Full wwPDB X-ray Structure Validation Report (i)

Dec 4, 2023 – 08:42 pm GMT

PDB ID	:	1GL6
Title	:	Plasmid coupling protein TrwB in complex with the non-hydrolysable GTP analogue GDPNP
Authors	:	Gomis-Ruth, F.X.; Moncalian, G.; De La cruz, F.; Coll, M.
Deposited on	:	2001-08-28
Resolution	:	2.80 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

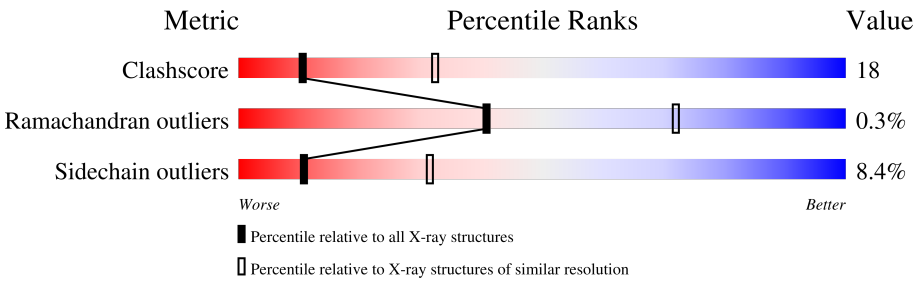
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	436	61% 31% • •
1	B	436	61% 32% • •
1	D	436	64% 27% • 5%
1	E	436	64% 25% 6% 5%
1	F	436	59% 33% • 5%
1	G	436	60% 30% • 5%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EPE	E	1505	-	-	X	-

2 Entry composition (i)

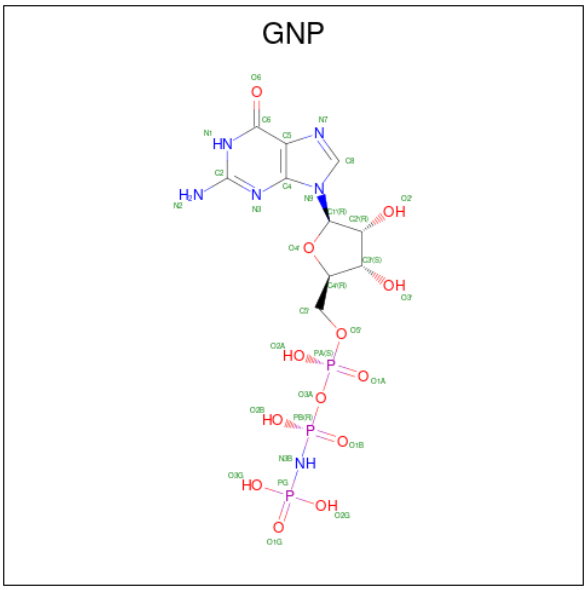
There are 5 unique types of molecules in this entry. The entry contains 20441 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	417	3270	2068	584	608	10	0	0	0
1	B	420	3294	2081	591	612	10	0	0	0
1	D	416	3269	2067	586	606	10	0	0	0
1	E	415	3265	2065	585	605	10	0	0	0
1	F	416	3265	2065	585	605	10	0	0	0
1	G	414	3249	2056	580	603	10	0	0	0

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

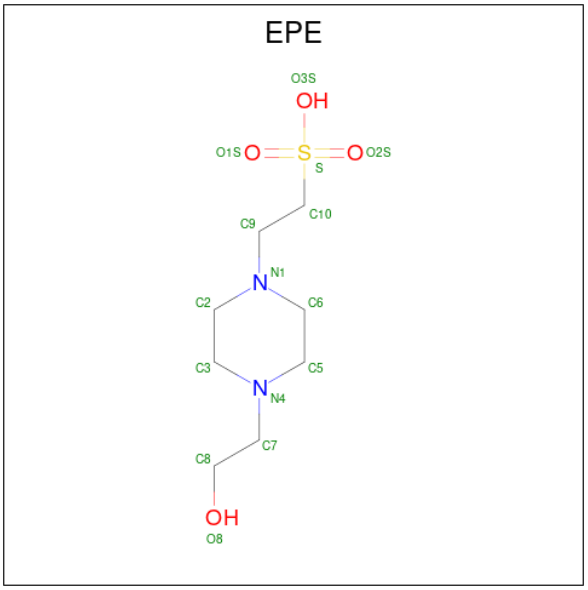


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	32	10	6	13	3	0	0
2	B	1	32	10	6	13	3	0	0
2	D	1	32	10	6	13	3	0	0
2	E	1	32	10	6	13	3	0	0
2	E	1	32	10	6	13	3	0	0
2	F	1	32	10	6	13	3	0	0
2	G	1	32	10	6	13	3	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	1	1	1	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	E	1	15	8	2	4	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	92	92	92	0	0
			Total	O		
5	B	98	98	98	0	0
			Total	O		
5	D	111	111	111	0	0
			Total	O		
5	E	115	115	115	0	0
			Total	O		
5	F	96	96	96	0	0
			Total	O		
5	G	77	77	77	0	0

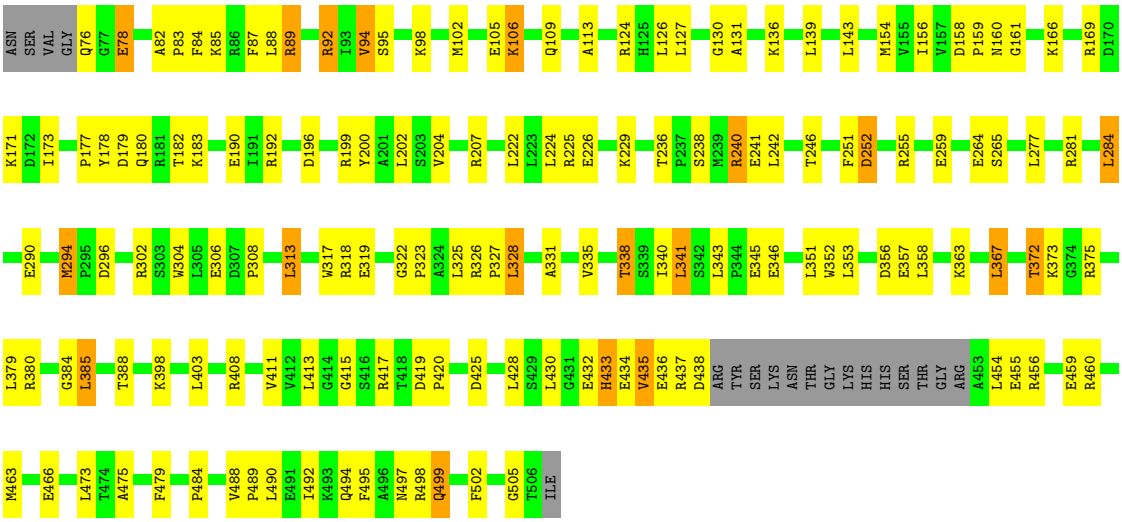
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

Note EDS was not executed.

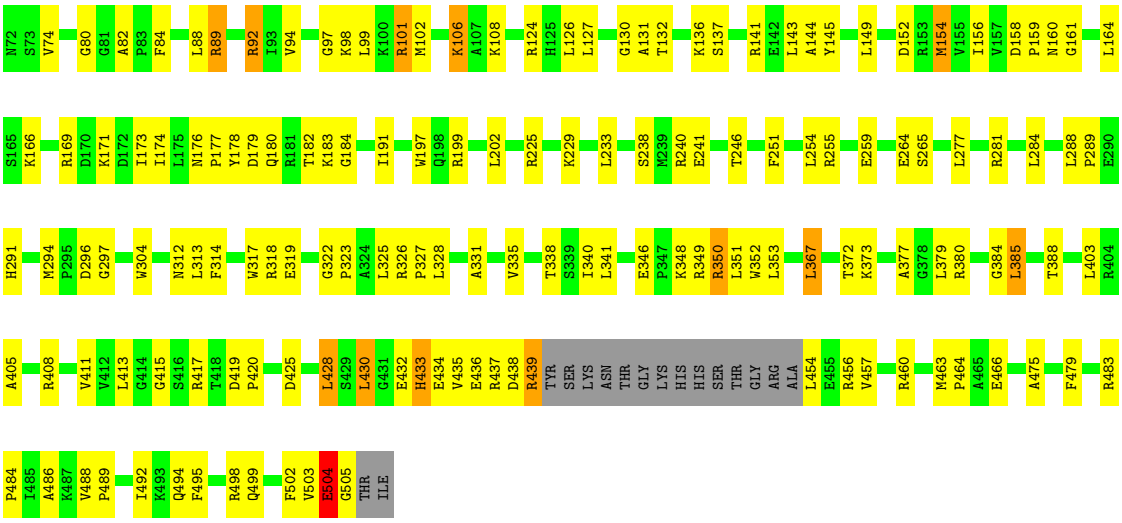
• Molecule 1: ATPASE

Chain A: 61% 31%



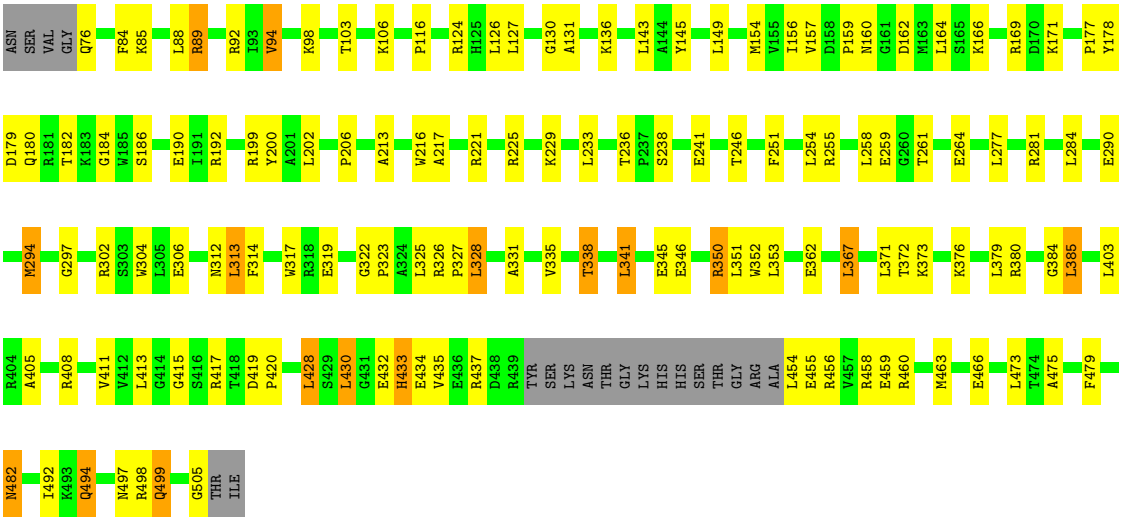
• Molecule 1: ATPASE

Chain B: 61% 32%



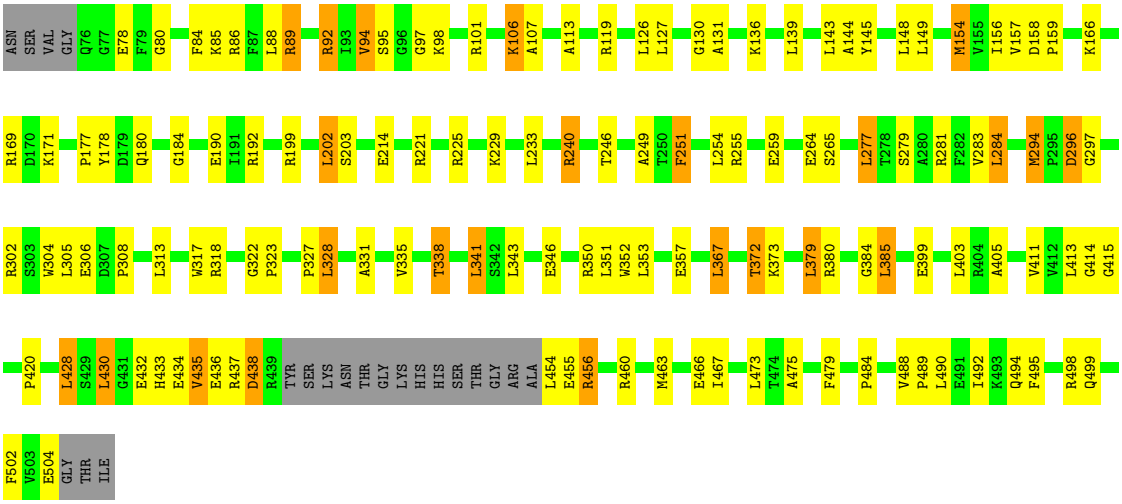
- Molecule 1: ATPASE

Chain D:



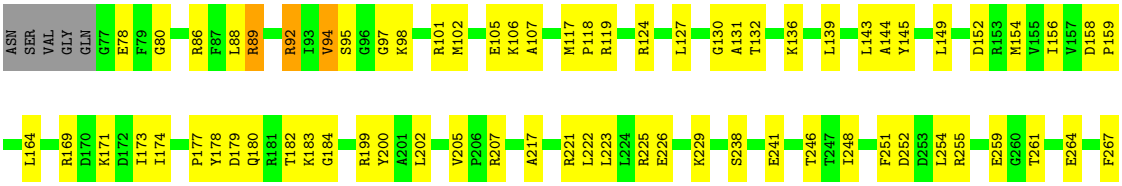
- Molecule 1: ATPASE

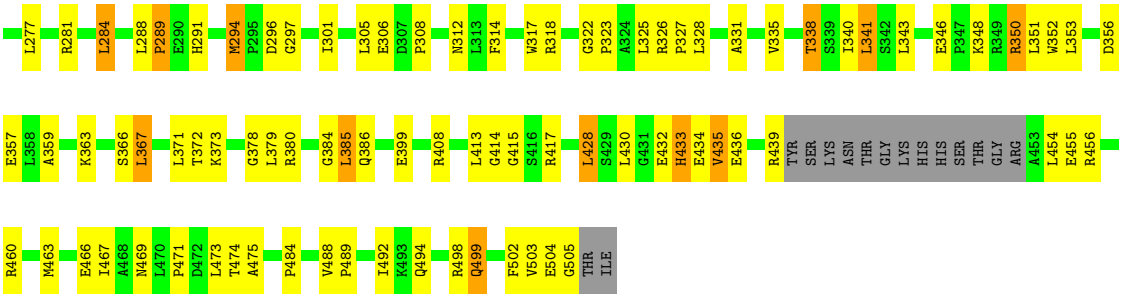
Chain E:



