



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 12:41 am BST

PDB ID : 2VNT  
Title : UROKINASE-TYPE PLASMINOGEN ACTIVATOR INHIBITOR COMPLEX WITH A 1-(7- SULPHOAMIDOISOQUINOLINYL)GUANIDINE  
Authors : Fish, P.V.; Barber, C.G.; Brown, D.G.; Butt, R.; Henry, B.T.; Horne, V.; Huggins, J.P.; Mccleverty, D.; Phillips, C.; Webster, R.; Dickinson, R.P.; Collis, M.G.; King, E.; O’Gara, M.; Mcintosh, F.  
Deposited on : 2008-02-07  
Resolution : 2.20 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)  
Xtrriage (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) : 2.11

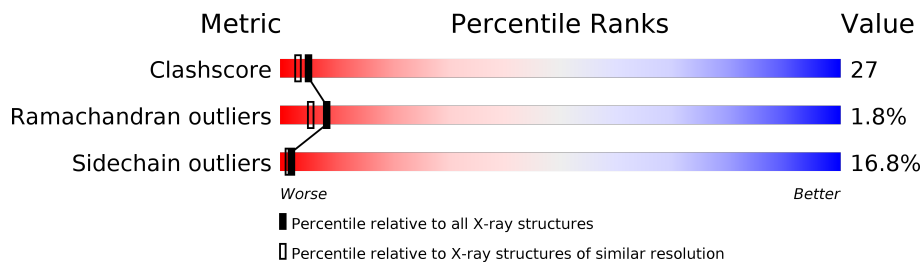
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	276	
1	B	276	
1	C	276	
1	D	276	
1	E	276	
1	F	276	

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

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
3	SO4	B	1262	-	-	X	-
3	SO4	E	1259	-	-	X	-

## 2 Entry composition [i](#)

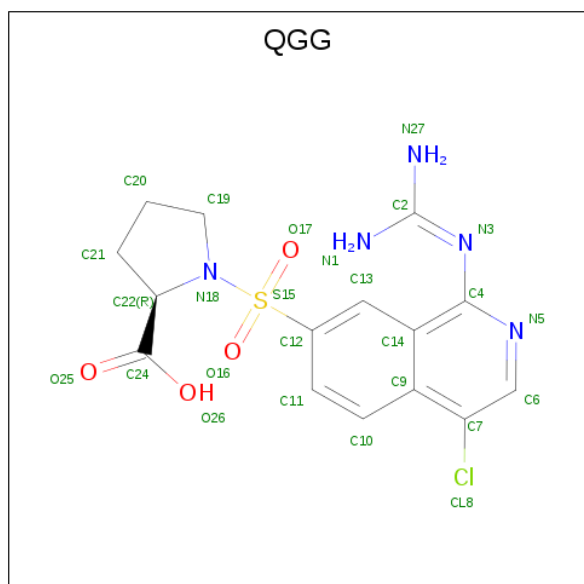
There are 4 unique types of molecules in this entry. The entry contains 13031 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UROKINASE-TYPE PLASMINOGEN ACTIVATOR.

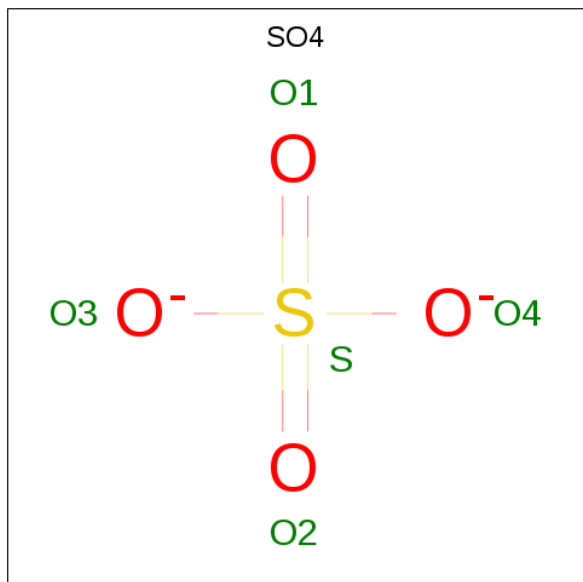
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	258	Total 2033	C 1280	N 356	O 379	S 18	0	0	1
1	B	259	Total 2041	C 1286	N 357	O 380	S 18	0	0	1
1	C	259	Total 2042	C 1285	N 359	O 380	S 18	0	0	1
1	D	259	Total 2041	C 1286	N 357	O 380	S 18	0	0	1
1	E	259	Total 2041	C 1286	N 357	O 380	S 18	0	0	1
1	F	257	Total 2022	C 1271	N 356	O 377	S 18	0	0	1

- Molecule 2 is 1-({4-CHLORO-1-[(DIAMINOMETHYLIDENE)AMINO]ISOQUINOLIN-7-YL}SULFONYL)-D-PROLINE (three-letter code: QGG) (formula: C<sub>15</sub>H<sub>16</sub>ClN<sub>5</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	Cl	N	O	S	0	0
			26	15	1	5	4	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			26	15	1	5	4	1		
2	C	1	Total	C	Cl	N	O	S	0	0
			26	15	1	5	4	1		
2	D	1	Total	C	Cl	N	O	S	0	0
			26	15	1	5	4	1		
2	E	1	Total	C	Cl	N	O	S	0	0
			26	15	1	5	4	1		
2	F	1	Total	C	Cl	N	O	S	0	0
			26	15	1	5	4	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		
3	D	1	Total	O S	0	0
			5	4 1		
3	D	1	Total	O S	0	0
			5	4 1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	90	Total O 90 90	0	0
4	B	86	Total O 86 86	0	0
4	C	106	Total O 106 106	0	0
4	D	113	Total O 113 113	0	0
4	E	124	Total O 124 124	0	0
4	F	91	Total O 91 91	0	0

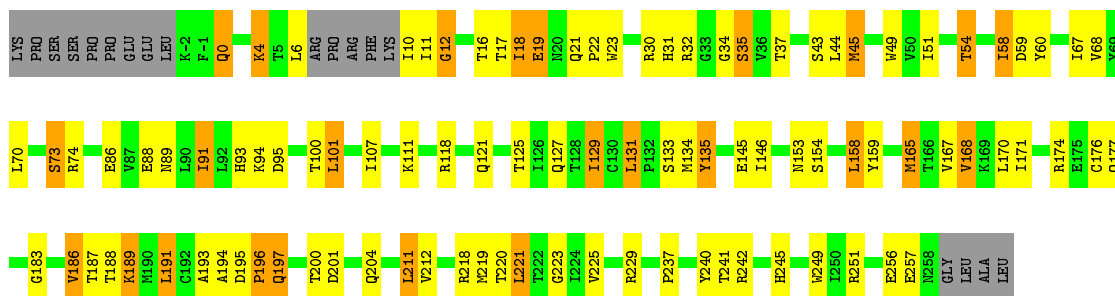
### 3 Residue-property plots

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. 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.

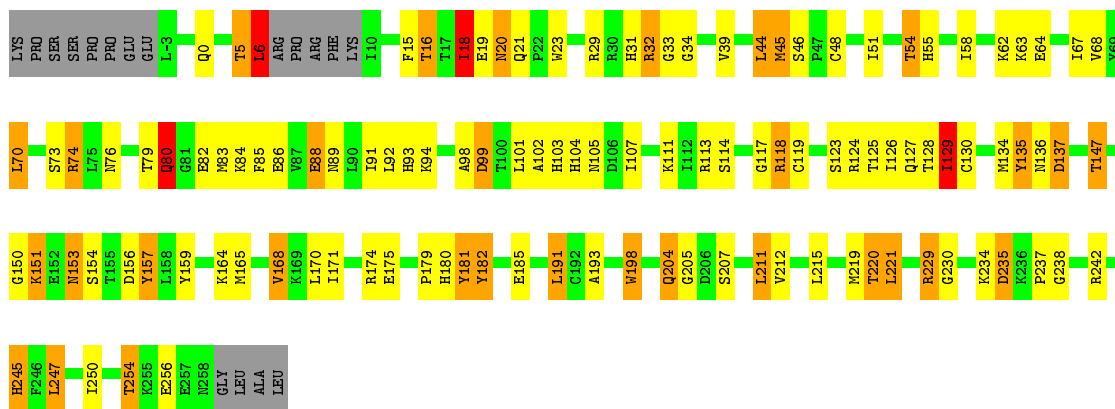
- Molecule 1: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

Chain A: 



- Molecule 1: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

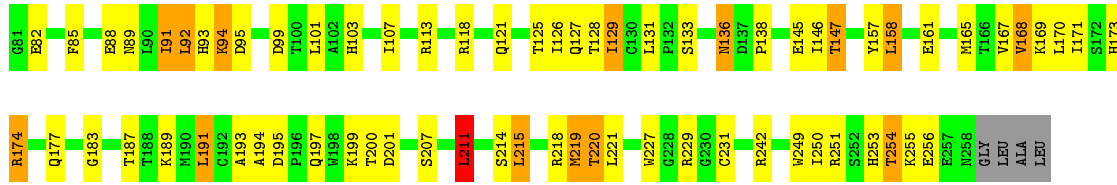
Chain B: 



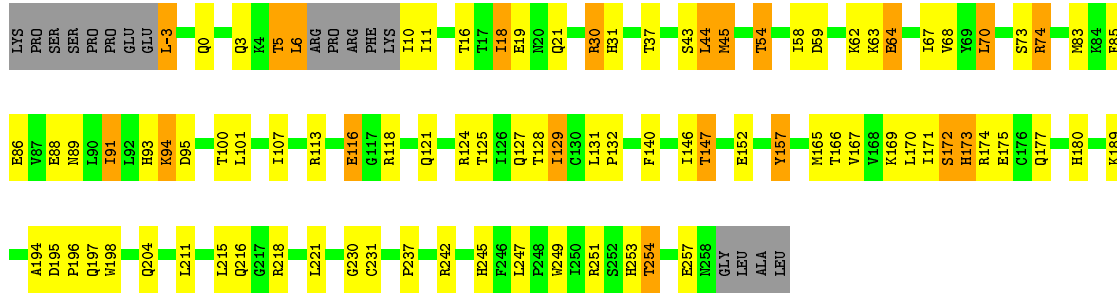
- Molecule 1: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

Chain C: 

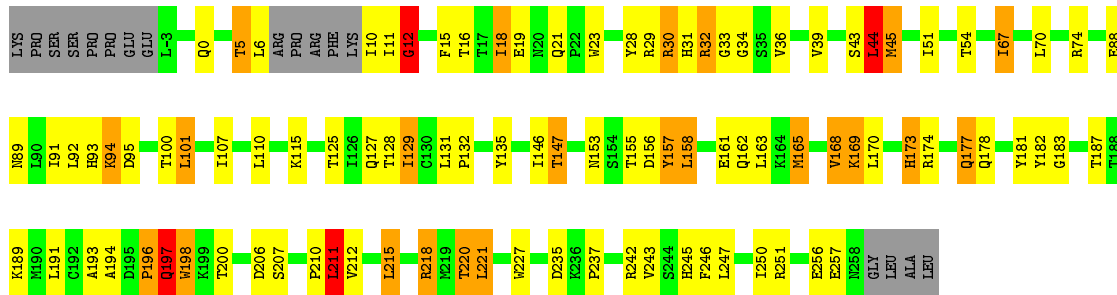




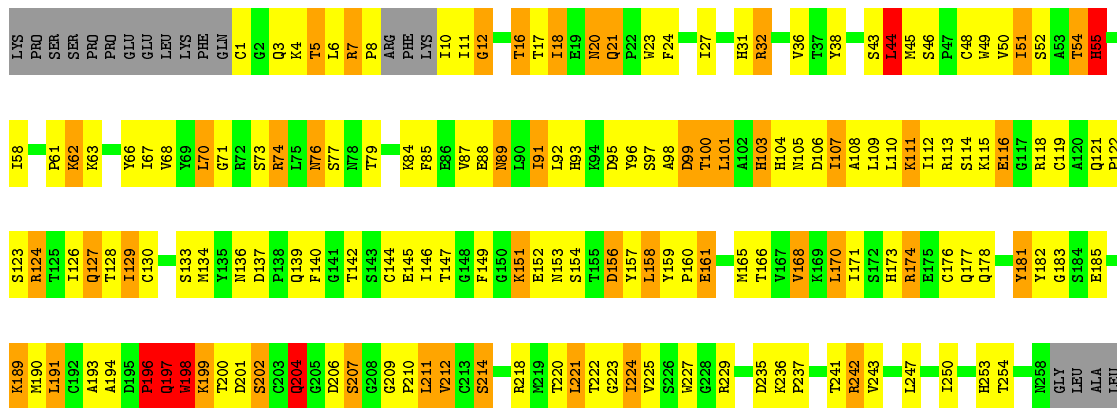
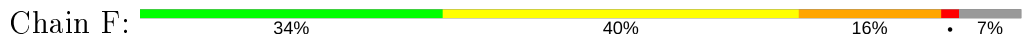
• Molecule 1: UROKINASE-TYPE PLASMINOGEN ACTIVATOR



• Molecule 1: UROKINASE-TYPE PLASMINOGEN ACTIVATOR



• Molecule 1: UROKINASE-TYPE PLASMINOGEN ACTIVATOR





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.56Å 181.11Å 104.36Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	35.00 – 2.20	Depositor
% Data completeness (in resolution range)	99.5 (35.00-2.20)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.241 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	13031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QGG, SO4

