



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:12 PM UTC

PDB ID : 2I2X / pdb_00002i2x
Title : Crystal structure of methanol:cobalamin methyltransferase complex MtaBC from *Methanosarcina barkeri*
Authors : Hagemeyer, C.H.; Kruer, M.; Thauer, R.K.; Warkentin, E.; Ermler, U.
Deposited on : 2006-08-17
Resolution : 2.50 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

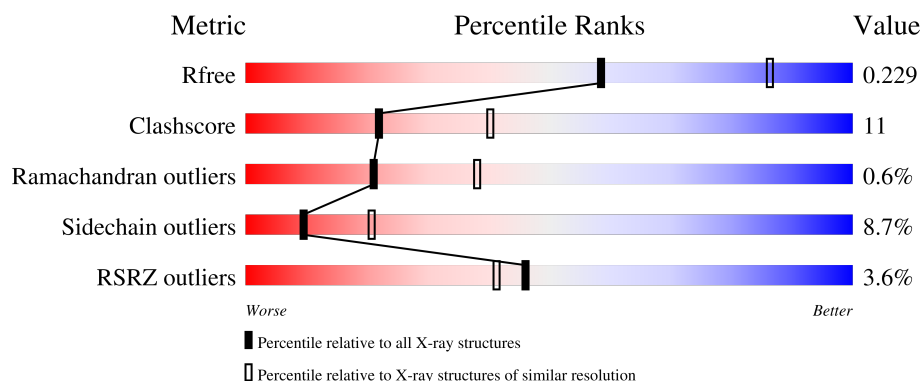
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	461	 83% 13% .
1	C	461	 79% 17% .
1	E	461	 77% 20% .
1	G	461	 77% 20% .
1	I	461	 82% 14% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	461	 80%17%.
1	M	461	 81%16%.
1	O	461	 78%19%..
2	B	258	 14%65%30%5%
2	D	258	 15%66%29%. .
2	F	258	 7%68%28%..
2	H	258	 4%71%25%..
2	J	258	 7%68%27%5%
2	L	258	 6%70%26%. .
2	N	258	 14%69%28%. .
2	P	258	 11%69%26%5%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 45566 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 Methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	C	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	E	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	G	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	I	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	K	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	M	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	O	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			

- Molecule 2 is a protein called Methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			
2	D	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			
2	F	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			
2	H	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			
2	J	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			
2	L	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	258	Total 1951	C 1238	N 311	O 389	S 13	0	0	0
2	P	258	Total 1951	C 1238	N 311	O 389	S 13	0	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Zn 2	0	0
3	C	1	Total 1	Zn 1	0	0
3	E	2	Total 2	Zn 2	0	0
3	G	1	Total 1	Zn 1	0	0
3	I	2	Total 2	Zn 2	0	0
3	K	1	Total 1	Zn 1	0	0
3	M	2	Total 2	Zn 2	0	0
3	O	1	Total 1	Zn 1	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

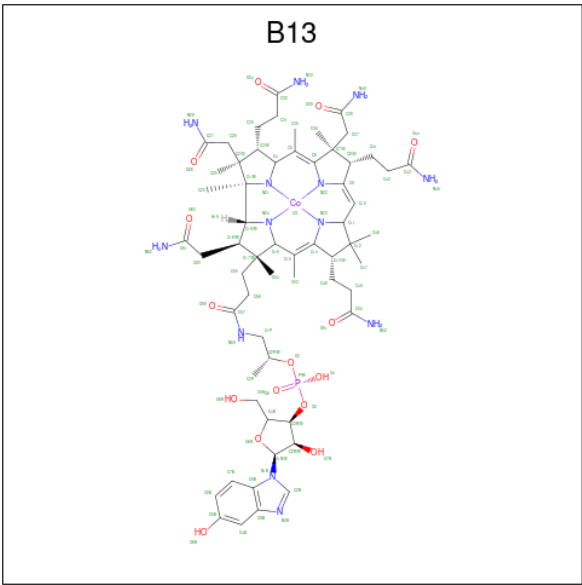
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	K 1	0	0
4	C	1	Total 1	K 1	0	0
4	E	1	Total 1	K 1	0	0
4	G	1	Total 1	K 1	0	0
4	I	1	Total 1	K 1	0	0
4	K	1	Total 1	K 1	0	0
4	M	1	Total 1	K 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	O	1	Total K 1 1	0	0

- Molecule 5 is 5-HYDROXYBENZIMIDAZOLYLCOB(III)AMIDE (CCD ID: B13) (formula: $C_{60}H_{88}CoN_{13}O_{15}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total 90	C 60	Co 1	N 13	O 15	P 1	0	0
5	D	1	Total 90	C 60	Co 1	N 13	O 15	P 1	0	0
5	F	1	Total 90	C 60	Co 1	N 13	O 15	P 1	0	0
5	H	1	Total 90	C 60	Co 1	N 13	O 15	P 1	0	0
5	J	1	Total 90	C 60	Co 1	N 13	O 15	P 1	0	0
5	L	1	Total 90	C 60	Co 1	N 13	O 15	P 1	0	0
5	N	1	Total 90	C 60	Co 1	N 13	O 15	P 1	0	0
5	P	1	Total 90	C 60	Co 1	N 13	O 15	P 1	0	0

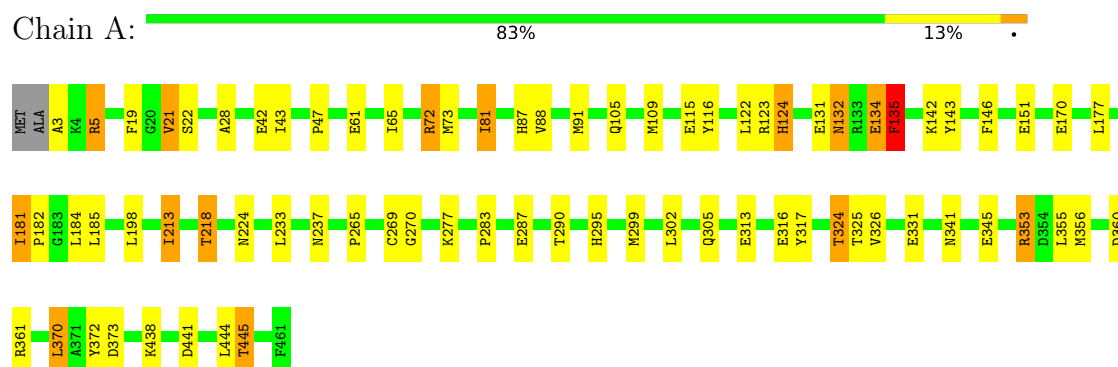
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	162	Total 162	O 162	0	0
6	B	36	Total 36	O 36	0	0
6	C	183	Total 183	O 183	0	0
6	D	27	Total 27	O 27	0	0
6	E	20	Total 20	O 20	0	0
6	F	6	Total 6	O 6	0	0
6	G	47	Total 47	O 47	0	0
6	H	1	Total 1	O 1	0	0
6	I	93	Total 93	O 93	0	0
6	J	15	Total 15	O 15	0	0
6	K	99	Total 99	O 99	0	0
6	L	18	Total 18	O 18	0	0
6	M	95	Total 95	O 95	0	0
6	N	18	Total 18	O 18	0	0
6	O	111	Total 111	O 111	0	0
6	P	15	Total 15	O 15	0	0