- Molecule 1: ATPASE

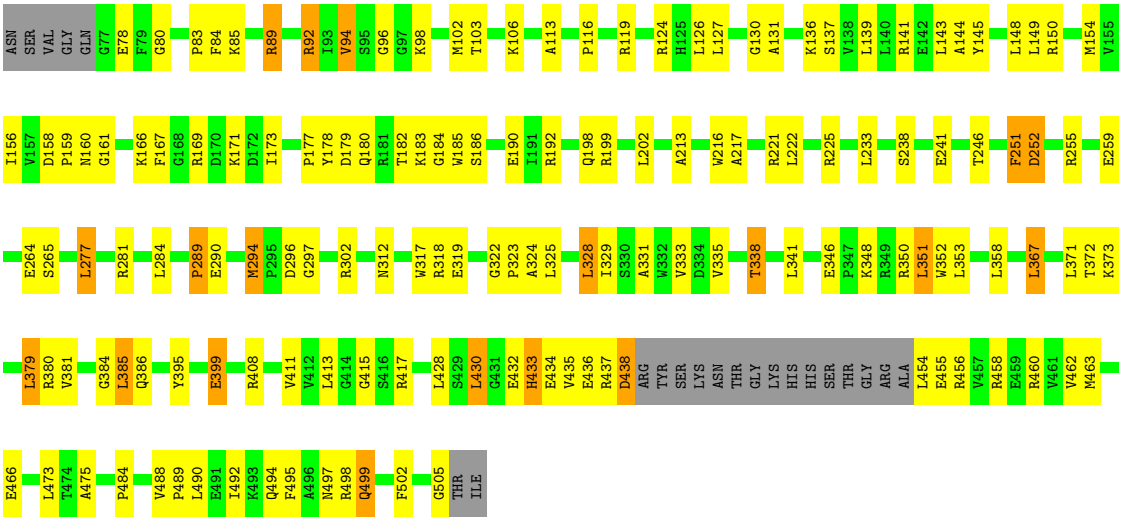
Chain F:





- Molecule 1: ATPASE

Chain G: 60% 30% • 5%



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	151.60Å 151.60Å 252.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80	Depositor
% Data completeness (in resolution range)	100.0 (50.00-2.80)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.214 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20441	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

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: GNP, CL, EPE

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	0.44	0/3334	0.68	0/4507
1	B	0.43	0/3358	0.68	0/4538
1	D	0.44	0/3333	0.70	0/4504
1	E	0.43	0/3329	0.70	0/4499
1	F	0.45	0/3329	0.70	0/4499
1	G	0.43	0/3313	0.68	0/4478
All	All	0.44	0/19996	0.69	0/27025