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	0.75	0/2082	0.91	6/2815 (0.2%)
1	B	0.79	1/2090 (0.0%)	0.95	7/2826 (0.2%)
1	C	0.70	0/2092	0.84	2/2830 (0.1%)
1	D	0.83	0/2090	0.97	4/2826 (0.1%)
1	E	0.85	0/2090	0.97	4/2826 (0.1%)
1	F	0.78	0/2071	0.90	4/2802 (0.1%)
All	All	0.78	1/12515 (0.0%)	0.93	27/16925 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
1	E	0	3
1	F	0	2
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	GLN	CG-CD	5.41	1.63	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	173	HIS	N-CA-C	-11.50	79.94	111.00
1	B	74	ARG	NE-CZ-NH2	-7.97	116.31	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	211	LEU	CA-CB-CG	7.45	132.42	115.30
1	B	211	LEU	CA-CB-CG	7.11	131.65	115.30
1	D	74	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	D	211	LEU	CA-CB-CG	6.75	130.82	115.30
1	A	201	ASP	CB-CG-OD1	6.38	124.04	118.30
1	E	44	LEU	CA-CB-CG	6.11	129.36	115.30
1	F	211	LEU	CA-CB-CG	6.06	129.25	115.30
1	B	191	LEU	CA-CB-CG	5.98	129.05	115.30
1	A	211	LEU	CA-CB-CG	5.98	129.05	115.30
1	B	74	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	196	PRO	N-CA-C	5.70	126.91	112.10
1	A	158	LEU	CA-CB-CG	5.56	128.09	115.30
1	E	74	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	F	44	LEU	CA-CB-CG	5.50	127.96	115.30
1	B	6	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	129	ILE	CB-CA-C	-5.49	100.63	111.60
1	C	99	ASP	CB-CG-OD2	5.42	123.18	118.30
1	E	211	LEU	CA-CB-CG	5.42	127.76	115.30
1	B	129	ILE	CB-CA-C	-5.15	101.30	111.60
1	E	110	LEU	CA-CB-CG	5.15	127.14	115.30
1	D	59	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	196	PRO	C-N-CA	5.09	134.43	121.70
1	B	18	ILE	CB-CA-C	-5.06	101.49	111.60
1	F	156	ASP	CB-CA-C	5.04	120.47	110.40
1	F	191	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	198	TRP	Peptide
1	D	172	SER	Peptide
1	E	12	GLY	Peptide
1	E	196	PRO	Peptide
1	E	197	GLN	Peptide
1	F	196	PRO	Peptide
1	F	198	TRP	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2033	0	1980	83	0
1	B	2041	0	1991	129	0
1	C	2042	0	1987	92	0
1	D	2041	0	1991	88	0
1	E	2041	0	1991	101	0
1	F	2022	0	1970	193	0
2	A	26	0	15	1	0
2	B	26	0	15	4	0
2	C	26	0	15	1	0
2	D	26	0	15	1	0
2	E	26	0	15	1	0
2	F	26	0	15	5	0
3	B	20	0	0	5	0
3	D	15	0	0	1	0
3	E	10	0	0	3	0
4	A	90	0	0	7	0
4	B	86	0	0	20	0
4	C	106	0	0	9	0
4	D	113	0	0	15	0
4	E	124	0	0	12	0
4	F	91	0	0	31	0
All	All	13031	0	12000	661	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 27.

All (661) 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:187:THR:OG1	1:A:189:LYS:HD2	1.35	1.24
1:D:94:LYS:H	1:D:94:LYS:CD	1.51	1.20
1:F:21:GLN:HE22	1:F:165:MET:CE	1.53	1.20
1:B:80:GLN:HG2	4:B:2030:HOH:O	1.42	1.20
1:B:45:MET:HE2	1:B:51:ILE:CG2	1.74	1.15
1:D:94:LYS:HD2	1:D:94:LYS:N	1.49	1.15

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:ASN:HD21	1:F:161:GLU:HG3	1.13	1.13
1:E:21:GLN:HG3	1:E:147:THR:HG21	1.20	1.12
1:F:146:ILE:HG22	4:F:2071:HOH:O	1.45	1.12
1:A:34:GLY:HA2	1:A:35:SER:CB	1.81	1.10
1:F:76:ASN:ND2	1:F:161:GLU:HG3	1.66	1.09
1:A:34:GLY:HA2	1:A:35:SER:HB3	1.18	1.08
1:F:21:GLN:HE22	1:F:165:MET:HE3	1.12	1.08
1:A:187:THR:OG1	1:A:189:LYS:CD	2.01	1.07
1:B:21:GLN:HG3	1:B:147:THR:HG21	1.33	1.07
1:C:7:ARG:HE	1:C:8:PRO:HD2	1.18	1.05
1:D:11:ILE:HD11	1:D:231:CYS:HB3	1.33	1.05
1:D:21:GLN:HG3	1:D:147:THR:HG21	1.34	1.04
1:B:136:ASN:HA	1:B:137:ASP:HB2	1.43	1.00
1:A:12:GLY:HA2	1:A:200:THR:OG1	1.61	1.00
1:F:38:TYR:HD1	4:F:2009:HOH:O	1.45	1.00
1:F:100:THR:HG23	4:F:2029:HOH:O	1.61	1.00
1:F:66:TYR:HB3	4:F:2021:HOH:O	1.59	0.99
1:B:123:SER:HB2	1:E:33:GLY:HA3	1.45	0.98
1:F:21:GLN:NE2	1:F:165:MET:HE3	1.78	0.97
1:B:119:CYS:HB2	4:B:2039:HOH:O	1.65	0.96
1:F:182:TYR:HE1	1:F:236:LYS:HD2	1.29	0.96
1:F:76:ASN:HD21	1:F:161:GLU:CG	1.79	0.96
1:E:11:ILE:O	1:E:12:GLY:O	1.82	0.96
1:D:43:SER:HB3	1:D:129:ILE:HD11	1.46	0.96
1:B:45:MET:HE2	1:B:51:ILE:HG21	1.45	0.95
1:F:18:ILE:HD11	1:F:79:THR:HG21	1.49	0.95
1:F:198:TRP:CB	1:F:199:LYS:HD2	1.98	0.93
1:B:45:MET:CE	1:B:51:ILE:CG2	2.45	0.93
1:F:21:GLN:NE2	1:F:165:MET:CE	2.32	0.92
1:B:45:MET:CE	1:B:51:ILE:HG21	1.99	0.92
1:F:250:ILE:HB	4:F:2089:HOH:O	1.70	0.92
1:A:93:HIS:HD2	1:A:95:ASP:H	1.18	0.92
1:E:93:HIS:HD2	1:E:95:ASP:H	1.09	0.92
1:C:94:LYS:HE2	1:C:249:TRP:HE1	1.34	0.91
1:F:130:CYS:HB2	4:F:2076:HOH:O	1.69	0.91
1:B:45:MET:HE3	1:B:221:LEU:HD12	1.53	0.91
1:E:54:THR:HG23	1:E:107:ILE:O	1.70	0.91
1:F:198:TRP:HB3	1:F:199:LYS:HD2	1.51	0.91
1:D:167:VAL:HB	4:D:2070:HOH:O	1.70	0.90
1:D:195:ASP:O	1:D:197:GLN:HA	1.70	0.90
1:F:207:SER:OG	2:F:1258:QGG:CL8	2.25	0.90

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:LEU:HD21	1:F:242:ARG:HE	1.35	0.89
1:C:35:SER:HA	1:C:36:VAL:HB	1.50	0.89
1:F:181:TYR:HD2	4:F:2056:HOH:O	1.55	0.89
1:F:10:ILE:CG2	1:F:12:GLY:HA3	2.03	0.88
1:A:187:THR:CB	1:A:189:LYS:HD2	2.03	0.88
1:F:145:GLU:HB2	4:F:2052:HOH:O	1.72	0.88
1:A:16:THR:HG21	1:A:165:MET:SD	2.13	0.88
1:F:76:ASN:HB3	4:F:2022:HOH:O	1.73	0.88
1:B:21:GLN:CG	1:B:147:THR:HG21	2.03	0.88
1:F:21:GLN:CD	1:F:147:THR:HG21	1.93	0.87
1:A:45:MET:CE	1:A:131:LEU:HD11	2.05	0.87
1:D:54:THR:HG23	1:D:107:ILE:O	1.75	0.87
1:E:21:GLN:CG	1:E:147:THR:HG21	2.05	0.86
1:B:45:MET:HE2	1:B:51:ILE:HG22	1.55	0.86
1:D:169:LYS:HD3	1:D:196:PRO:HG3	1.56	0.86
1:F:21:GLN:HE22	1:F:165:MET:HE2	1.39	0.86
1:D:196:PRO:HA	1:D:197:GLN:HG2	1.56	0.86
1:C:45:MET:HE2	1:C:131:LEU:HD21	1.56	0.86
1:F:197:GLN:HB3	1:F:198:TRP:CE3	2.11	0.85
1:B:101:LEU:O	1:B:101:LEU:HG	1.74	0.85
1:B:134:MET:O	1:B:135:TYR:HB2	1.74	0.85
1:E:197:GLN:OE1	1:E:198:TRP:HB3	1.76	0.85
1:D:16:THR:HG21	1:D:165:MET:HG2	1.58	0.84
1:F:182:TYR:CE1	1:F:236:LYS:HD2	2.11	0.84
1:D:11:ILE:CD1	1:D:231:CYS:HB3	2.07	0.84
1:C:54:THR:HG22	1:C:107:ILE:O	1.78	0.83
1:C:21:GLN:HG3	1:C:147:THR:HG21	1.58	0.83
1:B:207:SER:OG	2:B:1258:QGG:CL8	2.32	0.83
1:D:197:GLN:HB3	1:D:198:TRP:CD1	2.13	0.83
1:F:146:ILE:HG13	1:F:166:THR:HG22	1.61	0.83
1:E:221:LEU:HD13	1:E:243:VAL:HG21	1.60	0.82
1:A:195:ASP:OD1	1:A:197:GLN:HB3	1.79	0.82
1:C:35:SER:HA	1:C:36:VAL:CB	2.10	0.82
1:A:45:MET:HE3	1:A:131:LEU:HD11	1.62	0.81
1:B:80:GLN:HG3	1:E:36:VAL:HG22	1.63	0.81
1:C:168:VAL:HG13	1:C:193:ALA:HB1	1.61	0.81
1:F:176:CYS:SG	4:F:2056:HOH:O	2.37	0.81
1:D:54:THR:HG21	1:D:93:HIS:H	1.43	0.81
1:C:187:THR:OG1	1:C:189:LYS:HG2	1.81	0.80
1:A:11:ILE:O	1:A:12:GLY:O	1.99	0.80
1:A:18:ILE:HG23	1:A:73:SER:HB3	1.63	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:MET:SD	4:B:2011:HOH:O	2.38	0.80
1:E:54:THR:HG21	1:E:93:HIS:H	1.46	0.80
1:A:31:HIS:CE1	1:A:37:THR:OG1	2.34	0.80
1:E:12:GLY:CA	1:E:200:THR:OG1	2.29	0.80
1:C:145:GLU:HB3	4:C:2054:HOH:O	1.81	0.79
1:C:93:HIS:HD2	1:C:95:ASP:H	1.28	0.79
1:D:171:ILE:HD11	1:D:194:ALA:HB3	1.64	0.79
1:E:11:ILE:O	1:E:12:GLY:C	2.21	0.79
1:F:145:GLU:HB3	4:F:2044:HOH:O	1.81	0.79
1:C:161:GLU:HG2	4:C:2021:HOH:O	1.83	0.78
1:B:123:SER:HB2	1:E:33:GLY:CA	2.12	0.78
1:B:54:THR:HG23	1:B:107:ILE:O	1.82	0.78
1:F:76:ASN:ND2	1:F:161:GLU:OE1	2.18	0.77
1:B:16:THR:HG23	4:B:2009:HOH:O	1.85	0.77
1:C:94:LYS:CE	1:C:249:TRP:HE1	1.97	0.77
1:F:116:GLU:HB2	4:F:2034:HOH:O	1.83	0.77
1:F:91:ILE:HD12	1:F:253:HIS:HB3	1.64	0.77
1:C:11:ILE:HD11	1:C:231:CYS:HB3	1.65	0.77
1:D:21:GLN:CG	1:D:147:THR:HG21	2.13	0.77
1:D:172:SER:OG	1:D:174:ARG:HG2	1.85	0.77
1:D:196:PRO:HA	1:D:197:GLN:CG	2.15	0.77
1:F:38:TYR:CD1	4:F:2009:HOH:O	2.29	0.77
1:D:173:HIS:O	1:D:177:GLN:HG2	1.85	0.77
1:F:12:GLY:HA2	1:F:200:THR:OG1	1.85	0.77
1:F:76:ASN:ND2	1:F:161:GLU:CG	2.42	0.77
1:F:16:THR:HB	1:F:20:ASN:HD21	1.49	0.76
1:E:45:MET:HE3	1:E:131:LEU:HD21	1.66	0.76
1:F:18:ILE:HG21	1:F:71:GLY:HA2	1.68	0.75
1:B:45:MET:CE	1:B:51:ILE:HG22	2.13	0.74
1:F:99:ASP:HB2	4:F:2029:HOH:O	1.87	0.74
1:F:145:GLU:HG2	1:F:212:VAL:HG23	1.68	0.74
1:B:70:LEU:HD22	1:B:85:PHE:CE2	2.22	0.74
1:B:18:ILE:HG13	1:B:73:SER:OG	1.87	0.74
1:B:45:MET:CE	1:B:221:LEU:HD12	2.18	0.74
1:D:196:PRO:CA	1:D:197:GLN:HG2	2.16	0.74
1:E:168:VAL:HG13	1:E:193:ALA:HB1	1.69	0.73
1:B:32:ARG:NH1	3:B:1262:SO4:O1	2.22	0.73
1:E:93:HIS:CD2	1:E:95:ASP:H	2.00	0.73
1:F:214:SER:HA	4:F:2074:HOH:O	1.88	0.73
1:E:18:ILE:HD13	1:E:125:THR:HB	1.69	0.73
1:B:101:LEU:HB2	1:B:229:ARG:HH21	1.53	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:MET:CE	1:F:51:ILE:HB	2.19	0.73
1:A:34:GLY:HA3	4:A:2009:HOH:O	1.88	0.73
1:F:10:ILE:HG23	1:F:12:GLY:HA3	1.70	0.73
1:F:202:SER:OG	1:F:225:VAL:HG13	1.88	0.72
1:A:196:PRO:N	1:A:197:GLN:HB2	2.04	0.72
1:E:32:ARG:HD3	3:E:1259:SO4:O2	1.88	0.72
1:A:31:HIS:HE1	1:A:37:THR:OG1	1.72	0.72
1:F:93:HIS:CE1	1:F:95:ASP:HB2	2.24	0.72
2:B:1258:QGG:N27	4:B:2084:HOH:O	2.21	0.72
1:F:198:TRP:HB2	1:F:199:LYS:HD2	1.72	0.72
1:D:16:THR:CG2	1:D:165:MET:HG2	2.20	0.71
1:F:202:SER:HB3	2:F:1258:QGG:H1N1	1.55	0.71
1:E:197:GLN:OE1	1:E:198:TRP:CB	2.38	0.71
1:C:207:SER:OG	2:C:1258:QGG:CL8	2.45	0.71
1:E:12:GLY:HA3	1:E:200:THR:OG1	1.91	0.71
1:C:35:SER:CA	1:C:36:VAL:HB	2.20	0.71
1:B:93:HIS:CD2	1:B:105:ASN:HB3	2.25	0.70
1:D:45:MET:HE2	1:D:221:LEU:HD22	1.73	0.70
1:B:31:HIS:HD2	3:B:1262:SO4:O3	1.72	0.70
1:A:10:ILE:HG22	1:A:12:GLY:HA3	1.74	0.70
1:F:146:ILE:HG13	1:F:166:THR:CG2	2.21	0.70
1:F:45:MET:HE3	1:F:51:ILE:HB	1.73	0.69
1:A:45:MET:HE1	1:A:131:LEU:HD11	1.75	0.69
1:E:165:MET:SD	4:E:2063:HOH:O	2.49	0.69
1:A:34:GLY:CA	1:A:35:SER:CB	2.66	0.69
1:E:45:MET:CE	1:E:131:LEU:HD21	2.22	0.69
1:C:21:GLN:CG	1:C:147:THR:HG21	2.23	0.68
1:D:16:THR:HG21	1:D:165:MET:CG	2.24	0.68
1:F:11:ILE:O	1:F:12:GLY:O	2.12	0.68
1:B:54:THR:HG22	1:B:92:LEU:HG	1.76	0.68
1:A:187:THR:OG1	1:A:189:LYS:HD3	1.94	0.68
1:C:45:MET:CE	1:C:131:LEU:HD21	2.24	0.68
1:D:94:LYS:H	1:D:94:LYS:HD2	0.64	0.68
1:B:151:LYS:HG2	1:B:153:ASN:O	1.94	0.67
1:C:138:PRO:HD3	1:C:215:LEU:HD11	1.75	0.67
1:C:218:ARG:O	1:C:220:THR:HG22	1.94	0.67
1:E:168:VAL:CG1	1:E:193:ALA:HB1	2.24	0.67
1:F:62:LYS:HB3	1:F:62:LYS:HZ2	1.60	0.67
1:B:124:ARG:NH2	3:B:1259:SO4:O2	2.27	0.67
1:C:7:ARG:NE	1:C:8:PRO:HD2	2.02	0.67
1:D:45:MET:HE3	1:D:131:LEU:HD21	1.76	0.67