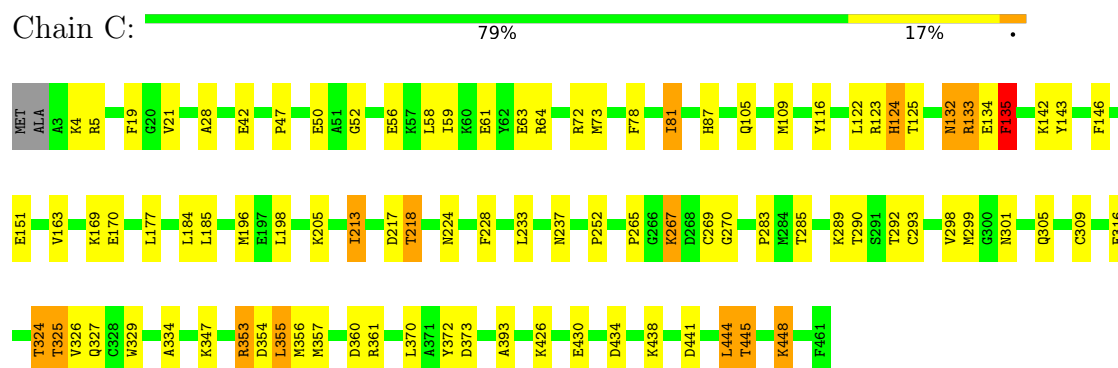
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

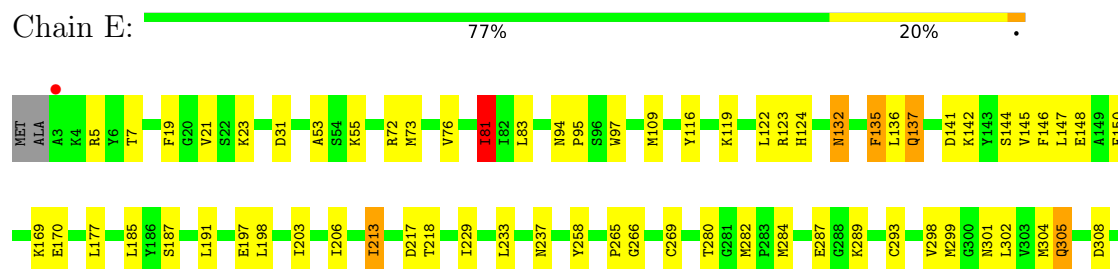
• Molecule 1: Methyltransferase 1

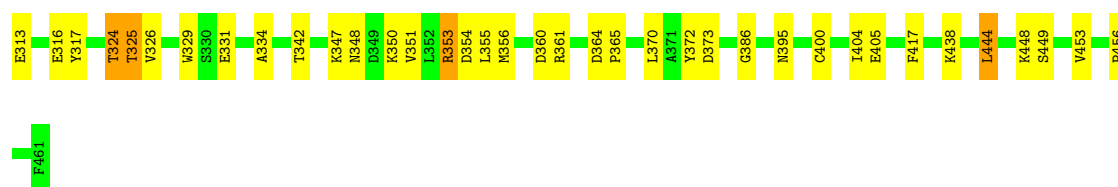


• Molecule 1: Methyltransferase 1



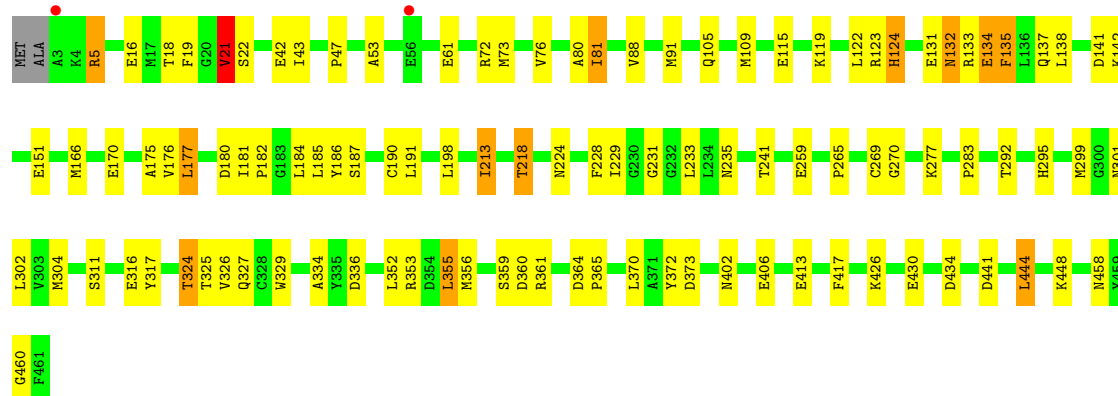
• Molecule 1: Methyltransferase 1





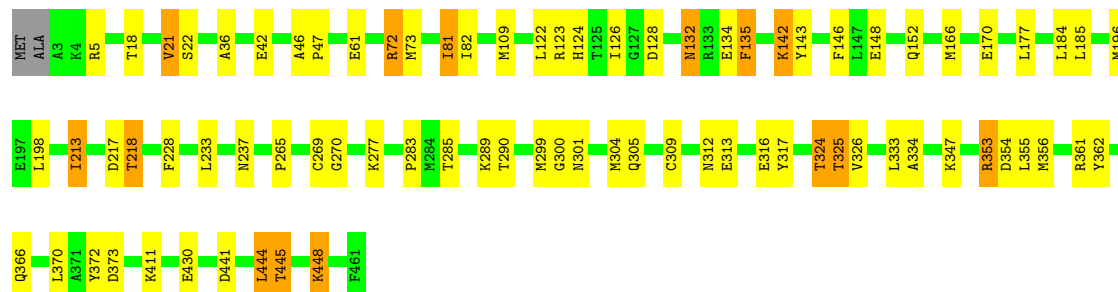
- Molecule 1: Methyltransferase 1

Chain G: 77% 20% .



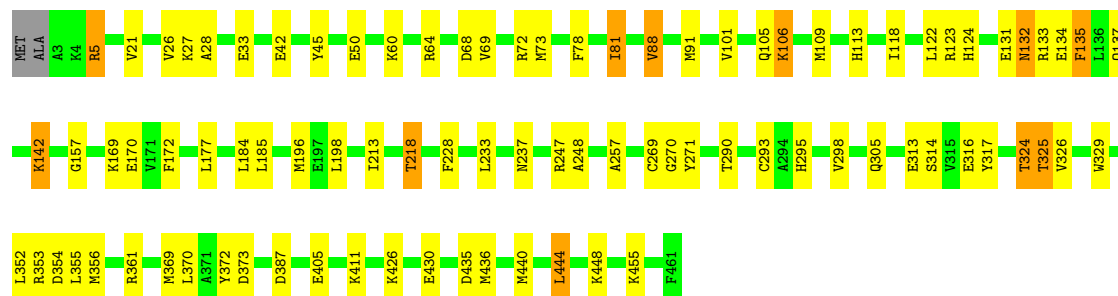
- Molecule 1: Methyltransferase 1

Chain I: 82% 14% .