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3270	0	3298	136	0
1	B	3294	0	3322	139	0
1	D	3269	0	3299	103	0
1	E	3265	0	3296	128	0
1	F	3265	0	3296	121	0
1	G	3249	0	3278	132	0
2	A	32	0	13	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	32	0	13	3	0
2	D	32	0	13	0	0
2	E	64	0	26	3	0
2	F	32	0	13	0	0
2	G	32	0	13	2	0
3	A	1	0	0	0	0
4	E	15	0	17	10	0
5	A	92	0	0	9	0
5	B	98	0	0	16	0
5	D	111	0	0	5	0
5	E	115	0	0	10	0
5	F	96	0	0	4	0
5	G	77	0	0	5	0
All	All	20441	0	19897	735	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (735) 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:F:92:ARG:HG3	1:F:484:PRO:HB3	1.43	0.96
1:E:372:THR:HG22	1:E:373:LYS:HG3	1.49	0.94
1:F:413:LEU:HD23	1:F:475:ALA:HB2	1.48	0.94
1:A:127:LEU:HD11	1:A:385:LEU:HD22	1.49	0.94
1:B:413:LEU:HD23	1:B:475:ALA:HB2	1.48	0.94
1:F:154:MET:HE2	1:F:156:ILE:HD11	1.47	0.94
1:B:169:ARG:HH11	1:B:171:LYS:HD3	1.31	0.92
1:B:503:VAL:O	1:B:504:GLU:HB2	1.68	0.91
1:E:498:ARG:O	1:E:499:GLN:HG3	1.72	0.90
1:G:432:GLU:HG2	1:G:460:ARG:HD3	1.51	0.90
1:D:413:LEU:HD23	1:D:475:ALA:HB2	1.52	0.89
1:F:246:THR:O	1:F:281:ARG:HD2	1.72	0.89
1:B:92:ARG:HG3	1:B:484:PRO:HB3	1.59	0.85
1:G:169:ARG:HH11	1:G:171:LYS:HD3	1.42	0.84
1:A:92:ARG:HG3	1:A:484:PRO:HB3	1.57	0.83
1:G:192:ARG:HD3	5:G:2028:HOH:O	1.76	0.83
1:E:246:THR:O	1:E:281:ARG:HD2	1.78	0.83
1:B:98:LYS:HA	1:B:101:ARG:NH2	1.94	0.83
1:F:331:ALA:O	1:F:335:VAL:HG23	1.81	0.81
1:A:192:ARG:HD2	5:A:2024:HOH:O	1.79	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:413:LEU:HD23	1:E:475:ALA:HB2	1.63	0.81
1:E:127:LEU:HD11	1:E:385:LEU:HD22	1.63	0.80
1:F:463:MET:HB2	1:F:466:GLU:HG3	1.65	0.78
1:A:76:GLN:HG2	1:A:83:PRO:HB3	1.66	0.78
1:D:498:ARG:O	1:D:499:GLN:HG3	1.85	0.77
1:G:92:ARG:HG3	1:G:484:PRO:HB3	1.66	0.77
1:F:127:LEU:HD11	1:F:385:LEU:HD22	1.67	0.77
1:B:498:ARG:O	1:B:499:GLN:HG3	1.83	0.77
1:A:255:ARG:HH21	1:A:255:ARG:HG3	1.50	0.76
1:E:85:LYS:HD2	1:E:454:LEU:HD21	1.66	0.76
1:G:154:MET:HE2	1:G:156:ILE:HD11	1.68	0.76
1:A:240:ARG:HB2	1:A:240:ARG:HH21	1.51	0.76
1:A:494:GLN:HE21	1:A:494:GLN:HA	1.51	0.76
1:G:413:LEU:HD23	1:G:475:ALA:HB2	1.67	0.76
1:D:463:MET:HB2	1:D:466:GLU:HG3	1.68	0.75
1:G:154:MET:HB3	1:G:352:TRP:HB2	1.66	0.75
1:A:437:ARG:O	1:A:438:ASP:HB2	1.86	0.75
1:B:246:THR:O	1:B:281:ARG:HD2	1.87	0.74
1:E:94:VAL:CG2	1:E:98:LYS:HG2	2.16	0.74
1:B:199:ARG:HE	1:B:338:THR:CG2	2.01	0.74
1:B:463:MET:HB2	1:B:466:GLU:HG3	1.69	0.74
1:G:199:ARG:HE	1:G:338:THR:CG2	2.00	0.74
1:D:413:LEU:CD2	1:D:475:ALA:HB2	2.17	0.74
1:E:199:ARG:HE	1:E:338:THR:CG2	2.00	0.74
1:D:154:MET:HE3	1:D:156:ILE:HD11	1.70	0.74
1:G:177:PRO:HG2	1:G:178:TYR:CD1	2.23	0.73
1:A:246:THR:O	1:A:281:ARG:HD2	1.89	0.73
1:F:199:ARG:HE	1:F:338:THR:CG2	2.02	0.73
1:F:159:PRO:HG3	1:F:317:TRP:CH2	2.24	0.72
1:G:94:VAL:CG2	1:G:98:LYS:HG2	2.20	0.72
1:B:106:LYS:HE2	5:B:2011:HOH:O	1.89	0.72
1:B:127:LEU:HD11	1:B:385:LEU:HD22	1.70	0.72
1:B:199:ARG:HE	1:B:338:THR:HG22	1.54	0.72
1:E:154:MET:HB3	1:E:352:TRP:HB2	1.72	0.72
1:E:380:ARG:HH21	1:E:380:ARG:HG3	1.54	0.72
1:D:246:THR:O	1:D:281:ARG:HD2	1.90	0.72
1:E:94:VAL:HG22	1:E:98:LYS:HG2	1.72	0.71
1:F:473:LEU:HD11	1:F:492:ILE:HD11	1.70	0.71
1:E:169:ARG:HH11	1:E:171:LYS:HD3	1.56	0.71
1:G:494:GLN:HA	1:G:494:GLN:HE21	1.54	0.70
1:A:492:ILE:HD11	2:A:701:GNP:H1'	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:463:MET:SD	1:G:89:ARG:HD3	2.30	0.70
1:G:94:VAL:HG22	1:G:98:LYS:HG2	1.73	0.70
1:A:463:MET:HB2	1:A:466:GLU:HG3	1.75	0.69
1:E:240:ARG:HH21	1:E:240:ARG:HB2	1.57	0.69
1:A:498:ARG:O	1:A:499:GLN:HG3	1.90	0.69
1:B:255:ARG:HH21	1:B:255:ARG:HG3	1.57	0.69
1:F:107:ALA:HB3	1:F:119:ARG:HD2	1.74	0.69
1:B:98:LYS:HA	1:B:101:ARG:HH21	1.54	0.68
1:D:169:ARG:HH11	1:D:171:LYS:HD3	1.58	0.68
1:A:494:GLN:HA	1:A:494:GLN:NE2	2.09	0.68
1:G:290:GLU:HB3	1:G:328:LEU:HD12	1.75	0.68
1:E:92:ARG:HG3	1:E:484:PRO:HB3	1.75	0.68
1:B:331:ALA:O	1:B:335:VAL:HG23	1.94	0.68
1:D:127:LEU:HD11	1:D:385:LEU:HD22	1.74	0.68
1:E:318:ARG:HD2	1:E:502:PHE:CE2	2.29	0.68
1:D:192:ARG:HD3	5:D:2032:HOH:O	1.95	0.67
1:D:281:ARG:NH2	1:E:265:SER:HB3	2.08	0.67
1:G:126:LEU:HD11	1:G:411:VAL:HG23	1.75	0.67
1:F:432:GLU:HG2	1:F:460:ARG:HD3	1.75	0.67
1:D:372:THR:HG22	1:D:373:LYS:HG3	1.75	0.67
1:F:357:GLU:HG3	5:F:2079:HOH:O	1.94	0.67
1:G:246:THR:O	1:G:281:ARG:HD2	1.95	0.67
1:E:156:ILE:HG22	1:E:158:ASP:HB2	1.77	0.67
1:G:180:GLN:HE21	1:G:505:GLY:HA2	1.60	0.67
1:B:154:MET:HE2	1:B:156:ILE:HD11	1.78	0.66
1:D:255:ARG:HH21	1:D:255:ARG:HG3	1.60	0.66
1:G:498:ARG:O	1:G:499:GLN:HG3	1.96	0.66
1:A:388:THR:HG22	5:A:2011:HOH:O	1.96	0.66
1:B:413:LEU:CD2	1:B:475:ALA:HB2	2.23	0.66
1:D:331:ALA:O	1:D:335:VAL:HG23	1.96	0.65
1:F:384:GLY:O	1:F:385:LEU:HD13	1.96	0.65
1:A:166:LYS:HE2	1:A:497:ASN:HD21	1.61	0.65
1:A:190:GLU:OE1	1:A:302:ARG:HG3	1.97	0.65
1:F:179:ASP:O	1:F:182:THR:HG22	1.97	0.65
1:A:154:MET:HE3	1:A:156:ILE:HD11	1.77	0.65
1:E:101:ARG:HH12	4:E:1505:EPE:H92	1.61	0.65
1:B:380:ARG:HH21	1:B:380:ARG:HG3	1.61	0.65
1:F:173:ILE:HG23	1:F:183:LYS:HG3	1.79	0.65
1:E:101:ARG:HH12	4:E:1505:EPE:H22	1.61	0.64
1:D:463:MET:SD	1:E:89:ARG:HD3	2.37	0.64
2:E:1506:GNP:H5'1	5:E:2114:HOH:O	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:498:ARG:O	1:F:499:GLN:HG3	1.98	0.64
1:B:183:LYS:HD3	5:B:2030:HOH:O	1.96	0.64
1:F:413:LEU:CD2	1:F:475:ALA:HB2	2.26	0.64
1:A:131:ALA:HB2	1:A:415:GLY:HA2	1.80	0.64
1:G:160:ASN:HD21	1:G:319:GLU:CD	2.01	0.64
1:A:259:GLU:HA	1:A:264:GLU:HG3	1.80	0.64
1:F:318:ARG:HD2	1:F:502:PHE:CE2	2.33	0.64
1:E:126:LEU:HD11	1:E:411:VAL:HG23	1.80	0.63
1:G:199:ARG:HE	1:G:338:THR:HG22	1.62	0.63
1:B:180:GLN:HE21	1:B:504:GLU:CG	2.11	0.63
1:A:255:ARG:HG3	1:A:255:ARG:NH2	2.13	0.63
1:B:439:ARG:NH2	1:B:439:ARG:HB3	2.13	0.63
1:E:413:LEU:CD2	1:E:475:ALA:HB2	2.28	0.63
1:E:456:ARG:HD2	5:E:2094:HOH:O	1.97	0.63
5:E:2097:HOH:O	1:F:92:ARG:HG2	1.98	0.63
1:G:463:MET:HB2	1:G:466:GLU:HG3	1.80	0.63
1:A:156:ILE:HG22	1:A:158:ASP:HB2	1.80	0.63
1:G:494:GLN:HA	1:G:494:GLN:NE2	2.13	0.63
1:A:199:ARG:HE	1:A:338:THR:CG2	2.11	0.63
1:D:177:PRO:HB3	1:D:294:MET:HG2	1.78	0.63
1:B:384:GLY:O	1:B:385:LEU:HD13	1.98	0.63
1:B:417:ARG:NH1	1:D:479:PHE:O	2.31	0.63
1:E:255:ARG:HH21	1:E:255:ARG:HG3	1.64	0.63
1:D:177:PRO:HG2	1:D:178:TYR:CD1	2.34	0.62
1:G:154:MET:CE	1:G:156:ILE:HD11	2.29	0.62
1:E:327:PRO:HG2	5:E:2067:HOH:O	1.98	0.62
1:F:255:ARG:HH21	1:F:255:ARG:HG3	1.64	0.62
1:D:162:ASP:HB2	5:D:2025:HOH:O	1.99	0.62
1:A:154:MET:HB3	1:A:352:TRP:HB2	1.80	0.62
1:F:184:GLY:HA3	1:F:297:GLY:HA3	1.81	0.62
1:G:166:LYS:HE2	1:G:497:ASN:HD21	1.65	0.62
1:A:154:MET:CE	1:A:156:ILE:HD11	2.29	0.62
1:E:463:MET:HB2	1:E:466:GLU:HG3	1.82	0.62
1:B:238:SER:HB3	1:B:241:GLU:HB2	1.81	0.61
1:B:154:MET:HB3	1:B:352:TRP:HB2	1.82	0.61
1:B:483:ARG:NH1	5:B:2093:HOH:O	2.32	0.61
1:E:488:VAL:HG13	1:E:489:PRO:HD2	1.81	0.61
1:F:154:MET:CE	1:F:156:ILE:HD11	2.26	0.61
1:A:388:THR:CG2	5:A:2011:HOH:O	2.48	0.61
1:A:473:LEU:HD11	1:A:492:ILE:HD11	1.81	0.61
1:F:199:ARG:HE	1:F:338:THR:HG22	1.64	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:SER:HB3	1:A:241:GLU:HB2	1.83	0.61
1:B:102:MET:HE2	5:B:2045:HOH:O	2.01	0.61
1:E:180:GLN:HB2	1:E:504:GLU:HB3	1.82	0.61
1:G:338:THR:O	1:G:341:LEU:HB2	2.01	0.61
1:B:318:ARG:HD2	1:B:502:PHE:CE2	2.35	0.61
1:D:89:ARG:HD2	1:D:434:GLU:OE1	2.00	0.61
1:F:177:PRO:HG2	1:F:178:TYR:CD1	2.36	0.61
1:A:456:ARG:HD2	1:A:456:ARG:N	2.15	0.61
1:F:88:LEU:HB2	1:F:434:GLU:O	2.01	0.61
1:E:372:THR:HG22	1:E:373:LYS:CG	2.27	0.60
1:G:413:LEU:CD2	1:G:475:ALA:HB2	2.30	0.60
1:E:131:ALA:HB2	1:E:415:GLY:HA2	1.84	0.60
1:A:199:ARG:HE	1:A:338:THR:HG22	1.65	0.60
1:B:372:THR:HG22	1:B:373:LYS:HG3	1.82	0.60
1:B:367:LEU:HD13	1:B:403:LEU:HD11	1.82	0.60
1:E:192:ARG:HD3	5:E:2030:HOH:O	1.99	0.60
1:F:494:GLN:HE21	1:F:494:GLN:HA	1.66	0.60
1:E:154:MET:HE2	1:E:156:ILE:HD11	1.83	0.60
1:B:177:PRO:HG2	1:B:178:TYR:CD1	2.37	0.60
1:D:259:GLU:HA	1:D:264:GLU:HG3	1.84	0.60
1:G:222:LEU:HA	1:G:225:ARG:NH1	2.17	0.60
1:B:98:LYS:O	1:B:102:MET:HG3	2.01	0.59
1:B:259:GLU:HA	1:B:264:GLU:HG3	1.84	0.59
1:A:331:ALA:O	1:A:335:VAL:HG23	2.02	0.59
2:A:701:GNP:H5'1	5:B:2067:HOH:O	2.00	0.59
1:D:180:GLN:NE2	1:D:505:GLY:HA2	2.18	0.59
1:D:473:LEU:HD11	1:D:492:ILE:HD11	1.84	0.59
1:A:413:LEU:HD23	1:A:475:ALA:HB2	1.85	0.59
1:A:432:GLU:HG2	1:A:460:ARG:HD3	1.83	0.59
1:B:92:ARG:HA	5:B:2005:HOH:O	2.01	0.59
1:D:124:ARG:HB3	1:D:408:ARG:HG3	1.85	0.59
1:D:131:ALA:HB2	1:D:415:GLY:HA2	1.84	0.59
1:F:106:LYS:H	1:F:106:LYS:HD2	1.68	0.59
1:F:136:LYS:HG2	1:F:413:LEU:HD12	1.84	0.59
1:A:127:LEU:HD11	1:A:385:LEU:CD2	2.29	0.59
1:A:436:GLU:HG2	1:A:454:LEU:HD13	1.84	0.59
1:B:92:ARG:HD2	5:B:2090:HOH:O	2.03	0.59
1:B:456:ARG:HD2	1:B:456:ARG:N	2.17	0.59
1:D:346:GLU:OE2	1:D:346:GLU:HA	2.03	0.59
1:B:102:MET:HB3	5:B:2045:HOH:O	2.01	0.59
1:B:432:GLU:HG2	1:B:460:ARG:HD3	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ILE:HG23	1:B:183:LYS:HG3	1.85	0.58
1:G:494:GLN:HE21	1:G:494:GLN:CA	2.16	0.58
1:G:190:GLU:OE1	1:G:302:ARG:HG3	2.03	0.58
1:G:380:ARG:HH21	1:G:380:ARG:HG3	1.67	0.58
1:E:251:PHE:CZ	1:E:277:LEU:HB3	2.39	0.58
1:A:437:ARG:HG2	1:A:438:ASP:H	1.67	0.58
1:B:145:TYR:CZ	1:B:149:LEU:HD11	2.38	0.58
1:F:131:ALA:HB2	1:F:415:GLY:HA2	1.85	0.58
1:G:169:ARG:NH2	1:G:312:ASN:ND2	2.50	0.58
1:G:437:ARG:O	1:G:454:LEU:HD22	2.04	0.58
1:B:132:THR:CG2	5:D:2094:HOH:O	2.51	0.58
1:E:145:TYR:CZ	1:E:149:LEU:HD11	2.39	0.58
1:A:328:LEU:O	1:A:331:ALA:HB3	2.03	0.57
1:A:384:GLY:O	1:A:385:LEU:HD13	2.04	0.57
1:E:177:PRO:HB3	1:E:294:MET:HG2	1.86	0.57
1:D:154:MET:HB3	1:D:352:TRP:HB2	1.87	0.57
1:G:198:GLN:HG2	5:G:2033:HOH:O	2.04	0.57
1:A:290:GLU:HG3	1:A:325:LEU:HD23	1.86	0.57
1:B:255:ARG:HG3	1:B:255:ARG:NH2	2.20	0.57
1:D:84:PHE:HA	1:D:437:ARG:HG2	1.86	0.57
1:E:159:PRO:HG3	1:E:317:TRP:CH2	2.40	0.57
1:D:184:GLY:HA3	1:D:297:GLY:HA3	1.86	0.56
1:A:89:ARG:HG2	1:G:80:GLY:O	2.04	0.56
1:A:179:ASP:O	1:A:182:THR:HG22	2.05	0.56
1:B:166:LYS:HD2	1:B:495:PHE:HB2	1.86	0.56
1:B:457:VAL:HG21	5:B:2085:HOH:O	2.03	0.56
1:D:180:GLN:HE21	1:D:505:GLY:HA2	1.71	0.56
1:D:255:ARG:HG3	1:D:255:ARG:NH2	2.20	0.56
1:B:433:HIS:HD2	1:B:433:HIS:O	1.88	0.56
1:B:84:PHE:CB	1:B:435:VAL:HG11	2.35	0.56
1:B:169:ARG:HH11	1:B:171:LYS:CD	2.12	0.56
1:E:473:LEU:HD11	1:E:492:ILE:HD11	1.86	0.56
1:D:432:GLU:OE1	1:D:458:ARG:HD2	2.05	0.56
1:F:92:ARG:HG3	1:F:484:PRO:CB	2.27	0.56
1:F:154:MET:HB3	1:F:352:TRP:HB2	1.87	0.56
1:G:173:ILE:HG23	1:G:183:LYS:HG3	1.86	0.56
1:F:340:ILE:HD12	1:F:341:LEU:N	2.21	0.56
1:F:456:ARG:HD3	1:F:456:ARG:N	2.21	0.56
1:G:433:HIS:HD2	1:G:433:HIS:O	1.89	0.56
1:D:433:HIS:HD2	1:D:433:HIS:O	1.89	0.55
1:E:331:ALA:O	1:E:335:VAL:HG23	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:HG3	1:A:484:PRO:CB	2.33	0.55
1:D:367:LEU:HD13	1:D:403:LEU:HD11	1.88	0.55
1:G:177:PRO:HG2	1:G:178:TYR:HD1	1.70	0.55
1:A:306:GLU:O	1:A:308:PRO:HD3	2.07	0.55
1:B:88:LEU:HB2	1:B:434:GLU:O	2.07	0.55
1:G:169:ARG:HH11	1:G:171:LYS:CD	2.17	0.55
1:G:238:SER:HB3	1:G:241:GLU:HB2	1.88	0.55
1:G:379:LEU:HD22	1:G:381:VAL:HG23	1.89	0.55
1:D:94:VAL:HG22	1:D:98:LYS:HG2	1.89	0.55
1:E:456:ARG:CD	5:E:2094:HOH:O	2.54	0.55
1:B:179:ASP:O	1:B:182:THR:HG22	2.07	0.55
1:D:85:LYS:HD2	1:D:454:LEU:HD11	1.89	0.55
1:E:94:VAL:HG21	1:E:98:LYS:HG2	1.88	0.55
1:B:346:GLU:OE1	1:B:348:LYS:HB2	2.07	0.54