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:ARG:HD3	1:F:77:SER:OG	1.95	0.67
1:A:168:VAL:HG13	1:A:193:ALA:HB1	1.76	0.67
1:E:45:MET:HE1	1:E:51:ILE:HG21	1.77	0.67
1:B:93:HIS:HD2	1:B:105:ASN:HB3	1.59	0.67
1:B:219:MET:CE	4:B:2073:HOH:O	2.43	0.67
1:B:151:LYS:HE2	1:B:156:ASP:O	1.95	0.66
1:D:93:HIS:HD2	1:D:95:ASP:H	1.42	0.66
1:E:165:MET:HG3	4:E:2063:HOH:O	1.95	0.66
1:B:44:LEU:HD13	1:B:128:THR:HG22	1.77	0.66
1:A:196:PRO:CA	1:A:197:GLN:HB2	2.24	0.66
1:C:136:ASN:CG	1:C:136:ASN:O	2.34	0.66
1:D:174:ARG:HG3	1:D:175:GLU:N	2.10	0.66
1:B:32:ARG:NH1	3:B:1262:SO4:S	2.70	0.65
1:D:94:LYS:HE2	1:D:249:TRP:HE1	1.61	0.65
1:B:134:MET:O	1:B:135:TYR:CB	2.43	0.65
1:F:242:ARG:O	1:F:242:ARG:HG3	1.97	0.65
1:F:181:TYR:CD2	4:F:2056:HOH:O	2.39	0.65
1:B:180:HIS:O	1:B:181:TYR:HB2	1.97	0.65
1:B:123:SER:CB	1:E:33:GLY:HA3	2.24	0.65
1:A:194:ALA:HB2	1:A:237:PRO:HB3	1.79	0.65
1:E:94:LYS:H	1:E:94:LYS:CD	2.08	0.65
1:E:207:SER:OG	2:E:1258:QGG:CL8	2.51	0.65
1:F:191:LEU:HD11	1:F:222:THR:HG22	1.79	0.65
1:C:147:THR:HG23	4:C:2053:HOH:O	1.96	0.64
1:F:10:ILE:HG22	1:F:12:GLY:HA3	1.79	0.64
1:F:76:ASN:CG	1:F:161:GLU:HG3	2.16	0.64
1:F:199:LYS:NZ	1:F:199:LYS:HA	2.13	0.64
1:E:182:TYR:CE2	1:E:237:PRO:HD2	2.32	0.64
1:F:68:VAL:HG11	1:F:112:ILE:HG21	1.80	0.64
1:A:18:ILE:HG23	1:A:73:SER:CB	2.27	0.64
1:B:165:MET:CE	4:B:2011:HOH:O	2.44	0.64
1:E:251:ARG:NH2	4:E:2120:HOH:O	2.30	0.64
1:C:18:ILE:HD13	1:C:125:THR:HB	1.79	0.63
1:C:145:GLU:CB	4:C:2054:HOH:O	2.41	0.63
1:E:94:LYS:HD3	1:E:94:LYS:H	1.62	0.63
1:A:45:MET:HE1	1:A:131:LEU:CD1	2.28	0.63
1:B:242:ARG:NH1	4:B:2081:HOH:O	2.31	0.63
1:A:34:GLY:CA	1:A:35:SER:HB3	2.12	0.63
1:C:214:SER:OG	1:C:219:MET:CE	2.47	0.63
1:F:16:THR:HG22	4:F:2007:HOH:O	1.98	0.63
1:D:132:PRO:O	1:D:247:LEU:HD11	1.99	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PRO:HB2	1:A:197:GLN:HG3	1.80	0.62
1:B:54:THR:HG21	1:B:93:HIS:H	1.64	0.62
1:D:18:ILE:HD13	1:D:125:THR:HB	1.79	0.62
1:D:43:SER:CB	1:D:129:ILE:HD11	2.26	0.62
1:B:250:ILE:O	1:B:254:THR:OG1	2.17	0.62
1:C:168:VAL:CG1	1:C:193:ALA:HB1	2.28	0.62
1:B:88:GLU:OE1	1:B:88:GLU:N	2.33	0.62
1:C:11:ILE:HD13	1:C:201:ASP:HB3	1.82	0.62
1:E:45:MET:HE3	1:E:131:LEU:CD2	2.30	0.62
1:E:45:MET:CE	1:E:51:ILE:HG21	2.30	0.62
1:F:153:ASN:OD1	1:F:154:SER:N	2.32	0.62
1:D:91:ILE:O	1:D:91:ILE:HG13	1.98	0.61
1:F:11:ILE:HD12	4:F:2049:HOH:O	1.99	0.61
1:D:194:ALA:HB2	1:D:237:PRO:HB3	1.82	0.61
1:F:21:GLN:CG	1:F:147:THR:HG21	2.29	0.61
1:A:58:ILE:HD11	1:D:100:THR:HG22	1.81	0.61
1:E:146:ILE:HG23	1:E:211:LEU:HD23	1.82	0.61
1:C:0:GLN:H	1:C:127:GLN:NE2	1.98	0.61
1:F:229:ARG:HG2	1:F:236:LYS:HE3	1.81	0.61
1:D:157:TYR:HE2	1:E:15:PHE:O	1.83	0.61
1:F:48:CYS:O	1:F:112:ILE:HG12	2.01	0.61
1:B:6:LEU:HD11	1:C:38:TYR:O	2.01	0.61
1:E:169:LYS:HE2	1:E:196:PRO:HG3	1.82	0.61
1:A:30:ARG:HE	1:A:67:ILE:HD11	1.66	0.61
1:D:204:GLN:HG2	4:D:2091:HOH:O	2.01	0.61
1:A:196:PRO:HB2	1:A:197:GLN:CG	2.31	0.61
1:C:133:SER:OG	1:C:136:ASN:ND2	2.34	0.61
1:D:62:LYS:HE2	1:D:64:GLU:HG3	1.82	0.61
1:B:33:GLY:HA3	4:B:2017:HOH:O	2.00	0.60
1:F:87:VAL:HG11	1:F:110:LEU:HD23	1.82	0.60
1:B:157:TYR:HB2	4:B:2055:HOH:O	2.00	0.60
1:E:191:LEU:HD11	1:E:242:ARG:HG3	1.82	0.60
1:B:5:THR:HG21	1:B:19:GLU:OE1	2.02	0.60
1:A:89:ASN:HB2	1:A:111:LYS:HB3	1.84	0.60
1:F:134:MET:HG2	1:F:247:LEU:HD12	1.84	0.60
1:F:27:ILE:HG23	4:F:2021:HOH:O	2.01	0.60
1:A:30:ARG:NH2	1:A:86:GLU:OE1	2.29	0.60
1:C:177:GLN:HG3	1:C:183:GLY:O	2.01	0.59
1:C:94:LYS:HE3	1:C:94:LYS:H	1.66	0.59
1:F:145:GLU:CG	1:F:212:VAL:HG23	2.30	0.59
1:C:20:ASN:HB3	1:C:165:MET:HE1	1.83	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:MET:CE	1:A:131:LEU:CD1	2.78	0.59
1:F:16:THR:HB	1:F:20:ASN:ND2	2.17	0.59
1:F:7:ARG:HB2	1:F:124:ARG:NH2	2.18	0.59
1:F:202:SER:HB3	2:F:1258:QGG:N1	2.17	0.59
1:F:218:ARG:O	1:F:220:THR:HG23	2.02	0.59
1:E:92:LEU:N	1:E:92:LEU:HD12	2.17	0.59
1:F:32:ARG:CG	1:F:32:ARG:HH11	2.15	0.59
1:E:89:ASN:ND2	4:E:2042:HOH:O	2.36	0.59
1:E:157:TYR:CD2	1:E:158:LEU:HD22	2.37	0.58
1:A:101:LEU:HG	1:A:229:ARG:NH1	2.18	0.58
1:C:0:GLN:H	1:C:127:GLN:HE22	1.51	0.58
1:F:191:LEU:CD2	1:F:242:ARG:HE	2.12	0.58
1:B:230:GLY:O	2:B:1258:QGG:H13	2.03	0.58
1:C:118:ARG:CZ	1:C:121:GLN:HE22	2.16	0.58
1:E:93:HIS:HE1	4:E:2044:HOH:O	1.85	0.58
1:D:70:LEU:HD22	1:D:85:PHE:CE2	2.38	0.58
1:F:54:THR:HG23	1:F:107:ILE:O	2.04	0.58
1:F:55:HIS:O	1:F:55:HIS:CD2	2.57	0.58
1:C:250:ILE:O	1:C:254:THR:HB	2.04	0.57
1:F:223:GLY:HA2	1:F:241:THR:O	2.03	0.57
1:B:185:GLU:HB2	4:B:2065:HOH:O	2.04	0.57
1:D:5:THR:HG23	1:D:6:LEU:N	2.19	0.57
1:C:35:SER:HA	1:C:36:VAL:CG2	2.34	0.57
1:E:242:ARG:HD3	1:E:245:HIS:CE1	2.40	0.57
1:E:54:THR:CG2	1:E:107:ILE:O	2.51	0.57
1:C:214:SER:OG	1:C:219:MET:HE3	2.04	0.57
1:C:242:ARG:HD3	4:C:2098:HOH:O	2.04	0.57
1:F:152:GLU:OE1	1:F:160:PRO:HB3	2.05	0.57
1:B:130:CYS:HB2	1:B:220:THR:HG22	1.87	0.57
1:F:21:GLN:NE2	1:F:165:MET:HE2	2.09	0.57
1:F:173:HIS:CE1	1:F:177:GLN:NE2	2.73	0.57
1:B:18:ILE:HD13	1:B:125:THR:HB	1.87	0.56
1:D:62:LYS:HD2	4:D:2026:HOH:O	2.04	0.56
1:A:45:MET:HE1	1:A:221:LEU:HD12	1.87	0.56
1:C:79:THR:O	1:C:82:GLU:HG2	2.05	0.56
1:F:181:TYR:HB3	4:F:2056:HOH:O	2.03	0.56
1:D:16:THR:HG21	1:D:165:MET:SD	2.46	0.56
1:B:157:TYR:CD1	1:B:157:TYR:N	2.74	0.56
1:C:43:SER:HB3	1:C:129:ILE:HD11	1.87	0.56
1:F:209:GLY:O	1:F:225:VAL:HG23	2.04	0.56
1:B:229:ARG:HH12	1:F:61:PRO:HG3	1.71	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:THR:CG2	1:C:107:ILE:O	2.51	0.56
1:F:62:LYS:NZ	1:F:62:LYS:HB3	2.19	0.56
1:B:114:SER:OG	1:B:118:ARG:HG3	2.04	0.56
1:B:80:GLN:H	1:B:80:GLN:CD	2.09	0.56
1:D:116:GLU:HB3	4:D:2060:HOH:O	2.05	0.56
1:D:147:THR:HG23	4:D:2071:HOH:O	2.06	0.56
1:F:7:ARG:HB2	1:F:124:ARG:HH21	1.70	0.56
1:F:1:CYS:SG	4:F:2076:HOH:O	2.57	0.56
1:C:70:LEU:HD22	1:C:85:PHE:CE2	2.40	0.56
1:F:43:SER:HB3	1:F:129:ILE:HD11	1.88	0.56
1:A:45:MET:HE2	1:A:51:ILE:HG21	1.87	0.56
1:D:0:GLN:H	1:D:127:GLN:HE22	1.53	0.56
1:E:153:ASN:ND2	1:E:155:THR:OG1	2.39	0.56
1:A:19:GLU:HG3	1:A:125:THR:HG22	1.88	0.56
1:A:91:ILE:HD11	1:A:249:TRP:CZ2	2.41	0.56
1:D:196:PRO:C	1:D:197:GLN:HG2	2.26	0.56
1:F:21:GLN:HG3	1:F:147:THR:HG21	1.87	0.56
1:D:242:ARG:HD3	1:D:245:HIS:ND1	2.21	0.55
1:F:146:ILE:CG1	1:F:166:THR:CG2	2.84	0.55
1:F:171:ILE:HD11	1:F:194:ALA:HB3	1.88	0.55
1:F:7:ARG:N	1:F:8:PRO:CD	2.70	0.55
1:C:29:ARG:HG3	1:C:39:VAL:HG21	1.89	0.55
1:B:101:LEU:O	1:B:101:LEU:CG	2.48	0.55
1:B:70:LEU:HD22	1:B:85:PHE:HE2	1.69	0.55
1:A:177:GLN:O	1:A:183:GLY:HA2	2.06	0.55
1:A:146:ILE:CG2	1:A:211:LEU:HD23	2.37	0.55
1:C:72:ARG:HD2	1:C:82:GLU:OE1	2.06	0.55
1:F:242:ARG:HH11	1:F:242:ARG:HG2	1.71	0.55
1:B:182:TYR:CE2	1:B:237:PRO:HG2	2.41	0.55
1:B:168:VAL:HG13	1:B:193:ALA:HB1	1.89	0.55
1:F:221:LEU:HD22	1:F:243:VAL:HG21	1.89	0.55
1:F:46:SER:HB3	1:F:49:TRP:H	1.71	0.55
1:B:83:MET:HG3	4:B:2040:HOH:O	2.06	0.55
1:F:76:ASN:ND2	1:F:161:GLU:CD	2.61	0.55
1:F:51:ILE:HD11	1:F:107:ILE:HD11	1.88	0.55
1:E:32:ARG:CD	3:E:1259:SO4:O2	2.54	0.55
1:F:242:ARG:NH1	1:F:242:ARG:HG2	2.22	0.55
1:F:55:HIS:HA	1:F:58:ILE:HG12	1.87	0.55
1:F:190:MET:O	4:F:2065:HOH:O	2.18	0.55
1:F:196:PRO:O	1:F:197:GLN:HB2	2.08	0.55
1:B:123:SER:CB	1:E:33:GLY:CA	2.85	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ARG:HD3	2:A:1258:QGG:O26	2.08	0.54
1:C:54:THR:HG21	1:C:93:HIS:H	1.72	0.54
1:C:255:LYS:HB2	4:C:2102:HOH:O	2.08	0.54
1:C:91:ILE:O	1:C:91:ILE:HG13	2.06	0.54
1:E:198:TRP:CD1	1:E:198:TRP:O	2.60	0.54
1:D:146:ILE:HG13	1:D:166:THR:HG22	1.90	0.54
1:B:198:TRP:CH2	1:B:235:ASP:HA	2.43	0.54
1:D:172:SER:OG	1:D:174:ARG:CG	2.55	0.54
1:F:45:MET:HE2	1:F:51:ILE:HB	1.89	0.54
1:D:174:ARG:HG3	1:D:175:GLU:H	1.73	0.54
1:D:180:HIS:CD2	1:D:180:HIS:H	2.24	0.54
1:C:147:THR:CG2	4:C:2053:HOH:O	2.54	0.53
1:B:99:ASP:HB3	1:F:96:TYR:O	2.09	0.53
1:E:54:THR:HG22	1:E:92:LEU:HA	1.88	0.53
1:B:94:LYS:H	1:B:94:LYS:HE2	1.72	0.53
1:F:45:MET:HE3	1:F:51:ILE:CG2	2.38	0.53
1:E:29:ARG:HG3	1:E:39:VAL:HG21	1.90	0.53
1:F:51:ILE:HA	1:F:108:ALA:O	2.07	0.53
1:C:214:SER:OG	1:C:219:MET:HE1	2.09	0.53
1:D:174:ARG:HB3	4:D:2082:HOH:O	2.08	0.53
1:E:12:GLY:HA2	1:E:200:THR:CB	2.39	0.53
1:F:23:TRP:CE3	1:F:129:ILE:HG23	2.43	0.53
1:E:5:THR:HG21	1:E:19:GLU:OE1	2.09	0.53
1:B:74:ARG:NH2	1:E:161:GLU:CD	2.62	0.53
1:B:0:GLN:H	1:B:127:GLN:HE22	1.57	0.52
1:B:127:GLN:HE21	1:B:128:THR:H	1.57	0.52
1:C:7:ARG:HA	1:C:7:ARG:NE	2.25	0.52
1:C:88:GLU:HG3	1:C:113:ARG:HE	1.74	0.52
1:F:31:HIS:HB3	1:F:32:ARG:HG2	1.90	0.52
1:A:118:ARG:HH12	1:A:121:GLN:NE2	2.08	0.52
1:E:44:LEU:HD13	1:E:128:THR:HG22	1.92	0.52
1:F:178:GLN:HB3	4:F:2057:HOH:O	2.08	0.52
1:E:45:MET:HE1	1:E:51:ILE:CG2	2.40	0.52
1:F:224:ILE:HG21	4:F:2015:HOH:O	2.08	0.52
1:A:93:HIS:CD2	1:A:95:ASP:H	2.10	0.52
1:B:19:GLU:HG3	4:B:2010:HOH:O	2.09	0.52
1:F:93:HIS:HD2	1:F:107:ILE:CG2	2.23	0.52
1:D:113:ARG:HD3	4:D:2057:HOH:O	2.09	0.52
1:D:0:GLN:H	1:D:127:GLN:NE2	2.07	0.52
1:B:101:LEU:HD22	1:B:229:ARG:HE	1.75	0.51
1:B:51:ILE:HD11	1:B:107:ILE:HD11	1.91	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:ARG:HG3	1:E:67:ILE:HD13	1.91	0.51
1:B:74:ARG:NH2	1:E:161:GLU:OE1	2.43	0.51
1:F:137:ASP:OD2	1:F:242:ARG:HD2	2.11	0.51
1:C:91:ILE:HD13	1:C:253:HIS:ND1	2.25	0.51
1:B:45:MET:HE3	1:B:221:LEU:CD1	2.32	0.51
1:E:196:PRO:O	1:E:197:GLN:HB2	2.10	0.51
1:B:165:MET:HE2	4:B:2011:HOH:O	2.09	0.51
1:D:54:THR:CG2	1:D:107:ILE:O	2.53	0.51
1:D:230:GLY:O	2:D:1258:QGG:H13	2.11	0.51
1:F:118:ARG:HG2	4:F:2034:HOH:O	2.10	0.51
1:D:19:GLU:HG3	1:D:125:THR:HG22	1.93	0.51
1:C:94:LYS:CE	1:C:94:LYS:H	2.23	0.51
1:A:197:GLN:HG2	4:A:2069:HOH:O	2.10	0.50
1:C:113:ARG:NH2	4:C:2036:HOH:O	2.44	0.50
1:E:12:GLY:HA2	1:E:200:THR:OG1	2.11	0.50
1:E:45:MET:CE	1:E:221:LEU:HD12	2.41	0.50
1:D:91:ILE:HD13	1:D:253:HIS:ND1	2.26	0.50
1:E:31:HIS:HD2	3:E:1259:SO4:O4	1.94	0.50
1:E:88:GLU:HG2	4:E:2047:HOH:O	2.11	0.50
1:F:151:LYS:HD3	1:F:159:TYR:HE1	1.76	0.50
1:B:182:TYR:CD2	1:B:237:PRO:HG2	2.46	0.50
1:A:21:GLN:HE21	1:A:165:MET:HE2	1.77	0.50
1:C:11:ILE:H	1:C:11:ILE:HD12	1.77	0.49
1:C:191:LEU:HD11	1:C:242:ARG:HA	1.93	0.49
1:E:0:GLN:H	1:E:127:GLN:HE22	1.59	0.49
1:E:165:MET:CG	4:E:2063:HOH:O	2.55	0.49
1:F:24:PHE:HD2	1:F:147:THR:HG1	1.60	0.49
1:F:52:SER:C	4:F:2015:HOH:O	2.51	0.49
1:A:18:ILE:HG22	4:A:2006:HOH:O	2.11	0.49
1:E:30:ARG:HH11	1:E:30:ARG:CB	2.25	0.49
1:B:58:ILE:HG23	1:F:100:THR:O	2.12	0.49
4:D:2006:HOH:O	1:F:32:ARG:HB2	2.12	0.49
1:B:79:THR:O	1:B:82:GLU:HG2	2.13	0.49
1:A:159:TYR:CE2	1:E:6:LEU:HD23	2.48	0.49
1:D:10:ILE:O	1:D:152:GLU:HA	2.12	0.49
1:B:74:ARG:HH22	1:E:161:GLU:CD	2.16	0.49
1:A:218:ARG:O	1:A:220:THR:HG23	2.12	0.49
1:D:140:PHE:HB3	1:D:172:SER:HB3	1.95	0.49
1:D:74:ARG:NH2	4:D:2030:HOH:O	2.45	0.49
1:E:30:ARG:HB3	1:E:30:ARG:HH11	1.78	0.49
1:F:204:GLN:HG2	2:F:1258:QGG:O17	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:GLN:HB2	4:F:2035:HOH:O	2.13	0.49
1:F:50:VAL:O	1:F:109:LEU:HA	2.12	0.49
1:A:21:GLN:NE2	1:A:145:GLU:HG2	2.28	0.49