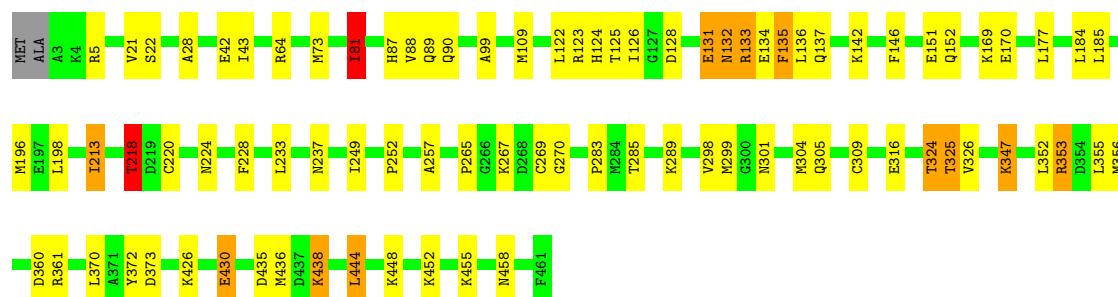
- Molecule 1: Methyltransferase 1

Chain K: 80% 17% .



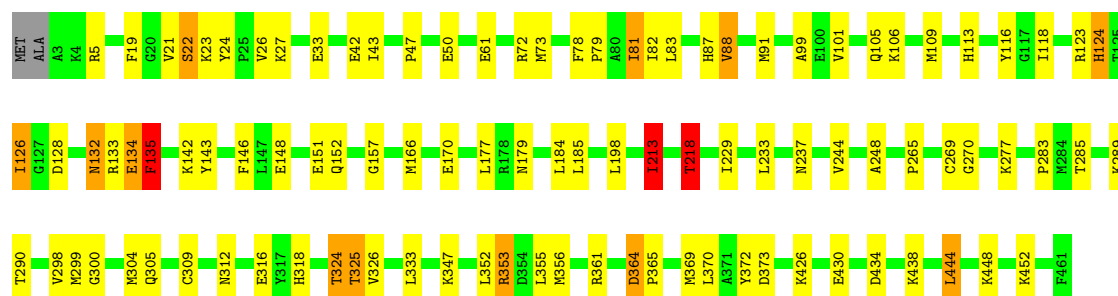
- Molecule 1: Methyltransferase 1

Chain M:  81% 16% .



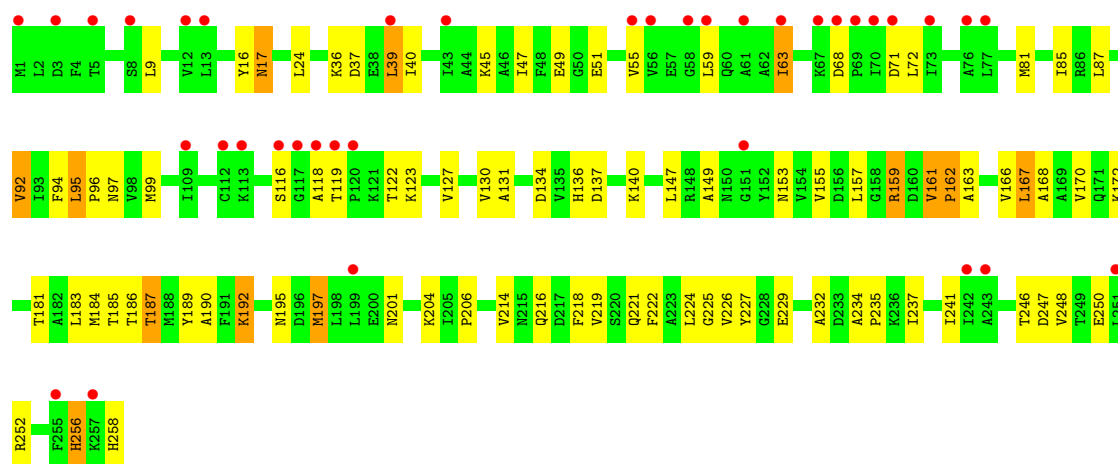
• Molecule 1: Methyltransferase 1

Chain O:  78% 19% . .



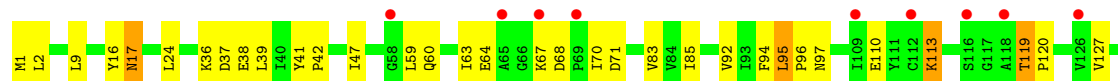
• Molecule 2: Methyltransferase 1

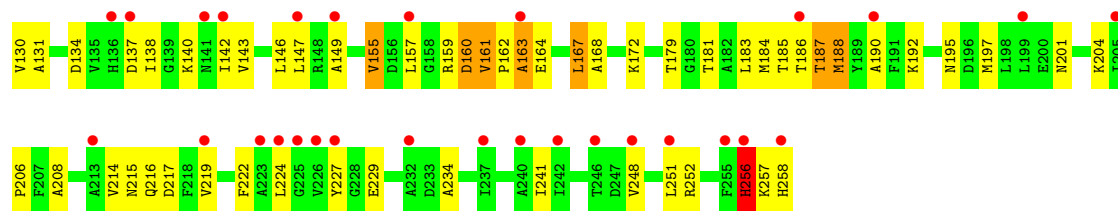
Chain B:  14% 65% 30% 5%



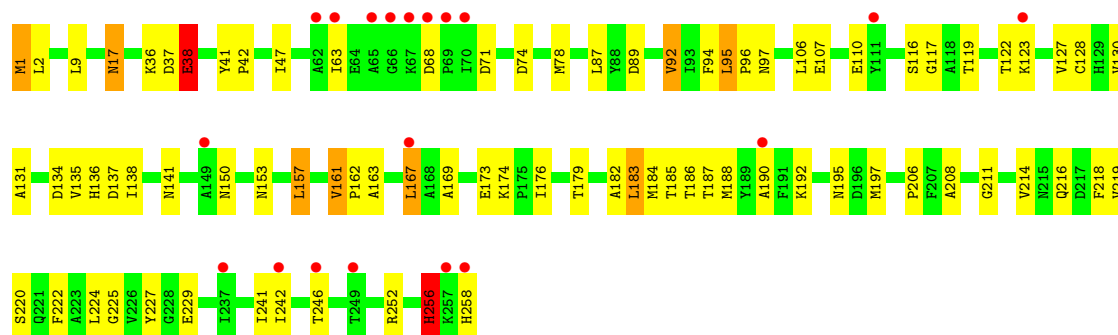
• Molecule 2: Methyltransferase 1

Chain D:  15% 66% 29% .

