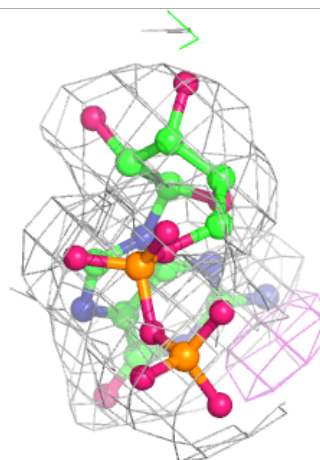
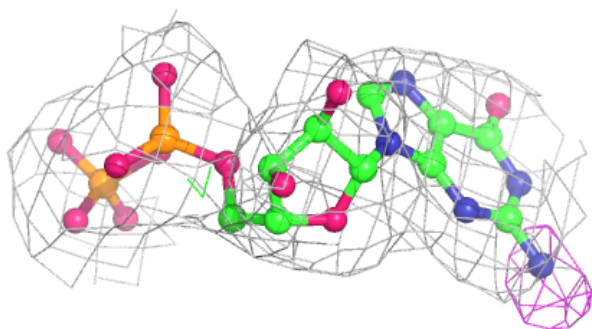
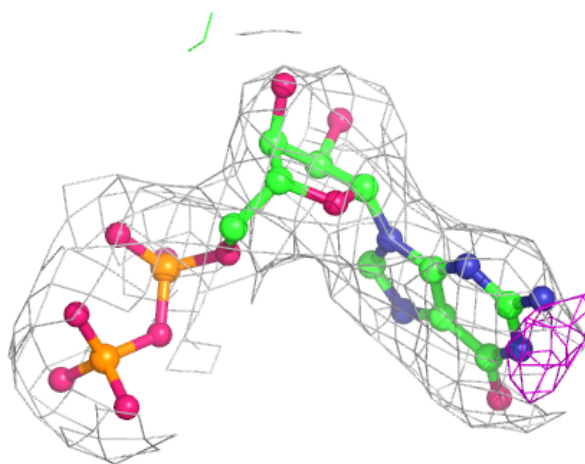
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





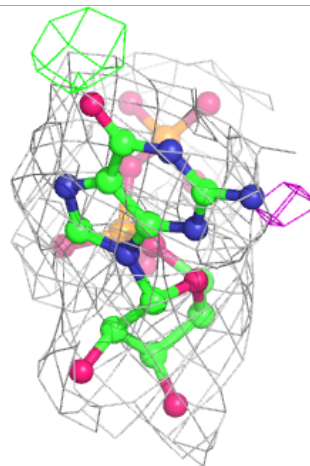
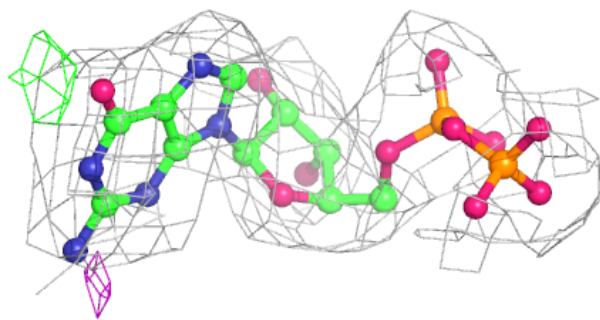
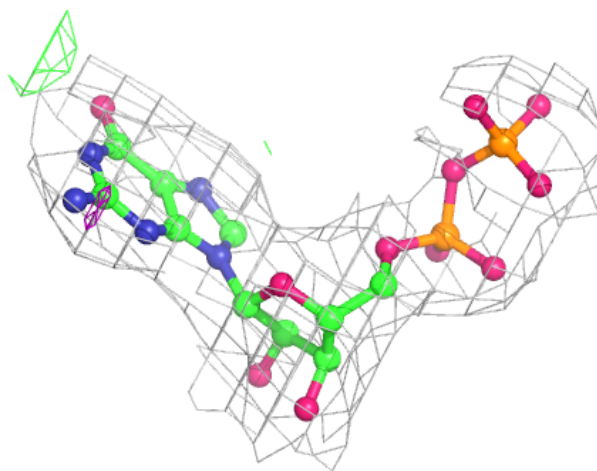
**Electron density around GDP C 3850:**

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



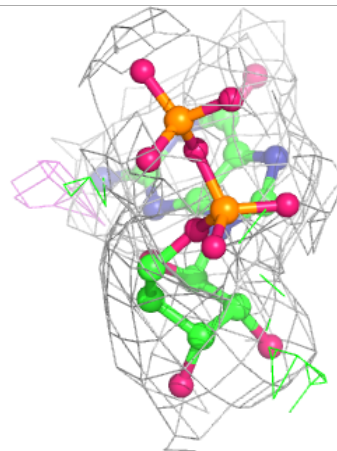
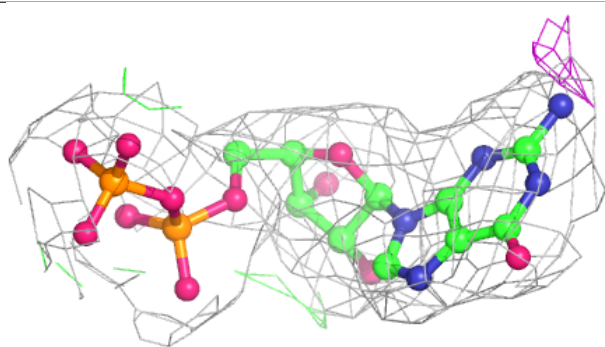
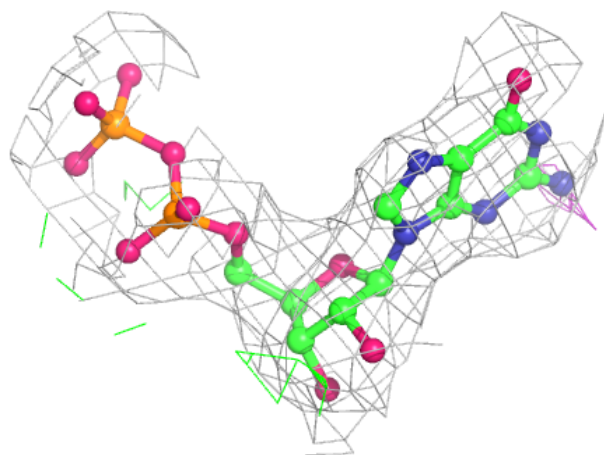
**Electron density around GDP E 3850:**

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



**Electron density around GDP G 3850:**

$2mF_o-DF_c$  (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.