1:E:10:ILE:N	1:E:206:ASP:OD2	2.46	0.49
1:F:146:ILE:CG1	1:F:166:THR:HG23	2.43	0.49
1:B:33:GLY:N	1:B:34:GLY:HA2	2.28	0.49
1:D:242:ARG:HD3	1:D:245:HIS:CE1	2.47	0.49
1:F:91:ILE:CD1	1:F:253:HIS:HB3	2.39	0.48
1:B:67:ILE:HG12	1:B:84:LYS:HE3	1.93	0.48
1:D:63:LYS:HE3	1:D:64:GLU:OE2	2.12	0.48
1:E:194:ALA:HB2	1:E:237:PRO:HB3	1.93	0.48
1:F:45:MET:HE3	1:F:51:ILE:CB	2.41	0.48
1:D:174:ARG:CG	1:D:175:GLU:N	2.76	0.48
1:D:197:GLN:HB3	1:D:198:TRP:NE1	2.28	0.48
1:E:18:ILE:HD13	1:E:125:THR:CB	2.42	0.48
1:F:38:TYR:CZ	1:F:149:PHE:HB2	2.49	0.48
1:E:94:LYS:HB2	4:E:2045:HOH:O	2.12	0.48
1:D:45:MET:CE	1:D:131:LEU:HD21	2.42	0.48
1:C:197:GLN:O	1:C:199:LYS:HE3	2.14	0.48
1:A:89:ASN:HB2	1:A:111:LYS:CB	2.43	0.48
1:B:135:TYR:HA	4:B:2048:HOH:O	2.14	0.48
1:B:88:GLU:CA	1:B:88:GLU:OE1	2.61	0.48
1:A:4:LYS:HD3	4:A:2003:HOH:O	2.13	0.48
1:D:245:HIS:HD2	4:D:2085:HOH:O	1.97	0.48
1:B:104:HIS:HB3	4:B:2037:HOH:O	2.13	0.47
1:F:229:ARG:HD3	2:F:1258:QGG:O25	2.14	0.47
1:F:250:ILE:O	1:F:254:THR:HB	2.14	0.47
1:F:7:ARG:HE	1:F:124:ARG:NH2	2.11	0.47
1:A:54:THR:HG22	1:A:107:ILE:N	2.29	0.47
1:B:151:LYS:HD3	1:B:204:GLN:HB3	1.97	0.47
1:F:23:TRP:CD2	1:F:129:ILE:HG23	2.49	0.47
1:B:21:GLN:CD	1:B:147:THR:HG21	2.35	0.47
1:A:101:LEU:HG	1:A:229:ARG:HH11	1.78	0.47
1:A:118:ARG:NH1	1:A:121:GLN:NE2	2.63	0.47
1:B:191:LEU:HD12	1:B:242:ARG:HD3	1.95	0.47
1:E:43:SER:HB3	1:E:129:ILE:HD11	1.96	0.47
1:A:171:ILE:HD11	1:A:194:ALA:HB3	1.96	0.47
1:B:153:ASN:HB2	1:B:156:ASP:CG	2.34	0.47
1:E:146:ILE:CG2	1:E:211:LEU:HD23	2.45	0.47
1:F:168:VAL:HG13	1:F:193:ALA:HB1	1.96	0.47
1:F:199:LYS:HZ2	1:F:199:LYS:HA	1.77	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:0:GLN:HB3	1:D:3:GLN:OE1	2.14	0.47
1:F:32:ARG:HG3	1:F:32:ARG:HH11	1.79	0.47
1:B:181:TYR:CG	1:B:235:ASP:HB3	2.49	0.47
1:B:45:MET:SD	1:B:129:ILE:CD1	3.02	0.47
1:D:167:VAL:CB	4:D:2070:HOH:O	2.43	0.47
1:F:68:VAL:HG13	1:F:85:PHE:HB2	1.95	0.47
1:B:70:LEU:HB3	1:B:126:ILE:HG12	1.96	0.47
1:E:210:PRO:HB2	1:E:212:VAL:HG23	1.96	0.47
1:A:146:ILE:HG23	1:A:211:LEU:HD23	1.96	0.47
1:F:147:THR:HG22	1:F:165:MET:HB2	1.96	0.47
1:F:197:GLN:O	1:F:198:TRP:HB2	2.14	0.47
1:F:235:ASP:HB2	4:F:2085:HOH:O	2.14	0.47
1:B:55:HIS:HB3	4:B:2038:HOH:O	2.15	0.47
1:C:58:ILE:HD11	1:E:100:THR:HG22	1.96	0.47
1:F:235:ASP:C	1:F:237:PRO:HD3	2.34	0.47
1:A:257:GLU:HG3	4:A:2089:HOH:O	2.14	0.47
1:F:54:THR:CG2	1:F:93:HIS:H	2.28	0.47
1:C:35:SER:HA	1:C:36:VAL:HG23	1.97	0.46
1:F:177:GLN:HA	1:F:183:GLY:O	2.16	0.46
1:C:21:GLN:HG3	1:C:147:THR:CG2	2.38	0.46
1:A:242:ARG:NH2	4:A:2085:HOH:O	2.49	0.46
1:C:30:ARG:NH1	1:C:64:GLU:O	2.39	0.46
1:B:157:TYR:HB3	1:F:32:ARG:NH1	2.29	0.46
1:A:0:GLN:H	1:A:127:GLN:HE22	1.62	0.46
1:B:45:MET:CE	1:B:221:LEU:CD1	2.89	0.46
1:C:146:ILE:HG23	1:C:211:LEU:HD23	1.98	0.46
1:C:187:THR:OG1	1:C:189:LYS:CG	2.56	0.46
1:C:94:LYS:CD	1:C:94:LYS:H	2.29	0.46
1:B:23:TRP:HA	1:B:127:GLN:O	2.16	0.46
1:B:20:ASN:HB3	1:B:165:MET:HE1	1.98	0.46
1:E:242:ARG:HD3	1:E:245:HIS:ND1	2.31	0.46
1:B:98:ALA:HB1	4:B:2034:HOH:O	2.15	0.46
1:F:88:GLU:HG3	1:F:113:ARG:HE	1.81	0.46
1:B:94:LYS:H	1:B:94:LYS:CE	2.29	0.46
1:C:157:TYR:CD2	1:C:158:LEU:HD13	2.50	0.46
1:E:153:ASN:O	1:E:156:ASP:HB2	2.15	0.46
1:F:16:THR:CB	1:F:20:ASN:HD21	2.26	0.46
1:C:18:ILE:HG13	1:C:73:SER:HB3	1.99	0.45
1:F:43:SER:OG	1:F:210:PRO:HB3	2.16	0.45
1:F:104:HIS:CE1	4:F:2032:HOH:O	2.68	0.45
1:B:44:LEU:HD13	1:B:128:THR:CG2	2.44	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PRO:HD2	1:A:23:TRP:CZ3	2.52	0.45
1:B:45:MET:HE1	1:B:51:ILE:HG22	1.98	0.45
1:B:94:LYS:HD3	1:B:94:LYS:N	2.31	0.45
1:E:93:HIS:HD2	1:E:95:ASP:N	1.93	0.45
1:A:21:GLN:HE21	1:A:165:MET:CE	2.29	0.45
1:B:6:LEU:HD21	1:C:38:TYR:HB3	1.97	0.45
1:E:165:MET:CE	4:E:2063:HOH:O	2.65	0.45
1:F:182:TYR:O	1:F:185:GLU:HB2	2.17	0.45
1:B:180:HIS:O	1:B:181:TYR:CB	2.64	0.45
1:E:173:HIS:HE1	1:E:187:THR:O	1.98	0.45
1:C:103:HIS:HD2	1:C:227:TRP:HB3	1.81	0.45
1:F:224:ILE:CG2	4:F:2015:HOH:O	2.63	0.45
1:F:89:ASN:CB	1:F:111:LYS:HB3	2.47	0.45
1:F:198:TRP:HB2	1:F:199:LYS:CD	2.45	0.45
1:C:11:ILE:HD12	1:C:11:ILE:N	2.31	0.44
1:F:191:LEU:HD11	1:F:222:THR:CG2	2.47	0.44
1:F:91:ILE:HD13	1:F:109:LEU:HB2	1.99	0.44
1:A:10:ILE:CG2	1:A:12:GLY:HA3	2.44	0.44
1:A:212:VAL:CG1	1:A:219:MET:HG3	2.47	0.44
1:B:238:GLY:HA2	2:B:1258:QGG:N1	2.32	0.44
1:C:127:GLN:HE21	1:C:128:THR:H	1.65	0.44
1:E:45:MET:SD	1:E:129:ILE:CD1	3.05	0.44
1:C:191:LEU:N	1:C:191:LEU:HD12	2.32	0.44
1:F:151:LYS:HG3	1:F:156:ASP:OD1	2.17	0.44
1:E:29:ARG:O	1:E:36:VAL:HA	2.16	0.44
1:F:153:ASN:HB2	4:F:2047:HOH:O	2.17	0.44
1:B:29:ARG:HG3	1:B:39:VAL:HG21	2.00	0.44
1:C:129:ILE:HD13	1:C:221:LEU:HB2	2.00	0.44
1:D:174:ARG:CG	1:D:175:GLU:H	2.30	0.44
1:B:48:CYS:O	1:B:111:LYS:HA	2.17	0.44
1:E:178:GLN:CG	4:E:2080:HOH:O	2.66	0.44
1:A:16:THR:CG2	1:A:165:MET:SD	2.97	0.44
1:A:223:GLY:HA2	1:A:241:THR:O	2.18	0.44
1:D:247:LEU:O	1:D:251:ARG:HG2	2.18	0.44
1:F:70:LEU:HB3	1:F:126:ILE:HG12	2.00	0.44
1:F:54:THR:HG21	1:F:93:HIS:H	1.83	0.44
1:A:188:THR:O	1:A:245:HIS:CE1	2.71	0.43
1:B:134:MET:HB2	1:B:247:LEU:HD12	2.00	0.43
1:F:18:ILE:HG21	1:F:71:GLY:CA	2.42	0.43
1:B:181:TYR:CD2	1:B:235:ASP:HB3	2.53	0.43
1:D:45:MET:HE2	1:D:221:LEU:CD2	2.44	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:ILE:H	1:F:18:ILE:HG13	1.43	0.43
1:F:51:ILE:HD11	1:F:107:ILE:CD1	2.48	0.43
1:B:151:LYS:CG	1:B:153:ASN:O	2.64	0.43
1:C:21:GLN:HE22	1:C:145:GLU:CD	2.21	0.43
1:E:162:GLN:HG3	1:E:163:LEU:N	2.33	0.43
1:D:86:GLU:HG3	4:D:2046:HOH:O	2.18	0.43
1:F:44:LEU:HD13	1:F:128:THR:HG22	2.00	0.43
1:A:225:VAL:HG22	1:A:240:TYR:HE2	1.84	0.43
1:B:212:VAL:CG1	1:B:219:MET:HG3	2.48	0.43
1:E:12:GLY:HA2	1:E:200:THR:HB	2.01	0.43
1:E:218:ARG:O	1:E:220:THR:HG22	2.18	0.43
1:F:63:LYS:HD3	1:F:88:GLU:O	2.18	0.43
1:B:159:TYR:OH	1:B:204:GLN:NE2	2.47	0.43
1:C:171:ILE:HD11	1:C:194:ALA:HB3	2.00	0.43
1:C:70:LEU:HB3	1:C:126:ILE:HG12	2.00	0.43
1:B:150:GLY:HA2	1:B:205:GLY:HA3	2.01	0.43
1:B:157:TYR:HB3	1:F:32:ARG:HH11	1.83	0.43
1:B:98:ALA:O	1:F:98:ALA:N	2.48	0.43
1:D:116:GLU:HG3	1:D:116:GLU:H	1.47	0.43
1:F:87:VAL:HG13	1:F:110:LEU:HB3	2.01	0.43
1:F:70:LEU:HD22	1:F:85:PHE:CE2	2.54	0.43
1:F:93:HIS:HD2	1:F:107:ILE:HG22	1.83	0.43
1:D:45:MET:CE	1:D:221:LEU:HD22	2.46	0.43
1:E:23:TRP:HA	1:E:127:GLN:O	2.18	0.43
1:A:153:ASN:OD1	1:A:154:SER:N	2.52	0.43
1:A:194:ALA:HB2	1:A:237:PRO:CB	2.46	0.43
1:D:254:THR:HG21	4:D:2048:HOH:O	2.19	0.43
1:D:30:ARG:NH2	1:D:86:GLU:OE1	2.52	0.43
1:E:101:LEU:HD22	1:E:227:TRP:CE3	2.54	0.43
1:E:246:PHE:O	1:E:250:ILE:HG13	2.19	0.43
1:E:28:TYR:HB2	1:E:67:ILE:HG22	2.00	0.43
1:F:121:GLN:HA	1:F:122:PRO:HD3	1.81	0.43
1:F:105:ASN:H	1:F:189:LYS:HE2	1.84	0.43
1:B:99:ASP:HA	1:F:97:SER:HA	2.01	0.43
1:B:151:LYS:CE	1:B:156:ASP:O	2.65	0.42
1:E:30:ARG:HD2	4:E:2013:HOH:O	2.19	0.42
1:F:55:HIS:C	1:F:55:HIS:CD2	2.92	0.42
1:F:45:MET:CE	1:F:51:ILE:CB	2.94	0.42
3:B:1260:SO4:O4	1:D:124:ARG:NH1	2.50	0.42
1:B:136:ASN:HA	1:B:137:ASP:CB	2.27	0.42
1:D:171:ILE:HD11	1:D:194:ALA:CB	2.43	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:ILE:O	1:F:165:MET:HA	2.20	0.42
1:F:89:ASN:HD22	1:F:91:ILE:HG22	1.83	0.42
1:A:21:GLN:HG2	1:A:165:MET:CE	2.49	0.42
1:A:54:THR:HG22	1:A:107:ILE:H	1.83	0.42
1:B:15:PHE:O	1:E:157:TYR:HE2	2.03	0.42
1:F:5:THR:OG1	1:F:124:ARG:HG2	2.20	0.42
1:B:94:LYS:H	1:B:94:LYS:CD	2.32	0.42
1:C:118:ARG:NH2	1:C:121:GLN:HE22	2.18	0.42
1:C:44:LEU:HD13	1:C:128:THR:HG22	2.02	0.42
1:F:10:ILE:N	1:F:206:ASP:OD2	2.52	0.42
1:B:102:ALA:C	1:B:103:HIS:HD2	2.23	0.42
1:C:118:ARG:HD2	4:C:2038:HOH:O	2.19	0.42
1:D:31:HIS:HD2	3:D:1260:SO4:O3	2.01	0.42
1:E:54:THR:CG2	1:E:93:HIS:H	2.24	0.42
1:F:18:ILE:HG13	1:F:73:SER:OG	2.19	0.42
1:A:100:THR:HG22	1:D:58:ILE:CD1	2.50	0.42
1:C:58:ILE:HD12	1:C:58:ILE:HA	1.83	0.42
1:D:88:GLU:HG3	4:D:2056:HOH:O	2.19	0.42
1:F:157:TYR:CD2	1:F:158:LEU:HD13	2.55	0.42
1:B:62:LYS:HD3	1:B:63:LYS:N	2.35	0.42
1:F:103:HIS:N	1:F:103:HIS:CD2	2.88	0.42
1:F:191:LEU:CD1	1:F:222:THR:HG22	2.47	0.42
1:D:44:LEU:HD13	1:D:128:THR:HG22	2.02	0.42
1:F:96:TYR:HA	1:F:105:ASN:HB2	2.02	0.42
1:E:178:GLN:HG3	4:E:2080:HOH:O	2.19	0.41
1:A:45:MET:HB2	1:A:49:TRP:O	2.19	0.41
1:B:136:ASN:N	1:B:136:ASN:OD1	2.50	0.41
1:B:32:ARG:HE	1:D:-3:LEU:HD12	1.85	0.41
1:F:10:ILE:HG23	1:F:12:GLY:CA	2.46	0.41
1:F:45:MET:CE	1:F:51:ILE:CG2	2.98	0.41
1:A:23:TRP:O	1:A:43:SER:HA	2.21	0.41
1:C:57:PHE:HB2	1:C:92:LEU:HD11	2.02	0.41
1:C:94:LYS:CD	1:C:94:LYS:N	2.83	0.41
1:D:31:HIS:HE1	1:D:37:THR:OG1	2.03	0.41
1:E:191:LEU:CD1	1:E:242:ARG:HA	2.50	0.41
1:A:170:LEU:HG	1:A:191:LEU:CD2	2.50	0.41
1:C:187:THR:OG1	1:C:189:LYS:HE2	2.20	0.41
1:F:10:ILE:HA	1:F:201:ASP:O	2.20	0.41
1:F:44:LEU:HD23	1:F:50:VAL:HG22	2.03	0.41
1:A:32:ARG:HD2	1:D:157:TYR:HB3	2.03	0.41
1:F:99:ASP:HB2	1:F:100:THR:H	1.48	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:54:THR:OG1	1:F:106:ASP:HA	2.20	0.41
1:C:174:ARG:HA	1:C:174:ARG:HD2	1.54	0.41
1:E:181:TYR:HA	1:E:235:ASP:O	2.21	0.41
1:A:177:GLN:HG2	1:A:186:VAL:HG23	2.03	0.41
1:E:177:GLN:O	1:E:183:GLY:HA2	2.21	0.41
1:E:247:LEU:O	1:E:251:ARG:HG2	2.21	0.41
1:F:144:CYS:HB2	1:F:211:LEU:HD22	2.02	0.41
1:F:76:ASN:HD21	1:F:161:GLU:CD	2.19	0.41
1:A:134:MET:O	1:A:135:TYR:HB2	2.21	0.41
1:B:0:GLN:H	1:B:127:GLN:NE2	2.19	0.41
1:B:99:ASP:N	1:B:99:ASP:OD1	2.54	0.41
1:C:195:ASP:HB2	1:C:200:THR:HG22	2.02	0.41
1:F:101:LEU:HD13	1:F:227:TRP:CZ3	2.56	0.41
1:F:7:ARG:H	1:F:8:PRO:HD3	1.86	0.41
1:A:18:ILE:HG13	1:A:125:THR:HB	2.03	0.41
1:F:197:GLN:OE1	1:F:197:GLN:HA	2.21	0.41
1:F:68:VAL:HG11	1:F:112:ILE:CG2	2.48	0.41
1:A:59:ASP:HB2	4:A:2017:HOH:O	2.20	0.40
1:B:245:HIS:HD2	4:B:2067:HOH:O	2.03	0.40
1:C:173:HIS:CE1	1:C:177:GLN:NE2	2.89	0.40
1:C:7:ARG:HA	1:C:8:PRO:HD2	1.69	0.40
1:F:67:ILE:HG12	1:F:84:LYS:HE3	2.03	0.40
1:B:21:GLN:NE2	4:B:2011:HOH:O	2.54	0.40
1:C:93:HIS:CD2	1:C:95:ASP:H	2.20	0.40
1:F:140:PHE:HA	1:F:170:LEU:HB3	2.03	0.40
1:A:196:PRO:CB	1:A:197:GLN:HB2	2.51	0.40
1:B:113:ARG:HD3	1:B:117:GLY:HA2	2.03	0.40
1:C:91:ILE:HD13	1:C:253:HIS:HD1	1.86	0.40
1:C:94:LYS:HD3	1:C:94:LYS:N	2.37	0.40
1:A:131:LEU:HD12	1:A:131:LEU:HA	1.89	0.40
1:B:171:ILE:HG23	1:B:175:GLU:HG3	2.03	0.40
1:B:32:ARG:HG2	1:B:32:ARG:H	1.61	0.40
1:E:242:ARG:CD	1:E:245:HIS:CE1	3.04	0.40
1:E:132:PRO:O	1:E:247:LEU:HD11	2.22	0.40
1:D:6:LEU:HD22	1:F:159:TYR:CE2	2.56	0.40
1:F:87:VAL:O	1:F:87:VAL:HG12	2.22	0.40
1:C:80:GLN:OE1	1:C:80:GLN:N	2.53	0.40
1:D:167:VAL:CG1	4:D:2070:HOH:O	2.68	0.40
1:D:196:PRO:HA	1:D:197:GLN:CD	2.42	0.40
1:E:215:LEU:HB3	1:E:220:THR:HG21	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/276 (92%)	234 (92%)	15 (6%)	5 (2%)	7	4
1	B	255/276 (92%)	230 (90%)	19 (8%)	6 (2%)	6	3
1	C	255/276 (92%)	235 (92%)	19 (8%)	1 (0%)	34	37
1	D	255/276 (92%)	232 (91%)	23 (9%)	0	100	100
1	E	255/276 (92%)	238 (93%)	12 (5%)	5 (2%)	7	4
1	F	253/276 (92%)	212 (84%)	31 (12%)	10 (4%)	3	1
All	All	1527/1656 (92%)	1381 (90%)	119 (8%)	27 (2%)	8	5