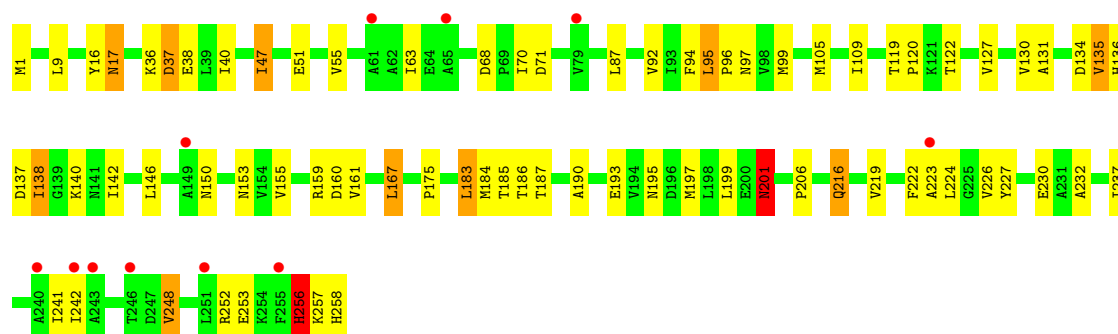




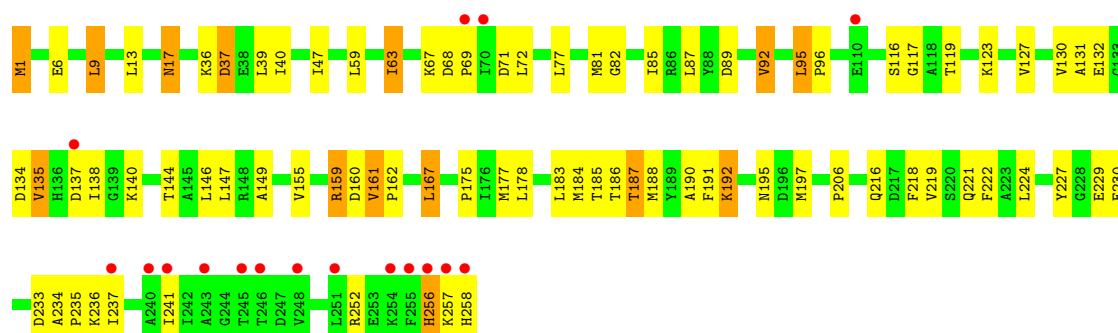
• Molecule 2: Methyltransferase 1



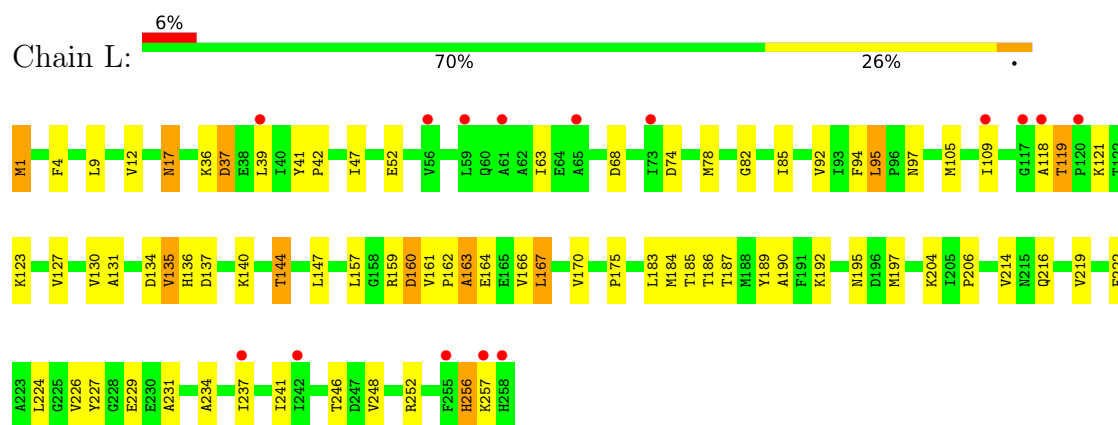
• Molecule 2: Methyltransferase 1



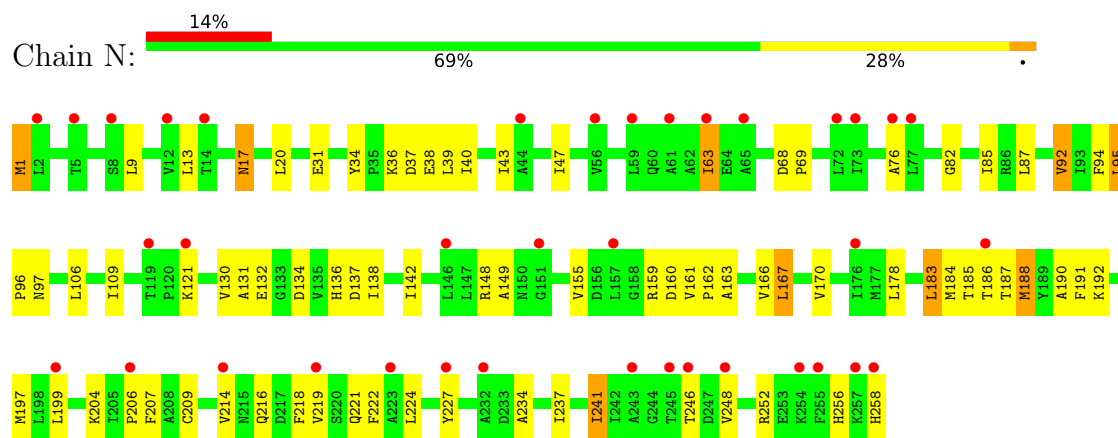
• Molecule 2: Methyltransferase 1



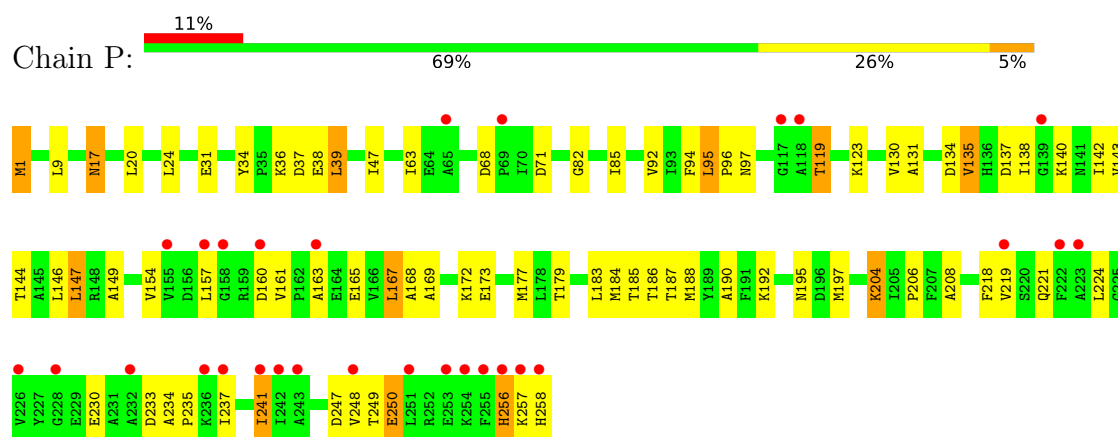
• Molecule 2: Methyltransferase 1



• Molecule 2: Methyltransferase 1



• Molecule 2: Methyltransferase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.75Å 172.85Å 190.54Å 90.00° 98.86° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-2.50) 98.3 (20.00-2.51)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.182 , 0.231 0.182 , 0.229	Depositor DCC
R_{free} test set	10921 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	45566	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, B13, K