1:E:184:GLY:HA3	1:E:297:GLY:HA3	1.89	0.54
1:F:359:ALA:HB3	5:F:2079:HOH:O	2.06	0.54
1:G:98:LYS:O	1:G:102:MET:HG3	2.07	0.54
1:A:492:ILE:CD1	2:A:701:GNP:H1'	2.38	0.54
1:B:108:LYS:HE3	5:B:2013:HOH:O	2.06	0.54
1:G:159:PRO:HG3	1:G:317:TRP:CH2	2.41	0.54
1:A:225:ARG:O	1:A:229:LYS:HB2	2.07	0.54
1:E:492:ILE:HD11	2:E:701:GNP:H1'	1.88	0.54
1:G:131:ALA:HB2	1:G:415:GLY:HA2	1.90	0.54
1:G:251:PHE:CZ	1:G:277:LEU:HB3	2.43	0.54
1:G:331:ALA:O	1:G:335:VAL:HG23	2.07	0.54
1:B:184:GLY:HA3	1:B:297:GLY:HA3	1.88	0.54
1:D:238:SER:HB3	1:D:241:GLU:CG	2.37	0.54
1:F:317:TRP:HB2	1:F:325:LEU:HD12	1.90	0.54
1:E:101:ARG:NH1	4:E:1505:EPE:H22	2.23	0.54
1:E:432:GLU:HG2	1:E:460:ARG:HD3	1.90	0.54
1:F:94:VAL:HG22	1:F:98:LYS:HG2	1.90	0.54
1:A:207:ARG:CB	1:A:363:LYS:HD3	2.38	0.54
1:B:439:ARG:HB3	1:B:439:ARG:HH21	1.72	0.54
1:D:124:ARG:HB3	1:D:408:ARG:CG	2.37	0.54
1:D:432:GLU:HG2	1:D:460:ARG:HD3	1.90	0.54
1:E:463:MET:SD	1:F:89:ARG:HD3	2.48	0.54
1:A:85:LYS:HE3	1:A:454:LEU:HD21	1.90	0.54
1:B:420:PRO:HB2	1:D:428:LEU:HD13	1.90	0.54
1:A:124:ARG:HB3	1:A:408:ARG:CG	2.38	0.54
1:D:130:GLY:HA3	1:D:413:LEU:HB2	1.88	0.54
1:D:419:ASP:HB2	1:E:405:ALA:CB	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:GLN:NE2	1:E:504:GLU:HG3	2.23	0.54
1:G:124:ARG:HB3	1:G:408:ARG:HG3	1.89	0.54
1:G:124:ARG:HB3	1:G:408:ARG:CG	2.38	0.54
1:A:159:PRO:HG3	1:A:317:TRP:CH2	2.43	0.53
1:E:166:LYS:HD2	1:E:495:PHE:HB2	1.90	0.53
1:G:386:GLN:HB2	5:G:2058:HOH:O	2.08	0.53
1:G:318:ARG:HD2	1:G:502:PHE:CE2	2.44	0.53
1:G:94:VAL:HG21	1:G:98:LYS:HG2	1.90	0.53
1:B:131:ALA:HB2	1:B:415:GLY:HA2	1.90	0.53
1:D:94:VAL:CG2	1:D:98:LYS:HG2	2.39	0.53
1:A:180:GLN:HE21	1:A:505:GLY:HA2	1.74	0.53
1:B:84:PHE:HB3	1:B:435:VAL:HG11	1.91	0.53
1:B:492:ILE:HD11	2:B:701:GNP:H1'	1.90	0.53
1:D:420:PRO:HB2	1:E:428:LEU:HD13	1.90	0.53
1:A:166:LYS:HE2	1:A:497:ASN:ND2	2.24	0.53
1:A:463:MET:SD	1:B:89:ARG:HD3	2.49	0.53
1:E:154:MET:CE	1:E:156:ILE:HD11	2.39	0.53
1:F:169:ARG:HH21	1:F:312:ASN:ND2	2.07	0.53
1:A:159:PRO:HG2	1:A:356:ASP:OD1	2.09	0.52
1:F:255:ARG:HG3	1:F:255:ARG:NH2	2.24	0.52
1:G:456:ARG:N	1:G:456:ARG:HD2	2.24	0.52
1:A:85:LYS:CE	1:A:454:LEU:HD21	2.40	0.52
1:A:94:VAL:HG13	1:A:98:LYS:HB3	1.91	0.52
1:A:177:PRO:HA	1:A:294:MET:HE1	1.91	0.52
1:F:378:GLY:O	1:F:380:ARG:NH2	2.42	0.52
1:G:199:ARG:HG3	1:G:338:THR:HG21	1.91	0.52
1:A:130:GLY:HA3	1:A:413:LEU:HB2	1.91	0.52
1:A:433:HIS:HD2	1:A:433:HIS:O	1.91	0.52
1:D:482:ASN:C	1:D:482:ASN:HD22	2.13	0.52
1:E:88:LEU:HB2	1:E:434:GLU:O	2.09	0.52
1:B:435:VAL:CG1	1:B:436:GLU:N	2.72	0.52
1:B:488:VAL:HG13	1:B:489:PRO:HD2	1.92	0.52
1:E:436:GLU:OE2	5:E:2094:HOH:O	2.19	0.52
1:A:136:LYS:HG2	1:A:413:LEU:HD12	1.91	0.52
1:A:200:TYR:O	1:A:204:VAL:HG23	2.09	0.52
1:B:101:ARG:HH21	1:B:101:ARG:CG	2.22	0.52
1:B:152:ASP:OD1	1:B:350:ARG:NH2	2.43	0.52
1:G:346:GLU:OE1	1:G:348:LYS:HB2	2.09	0.52
1:B:225:ARG:O	1:B:229:LYS:HB2	2.09	0.52
1:F:124:ARG:HB3	1:F:408:ARG:HB2	1.91	0.52
1:F:380:ARG:HH21	1:F:380:ARG:HG3	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:322:GLY:N	1:G:323:PRO:HD2	2.24	0.52
1:A:281:ARG:NH2	1:B:265:SER:HB3	2.25	0.52
1:B:92:ARG:CD	5:B:2090:HOH:O	2.58	0.52
1:B:456:ARG:HD2	1:B:456:ARG:H	1.75	0.52
1:E:130:GLY:HA3	1:E:413:LEU:HB2	1.91	0.52
1:G:103:THR:OG1	1:G:116:PRO:HG2	2.10	0.52
1:A:98:LYS:O	1:A:102:MET:HG3	2.10	0.52
1:B:126:LEU:HD11	1:B:411:VAL:HG23	1.92	0.52
1:G:255:ARG:HH21	1:G:255:ARG:HG3	1.75	0.52
1:A:375:ARG:NH1	2:G:701:GNP:O3G	2.44	0.51
1:F:124:ARG:HB3	1:F:408:ARG:CG	2.40	0.51
1:F:259:GLU:HA	1:F:264:GLU:HG3	1.91	0.51
1:G:166:LYS:HD2	1:G:495:PHE:HB2	1.92	0.51
1:A:84:PHE:HB3	1:A:435:VAL:HG11	1.93	0.51
1:A:494:GLN:HE21	1:A:494:GLN:CA	2.15	0.51
1:E:322:GLY:N	1:E:323:PRO:HD2	2.26	0.51
1:G:199:ARG:CG	1:G:338:THR:HG21	2.39	0.51
1:B:180:GLN:HE21	1:B:504:GLU:HG3	1.74	0.51
1:D:169:ARG:NH2	1:D:312:ASN:ND2	2.59	0.51
1:E:78:GLU:HA	5:E:2002:HOH:O	2.10	0.51
1:F:338:THR:O	1:F:341:LEU:HB2	2.09	0.51
1:E:95:SER:OG	4:E:1505:EPE:H52	2.10	0.51
1:E:199:ARG:HE	1:E:338:THR:HG22	1.74	0.51
1:A:89:ARG:HD2	1:A:434:GLU:OE1	2.11	0.51
1:F:225:ARG:O	1:F:229:LYS:HB2	2.11	0.51
1:F:288:LEU:O	1:F:291:HIS:HB2	2.11	0.51
1:G:438:ASP:O	1:G:454:LEU:HA	2.11	0.51
1:A:265:SER:HB3	1:G:281:ARG:NH2	2.25	0.51
1:B:180:GLN:HE21	1:B:504:GLU:HG2	1.74	0.51
1:D:136:LYS:HG2	1:D:413:LEU:HD12	1.93	0.51
1:G:184:GLY:HA3	1:G:297:GLY:HA3	1.92	0.51
1:A:124:ARG:HB3	1:A:408:ARG:HG3	1.91	0.51
1:D:290:GLU:HG3	1:D:325:LEU:HD23	1.93	0.51
1:F:281:ARG:NH2	1:G:265:SER:HB3	2.26	0.51
1:A:88:LEU:HB2	1:A:434:GLU:O	2.11	0.50
1:E:101:ARG:HH22	4:E:1505:EPE:H22	1.76	0.50
1:F:78:GLU:HG2	1:F:95:SER:HB3	1.92	0.50
1:G:473:LEU:HD11	1:G:492:ILE:HD11	1.93	0.50
1:A:158:ASP:OD2	1:A:161:GLY:HA2	2.12	0.50
1:B:89:ARG:HD2	1:B:434:GLU:OE1	2.10	0.50
1:B:159:PRO:HG3	1:B:317:TRP:CH2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ARG:HG3	1:B:484:PRO:CB	2.37	0.50
1:E:144:ALA:O	1:E:148:LEU:HG	2.12	0.50
1:A:437:ARG:HG2	1:A:438:ASP:N	2.26	0.50
1:G:92:ARG:HG3	1:G:484:PRO:CB	2.40	0.50
1:B:106:LYS:HE2	5:B:2012:HOH:O	2.12	0.50
1:E:338:THR:O	1:E:341:LEU:HB2	2.12	0.50
1:B:137:SER:HB2	2:B:701:GNP:O1A	2.12	0.50
1:B:322:GLY:N	1:B:323:PRO:HD2	2.27	0.50
1:G:180:GLN:NE2	1:G:505:GLY:HA2	2.24	0.50
1:G:492:ILE:HD11	2:G:701:GNP:H1'	1.93	0.50
1:B:180:GLN:HB2	1:B:504:GLU:HG2	1.93	0.50
1:D:154:MET:CE	1:D:156:ILE:HD11	2.38	0.50
1:F:80:GLY:O	1:G:89:ARG:HG2	2.10	0.50
1:F:301:ILE:O	1:F:305:LEU:HG	2.11	0.50
1:F:494:GLN:HA	1:F:494:GLN:NE2	2.26	0.50
1:B:145:TYR:CE2	1:B:149:LEU:HD11	2.47	0.50
1:D:326:ARG:N	1:D:327:PRO:HD2	2.27	0.50
1:F:152:ASP:OD1	1:F:350:ARG:NH2	2.45	0.50
1:G:166:LYS:CE	1:G:497:ASN:HD21	2.24	0.50
1:G:259:GLU:HA	1:G:264:GLU:HG3	1.93	0.50
1:A:236:THR:O	1:A:238:SER:N	2.42	0.49
1:A:338:THR:O	1:A:341:LEU:HB2	2.11	0.49
1:D:217:ALA:O	1:D:221:ARG:HG3	2.11	0.49
1:F:86:ARG:HG3	1:F:86:ARG:HH11	1.77	0.49
1:A:126:LEU:HD11	1:A:411:VAL:HG23	1.94	0.49
1:D:372:THR:HG22	1:D:373:LYS:CG	2.42	0.49
1:A:358:LEU:HB3	1:A:385:LEU:CD1	2.42	0.49
1:B:177:PRO:HG2	1:B:178:TYR:CE1	2.47	0.49
1:F:159:PRO:HG2	1:F:356:ASP:OD1	2.12	0.49
1:A:89:ARG:HD3	1:G:463:MET:SD	2.52	0.49
1:A:388:THR:HG21	1:A:425:ASP:OD1	2.13	0.49
1:B:317:TRP:HB2	1:B:325:LEU:HD12	1.93	0.49
1:E:255:ARG:HG3	1:E:255:ARG:NH2	2.27	0.49
1:D:338:THR:O	1:D:341:LEU:HB2	2.12	0.49
1:F:199:ARG:HE	1:F:338:THR:HG21	1.78	0.49
1:F:471:PRO:HG2	1:F:474:THR:OG1	2.13	0.49
1:E:455:GLU:O	1:E:455:GLU:HG3	2.12	0.49
1:E:199:ARG:HE	1:E:338:THR:HG21	1.72	0.49
1:A:222:LEU:HA	1:A:225:ARG:NH1	2.28	0.49
1:E:101:ARG:HH22	4:E:1505:EPE:C2	2.26	0.49
1:E:380:ARG:HG3	1:E:380:ARG:NH2	2.24	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:ARG:HB3	1:F:327:PRO:CD	2.42	0.49
1:B:435:VAL:HG13	1:B:436:GLU:N	2.28	0.48
1:D:322:GLY:N	1:D:323:PRO:HD2	2.28	0.48
1:E:80:GLY:O	1:F:89:ARG:HG2	2.13	0.48
1:B:349:ARG:HD2	1:B:377:ALA:O	2.13	0.48
1:E:384:GLY:O	1:E:385:LEU:HD13	2.13	0.48
1:B:199:ARG:HE	1:B:338:THR:HG21	1.77	0.48
1:E:177:PRO:HG2	1:E:178:TYR:CD1	2.49	0.48
1:E:328:LEU:O	1:E:331:ALA:HB3	2.13	0.48
1:F:322:GLY:N	1:F:323:PRO:HD2	2.28	0.48
1:A:479:PHE:O	1:G:417:ARG:NH1	2.46	0.48
1:F:156:ILE:HG22	1:F:158:ASP:HB2	1.96	0.48
1:F:217:ALA:O	1:F:221:ARG:HG3	2.14	0.48
1:D:417:ARG:NH1	1:E:479:PHE:O	2.44	0.48
1:F:169:ARG:NH1	1:F:171:LYS:HD3	2.28	0.48
1:G:251:PHE:CE1	1:G:277:LEU:HD13	2.49	0.48
1:A:173:ILE:HG23	1:A:183:LYS:HG3	1.96	0.48
1:B:164:LEU:HD11	1:B:174:ILE:HD11	1.95	0.48
1:E:225:ARG:O	1:E:229:LYS:HB2	2.14	0.48
1:F:386:GLN:HB2	5:F:2076:HOH:O	2.13	0.48
1:A:437:ARG:HG3	1:A:437:ARG:HH21	1.78	0.48
1:F:106:LYS:NZ	5:F:2013:HOH:O	2.47	0.48
1:B:191:ILE:HG13	1:B:197:TRP:CZ3	2.49	0.48
1:B:346:GLU:OE2	1:B:346:GLU:HA	2.14	0.48
1:D:199:ARG:HE	1:D:338:THR:CG2	2.27	0.48
1:D:380:ARG:HH21	1:D:380:ARG:HG3	1.79	0.48
1:E:169:ARG:NH1	1:E:171:LYS:HD3	2.25	0.47
1:G:328:LEU:O	1:G:331:ALA:HB3	2.14	0.47
1:G:455:GLU:O	1:G:455:GLU:HG3	2.13	0.47
1:G:166:LYS:HE2	1:G:497:ASN:ND2	2.29	0.47
1:F:139:LEU:C	1:F:139:LEU:HD23	2.35	0.47
1:A:372:THR:HG22	1:A:373:LYS:HG3	1.95	0.47
1:D:103:THR:OG1	1:D:116:PRO:HG2	2.14	0.47
1:D:126:LEU:HD11	1:D:411:VAL:HG23	1.96	0.47
1:D:164:LEU:HA	1:D:314:PHE:CE2	2.49	0.47
1:D:179:ASP:O	1:D:182:THR:HG22	2.14	0.47
1:E:305:LEU:HB3	1:E:343:LEU:HD21	1.95	0.47
1:F:417:ARG:NH2	1:F:469:ASN:OD1	2.47	0.47
1:F:455:GLU:HG3	1:F:455:GLU:O	2.13	0.47
1:A:207:ARG:HB2	1:A:363:LYS:HD3	1.96	0.47
1:B:80:GLY:O	1:D:89:ARG:HG2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:367:LEU:HD22	1:F:371:LEU:HG	1.97	0.47
1:B:82:ALA:O	1:B:437:ARG:NH1	2.47	0.47
1:B:164:LEU:HA	1:B:314:PHE:CE2	2.50	0.47
1:B:433:HIS:O	1:B:433:HIS:CD2	2.67	0.47
1:F:502:PHE:CE2	1:F:504:GLU:HB2	2.50	0.47
1:E:92:ARG:CG	1:E:484:PRO:HB3	2.42	0.47
1:F:340:ILE:HD12	1:F:340:ILE:C	2.35	0.47
1:G:169:ARG:NH2	1:G:312:ASN:HD21	2.13	0.47
1:G:384:GLY:O	1:G:385:LEU:HD13	2.15	0.47
1:F:306:GLU:O	1:F:308:PRO:HD3	2.15	0.47
1:A:166:LYS:CE	1:A:497:ASN:HD21	2.27	0.47
1:D:225:ARG:O	1:D:229:LYS:HB2	2.14	0.47
1:D:482:ASN:C	1:D:482:ASN:ND2	2.68	0.47
1:E:97:GLY:HA3	4:E:1505:EPE:H91	1.97	0.47
1:B:259:GLU:HA	1:B:264:GLU:CG	2.44	0.47
1:E:494:GLN:HE21	1:E:494:GLN:HA	1.80	0.47
1:A:85:LYS:HE3	5:A:2002:HOH:O	2.16	0.46
1:B:433:HIS:CD2	1:B:433:HIS:C	2.89	0.46
1:D:190:GLU:OE1	1:D:302:ARG:HG3	2.14	0.46
1:E:259:GLU:HA	1:E:264:GLU:HG3	1.96	0.46
1:A:139:LEU:C	1:A:139:LEU:HD23	2.36	0.46
1:A:207:ARG:HB3	1:A:363:LYS:HD3	1.97	0.46
1:A:340:ILE:HA	1:A:343:LEU:HG	1.96	0.46
1:B:388:THR:HG21	1:B:425:ASP:OD1	2.15	0.46
1:G:131:ALA:HA	1:G:386:GLN:HG3	1.96	0.46
1:B:338:THR:O	1:B:341:LEU:HB2	2.15	0.46
1:D:145:TYR:CZ	1:D:149:LEU:HD11	2.51	0.46
1:E:498:ARG:O	1:E:499:GLN:CG	2.56	0.46
1:G:433:HIS:C	1:G:433:HIS:CD2	2.89	0.46
1:B:124:ARG:HB3	1:B:408:ARG:HB2	1.97	0.46
1:G:177:PRO:HG2	1:G:178:TYR:CE1	2.50	0.46
1:G:217:ALA:O	1:G:221:ARG:HG3	2.16	0.46
1:G:395:TYR:HB3	1:G:399:GLU:HB3	1.98	0.46
1:D:419:ASP:HB2	1:E:405:ALA:HB2	1.98	0.46
1:B:169:ARG:NH2	1:B:312:ASN:ND2	2.63	0.46
1:D:384:GLY:O	1:D:385:LEU:HD13	2.15	0.46
1:A:196:ASP:O	1:A:200:TYR:HD1	1.99	0.46
1:D:192:ARG:HH12	1:D:306:GLU:CD	2.19	0.46
1:D:494:GLN:CA	1:D:494:GLN:HE21	2.28	0.46
1:E:101:ARG:HH22	4:E:1505:EPE:C3	2.29	0.46
1:F:372:THR:HG22	1:F:373:LYS:HG3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LYS:H	1:A:106:LYS:HG2	1.29	0.46
1:B:428:LEU:O	1:B:428:LEU:HD22	2.16	0.46
1:D:455:GLU:O	1:D:455:GLU:HG3	2.15	0.46
1:F:223:LEU:HD23	1:F:284:LEU:CD2	2.45	0.46
1:D:199:ARG:HE	1:D:338:THR:HG22	1.80	0.46
1:G:156:ILE:HG22	1:G:158:ASP:HB2	1.97	0.46
1:B:169:ARG:NH1	1:B:171:LYS:HD3	2.15	0.46
1:F:130:GLY:HA3	1:F:413:LEU:HB2	1.97	0.46
1:G:127:LEU:HD11	1:G:385:LEU:HD22	1.97	0.46
1:G:158:ASP:OD2	1:G:161:GLY:HA2	2.16	0.46
1:G:177:PRO:HB3	1:G:294:MET:HG2	1.98	0.46
1:A:252:ASP:N	1:A:252:ASP:OD2	2.48	0.45
1:A:367:LEU:HD13	1:A:403:LEU:HD11	1.98	0.45
1:A:417:ARG:NH1	1:B:479:PHE:O	2.49	0.45
1:A:488:VAL:HG13	1:A:489:PRO:HD2	1.98	0.45
1:B:84:PHE:CB	1:B:435:VAL:CG1	2.94	0.45
1:E:85:LYS:CD	1:E:454:LEU:HD21	2.41	0.45
1:E:101:ARG:NH1	4:E:1505:EPE:H92	2.31	0.45
1:B:439:ARG:HD2	1:B:454:LEU:N	2.31	0.45
1:D:367:LEU:HD22	1:D:371:LEU:HG	1.98	0.45
1:A:408:ARG:NH2	5:A:2078:HOH:O	2.43	0.45
1:D:200:TYR:HE2	1:D:335:VAL:HG13	1.81	0.45
1:F:238:SER:HB3	1:F:241:GLU:HB2	1.98	0.45