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	GLY
1	A	197	GLN
1	B	135	TYR
1	C	36	VAL
1	E	12	GLY
1	E	34	GLY
1	F	12	GLY
1	A	135	TYR
1	B	181	TYR
1	B	256	GLU
1	F	55	HIS
1	F	119	CYS
1	F	197	GLN
1	F	198	TRP
1	F	207	SER
1	A	35	SER
1	B	137	ASP
1	E	135	TYR
1	E	256	GLU
1	F	174	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	181	TYR
1	F	204	GLN
1	A	256	GLU
1	B	151	LYS
1	E	257	GLU
1	B	179	PRO
1	F	196	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	225/242 (93%)	191 (85%)	34 (15%)	3	2
1	B	226/242 (93%)	184 (81%)	42 (19%)	1	1
1	C	226/242 (93%)	194 (86%)	32 (14%)	3	2
1	D	226/242 (93%)	195 (86%)	31 (14%)	3	3
1	E	226/242 (93%)	194 (86%)	32 (14%)	3	2
1	F	224/242 (93%)	168 (75%)	56 (25%)	0	0
All	All	1353/1452 (93%)	1126 (83%)	227 (17%)	2	1

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	GLN
1	A	4	LYS
1	A	6	LEU
1	A	17	THR
1	A	18	ILE
1	A	19	GLU
1	A	44	LEU
1	A	45	MET
1	A	54	THR
1	A	58	ILE
1	A	60	TYR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	68	VAL
1	A	70	LEU
1	A	73	SER
1	A	74	ARG
1	A	88	GLU
1	A	91	ILE
1	A	94	LYS
1	A	101	LEU
1	A	129	ILE
1	A	131	LEU
1	A	133	SER
1	A	158	LEU
1	A	165	MET
1	A	167	VAL
1	A	168	VAL
1	A	174	ARG
1	A	176	CYS
1	A	186	VAL
1	A	189	LYS
1	A	191	LEU
1	A	204	GLN
1	A	221	LEU
1	A	251	ARG
1	B	5	THR
1	B	6	LEU
1	B	16	THR
1	B	18	ILE
1	B	20	ASN
1	B	32	ARG
1	B	44	LEU
1	B	45	MET
1	B	46	SER
1	B	54	THR
1	B	64	GLU
1	B	68	VAL
1	B	70	LEU
1	B	76	ASN
1	B	80	GLN
1	B	86	GLU
1	B	88	GLU
1	B	89	ASN
1	B	91	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	99	ASP
1	B	118	ARG
1	B	129	ILE
1	B	147	THR
1	B	153	ASN
1	B	154	SER
1	B	157	TYR
1	B	164	LYS
1	B	168	VAL
1	B	170	LEU
1	B	174	ARG
1	B	182	TYR
1	B	204	GLN
1	B	211	LEU
1	B	215	LEU
1	B	220	THR
1	B	221	LEU
1	B	229	ARG
1	B	234	LYS
1	B	235	ASP
1	B	245	HIS
1	B	247	LEU
1	B	254	THR
1	C	4	LYS
1	C	6	LEU
1	C	14	GLU
1	C	18	ILE
1	C	32	ARG
1	C	37	THR
1	C	44	LEU
1	C	54	THR
1	C	58	ILE
1	C	89	ASN
1	C	91	ILE
1	C	92	LEU
1	C	94	LYS
1	C	101	LEU
1	C	129	ILE
1	C	136	ASN
1	C	147	THR
1	C	158	LEU
1	C	167	VAL