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	0.87	2/3595 (0.1%)	1.01	2/4852 (0.0%)
1	C	0.86	1/3595 (0.0%)	1.00	3/4852 (0.1%)
1	E	0.62	0/3595	0.94	4/4852 (0.1%)
1	G	0.65	1/3595 (0.0%)	0.92	3/4852 (0.1%)
1	I	0.74	0/3595	0.94	3/4852 (0.1%)
1	K	0.72	0/3595	0.94	6/4852 (0.1%)
1	M	0.72	0/3595	0.94	4/4852 (0.1%)
1	O	0.76	0/3595	0.96	7/4852 (0.1%)
2	B	0.66	0/1980	1.00	7/2682 (0.3%)
2	D	0.63	0/1980	0.95	1/2682 (0.0%)
2	F	0.62	0/1980	0.95	2/2682 (0.1%)
2	H	0.63	0/1980	0.92	2/2682 (0.1%)
2	J	0.64	0/1980	0.95	1/2682 (0.0%)
2	L	0.62	0/1980	0.94	1/2682 (0.0%)
2	N	0.67	0/1980	0.93	0/2682
2	P	0.63	0/1980	0.98	1/2682 (0.0%)
All	All	0.71	4/44600 (0.0%)	0.96	47/60272 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	21	VAL	CA-CB	5.82	1.61	1.54
1	C	163	VAL	CA-CB	5.76	1.61	1.55
1	A	181	ILE	CA-CB	-5.66	1.51	1.54
1	A	21	VAL	CA-CB	5.22	1.62	1.54

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	THR	CB-CA-C	-8.97	93.72	109.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	218	THR	CB-CA-C	-8.76	94.09	109.86
1	C	218	THR	CB-CA-C	-7.59	96.20	109.86
1	I	218	THR	CB-CA-C	-7.43	96.49	109.86
1	O	364	ASP	CA-C-N	-7.40	112.08	119.56
1	O	364	ASP	C-N-CA	-7.40	112.08	119.56
2	P	161	VAL	N-CA-C	7.06	113.99	107.56
2	F	225	GLY	N-CA-C	6.75	120.72	111.54
1	O	135	PHE	N-CA-C	6.72	118.97	108.96
1	G	213	ILE	N-CA-C	6.66	117.46	107.80
2	H	37	ASP	N-CA-C	6.64	118.52	111.28
1	K	135	PHE	N-CA-C	6.53	118.69	108.96
2	B	161	VAL	N-CA-C	6.47	115.02	107.77
2	B	162	PRO	N-CA-C	6.45	121.94	114.20
1	A	135	PHE	N-CA-C	6.44	118.55	108.96
2	B	161	VAL	CA-C-N	6.21	127.02	120.12
2	B	161	VAL	C-N-CA	6.21	127.02	120.12
1	K	218	THR	CB-CA-C	-6.18	98.73	109.86
2	F	161	VAL	N-CA-C	6.03	113.05	107.56
1	E	213	ILE	N-CA-C	5.96	116.60	107.77
1	O	213	ILE	N-CA-C	5.96	116.43	107.80
1	C	135	PHE	N-CA-C	5.90	117.75	108.96
1	I	213	ILE	N-CA-C	5.80	116.29	108.17
1	K	88	VAL	N-CA-C	-5.80	103.73	110.05
2	D	161	VAL	N-CA-C	5.77	112.81	107.56
2	B	136	HIS	CA-C-N	5.76	128.46	120.29
2	B	136	HIS	C-N-CA	5.76	128.46	120.29
1	M	88	VAL	N-CA-C	-5.60	103.95	110.05
1	G	218	THR	CB-CA-C	-5.53	99.90	109.86
1	M	218	THR	CB-CA-C	-5.51	98.77	109.68
1	I	300	GLY	N-CA-C	5.51	119.34	112.73
1	O	88	VAL	N-CA-C	-5.41	104.15	110.05
1	K	455	LYS	CA-C-N	5.38	125.20	119.28
1	K	455	LYS	C-N-CA	5.38	125.20	119.28
2	J	161	VAL	N-CA-C	5.37	112.86	107.55
1	K	435	ASP	N-CA-C	5.35	116.86	109.15
1	M	436	MET	N-CA-C	5.31	116.75	111.07
1	E	308	ASP	N-CA-C	-5.27	107.52	114.31
1	E	135	PHE	N-CA-C	5.25	116.78	108.96
1	M	81	ILE	N-CA-C	5.24	114.77	108.06
1	C	298	VAL	CB-CA-C	5.23	118.03	111.65
2	B	225	GLY	N-CA-C	5.22	118.34	111.03
1	G	135	PHE	N-CA-C	5.16	116.14	108.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	12	VAL	N-CA-C	5.14	116.61	111.00
1	E	386	GLY	N-CA-C	5.08	120.02	113.27
2	H	138	ILE	N-CA-C	5.05	115.66	110.36
1	O	300	GLY	N-CA-C	5.04	118.78	112.73

There are no chirality outliers.

There are no planarity outliers.

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	3534	0	3462	52	0
1	C	3534	0	3462	63	0
1	E	3534	0	3462	65	0
1	G	3534	0	3462	70	0
1	I	3534	0	3462	57	0
1	K	3534	0	3462	70	0
1	M	3534	0	3462	60	0
1	O	3534	0	3462	67	0
2	B	1951	0	1952	67	0
2	D	1951	0	1952	59	0
2	F	1951	0	1952	60	0
2	H	1951	0	1952	56	0
2	J	1951	0	1952	56	0
2	L	1951	0	1952	52	0
2	N	1951	0	1952	54	0
2	P	1951	0	1952	48	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	E	2	0	0	0	0
3	G	1	0	0	0	0
3	I	2	0	0	0	0
3	K	1	0	0	0	0
3	M	2	0	0	0	0
3	O	1	0	0	0	0
4	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
5	B	90	0	81	11	0
5	D	90	0	81	15	0
5	F	90	0	81	7	0
5	H	90	0	81	10	0
5	J	90	0	81	14	0
5	L	90	0	81	10	0
5	N	90	0	81	11	0
5	P	90	0	81	9	0
6	A	162	0	0	4	0
6	B	36	0	0	1	0
6	C	183	0	0	3	0
6	D	27	0	0	0	0
6	E	20	0	0	0	0
6	F	6	0	0	0	0
6	G	47	0	0	3	0
6	H	1	0	0	0	0
6	I	93	0	0	3	0
6	J	15	0	0	0	0
6	K	99	0	0	4	0
6	L	18	0	0	1	0
6	M	95	0	0	4	0
6	N	18	0	0	0	0
6	O	111	0	0	4	0
6	P	15	0	0	0	0
All	All	45566	0	43960	947	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 11.