1:G:358:LEU:HB3	1:G:385:LEU:CD1	2.47	0.45
1:G:488:VAL:HG13	1:G:489:PRO:HD2	1.98	0.45
1:B:154:MET:CE	1:B:156:ILE:HD11	2.44	0.45
1:D:200:TYR:CE2	1:D:335:VAL:HG13	2.51	0.45
1:D:498:ARG:O	1:D:499:GLN:CG	2.60	0.45
1:E:346:GLU:HA	1:E:346:GLU:OE2	2.16	0.45
1:E:438:ASP:OD2	1:E:454:LEU:HD23	2.16	0.45
1:F:488:VAL:HG13	1:F:489:PRO:HD2	1.99	0.45
1:G:136:LYS:HG2	1:G:413:LEU:HD12	1.98	0.45
1:A:326:ARG:HD2	5:A:2061:HOH:O	2.16	0.45
1:B:132:THR:HG22	5:D:2094:HOH:O	2.15	0.45
1:D:430:LEU:HD12	1:D:430:LEU:HA	1.80	0.45
1:G:124:ARG:HB3	1:G:408:ARG:HB2	1.99	0.45
1:G:346:GLU:HA	1:G:346:GLU:OE2	2.16	0.45
1:A:317:TRP:HB2	1:A:325:LEU:HD12	1.99	0.45
1:B:259:GLU:HB3	5:B:2048:HOH:O	2.16	0.45
1:E:86:ARG:HG3	1:E:86:ARG:HH11	1.81	0.45
1:F:222:LEU:HD23	1:F:267: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:A:420:PRO:HB2	1:B:428:LEU:HD13	1.99	0.45
1:A:433:HIS:NE2	1:A:459:GLU:HG3	2.32	0.45
1:A:326:ARG:N	1:A:327:PRO:HD2	2.32	0.44
1:B:99:LEU:HD22	1:B:486:ALA:HB3	1.97	0.44
1:E:144:ALA:HB1	1:E:154:MET:HE1	2.00	0.44
1:E:357:GLU:HG3	5:E:2082:HOH:O	2.15	0.44
1:G:497:ASN:N	1:G:497:ASN:HD22	2.14	0.44
1:A:437:ARG:NH1	1:A:459:GLU:OE2	2.45	0.44
1:D:88:LEU:HB2	1:D:434:GLU:O	2.17	0.44
1:E:84:PHE:HB3	1:E:437:ARG:HG3	1.98	0.44
1:F:346:GLU:OE2	1:F:346:GLU:HA	2.18	0.44
1:A:78:GLU:HG3	1:A:94:VAL:HA	1.99	0.44
5:A:2026:HOH:O	1:G:324:ALA:HB2	2.16	0.44
1:D:159:PRO:HG3	1:D:317:TRP:CH2	2.52	0.44
1:F:340:ILE:CD1	1:F:341:LEU:HD13	2.47	0.44
1:A:497:ASN:N	1:A:497:ASN:HD22	2.15	0.44
1:B:240:ARG:HH21	1:B:240:ARG:HB2	1.82	0.44
1:D:456:ARG:HD2	1:D:456:ARG:N	2.32	0.44
1:F:252:ASP:O	1:F:255:ARG:HB2	2.17	0.44
1:D:433:HIS:C	1:D:433:HIS:CD2	2.90	0.44
1:A:166:LYS:CE	1:A:497:ASN:ND2	2.80	0.44
1:F:164:LEU:HA	1:F:314:PHE:CE2	2.53	0.44
1:G:433:HIS:O	1:G:433:HIS:CD2	2.70	0.44
1:B:160:ASN:HD21	1:B:319:GLU:CD	2.21	0.44
1:B:304:TRP:CH2	1:B:313:LEU:HB2	2.52	0.44
1:B:326:ARG:N	1:B:327:PRO:HD2	2.33	0.44
1:E:246:THR:HB	1:E:284:LEU:HD23	2.00	0.44
1:D:304:TRP:CH2	1:D:313:LEU:HB2	2.53	0.44
1:D:433:HIS:O	1:D:433:HIS:CD2	2.69	0.44
1:E:107:ALA:HB3	1:E:119:ARG:CD	2.48	0.44
1:F:124:ARG:HB3	1:F:408:ARG:HG3	2.00	0.44
1:G:130:GLY:O	1:G:136:LYS:NZ	2.50	0.44
1:G:435:VAL:CG1	1:G:436:GLU:N	2.80	0.44
1:A:388:THR:HA	5:A:2076:HOH:O	2.16	0.44
1:D:313:LEU:HD23	1:D:314:PHE:N	2.33	0.44
1:E:306:GLU:O	1:E:308:PRO:HD3	2.18	0.44
1:E:414:GLY:HA2	1:E:467:ILE:CG2	2.48	0.44
1:G:179:ASP:O	1:G:182:THR:HG22	2.18	0.44
1:A:433:HIS:CD2	1:A:433:HIS:C	2.91	0.43
1:E:180:GLN:HB2	1:E:504:GLU:CB	2.46	0.43
1:F:105:GLU:OE1	1:F:119:ARG:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:430:LEU:HD12	1:E:430:LEU:HA	1.69	0.43
1:F:200:TYR:HE2	1:F:335:VAL:HG13	1.83	0.43
1:G:251:PHE:CZ	1:G:277:LEU:HD13	2.53	0.43
1:B:438:ASP:HB3	1:B:439:ARG:H	1.72	0.43
1:E:202:LEU:HD13	1:E:221:ARG:CD	2.49	0.43
1:E:240:ARG:HB2	1:E:240:ARG:NH2	2.31	0.43
1:A:352:TRP:CZ2	1:A:380:ARG:HD3	2.53	0.43
1:D:124:ARG:HB3	1:D:408:ARG:HB2	2.01	0.43
1:E:84:PHE:HA	1:E:437:ARG:CG	2.48	0.43
1:E:304:TRP:CH2	1:E:313:LEU:HB2	2.54	0.43
1:F:144:ALA:HB1	1:F:154:MET:CE	2.48	0.43
1:F:184:GLY:HA3	1:F:297:GLY:CA	2.48	0.43
1:G:173:ILE:HG23	1:G:183:LYS:CG	2.49	0.43
1:D:433:HIS:NE2	1:D:459:GLU:HG3	2.33	0.43
1:F:98:LYS:O	1:F:102:MET:HG3	2.18	0.43
1:A:346:GLU:OE2	1:A:346:GLU:HA	2.19	0.43
1:A:413:LEU:CD2	1:A:475:ALA:HB2	2.48	0.43
1:G:222:LEU:HD12	1:G:225:ARG:NH1	2.34	0.43
1:A:95:SER:OG	1:A:98:LYS:HB2	2.19	0.43
1:A:177:PRO:HG2	1:A:178:TYR:CD1	2.53	0.43
1:A:84:PHE:CB	1:A:435:VAL:HG11	2.49	0.43
1:A:160:ASN:HD21	1:A:319:GLU:CD	2.22	0.43
1:B:158:ASP:OD2	1:B:161:GLY:HA2	2.18	0.43
1:B:430:LEU:HD12	1:B:430:LEU:HA	1.91	0.43
1:D:238:SER:HB3	1:D:241:GLU:HB2	2.01	0.43
1:G:367:LEU:HD22	1:G:371:LEU:HD11	2.01	0.43
1:A:259:GLU:HA	1:A:264:GLU:CG	2.45	0.43
1:E:177:PRO:HG2	1:E:178:TYR:CE1	2.54	0.43
1:F:494:GLN:HE21	1:F:494:GLN:CA	2.28	0.43
1:F:503:VAL:HG12	1:F:503:VAL:O	2.19	0.43
1:A:136:LYS:HE3	1:A:357:GLU:OE2	2.19	0.43
1:D:236:THR:O	1:D:238:SER:N	2.50	0.43
1:E:84:PHE:HA	1:E:437:ARG:HG3	2.01	0.43
1:E:136:LYS:HG2	1:E:413:LEU:HD12	2.01	0.43
1:E:249:ALA:O	1:E:281:ARG:NH2	2.36	0.43
1:F:352:TRP:CE2	1:F:380:ARG:HD3	2.54	0.43
1:G:145:TYR:CZ	1:G:149:LEU:HD11	2.54	0.43
1:A:166:LYS:HD2	1:A:495:PHE:HB2	2.00	0.42
1:A:322:GLY:N	1:A:323:PRO:HD2	2.34	0.42
1:B:504:GLU:HB3	1:B:505:GLY:H	1.54	0.42
1:D:177:PRO:HG2	1:D:178:TYR:CE1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:LEU:HD23	1:D:413:LEU:HA	1.84	0.42
1:E:304:TRP:CZ2	1:E:313:LEU:HB2	2.54	0.42
1:F:356:ASP:OD2	1:F:357:GLU:N	2.52	0.42
1:G:84:PHE:HB3	1:G:435:VAL:HG11	2.00	0.42
1:G:130:GLY:HA3	1:G:413:LEU:HB2	2.00	0.42
1:A:255:ARG:NH2	1:A:255:ARG:CG	2.81	0.42
1:D:84:PHE:HB3	1:D:437:ARG:HG3	2.00	0.42
1:D:186:SER:HA	5:D:2064:HOH:O	2.19	0.42
1:D:328:LEU:O	1:D:331:ALA:HB3	2.19	0.42
1:E:488:VAL:CG1	1:E:489:PRO:HD2	2.46	0.42
1:F:200:TYR:CE2	1:F:335:VAL:HG13	2.55	0.42
1:F:226:GLU:OE1	1:F:261:THR:HB	2.18	0.42
1:A:113:ALA:HA	1:A:490:LEU:HD23	2.01	0.42
1:E:157:VAL:O	1:E:159:PRO:HD3	2.18	0.42
1:F:248:ILE:O	1:G:265:SER:OG	2.26	0.42
1:B:101:ARG:NH2	1:B:101:ARG:CG	2.81	0.42
1:B:144:ALA:HB1	1:B:154:MET:HE1	2.01	0.42
1:B:173:ILE:HG23	1:B:183:LYS:CG	2.49	0.42
1:B:419:ASP:HB2	1:D:405:ALA:CB	2.50	0.42
1:E:84:PHE:CB	1:E:437:ARG:HG3	2.50	0.42
1:E:203:SER:O	1:E:331:ALA:HA	2.18	0.42
1:A:284:LEU:HD12	1:A:284:LEU:HA	1.83	0.42
1:B:372:THR:HG22	1:B:373:LYS:CG	2.49	0.42
1:D:497:ASN:N	1:D:497:ASN:HD22	2.18	0.42
1:E:139:LEU:HD23	1:E:139:LEU:C	2.40	0.42
1:F:89:ARG:HD2	1:F:434:GLU:OE1	2.20	0.42
1:A:84:PHE:HE2	1:A:87:PHE:HB2	1.84	0.42
1:B:101:ARG:NH1	5:B:2010:HOH:O	2.52	0.42
1:B:130:GLY:HA3	1:B:413:LEU:HB2	2.02	0.42
1:B:304:TRP:CZ2	1:B:313:LEU:HB2	2.55	0.42
1:F:173:ILE:HG22	1:F:174:ILE:N	2.34	0.42
1:G:255:ARG:HG3	1:G:255:ARG:NH2	2.34	0.42
1:A:89:ARG:HG2	1:G:80:GLY:C	2.40	0.42
1:B:97:GLY:O	1:B:101:ARG:HD3	2.20	0.42
1:B:101:ARG:HH21	1:B:101:ARG:HG2	1.84	0.42
1:D:350:ARG:HH21	1:D:350:ARG:HB2	1.84	0.42
1:F:180:GLN:NE2	1:F:505:GLY:HA3	2.35	0.42
1:G:166:LYS:CE	1:G:497:ASN:ND2	2.82	0.42
1:G:252:ASP:OD2	1:G:252:ASP:N	2.53	0.42
1:A:398:LYS:HB2	5:A:2071:HOH:O	2.20	0.42
1:E:350:ARG:HG2	1:E:380:ARG:NH1	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:LEU:HD22	1:E:380:ARG:N	2.35	0.42
2:E:1506:GNP:HN22	2:E:1506:GNP:PA	2.43	0.42
1:F:173:ILE:HG23	1:F:183:LYS:CG	2.49	0.42
1:G:113:ALA:HA	1:G:490:LEU:HD23	2.00	0.42
1:A:318:ARG:HD2	1:A:502:PHE:CE2	2.55	0.42
1:B:340:ILE:HD12	1:B:341:LEU:HD12	2.02	0.42
1:E:367:LEU:HD13	1:E:403:LEU:HD11	2.01	0.42
1:G:83:PRO:HA	5:G:2004:HOH:O	2.19	0.42
1:G:372:THR:HG22	1:G:373:LYS:HG3	2.00	0.42
1:A:224:LEU:CD1	1:A:242:LEU:HD21	2.49	0.42
1:A:225:ARG:HG3	1:A:226:GLU:N	2.35	0.42
1:B:288:LEU:O	1:B:291:HIS:HB2	2.20	0.42
1:D:169:ARG:HH11	1:D:171:LYS:CD	2.28	0.42
1:D:213:ALA:HA	1:D:216:TRP:CE3	2.55	0.42
1:F:92:ARG:HG2	1:F:92:ARG:H	1.76	0.42
1:F:199:ARG:HG3	1:F:338:THR:HG21	2.01	0.42
1:F:414:GLY:HA2	1:F:467:ILE:CG2	2.50	0.42
1:G:494:GLN:NE2	1:G:494:GLN:CA	2.79	0.42
1:A:105:GLU:HB2	1:A:109:GLN:NE2	2.35	0.41
1:A:433:HIS:O	1:A:433:HIS:CD2	2.72	0.41
1:A:454:LEU:O	1:A:455:GLU:HB3	2.20	0.41
1:B:492:ILE:CD1	2:B:701:GNP:H1'	2.50	0.41
1:E:233:LEU:HD23	1:E:233:LEU:HA	1.80	0.41
1:F:340:ILE:HA	1:F:343:LEU:HG	2.02	0.41
1:F:346:GLU:OE1	1:F:348:LYS:HB2	2.20	0.41
1:F:352:TRP:CZ2	1:F:380:ARG:HD3	2.55	0.41
1:F:433:HIS:HD2	1:F:433:HIS:O	2.02	0.41
1:G:169:ARG:HH21	1:G:312:ASN:ND2	2.18	0.41
1:A:358:LEU:HB3	1:A:385:LEU:HD11	2.02	0.41
1:B:136:LYS:HG2	1:B:413:LEU:HD12	2.02	0.41
1:F:144:ALA:HB1	1:F:154:MET:HE1	2.01	0.41
1:G:144:ALA:HB1	1:G:154:MET:HE1	2.02	0.41
1:G:148:LEU:HD23	1:G:148:LEU:HA	1.87	0.41
1:A:169:ARG:HG2	1:A:498:ARG:NH2	2.35	0.41
1:A:304:TRP:CH2	1:A:313:LEU:HB2	2.54	0.41
1:F:145:TYR:CZ	1:F:149:LEU:HD11	2.55	0.41
1:G:352:TRP:CE2	1:G:380:ARG:HD3	2.54	0.41
1:D:160:ASN:HD21	1:D:319:GLU:CD	2.24	0.41
1:E:190:GLU:OE1	1:E:302:ARG:HG3	2.21	0.41
1:G:137:SER:O	1:G:141:ARG:HB2	2.20	0.41
1:G:233:LEU:HD23	1:G:233:LEU:HA	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ALA:O	1:A:437:ARG:NH2	2.54	0.41
1:B:288:LEU:N	1:B:289:PRO:CD	2.84	0.41
1:B:494:GLN:HA	1:B:494:GLN:HE21	1.85	0.41
1:F:97:GLY:O	1:F:101:ARG:HG3	2.20	0.41
1:G:119:ARG:HH11	1:G:150:ARG:NH1	2.19	0.41
1:G:380:ARG:HG3	1:G:380:ARG:NH2	2.34	0.41
1:B:380:ARG:CG	1:B:380:ARG:NH2	2.82	0.41
1:F:117:MET:HA	1:F:118:PRO:HD3	1.98	0.41
1:F:340:ILE:HD11	1:F:341:LEU:HD13	2.02	0.41
1:B:102:MET:CE	5:B:2024:HOH:O	2.68	0.41
1:B:124:ARG:HB3	1:B:408:ARG:CG	2.50	0.41
1:D:258:LEU:O	1:D:261:THR:OG1	2.30	0.41
1:E:101:ARG:NH2	4:E:1505:EPE:H22	2.34	0.41
1:F:177:PRO:HA	1:F:294:MET:HE1	2.01	0.41
1:F:205:VAL:HB	1:F:221:ARG:HG2	2.02	0.41
1:B:380:ARG:HH21	1:B:380:ARG:CG	2.27	0.41
1:E:101:ARG:HD3	5:E:2008:HOH:O	2.19	0.41
1:E:106:LYS:H	1:E:106:LYS:HG2	1.27	0.41
1:A:419:ASP:HB2	1:B:405:ALA:CB	2.50	0.41
1:B:137:SER:HB3	1:B:141:ARG:NH2	2.36	0.41
1:B:494:GLN:HA	1:B:494:GLN:NE2	2.36	0.41
1:D:166:LYS:HE2	1:D:497:ASN:HD21	1.86	0.41
1:E:145:TYR:CE2	1:E:149:LEU:HD11	2.55	0.41
1:E:251:PHE:HZ	1:E:277:LEU:HB3	1.84	0.41
1:E:435:VAL:HG13	1:E:436:GLU:N	2.36	0.41
1:F:86:ARG:HD3	1:F:436:GLU:OE1	2.21	0.41
1:F:435:VAL:HG13	1:F:436:GLU:N	2.36	0.41
1:G:154:MET:HA	1:G:351:LEU:CD2	2.50	0.41
1:G:185:TRP:CG	1:G:186:SER:N	2.88	0.41
1:G:329:ILE:O	1:G:333:VAL:HG23	2.21	0.41
1:D:157:VAL:O	1:D:159:PRO:HD3	2.21	0.41
1:D:206:PRO:HG2	1:D:362:GLU:OE2	2.21	0.41
1:E:420:PRO:HB2	1:F:428:LEU:HD13	2.02	0.41
1:G:148:LEU:CD1	1:G:167:PHE:HB3	2.51	0.41
1:A:437:ARG:O	1:A:438:ASP:CB	2.61	0.40
1:E:279:SER:O	1:E:283:VAL:HG23	2.21	0.40
1:E:284:LEU:HD12	1:E:284:LEU:HA	1.87	0.40
1:G:89:ARG:HD2	1:G:434:GLU:OE1	2.21	0.40
1:G:96:GLY:HA3	5:G:2009:HOH:O	2.21	0.40
1:G:277:LEU:HD23	1:G:277:LEU:HA	1.85	0.40
1:A:169:ARG:NH1	1:A:171:LYS:HD3	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ASN:O	1:B:182:THR:HB	2.21	0.40
1:B:191:ILE:HG21	1:B:197:TRP:CZ2	2.57	0.40
1:B:464:PRO:HD2	5:B:2086:HOH:O	2.20	0.40
1:E:113:ALA:HA	1:E:490:LEU:HD23	2.03	0.40
1:E:184:GLY:HA3	1:E:296:ASP:C	2.41	0.40
1:E:192:ARG:HG3	1:E:302:ARG:NH1	2.36	0.40
1:F:98:LYS:HA	1:F:101:ARG:NH2	2.36	0.40
1:F:439:ARG:HE	1:F:439:ARG:HA	1.86	0.40
1:G:139:LEU:HD23	1:G:139:LEU:C	2.42	0.40
1:G:290:GLU:HG3	1:G:325:LEU:HD23	2.02	0.40
1:A:84:PHE:CB	1:A:435:VAL:CG1	2.99	0.40
1:D:169:ARG:HH21	1:D:312:ASN:ND2	2.19	0.40
1:E:494:GLN:HA	1:E:494:GLN:NE2	2.36	0.40
1:F:207:ARG:HB2	1:F:363:LYS:HB3	2.04	0.40
1:G:430:LEU:HD23	1:G:462:VAL:HB	2.04	0.40
1:E:380:ARG:NH2	1:E:380:ARG:CG	2.83	0.40
1:E:214:GLU:HA	1:E:214:GLU:OE1	2.22	0.40
1:G:213:ALA:HA	1:G:216:TRP:CE3	2.56	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	413/436 (95%)	394 (95%)	18 (4%)	1 (0%)	47 78
1	B	416/436 (95%)	395 (95%)	20 (5%)	1 (0%)	47 78
1	D	412/436 (94%)	390 (95%)	21 (5%)	1 (0%)	47 78
1	E	411/436 (94%)	389 (95%)	22 (5%)	0	100 100
1	F	412/436 (94%)	392 (95%)	17 (4%)	3 (1%)	22 53
1	G	410/436 (94%)	387 (94%)	21 (5%)	2 (0%)	29 61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2474/2616 (95%)	2347 (95%)	119 (5%)	8 (0%)	41 72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	504	GLU
1	F	454	LEU
1	G	499	GLN
1	A	499	GLN
1	D	499	GLN
1	F	499	GLN
1	F	289	PRO
1	G	289	PRO