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	168	VAL
1	C	169	LYS
1	C	170	LEU
1	C	174	ARG
1	C	191	LEU
1	C	211	LEU
1	C	215	LEU
1	C	219	MET
1	C	220	THR
1	C	229	ARG
1	C	251	ARG
1	C	254	THR
1	C	256	GLU
1	D	-3	LEU
1	D	5	THR
1	D	6	LEU
1	D	18	ILE
1	D	30	ARG
1	D	44	LEU
1	D	45	MET
1	D	54	THR
1	D	64	GLU
1	D	67	ILE
1	D	68	VAL
1	D	70	LEU
1	D	73	SER
1	D	83	MET
1	D	89	ASN
1	D	91	ILE
1	D	94	LYS
1	D	101	LEU
1	D	116	GLU
1	D	118	ARG
1	D	121	GLN
1	D	129	ILE
1	D	147	THR
1	D	157	TYR
1	D	170	LEU
1	D	189	LYS
1	D	215	LEU
1	D	216	GLN
1	D	218	ARG

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	254	THR
1	D	257	GLU
1	E	5	THR
1	E	16	THR
1	E	18	ILE
1	E	30	ARG
1	E	32	ARG
1	E	44	LEU
1	E	45	MET
1	E	67	ILE
1	E	70	LEU
1	E	91	ILE
1	E	94	LYS
1	E	101	LEU
1	E	115	LYS
1	E	129	ILE
1	E	147	THR
1	E	157	TYR
1	E	158	LEU
1	E	165	MET
1	E	168	VAL
1	E	169	LYS
1	E	170	LEU
1	E	173	HIS
1	E	174	ARG
1	E	177	GLN
1	E	189	LYS
1	E	197	GLN
1	E	198	TRP
1	E	211	LEU
1	E	215	LEU
1	E	218	ARG
1	E	220	THR
1	E	221	LEU
1	F	3	GLN
1	F	4	LYS
1	F	5	THR
1	F	6	LEU
1	F	7	ARG
1	F	16	THR
1	F	17	THR
1	F	18	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	20	ASN
1	F	21	GLN
1	F	32	ARG
1	F	36	VAL
1	F	44	LEU
1	F	51	ILE
1	F	54	THR
1	F	55	HIS
1	F	62	LYS
1	F	70	LEU
1	F	74	ARG
1	F	76	ASN
1	F	89	ASN
1	F	91	ILE
1	F	92	LEU
1	F	99	ASP
1	F	100	THR
1	F	101	LEU
1	F	103	HIS
1	F	107	ILE
1	F	111	LYS
1	F	114	SER
1	F	115	LYS
1	F	116	GLU
1	F	123	SER
1	F	124	ARG
1	F	127	GLN
1	F	129	ILE
1	F	133	SER
1	F	136	ASN
1	F	139	GLN
1	F	142	THR
1	F	151	LYS
1	F	158	LEU
1	F	161	GLU
1	F	168	VAL
1	F	170	LEU
1	F	174	ARG
1	F	189	LYS
1	F	197	GLN
1	F	199	LYS
1	F	202	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	204	GLN
1	F	212	VAL
1	F	214	SER
1	F	221	LEU
1	F	224	ILE
1	F	242	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	GLN
1	A	31	HIS
1	A	78	ASN
1	A	93	HIS
1	A	121	GLN
1	A	127	GLN
1	A	178	GLN
1	A	245	HIS
1	B	21	GLN
1	B	31	HIS
1	B	103	HIS
1	B	127	GLN
1	B	153	ASN
1	B	177	GLN
1	B	180	HIS
1	B	204	GLN
1	B	245	HIS
1	C	0	GLN
1	C	3	GLN
1	C	89	ASN
1	C	93	HIS
1	C	121	GLN
1	C	127	GLN
1	C	136	ASN
1	C	153	ASN
1	C	178	GLN
1	C	245	HIS
1	D	20	ASN
1	D	31	HIS
1	D	80	GLN
1	D	89	ASN
1	D	93	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	121	GLN
1	D	127	GLN
1	D	139	GLN
1	D	153	ASN
1	D	177	GLN
1	D	178	GLN
1	D	180	HIS
1	E	31	HIS
1	E	93	HIS
1	E	127	GLN
1	E	153	ASN
1	E	173	HIS
1	E	178	GLN
1	E	204	GLN
1	E	253	HIS
1	F	3	GLN
1	F	20	ASN
1	F	21	GLN
1	F	76	ASN
1	F	89	ASN
1	F	127	GLN
1	F	177	GLN
1	F	253	HIS

### 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](#)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	B	1261	-	4,4,4	0.23	0	6,6,6	0.39	0
3	SO4	D	1260	-	4,4,4	0.29	0	6,6,6	1.00	0
2	QGG	D	1258	-	25,28,28	1.42	5 (20%)	36,42,42	1.90	10 (27%)
2	QGG	F	1258	-	25,28,28	1.17	3 (12%)	36,42,42	1.97	13 (36%)
2	QGG	B	1258	-	25,28,28	1.21	3 (12%)	36,42,42	1.57	9 (25%)
2	QGG	C	1258	-	25,28,28	1.19	3 (12%)	36,42,42	1.43	7 (19%)
3	SO4	E	1259	-	4,4,4	0.26	0	6,6,6	0.51	0
3	SO4	B	1262	-	4,4,4	0.18	0	6,6,6	0.50	0
3	SO4	D	1261	-	4,4,4	0.20	0	6,6,6	0.28	0
2	QGG	E	1258	-	25,28,28	1.44	4 (16%)	36,42,42	2.03	11 (30%)
3	SO4	D	1259	-	4,4,4	0.17	0	6,6,6	0.29	0
3	SO4	B	1259	-	4,4,4	0.23	0	6,6,6	0.30	0
2	QGG	A	1258	-	25,28,28	1.70	3 (12%)	36,42,42	2.34	11 (30%)
3	SO4	E	1260	-	4,4,4	0.27	0	6,6,6	0.44	0
3	SO4	B	1260	-	4,4,4	0.21	0	6,6,6	0.29	0

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	QGG	D	1258	-	-	2/15/30/30	0/3/3/3
2	QGG	F	1258	-	-	1/15/30/30	0/3/3/3
2	QGG	B	1258	-	-	1/15/30/30	0/3/3/3
2	QGG	C	1258	-	-	0/15/30/30	0/3/3/3
2	QGG	E	1258	-	-	1/15/30/30	0/3/3/3
2	QGG	A	1258	-	-	1/15/30/30	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1258	QGG	O17-S15	-4.87	1.38	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1258	QGG	C6-C7	-4.72	1.34	1.39
2	D	1258	QGG	C6-C7	-4.64	1.34	1.39
2	A	1258	QGG	S15-N18	3.88	1.69	1.63
2	B	1258	QGG	S15-N18	2.91	1.67	1.63
2	A	1258	QGG	C2-N3	-2.86	1.30	1.34
2	F	1258	QGG	S15-N18	2.78	1.67	1.63
2	C	1258	QGG	O17-S15	-2.73	1.40	1.43
2	F	1258	QGG	C2-N27	2.69	1.38	1.33
2	B	1258	QGG	C6-C7	-2.52	1.36	1.39
2	D	1258	QGG	S15-N18	2.46	1.67	1.63
2	E	1258	QGG	C2-N1	2.44	1.38	1.33
2	D	1258	QGG	C2-N1	2.29	1.37	1.33
2	E	1258	QGG	C2-N27	2.27	1.37	1.33
2	C	1258	QGG	C6-C7	-2.26	1.36	1.39
2	F	1258	QGG	C2-N1	2.26	1.37	1.33
2	E	1258	QGG	S15-N18	2.16	1.66	1.63
2	D	1258	QGG	C2-N27	2.14	1.37	1.33
2	C	1258	QGG	C22-N18	-2.08	1.46	1.49
2	B	1258	QGG	C2-N27	2.04	1.37	1.33
2	D	1258	QGG	C2-N3	-2.03	1.31	1.34