All (947) 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)
2:P:233:ASP:O	2:P:237:ILE:HG22	1.56	1.05
1:M:353:ARG:HA	1:M:356:MET:CE	1.92	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:353:ARG:HA	1:K:356:MET:CE	1.95	0.97
1:C:353:ARG:HA	1:C:356:MET:HE2	1.49	0.95
1:A:109:MET:HE1	1:A:122:LEU:HD13	1.49	0.94
2:L:134:ASP:HB2	2:L:187:THR:HG21	1.46	0.94
1:A:353:ARG:HA	1:A:356:MET:HE2	1.51	0.92
2:B:17:ASN:HD22	2:B:17:ASN:H	1.14	0.91
2:F:134:ASP:HB2	2:F:187:THR:HG21	1.54	0.90
1:A:305:GLN:HA	1:A:356:MET:HE3	1.52	0.89
2:H:219:VAL:HG21	2:H:227:TYR:HB2	1.54	0.89
2:D:167:LEU:HB2	2:D:197:MET:HE3	1.53	0.89
2:F:37:ASP:O	2:F:38:GLU:HB3	1.73	0.88
2:F:68:ASP:HB3	2:F:71:ASP:HB2	1.54	0.88
2:L:184:MET:HG2	5:L:500:B13:H302	1.55	0.87
1:A:72:ARG:NH2	6:A:681:HOH:O	2.09	0.85
2:F:184:MET:HG2	5:F:500:B13:H302	1.58	0.85
2:L:219:VAL:HG21	2:L:227:TYR:HB2	1.57	0.85
1:O:218:THR:HG21	1:O:269:CYS:SG	2.17	0.85
1:E:354:ASP:OD2	2:F:1:MET:HA	1.77	0.85
1:O:316:GLU:O	1:O:325:THR:HG21	1.77	0.84
2:J:17:ASN:H	2:J:17:ASN:HD22	1.24	0.84
2:H:134:ASP:HB2	2:H:187:THR:HG21	1.58	0.84
1:C:305:GLN:HA	1:C:356:MET:HE3	1.61	0.83
2:B:226:VAL:HG11	2:B:237:ILE:HD11	1.59	0.82
1:G:218:THR:HG21	1:G:269:CYS:SG	2.18	0.82
2:D:17:ASN:HD22	2:D:17:ASN:H	1.26	0.81
2:P:167:LEU:HB2	2:P:197:MET:HE3	1.63	0.81
1:O:229:ILE:HD11	2:P:138:ILE:HD13	1.63	0.80
5:D:500:B13:H363	5:D:500:B13:H401	1.45	0.80
2:L:137:ASP:HB2	5:L:500:B13:H522	1.47	0.79
1:M:353:ARG:HA	1:M:356:MET:HE2	1.64	0.79
2:N:134:ASP:HB2	2:N:187:THR:HG21	1.65	0.79
1:A:305:GLN:HA	1:A:356:MET:CE	2.12	0.78
1:I:218:THR:HG21	1:I:269:CYS:SG	2.24	0.77
1:C:316:GLU:O	1:C:325:THR:HG21	1.85	0.77
1:A:316:GLU:O	1:A:325:THR:HG21	1.84	0.77
1:I:73:MET:HE1	1:I:334:ALA:HB2	1.66	0.76
1:G:353:ARG:HA	1:G:356:MET:CE	2.16	0.76
1:E:316:GLU:O	1:E:325:THR:HG21	1.85	0.76
1:M:218:THR:HG21	1:M:269:CYS:SG	2.24	0.76
1:O:353:ARG:HA	1:O:356:MET:CE	2.14	0.76
1:C:109:MET:HE1	1:C:122:LEU:HD13	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:137:ASP:HB2	5:N:500:B13:H522	1.50	0.76
1:E:280:THR:HB	1:E:282:MET:HG3	1.69	0.75
2:B:85:ILE:HD11	2:B:149:ALA:HB1	1.67	0.75
1:E:218:THR:HG21	1:E:269:CYS:SG	2.26	0.75
1:C:324:THR:HG22	1:C:327:GLN:HG3	1.68	0.74
2:P:195:ASN:HD21	2:P:224:LEU:H	1.35	0.74
1:G:353:ARG:HD3	1:G:372:TYR:CE1	2.22	0.74
1:E:305:GLN:HA	1:E:356:MET:HE3	1.69	0.73
2:J:68:ASP:HB3	2:J:71:ASP:HB2	1.68	0.73
2:F:167:LEU:HB2	2:F:197:MET:HE3	1.71	0.73
1:C:324:THR:CG2	1:C:326:VAL:HG22	2.18	0.73
1:C:218:THR:HG21	1:C:269:CYS:SG	2.29	0.73
1:E:444:LEU:O	1:E:448:LYS:HB2	1.89	0.73
1:K:218:THR:HG21	1:K:269:CYS:SG	2.29	0.73
2:B:216:GLN:HE21	2:B:258:HIS:HD2	1.34	0.73
2:H:137:ASP:HB2	5:H:500:B13:H522	1.53	0.72
1:M:109:MET:HE1	1:M:122:LEU:HD13	1.71	0.72
1:K:316:GLU:O	1:K:325:THR:HG21	1.88	0.72
1:E:73:MET:HE2	1:E:81:ILE:HG12	1.72	0.72
2:N:191:PHE:HE2	2:N:209:CYS:HB3	1.52	0.72
2:L:131:ALA:HB1	2:L:190:ALA:HB3	1.71	0.72
1:K:72:ARG:NH2	6:K:587:HOH:O	2.22	0.72
1:I:353:ARG:HA	1:I:356:MET:HE2	1.70	0.71
2:P:177:MET:HE1	2:P:237:ILE:HG13	1.72	0.71
1:E:83:LEU:HD13	1:E:109:MET:HE2	1.72	0.71
1:K:353:ARG:HA	1:K:356:MET:HE2	1.71	0.71
2:F:185:THR:HG23	5:F:500:B13:H332	1.55	0.71
2:H:17:ASN:H	2:H:17:ASN:HD22	1.39	0.71
1:K:317:TYR:HE1	1:K:324:THR:HG21	1.56	0.71
2:P:94:PHE:H	2:P:97:ASN:HD22	1.37	0.71
1:A:218:THR:HG21	1:A:269:CYS:SG	2.31	0.70
2:H:219:VAL:CG2	2:H:227:TYR:HB2	2.22	0.70
1:I:361:ARG:NH2	1:I:373:ASP:OD1	2.24	0.70
1:M:316:GLU:O	1:M:325:THR:HG21	1.90	0.70
2:D:85:ILE:HD11	2:D:149:ALA:O	1.90	0.70
2:D:184:MET:HE3	5:D:500:B13:H353	1.72	0.70
2:N:219:VAL:HG21	2:N:227:TYR:HB2	1.73	0.70
2:D:137:ASP:HB2	5:D:500:B13:H522	1.57	0.69
2:P:68:ASP:HB3	2:P:71:ASP:HB2	1.72	0.69
1:K:352:LEU:O	1:K:356:MET:HE2	1.92	0.69
2:N:17:ASN:HD22	2:N:17:ASN:H	1.38	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:316:GLU:O	1:G:325:THR:HG21	1.91	0.69