5.3.2 Protein sidechains (i)

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	347/363 (96%)	318 (92%)	29 (8%)	11 31
1	B	350/363 (96%)	322 (92%)	28 (8%)	12 34
1	D	347/363 (96%)	316 (91%)	31 (9%)	9 28
1	E	347/363 (96%)	317 (91%)	30 (9%)	10 30
1	F	346/363 (95%)	318 (92%)	28 (8%)	11 33
1	G	345/363 (95%)	316 (92%)	29 (8%)	11 31
All	All	2082/2178 (96%)	1907 (92%)	175 (8%)	11 31

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLU
1	A	89	ARG
1	A	92	ARG
1	A	94	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	106	LYS
1	A	143	LEU
1	A	202	LEU
1	A	240	ARG
1	A	251	PHE
1	A	252	ASP
1	A	277	LEU
1	A	284	LEU
1	A	294	MET
1	A	296	ASP
1	A	313	LEU
1	A	328	LEU
1	A	338	THR
1	A	341	LEU
1	A	345	GLU
1	A	351	LEU
1	A	353	LEU
1	A	367	LEU
1	A	372	THR
1	A	379	LEU
1	A	385	LEU
1	A	428	LEU
1	A	430	LEU
1	A	433	HIS
1	A	435	VAL
1	B	74	VAL
1	B	89	ARG
1	B	92	ARG
1	B	94	VAL
1	B	101	ARG
1	B	106	LYS
1	B	143	LEU
1	B	154	MET
1	B	202	LEU
1	B	233	LEU
1	B	251	PHE
1	B	254	LEU
1	B	277	LEU
1	B	284	LEU
1	B	294	MET
1	B	296	ASP
1	B	328	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	350	ARG
1	B	351	LEU
1	B	353	LEU
1	B	367	LEU
1	B	379	LEU
1	B	385	LEU
1	B	428	LEU
1	B	430	LEU
1	B	433	HIS
1	B	439	ARG
1	B	504	GLU
1	D	76	GLN
1	D	89	ARG
1	D	92	ARG
1	D	94	VAL
1	D	106	LYS
1	D	143	LEU
1	D	202	LEU
1	D	233	LEU
1	D	251	PHE
1	D	254	LEU
1	D	277	LEU
1	D	284	LEU
1	D	294	MET
1	D	313	LEU
1	D	328	LEU
1	D	338	THR
1	D	341	LEU
1	D	345	GLU
1	D	350	ARG
1	D	351	LEU
1	D	353	LEU
1	D	367	LEU
1	D	376	LYS
1	D	379	LEU
1	D	385	LEU
1	D	428	LEU
1	D	430	LEU
1	D	433	HIS
1	D	435	VAL
1	D	482	ASN
1	D	494	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	89	ARG
1	E	92	ARG
1	E	94	VAL
1	E	106	LYS
1	E	143	LEU
1	E	154	MET
1	E	202	LEU
1	E	240	ARG
1	E	251	PHE
1	E	254	LEU
1	E	277	LEU
1	E	284	LEU
1	E	294	MET
1	E	296	ASP
1	E	328	LEU
1	E	338	THR
1	E	341	LEU
1	E	351	LEU
1	E	353	LEU
1	E	367	LEU
1	E	372	THR
1	E	379	LEU
1	E	385	LEU
1	E	399	GLU
1	E	428	LEU
1	E	430	LEU
1	E	433	HIS
1	E	435	VAL
1	E	438	ASP
1	E	456	ARG
1	F	89	ARG
1	F	92	ARG
1	F	94	VAL
1	F	132	THR
1	F	143	LEU
1	F	202	LEU
1	F	251	PHE
1	F	254	LEU
1	F	277	LEU
1	F	284	LEU
1	F	289	PRO
1	F	294	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	296	ASP
1	F	328	LEU
1	F	338	THR
1	F	341	LEU
1	F	350	ARG
1	F	351	LEU
1	F	353	LEU
1	F	366	SER
1	F	367	LEU
1	F	379	LEU
1	F	385	LEU
1	F	399	GLU
1	F	428	LEU
1	F	430	LEU
1	F	433	HIS
1	F	435	VAL
1	G	78	GLU
1	G	85	LYS
1	G	89	ARG
1	G	92	ARG
1	G	94	VAL
1	G	106	LYS
1	G	143	LEU
1	G	202	LEU
1	G	251	PHE
1	G	252	ASP
1	G	277	LEU
1	G	284	LEU
1	G	289	PRO
1	G	294	MET
1	G	296	ASP
1	G	328	LEU
1	G	338	THR
1	G	350	ARG
1	G	351	LEU
1	G	353	LEU
1	G	367	LEU
1	G	379	LEU
1	G	385	LEU
1	G	399	GLU
1	G	428	LEU
1	G	430	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	433	HIS
1	G	438	ASP
1	G	458	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	160	ASN
1	A	180	GLN
1	A	433	HIS
1	A	494	GLN
1	A	497	ASN
1	A	499	GLN
1	B	160	ASN
1	B	180	GLN
1	B	433	HIS
1	B	494	GLN
1	B	497	ASN
1	B	499	GLN
1	D	160	ASN
1	D	180	GLN
1	D	312	ASN
1	D	423	ASN
1	D	433	HIS
1	D	482	ASN
1	D	494	GLN
1	D	497	ASN
1	D	499	GLN
1	E	160	ASN
1	E	180	GLN
1	E	494	GLN
1	E	497	ASN
1	E	499	GLN
1	F	180	GLN
1	F	386	GLN
1	F	494	GLN
1	F	497	ASN
1	F	499	GLN
1	G	129	ASN
1	G	160	ASN
1	G	180	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	312	ASN
1	G	433	HIS
1	G	494	GLN
1	G	497	ASN
1	G	499	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	GNP	E	701	-	29,34,34	2.26	12 (41%)	33,54,54	2.91	6 (18%)
2	GNP	A	701	-	29,34,34	2.05	12 (41%)	33,54,54	3.08	8 (24%)
4	EPE	E	1505	-	15,15,15	1.28	2 (13%)	18,20,20	0.90	1 (5%)
2	GNP	D	701	-	29,34,34	2.32	12 (41%)	33,54,54	2.89	8 (24%)
2	GNP	G	701	-	29,34,34	2.23	11 (37%)	33,54,54	2.89	7 (21%)
2	GNP	B	701	-	29,34,34	2.25	12 (41%)	33,54,54	2.94	8 (24%)
2	GNP	F	701	-	29,34,34	2.25	11 (37%)	33,54,54	2.89	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GNP	E	1506	-	29,34,34	2.20	11 (37%)	33,54,54	2.89	9 (27%)

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	GNP	E	701	-	-	3/14/38/38	0/3/3/3
2	GNP	A	701	-	-	1/14/38/38	0/3/3/3
4	EPE	E	1505	-	-	2/9/19/19	0/1/1/1
2	GNP	D	701	-	-	3/14/38/38	0/3/3/3
2	GNP	G	701	-	-	1/14/38/38	0/3/3/3
2	GNP	B	701	-	-	3/14/38/38	0/3/3/3
2	GNP	F	701	-	-	3/14/38/38	0/3/3/3
2	GNP	E	1506	-	-	3/14/38/38	0/3/3/3

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1506	GNP	C2-N2	5.08	1.44	1.33
2	D	701	GNP	PG-N3B	4.94	1.76	1.63
2	F	701	GNP	C2-N2	4.93	1.43	1.33
2	G	701	GNP	C2-N2	4.84	1.43	1.33
2	D	701	GNP	C2-N2	4.73	1.43	1.33
2	B	701	GNP	C2-N2	4.68	1.43	1.33
2	E	701	GNP	PG-N3B	4.58	1.75	1.63
2	E	701	GNP	C2-N2	4.54	1.43	1.33
2	B	701	GNP	PG-N3B	4.37	1.74	1.63
2	F	701	GNP	PG-N3B	4.36	1.74	1.63
2	A	701	GNP	PG-N3B	4.14	1.74	1.63
2	G	701	GNP	PG-N3B	4.08	1.74	1.63
2	E	1506	GNP	PG-N3B	4.02	1.73	1.63
2	E	701	GNP	C6-N1	3.91	1.39	1.33
2	G	701	GNP	C6-N1	3.82	1.39	1.33
2	F	701	GNP	C6-N1	3.77	1.39	1.33
2	D	701	GNP	C6-N1	3.75	1.39	1.33
2	F	701	GNP	C5-C6	3.74	1.47	1.41
2	E	1506	GNP	C6-N1	3.72	1.39	1.33
2	B	701	GNP	C6-N1	3.69	1.39	1.33
2	A	701	GNP	C2-N2	3.69	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1506	GNP	C5-C6	3.63	1.47	1.41
2	A	701	GNP	C5-C6	3.58	1.47	1.41
2	D	701	GNP	PB-O3A	3.56	1.63	1.59
2	G	701	GNP	C5-C6	3.46	1.47	1.41
2	B	701	GNP	C5-C6	3.42	1.47	1.41
2	D	701	GNP	C5-C6	3.39	1.47	1.41
2	E	701	GNP	C5-C6	3.36	1.47	1.41
2	G	701	GNP	PB-O3A	3.24	1.63	1.59
2	F	701	GNP	PB-O3A	3.14	1.63	1.59
2	B	701	GNP	PB-O3A	3.10	1.63	1.59
2	E	1506	GNP	PB-O3A	3.09	1.63	1.59
2	E	701	GNP	O4'-C4'	-3.08	1.38	1.45
2	G	701	GNP	PG-O3G	-3.07	1.48	1.56
2	B	701	GNP	PG-O3G	-3.01	1.48	1.56
2	B	701	GNP	O4'-C4'	-2.92	1.38	1.45
2	D	701	GNP	PB-O2B	-2.92	1.48	1.56
2	E	701	GNP	PB-O2B	-2.86	1.49	1.56
2	F	701	GNP	PG-O3G	-2.85	1.49	1.56
2	A	701	GNP	O4'-C4'	-2.85	1.38	1.45
2	E	701	GNP	PB-O3A	2.82	1.62	1.59
2	A	701	GNP	O6-C6	-2.81	1.17	1.24
2	G	701	GNP	O4'-C4'	-2.79	1.38	1.45
2	E	701	GNP	PG-O3G	-2.78	1.49	1.56
2	B	701	GNP	PB-O2B	-2.77	1.49	1.56
2	D	701	GNP	O4'-C4'	-2.75	1.38	1.45
2	E	1506	GNP	PG-O3G	-2.74	1.49	1.56
2	A	701	GNP	PG-O3G	-2.68	1.49	1.56
2	F	701	GNP	PB-O2B	-2.68	1.49	1.56
2	D	701	GNP	PB-N3B	2.66	1.70	1.63
2	F	701	GNP	PG-O1G	2.65	1.50	1.46
2	G	701	GNP	PB-O2B	-2.60	1.49	1.56
2	D	701	GNP	PG-O1G	2.60	1.50	1.46
2	D	701	GNP	PG-O3G	-2.58	1.49	1.56
2	A	701	GNP	PB-O3A	2.57	1.62	1.59
2	G	701	GNP	O6-C6	-2.56	1.18	1.24
2	A	701	GNP	PB-O2B	-2.54	1.49	1.56
4	E	1505	EPE	C6-N1	2.53	1.53	1.46
2	E	701	GNP	O6-C6	-2.52	1.18	1.24
2	E	1506	GNP	PG-O1G	2.51	1.50	1.46
2	F	701	GNP	O6-C6	-2.50	1.18	1.24
2	E	1506	GNP	O6-C6	-2.48	1.18	1.24
2	B	701	GNP	O6-C6	-2.48	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1506	GNP	O4'-C4'	-2.47	1.39	1.45
2	F	701	GNP	O4'-C4'	-2.45	1.39	1.45
2	E	701	GNP	PB-N3B	2.43	1.69	1.63
2	B	701	GNP	PB-N3B	2.42	1.69	1.63
2	A	701	GNP	PB-N3B	2.41	1.69	1.63
2	D	701	GNP	O6-C6	-2.40	1.18	1.24
2	G	701	GNP	PB-N3B	2.39	1.69	1.63
2	B	701	GNP	PG-O1G	2.38	1.49	1.46
2	E	701	GNP	PG-O1G	2.38	1.49	1.46
2	F	701	GNP	PB-N3B	2.33	1.69	1.63
2	A	701	GNP	PG-O1G	2.31	1.49	1.46
2	A	701	GNP	C6-N1	2.28	1.37	1.33
4	E	1505	EPE	C10-S	2.27	1.80	1.77
2	B	701	GNP	C2'-C1'	-2.26	1.50	1.53
2	E	1506	GNP	PB-O2B	-2.22	1.50	1.56
2	E	1506	GNP	PB-N3B	2.18	1.69	1.63
2	A	701	GNP	PA-O5'	-2.13	1.50	1.59
2	D	701	GNP	C2-N1	2.07	1.39	1.35
2	G	701	GNP	C2-N1	2.03	1.39	1.35
2	E	701	GNP	C2'-C1'	-2.02	1.50	1.53