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1258	QGG	O17-S15-C12	-7.74	98.25	108.05
2	A	1258	QGG	C21-C22-N18	6.26	110.82	102.89
2	D	1258	QGG	O17-S15-C12	-5.19	101.48	108.05
2	F	1258	QGG	C6-C7-C9	-4.86	116.74	121.40
2	E	1258	QGG	O17-S15-C12	-4.82	101.95	108.05
2	F	1258	QGG	C21-C22-N18	4.09	108.07	102.89
2	E	1258	QGG	C21-C22-N18	3.93	107.88	102.89
2	D	1258	QGG	C11-C12-S15	-3.78	115.78	119.76
2	A	1258	QGG	C19-N18-S15	3.64	127.86	119.16
2	A	1258	QGG	C19-N18-C22	-3.55	106.45	111.22
2	E	1258	QGG	C19-N18-C22	-3.55	106.46	111.22
2	C	1258	QGG	C19-N18-S15	3.40	127.30	119.16
2	E	1258	QGG	C12-S15-N18	-3.37	101.36	107.36
2	D	1258	QGG	O17-S15-O16	3.35	124.95	119.52
2	B	1258	QGG	O17-S15-C12	-3.28	103.90	108.05
2	E	1258	QGG	C19-N18-S15	3.17	126.75	119.16
2	A	1258	QGG	N27-C2-N1	3.07	122.47	118.24
2	D	1258	QGG	C6-N5-C4	3.03	125.05	115.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1258	QGG	C4-C14-C9	2.96	120.90	114.19
2	D	1258	QGG	O16-S15-C12	2.93	111.75	108.05
2	E	1258	QGG	O16-S15-C12	-2.83	104.47	108.05
2	E	1258	QGG	C11-C12-S15	-2.75	116.87	119.76
2	F	1258	QGG	O17-S15-C12	-2.68	104.65	108.05
2	F	1258	QGG	C14-C4-N5	-2.66	116.00	122.13
2	D	1258	QGG	C7-C6-N5	-2.66	120.56	122.84
2	E	1258	QGG	C6-N5-C4	2.65	123.85	115.35
2	E	1258	QGG	O17-S15-N18	2.60	111.72	106.97
2	F	1258	QGG	C19-N18-S15	2.59	125.36	119.16
2	B	1258	QGG	C19-N18-C22	-2.58	107.76	111.22
2	C	1258	QGG	C21-C22-N18	2.57	106.14	102.89
2	D	1258	QGG	C21-C22-N18	2.54	106.11	102.89
2	A	1258	QGG	C6-N5-C4	2.54	123.49	115.35
2	D	1258	QGG	N27-C2-N1	2.52	121.72	118.24
2	A	1258	QGG	C7-C6-N5	-2.52	120.67	122.84
2	C	1258	QGG	O17-S15-N18	2.51	111.55	106.97
2	F	1258	QGG	C6-N5-C4	2.50	123.35	115.35
2	F	1258	QGG	C19-N18-C22	-2.49	107.88	111.22
2	B	1258	QGG	C21-C22-N18	2.48	106.04	102.89
2	F	1258	QGG	C6-C7-CL8	2.48	121.96	118.60
2	E	1258	QGG	O16-S15-N18	2.47	111.47	106.97
2	F	1258	QGG	C11-C12-S15	2.46	122.34	119.76
2	A	1258	QGG	C11-C12-S15	-2.41	117.22	119.76
2	A	1258	QGG	O17-S15-N18	2.40	111.35	106.97
2	C	1258	QGG	C19-N18-C22	-2.39	108.02	111.22
2	F	1258	QGG	C7-C9-C14	2.35	119.49	117.66
2	B	1258	QGG	C6-C7-CL8	2.35	121.79	118.60
2	E	1258	QGG	C10-C9-C7	-2.32	120.92	125.06
2	F	1258	QGG	C20-C19-N18	2.31	107.45	103.28
2	D	1258	QGG	C19-N18-C22	-2.25	108.21	111.22
2	C	1258	QGG	O17-S15-C12	-2.22	105.24	108.05
2	B	1258	QGG	C21-C22-C24	-2.19	108.14	113.98
2	A	1258	QGG	C21-C22-C24	-2.18	108.16	113.98
2	D	1258	QGG	C22-N18-S15	2.17	128.63	118.98
2	F	1258	QGG	O17-S15-O16	2.09	122.91	119.52
2	B	1258	QGG	C4-C14-C9	2.09	118.91	114.19
2	B	1258	QGG	C19-N18-S15	2.08	124.14	119.16
2	B	1258	QGG	C6-N5-C4	2.06	121.96	115.35
2	A	1258	QGG	O16-S15-C12	2.05	110.64	108.05
2	C	1258	QGG	C6-C7-CL8	2.05	121.38	118.60
2	B	1258	QGG	C22-N18-S15	2.03	128.04	118.98

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1258	QGG	C4-C14-C9	2.03	118.80	114.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

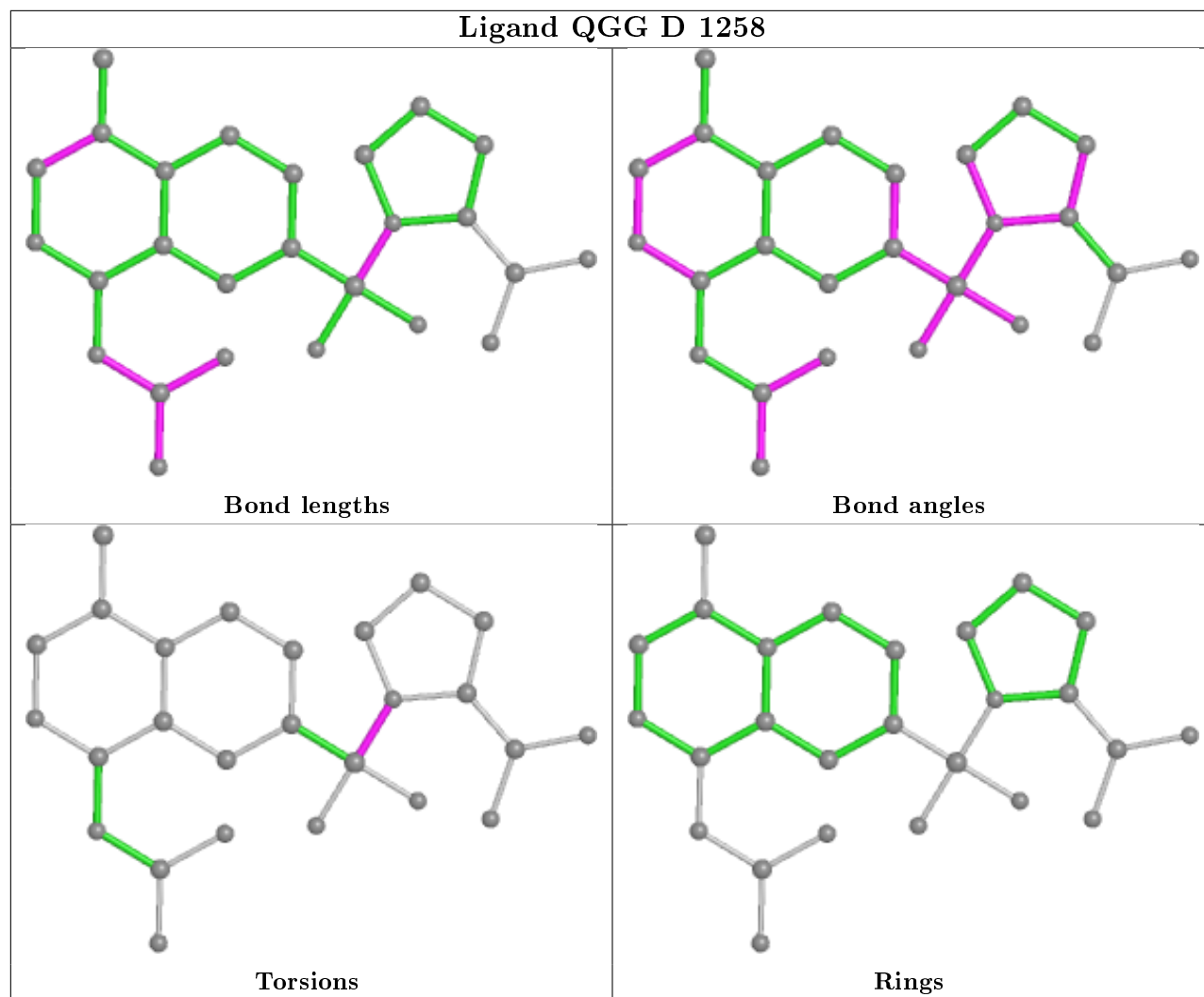
Mol	Chain	Res	Type	Atoms
2	D	1258	QGG	C19-N18-S15-O17
2	A	1258	QGG	C19-N18-S15-O17
2	B	1258	QGG	C22-N18-S15-O16
2	E	1258	QGG	C19-N18-S15-O17
2	F	1258	QGG	C19-N18-S15-O17
2	D	1258	QGG	C19-N18-S15-O16

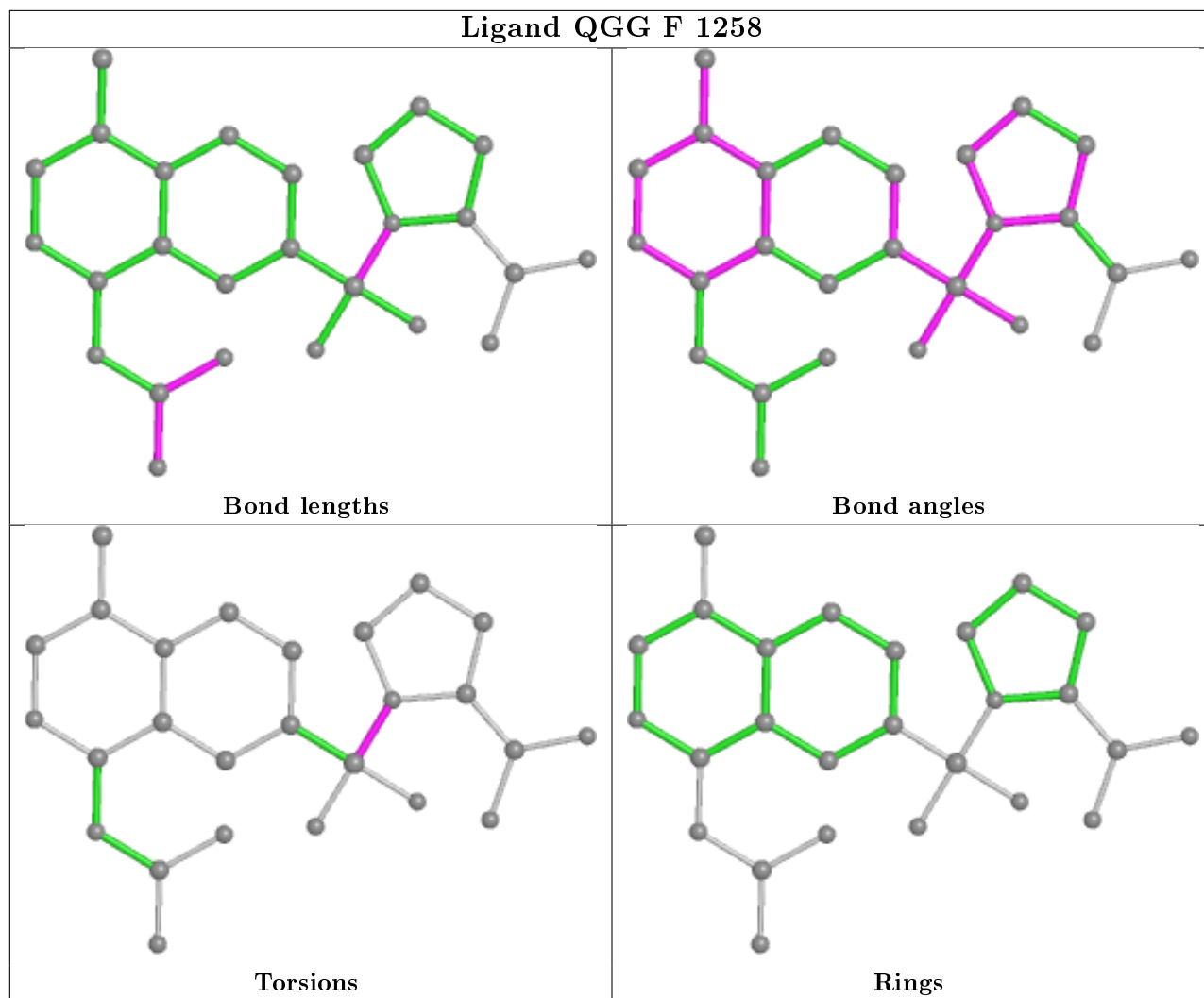
There are no ring outliers.