1:K:28:ALA:HB2	1:K:213:ILE:HD12	1.74	0.69
2:F:219:VAL:HG21	2:F:227:TYR:HB2	1.74	0.69
2:H:94:PHE:H	2:H:97:ASN:HD22	1.41	0.69
2:B:134:ASP:OD2	2:B:187:THR:HG21	1.92	0.69
2:J:184:MET:HG2	5:J:500:B13:H302	1.73	0.69
2:B:17:ASN:H	2:B:17:ASN:ND2	1.86	0.69
2:B:130:VAL:HG23	2:B:140:LYS:HD3	1.74	0.69
2:P:17:ASN:H	2:P:17:ASN:HD22	1.39	0.69
2:P:134:ASP:HB2	2:P:187:THR:HG21	1.74	0.69
1:I:316:GLU:O	1:I:325:THR:HG21	1.91	0.69
1:I:361:ARG:HH22	1:I:373:ASP:CG	2.00	0.68
5:P:500:B13:H262	5:P:500:B13:H601	1.75	0.68
1:C:28:ALA:HB2	1:C:213:ILE:HD13	1.76	0.68
1:I:354:ASP:OD2	2:J:1:MET:HA	1.94	0.68
2:B:185:THR:H	5:B:500:B13:H332	1.40	0.68
1:K:26:VAL:CG1	1:K:213:ILE:HD13	2.23	0.68
2:H:195:ASN:ND2	2:H:224:LEU:HB2	2.09	0.68
1:G:132:ASN:C	1:G:132:ASN:HD22	2.01	0.68
2:P:206:PRO:HG2	2:P:241:ILE:HD12	1.76	0.68
1:G:16:GLU:OE2	1:M:347:LYS:NZ	2.25	0.68
2:J:131:ALA:HB1	2:J:190:ALA:HB3	1.75	0.68
5:L:500:B13:H601	5:L:500:B13:H262	1.76	0.67
2:B:216:GLN:HE22	2:B:258:HIS:H	1.41	0.67
2:F:184:MET:HE3	5:F:500:B13:H353	1.76	0.67
1:M:361:ARG:NH2	1:M:373:ASP:OD1	2.27	0.67
1:G:361:ARG:HH22	1:G:373:ASP:CG	2.03	0.67
2:J:192:LYS:HG2	2:J:222:PHE:CE2	2.29	0.67
2:B:168:ALA:O	2:B:172:LYS:HG2	1.94	0.67
1:G:109:MET:HE1	1:G:122:LEU:HD13	1.77	0.67
2:F:131:ALA:HB1	2:F:190:ALA:HB3	1.76	0.67
2:D:41:TYR:HB3	2:D:42:PRO:HD3	1.76	0.67
1:G:301:ASN:HD22	1:G:304:MET:CE	2.07	0.67
2:F:17:ASN:H	2:F:17:ASN:HD22	1.41	0.66
1:O:132:ASN:HD22	1:O:134:GLU:H	1.43	0.66
1:G:426:LYS:O	1:G:430:GLU:HG3	1.95	0.66
1:I:353:ARG:HD3	1:I:372:TYR:CE1	2.30	0.66
2:P:37:ASP:O	2:P:39:LEU:N	2.25	0.66
5:F:500:B13:H252	5:F:500:B13:H601	1.76	0.66
5:H:500:B13:H252	5:H:500:B13:H601	1.75	0.66
5:B:500:B13:H351	5:B:500:B13:H361	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:134:ASP:HB2	2:D:187:THR:HG21	1.77	0.66
1:C:132:ASN:ND2	1:C:135:PHE:H	1.94	0.66
1:I:317:TYR:HE1	1:I:324:THR:HG21	1.59	0.66
1:M:123:ARG:NH2	1:M:265:PRO:O	2.28	0.66
1:G:417:PHE:HZ	2:H:97:ASN:HD21	1.43	0.65
2:B:192:LYS:HG2	2:B:222:PHE:HE2	1.62	0.65
1:O:43:ILE:HG22	1:O:81:ILE:HD11	1.79	0.65
2:B:206:PRO:HG2	2:B:241:ILE:HD12	1.79	0.65
1:M:353:ARG:HD3	1:M:372:TYR:CE1	2.31	0.65
2:B:166:VAL:O	2:B:170:VAL:HG23	1.97	0.65
1:G:5:ARG:HA	1:G:259:GLU:HG2	1.80	0.64
2:F:195:ASN:HD21	2:F:224:LEU:H	1.43	0.64
2:N:184:MET:HG2	5:N:500:B13:H302	1.78	0.64
2:D:185:THR:H	5:D:500:B13:H332	1.46	0.64
1:I:305:GLN:HA	1:I:356:MET:CE	2.28	0.64
1:O:353:ARG:HA	1:O:356:MET:HE2	1.77	0.64
2:P:85:ILE:HD11	2:P:149:ALA:HB1	1.79	0.64
1:A:5:ARG:HD2	6:A:657:HOH:O	1.97	0.64
6:G:530:HOH:O	2:H:1:MET:HB3	1.97	0.64
2:J:17:ASN:HD22	2:J:17:ASN:N	1.94	0.64
2:J:87:LEU:HB3	2:J:92:VAL:HG22	1.79	0.63
2:D:216:GLN:HE21	2:D:258:HIS:HD2	1.46	0.63
1:G:302:LEU:HB2	1:G:360:ASP:HB2	1.81	0.63
5:J:500:B13:H361	5:J:500:B13:H351	1.80	0.63
2:F:17:ASN:HD22	2:F:17:ASN:N	1.96	0.63
1:I:109:MET:HE1	1:I:122:LEU:HD13	1.81	0.63
2:F:216:GLN:HE22	2:F:258:HIS:H	1.45	0.63
2:B:137:ASP:HB2	5:B:500:B13:H522	1.64	0.63
5:D:500:B13:H363	5:D:500:B13:N40	2.14	0.63
2:B:216:GLN:HE21	2:B:258:HIS:CD2	2.16	0.62
2:N:185:THR:HG23	5:N:500:B13:H332	1.64	0.62
1:E:73:MET:HE1	1:E:334:ALA:HB2	1.80	0.62
1:K:109:MET:HE1	1:K:122:LEU:HD13	1.81	0.62
2:D:222:PHE:O	2:D:252:ARG:NH2	2.32	0.62
1:I:305:GLN:HA	1:I:356:MET:HE3	1.82	0.62
6:M:611:HOH:O	2:N:138:ILE:HG12	1.99	0.62
2:P:247:ASP:HB3	2:P:250:GLU:HB2	1.81	0.62
2:D:131:ALA:HB1	2:D:190:ALA:HB3	1.81	0.62
2:H:199:LEU:C	2:H:201:ASN:H	2.07	0.62
2:P:168:ALA:O	2:P:172:LYS:HG2	1.99	0.62
1:M:353:ARG:CA	1:M:356:MET:HE2	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:132:ASN:HD22	1:K:132:ASN:C	2.07	0.62
2:B:192:LYS:HG2	2:B:222:PHE:CE2	2.34	0.61
2:B:195:ASN:HD21	2:B:224:LEU:H	1.47	0.61
2:D:168:ALA:O	2:D:172:LYS:HG2	2.00	0.61
2:D:215:ASN:HD22	2:D:217:ASP:H	1.48	0.61