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	GNP	C5-C6-N1	-9.36	110.63	123.43
2	B	701	GNP	C5-C6-N1	-9.25	110.78	123.43
2	D	701	GNP	C5-C6-N1	-9.24	110.79	123.43
2	F	701	GNP	C5-C6-N1	-9.12	110.96	123.43
2	E	701	GNP	C5-C6-N1	-9.05	111.05	123.43
2	G	701	GNP	C5-C6-N1	-9.02	111.10	123.43
2	E	1506	GNP	C5-C6-N1	-8.95	111.19	123.43
2	A	701	GNP	C2-N3-C4	-7.70	106.56	115.36
2	E	701	GNP	O1G-PG-N3B	-7.51	100.72	111.77
2	B	701	GNP	O1G-PG-N3B	-7.48	100.75	111.77
2	B	701	GNP	C2-N3-C4	-7.33	106.98	115.36
2	F	701	GNP	O1G-PG-N3B	-7.22	101.14	111.77
2	G	701	GNP	O1G-PG-N3B	-7.20	101.16	111.77
2	E	701	GNP	C2-N3-C4	-7.20	107.13	115.36
2	D	701	GNP	C2-N3-C4	-7.19	107.14	115.36
2	F	701	GNP	C2-N3-C4	-7.19	107.15	115.36
2	D	701	GNP	O1G-PG-N3B	-7.16	101.22	111.77
2	G	701	GNP	C2-N3-C4	-7.12	107.22	115.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1506	GNP	C2-N3-C4	-6.96	107.41	115.36
2	E	1506	GNP	O1G-PG-N3B	-6.75	101.83	111.77
2	A	701	GNP	O1G-PG-N3B	-6.57	102.09	111.77
2	A	701	GNP	N3-C2-N1	5.93	135.13	127.22
2	A	701	GNP	N2-C2-N1	-5.78	108.27	117.25
2	E	1506	GNP	N2-C2-N1	-5.30	109.00	117.25
2	E	701	GNP	N2-C2-N1	-5.30	109.01	117.25
2	B	701	GNP	N2-C2-N1	-5.24	109.10	117.25
2	G	701	GNP	N2-C2-N1	-5.15	109.24	117.25
2	F	701	GNP	N2-C2-N1	-5.14	109.25	117.25
2	B	701	GNP	N3-C2-N1	5.12	134.06	127.22
2	D	701	GNP	N2-C2-N1	-5.05	109.40	117.25
2	E	701	GNP	N3-C2-N1	5.02	133.92	127.22
2	G	701	GNP	N3-C2-N1	5.00	133.90	127.22
2	D	701	GNP	N3-C2-N1	4.98	133.87	127.22
2	F	701	GNP	N3-C2-N1	4.93	133.80	127.22
2	E	1506	GNP	N3-C2-N1	4.84	133.68	127.22
2	E	1506	GNP	O2B-PB-O1B	4.05	118.40	109.92
2	F	701	GNP	O2B-PB-O1B	3.72	117.72	109.92
2	E	701	GNP	O2B-PB-O1B	3.69	117.66	109.92
2	G	701	GNP	O2B-PB-O1B	3.69	117.65	109.92
2	A	701	GNP	O2B-PB-O1B	3.60	117.47	109.92
2	D	701	GNP	O2B-PB-O1B	3.57	117.40	109.92
2	B	701	GNP	O2B-PB-O1B	3.36	116.96	109.92
2	A	701	GNP	C1'-N9-C4	3.08	132.06	126.64
2	A	701	GNP	O4'-C4'-C5'	2.78	118.53	109.37
2	E	1506	GNP	O4'-C4'-C5'	2.61	117.98	109.37
2	F	701	GNP	O4'-C4'-C5'	2.29	116.90	109.37
2	G	701	GNP	O4'-C4'-C5'	2.26	116.81	109.37
2	E	1506	GNP	C1'-N9-C4	2.22	130.54	126.64
4	E	1505	EPE	C7-N4-C5	-2.21	105.58	111.23
2	B	701	GNP	O4'-C4'-C5'	2.19	116.57	109.37
2	D	701	GNP	O4'-C4'-C5'	2.16	116.48	109.37
2	E	1506	GNP	C2-N1-C6	2.14	119.33	115.93
2	B	701	GNP	C2-N1-C6	2.07	119.22	115.93
2	F	701	GNP	C2-N1-C6	2.04	119.17	115.93
2	D	701	GNP	C2-N1-C6	2.03	119.15	115.93

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	GNP	PG-N3B-PB-O1B
2	B	701	GNP	PG-N3B-PB-O1B
2	D	701	GNP	PG-N3B-PB-O1B
2	E	701	GNP	PG-N3B-PB-O1B
2	E	1506	GNP	PA-O3A-PB-O2B
2	F	701	GNP	PG-N3B-PB-O1B
2	G	701	GNP	PG-N3B-PB-O1B
4	E	1505	EPE	C10-C9-N1-C6
4	E	1505	EPE	N4-C7-C8-O8
2	E	1506	GNP	O4'-C4'-C5'-O5'
2	D	701	GNP	O4'-C4'-C5'-O5'
2	B	701	GNP	O4'-C4'-C5'-O5'
2	E	701	GNP	O4'-C4'-C5'-O5'
2	F	701	GNP	O4'-C4'-C5'-O5'
2	D	701	GNP	C3'-C4'-C5'-O5'
2	E	1506	GNP	C3'-C4'-C5'-O5'
2	F	701	GNP	C3'-C4'-C5'-O5'
2	E	701	GNP	C3'-C4'-C5'-O5'
2	B	701	GNP	C3'-C4'-C5'-O5'

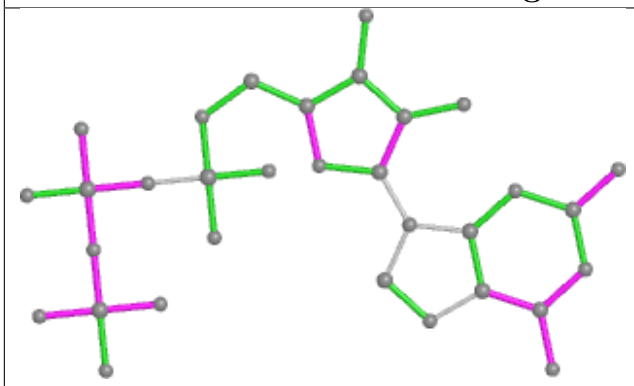
There are no ring outliers.

6 monomers are involved in 21 short contacts:

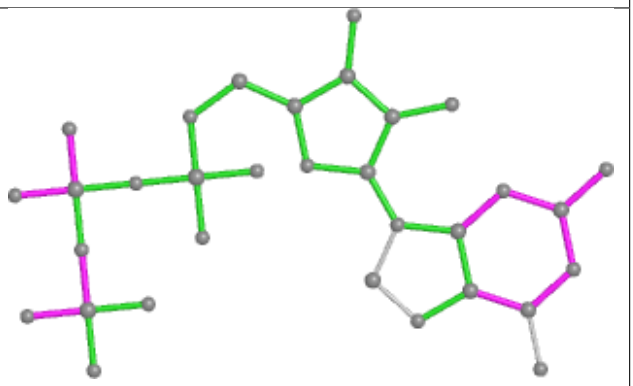
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	701	GNP	1	0
2	A	701	GNP	3	0
4	E	1505	EPE	10	0
2	G	701	GNP	2	0
2	B	701	GNP	3	0
2	E	1506	GNP	2	0

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 then 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.