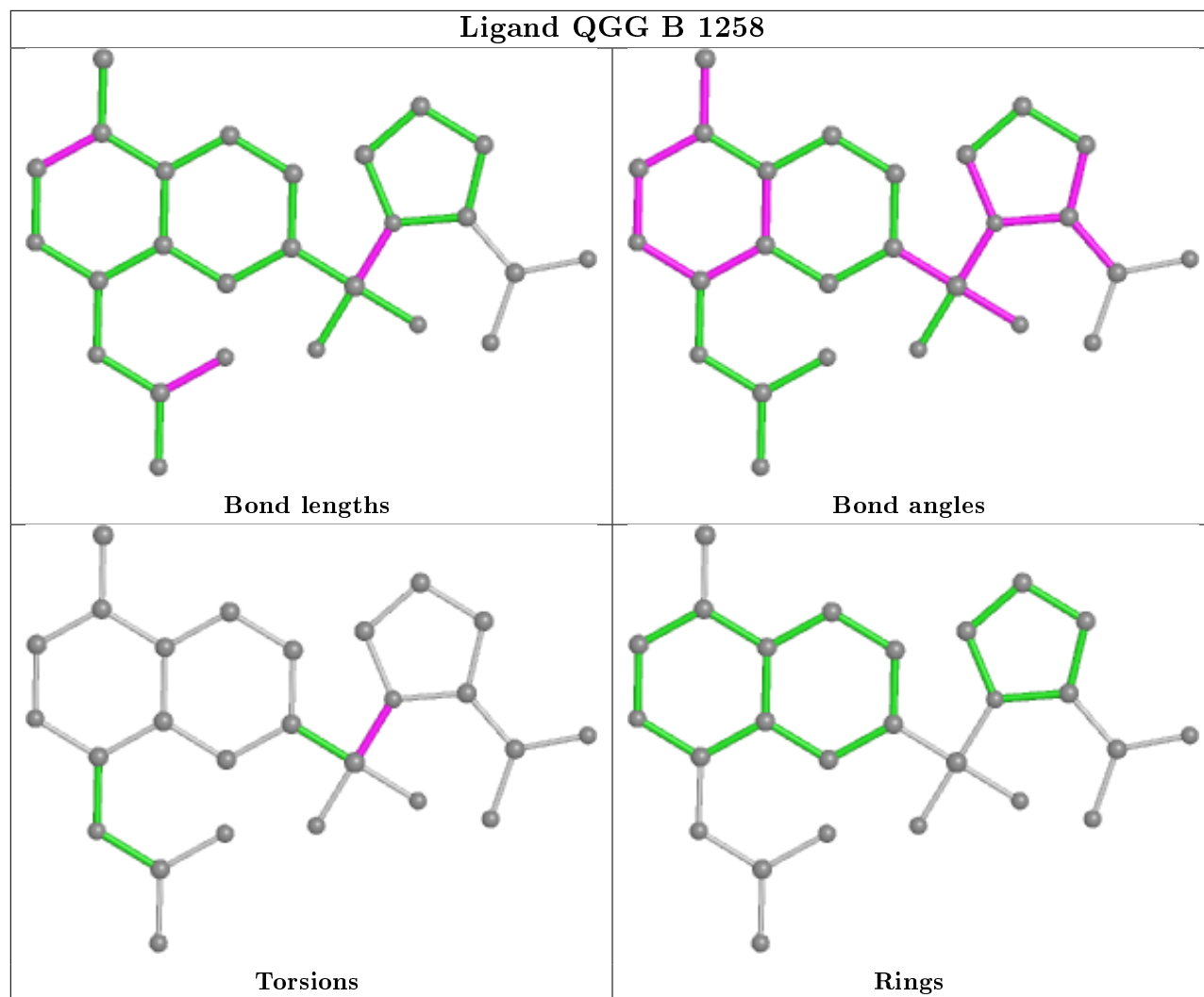
11 monomers are involved in 22 short contacts:

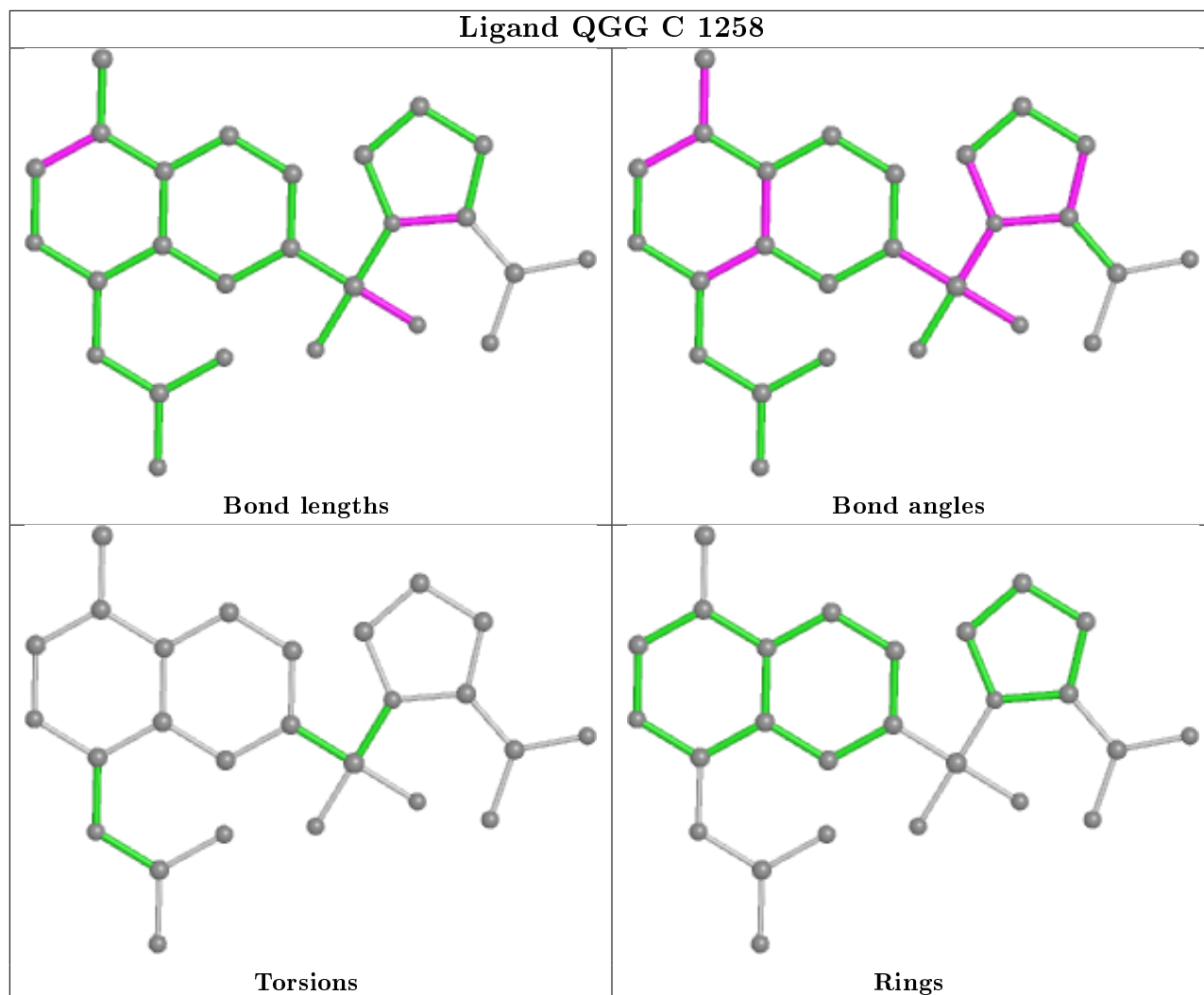
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1260	SO4	1	0
2	D	1258	QGG	1	0
2	F	1258	QGG	5	0
2	B	1258	QGG	4	0
2	C	1258	QGG	1	0
3	E	1259	SO4	3	0
3	B	1262	SO4	3	0
2	E	1258	QGG	1	0
3	B	1259	SO4	1	0
2	A	1258	QGG	1	0
3	B	1260	SO4	1	0

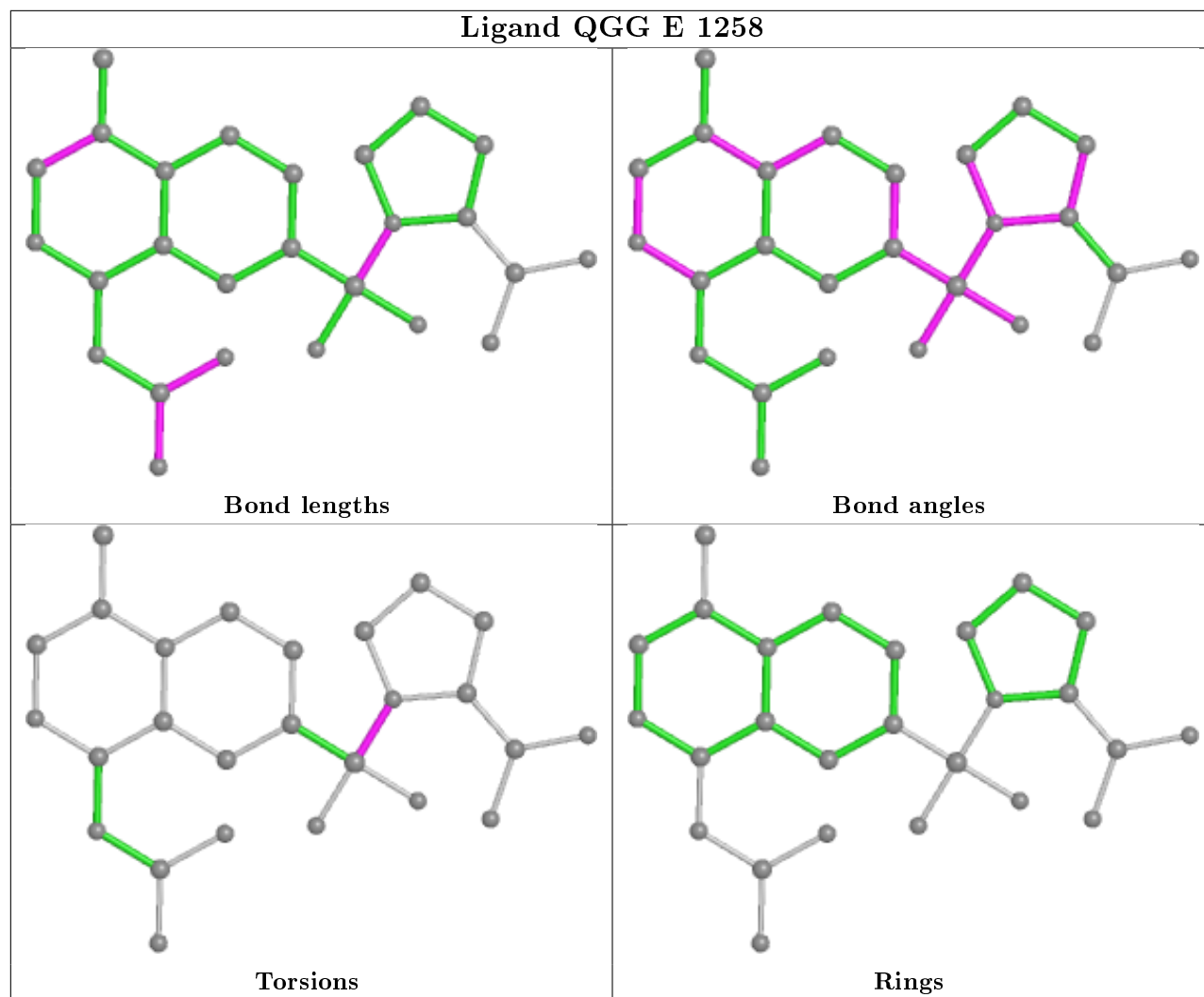
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

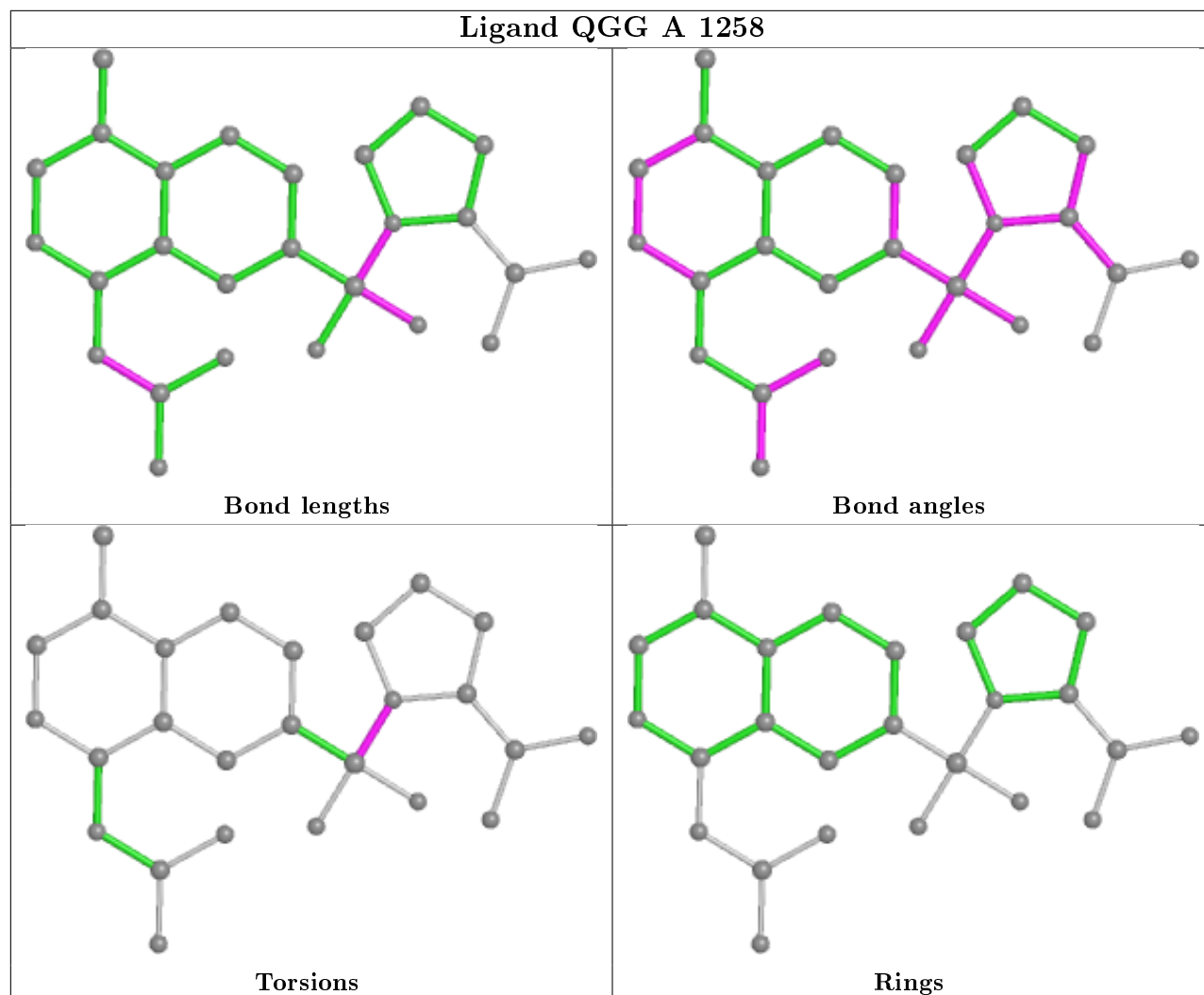












## 5.7 Other polymers [i](#)

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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.