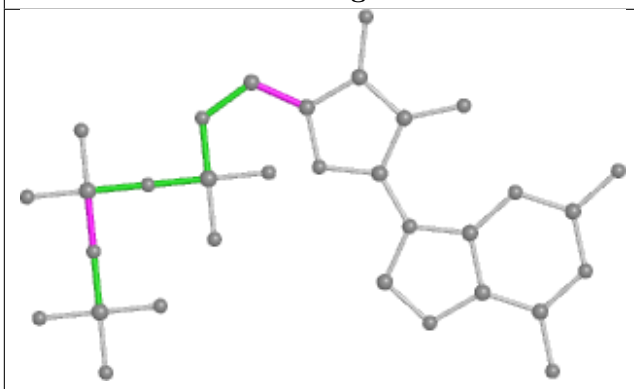
Ligand GNP E 701



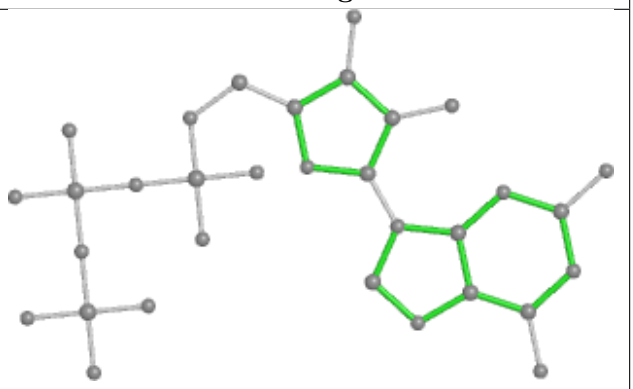
Bond lengths



Bond angles

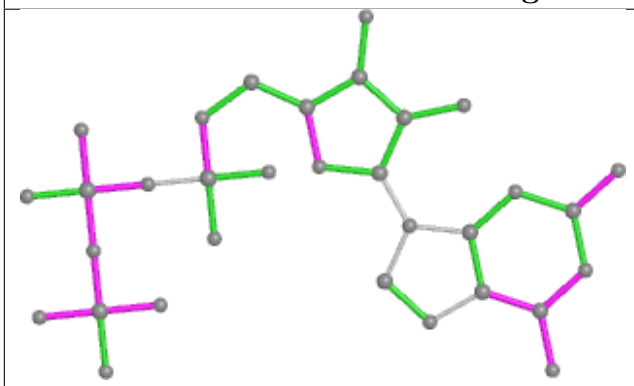


Torsions

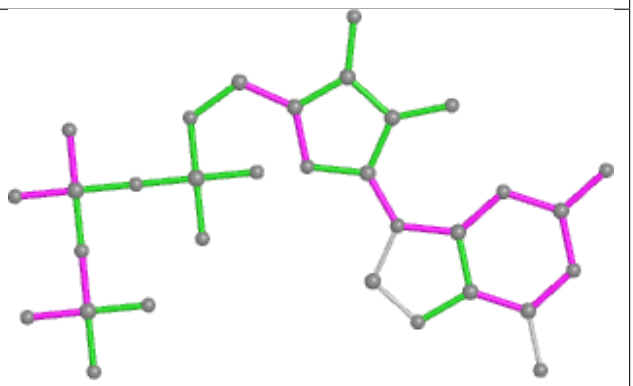


Rings

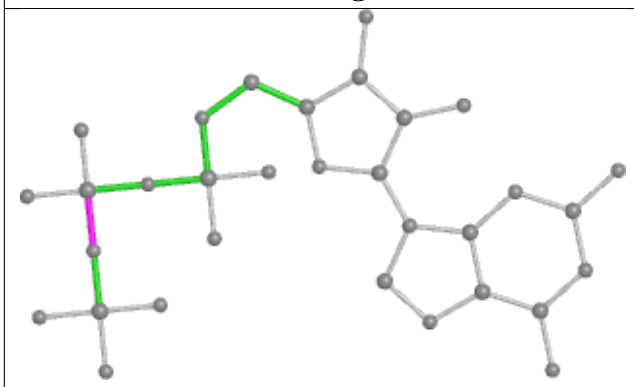
Ligand GNP A 701



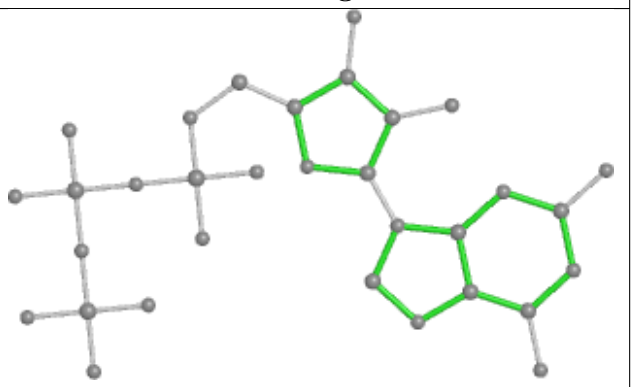
Bond lengths



Bond angles

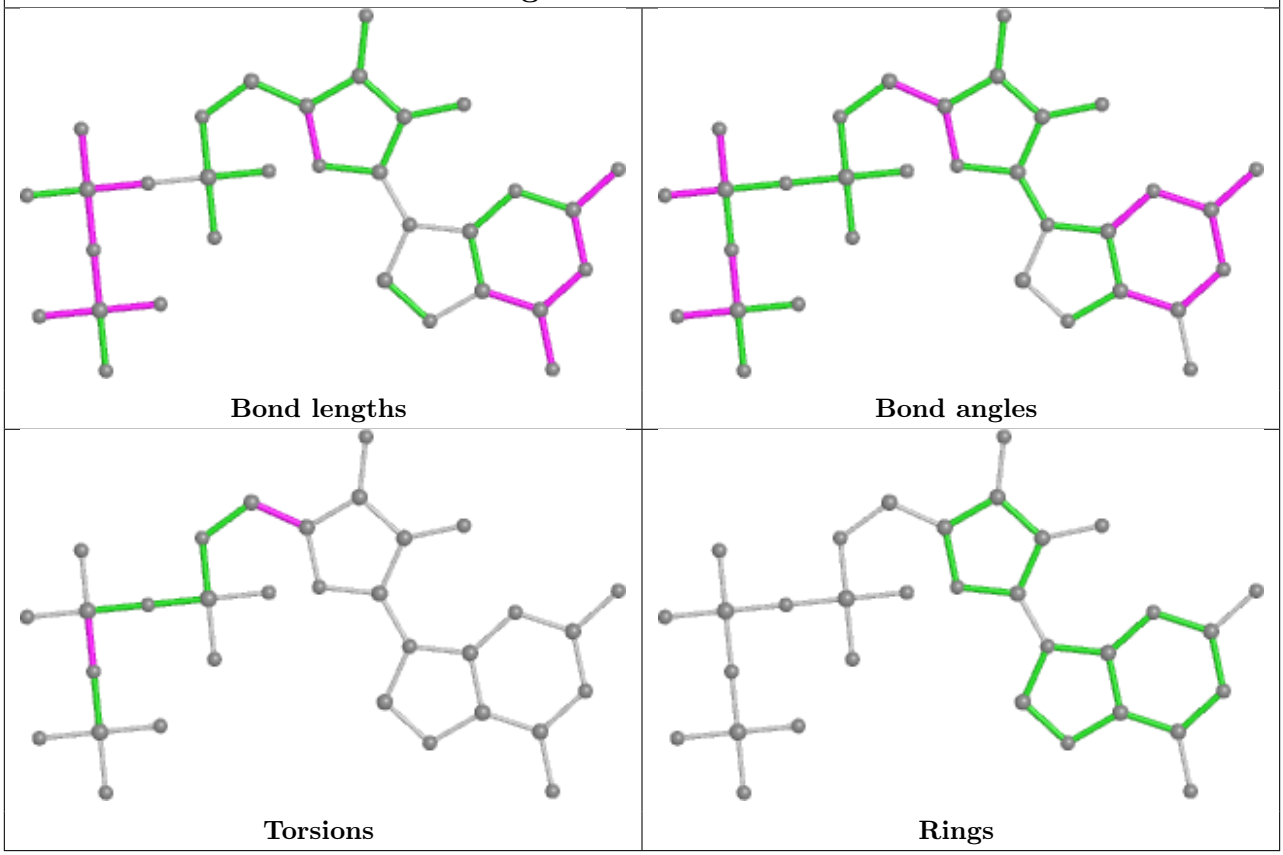


Torsions

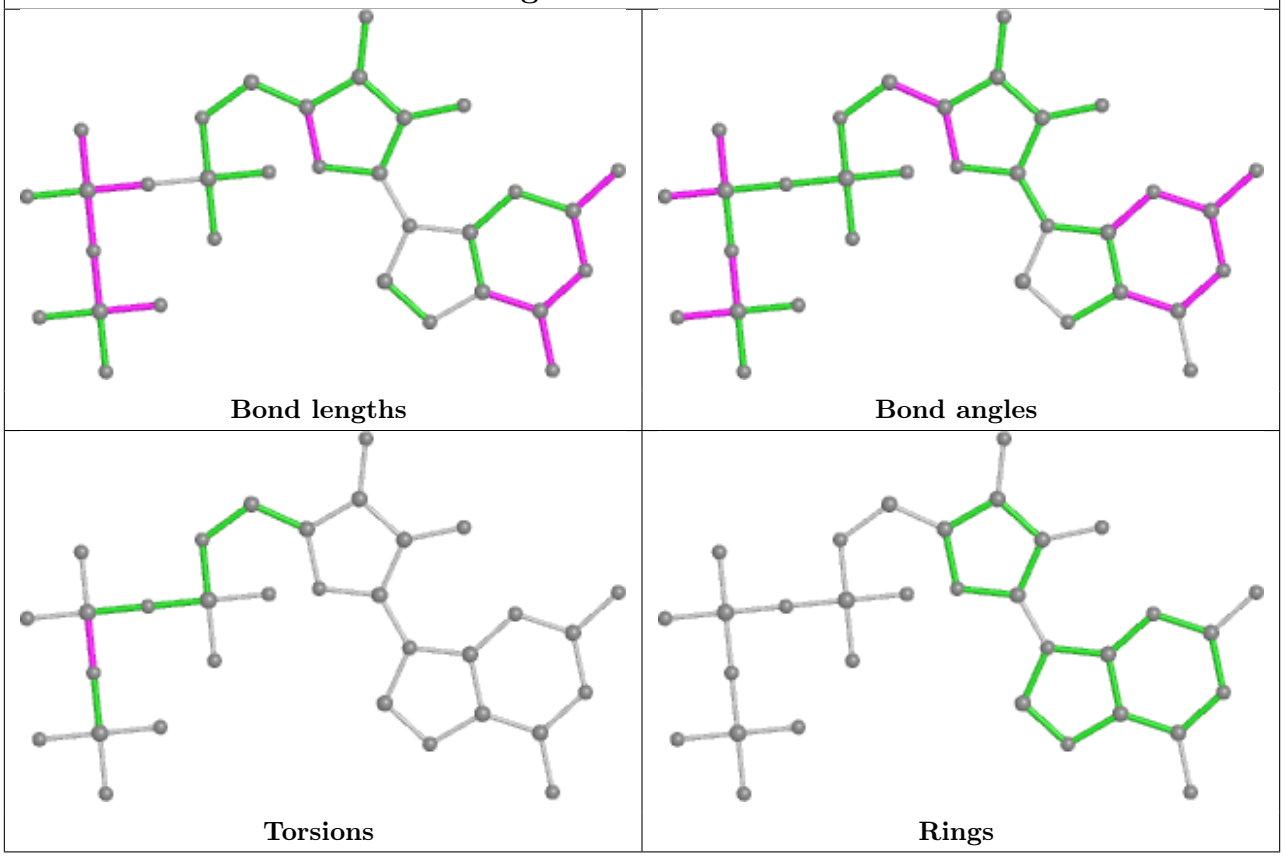


Rings

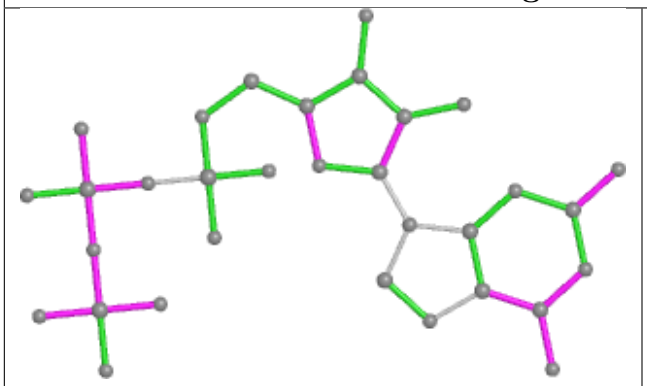
Ligand GNP D 701



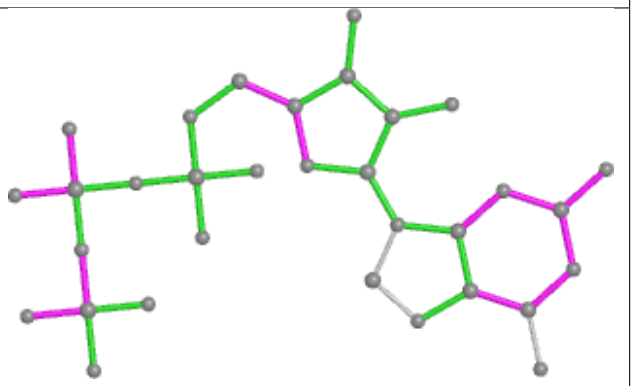
Ligand GNP G 701



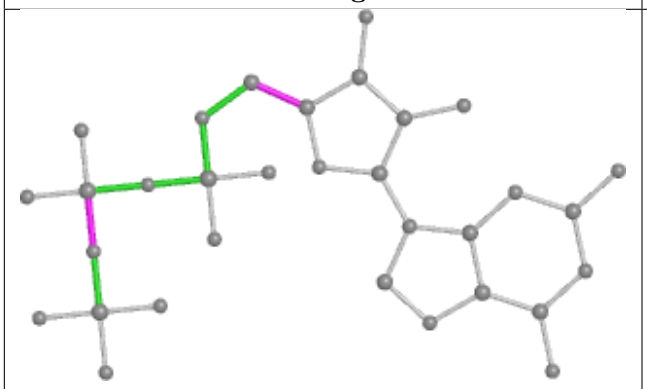
Ligand GNP B 701



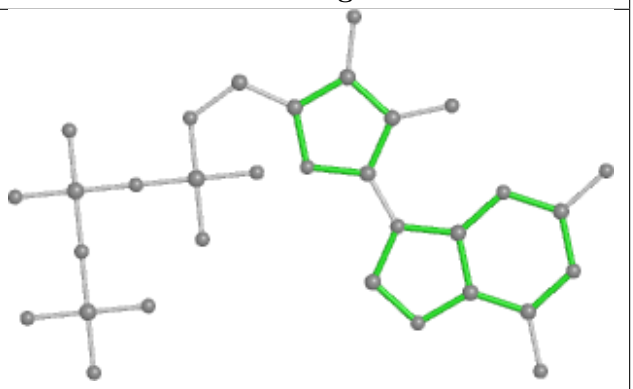
Bond lengths



Bond angles

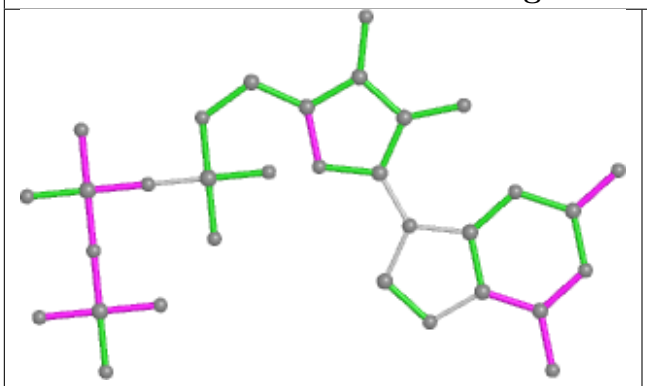


Torsions

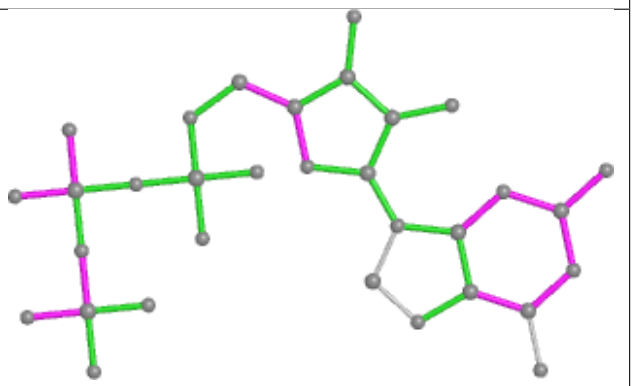


Rings

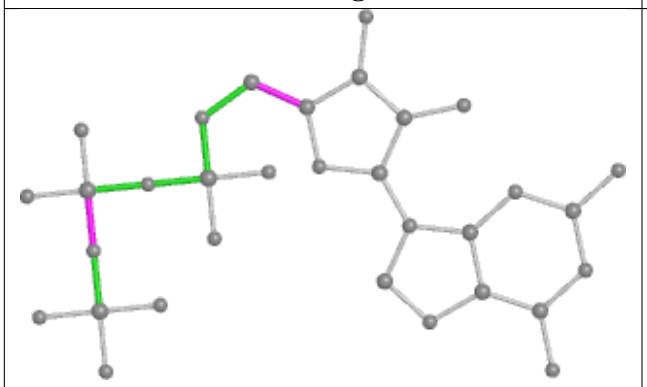
Ligand GNP F 701



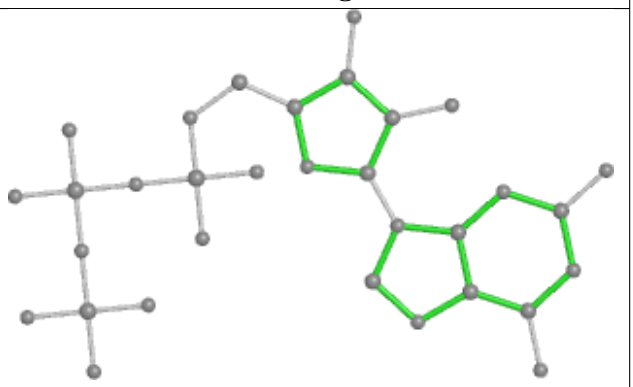
Bond lengths



Bond angles

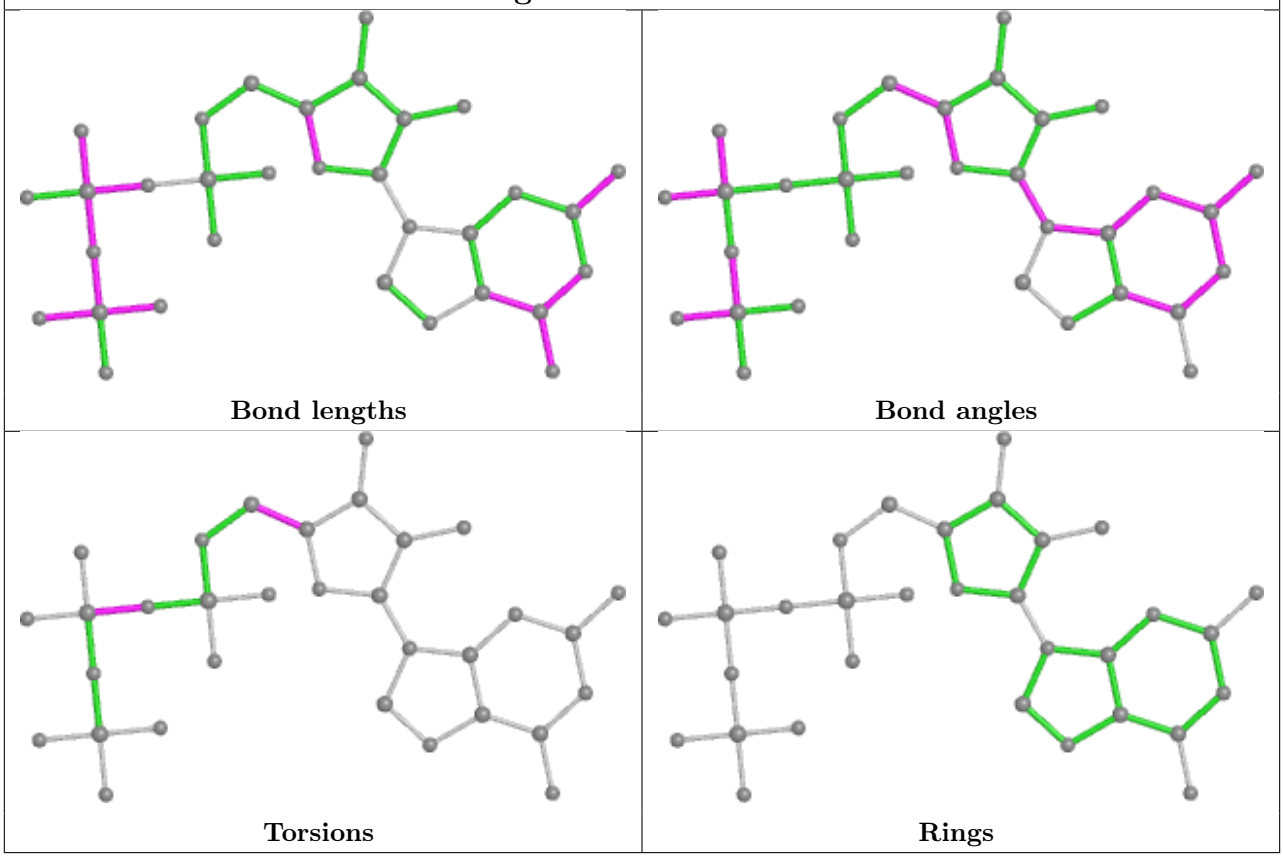


Torsions



Rings

Ligand GNP E 1506



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.