2:P:185:THR:HG23	5:P:500:B13:H332	1.65	0.61
1:K:133:ARG:HD2	2:L:160:ASP:HB3	1.80	0.61
1:C:42:GLU:OE2	1:C:123:ARG:HD2	2.00	0.61
1:O:72:ARG:NH2	6:O:616:HOH:O	2.33	0.61
1:G:460:GLY:HA2	6:G:554:HOH:O	2.00	0.61
2:P:177:MET:CE	2:P:237:ILE:HG13	2.30	0.61
2:J:195:ASN:HD21	2:J:224:LEU:H	1.47	0.61
1:M:426:LYS:HE3	1:M:430:GLU:OE2	2.00	0.61
1:O:132:ASN:ND2	1:O:134:GLU:H	1.98	0.61
2:P:131:ALA:HB1	2:P:190:ALA:HB3	1.81	0.61
1:C:426:LYS:O	1:C:430:GLU:HG3	2.01	0.61
2:J:184:MET:HE3	5:J:500:B13:H353	1.82	0.61
2:N:94:PHE:H	2:N:97:ASN:HD22	1.49	0.61
5:D:500:B13:H351	5:D:500:B13:H361	1.83	0.61
2:F:94:PHE:H	2:F:97:ASN:HD22	1.48	0.60
2:H:135:VAL:HG22	2:H:159:ARG:HE	1.66	0.60
2:L:82:GLY:HA2	2:L:85:ILE:HD12	1.81	0.60
2:N:94:PHE:H	2:N:97:ASN:ND2	1.98	0.60
1:G:73:MET:HE1	1:G:334:ALA:HB2	1.81	0.60
2:N:166:VAL:O	2:N:170:VAL:HG23	2.01	0.60
1:C:289:LYS:HD3	1:C:301:ASN:ND2	2.16	0.60
1:E:237:ASN:HA	2:F:95:LEU:HB2	1.83	0.60
1:C:4:LYS:HG2	6:O:629:HOH:O	2.02	0.60
1:O:132:ASN:ND2	1:O:135:PHE:H	1.98	0.60
2:F:252:ARG:O	2:F:256:HIS:HB2	2.00	0.60
1:M:133:ARG:HH11	1:M:133:ARG:CG	2.14	0.60
2:P:163:ALA:C	2:P:197:MET:HE1	2.27	0.60
1:G:224:ASN:O	1:G:228:PHE:HD2	1.84	0.60
2:L:167:LEU:HB2	2:L:197:MET:HE3	1.84	0.60
1:C:353:ARG:HA	1:C:356:MET:CE	2.29	0.60
2:J:37:ASP:HB3	2:J:40:ILE:HB	1.84	0.60
2:L:224:LEU:HA	2:L:248:VAL:HG21	1.83	0.59
2:B:167:LEU:HB2	2:B:197:MET:HE1	1.83	0.59
1:O:132:ASN:HD22	1:O:132:ASN:C	2.10	0.59
1:A:73:MET:HE2	1:A:81:ILE:HB	1.85	0.59
1:A:42:GLU:OE2	1:A:123:ARG:HD2	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:179:THR:HG22	2:F:208:ALA:HB3	1.85	0.59
1:I:312:ASN:HB3	1:I:333:LEU:HD11	1.85	0.59
2:F:163:ALA:C	2:F:197:MET:HE1	2.28	0.59
2:L:222:PHE:O	2:L:252:ARG:NH2	2.36	0.59
1:C:324:THR:HG23	1:C:326:VAL:HG22	1.85	0.59
2:N:40:ILE:HA	2:N:43:ILE:HD12	1.85	0.59
2:N:224:LEU:HA	2:N:248:VAL:HG21	1.83	0.59
5:H:500:B13:O58	5:H:500:B13:H532	2.02	0.59
2:N:219:VAL:CG2	2:N:227:TYR:HB2	2.33	0.59
2:B:206:PRO:HG2	2:B:241:ILE:CD1	2.33	0.58
2:D:185:THR:O	2:D:188:MET:HE2	2.03	0.58
2:J:216:GLN:HE21	2:J:258:HIS:HD2	1.49	0.58
1:K:317:TYR:CE1	1:K:324:THR:HG21	2.35	0.58
2:P:184:MET:HG2	5:P:500:B13:H302	1.85	0.58
1:E:444:LEU:CD2	1:E:448:LYS:HD2	2.32	0.58
2:J:185:THR:HG23	5:J:500:B13:H332	1.68	0.58
2:N:137:ASP:HB2	5:N:500:B13:N52	2.18	0.58
2:B:94:PHE:H	2:B:97:ASN:HD22	1.51	0.58
2:L:17:ASN:HD22	2:L:17:ASN:H	1.52	0.58
1:M:42:GLU:OE2	1:M:123:ARG:HD2	2.03	0.58
2:D:94:PHE:H	2:D:97:ASN:HD22	1.51	0.58
2:H:130:VAL:HG23	2:H:140:LYS:HD3	1.86	0.58
1:K:293:CYS:HB3	1:K:329:TRP:CZ2	2.39	0.58
1:O:373:ASP:HB3	2:P:1:MET:HE1	1.86	0.58
1:E:132:ASN:ND2	1:E:135:PHE:H	2.02	0.58
1:G:18:THR:HG23	1:G:21:VAL:HG13	1.86	0.58
1:I:444:LEU:HD22	1:I:448:LYS:HD2	1.85	0.58
2:J:185:THR:H	5:J:500:B13:H332	1.50	0.58
1:O:361:ARG:HH22	1:O:373:ASP:CG	2.11	0.58
2:B:189:TYR:O	2:B:192:LYS:HB2	2.04	0.58
2:P:234:ALA:HB3	2:P:235:PRO:HD3	1.85	0.58
2:B:184:MET:HG2	5:B:500:B13:H302	1.84	0.57
1:I:444:LEU:O	1:I:448:LYS:HB2	2.04	0.57
2:H:37:ASP:O	2:H:38:GLU:HB3	2.04	0.57
2:B:36:LYS:H	2:B:36:LYS:HD3	1.69	0.57
2:H:185:THR:HG23	5:H:500:B13:H332	1.68	0.57
1:E:444:LEU:HD22	1:E:448:LYS:HD2	1.85	0.57
2:H:17:ASN:HD22	2:H:17:ASN:N	2.03	0.57
2:J:216:GLN:HE21	2:J:258:HIS:CD2	2.21	0.57
1:O:42:GLU:OE2	1:O:123:ARG:HD2	2.04	0.57
2:P:138:ILE:O	2:P:142:ILE:HG13	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:185:THR:H	5:P:500:B13:H332	1.51	0.57
1:G:231:GLY:HA3	1:G:235:ASN:ND2	2.20	0.57
2:L:130:VAL:HG12	2:L:134:ASP:HB3	1.87	0.57
5:N:500:B13:H262	5:N:500:B13:H601	1.87	0.57
2:B:195:ASN:ND2	2:B:224:LEU:H	2.03	0.57
2:H:197:MET:HG2	2:H:197:MET:O	2.04	0.57
2:H:184:MET:HG2	5:H:500:B13:H302	1.86	0.57
1:K:169:LYS:HD2	5:L:500:B13:H473	1.87	0.57
2:L:127:VAL:HG23	2:L:175:PRO:HG3	1.85	0.57
2:B:94:PHE:H	2:B:97:ASN:ND2	2.03	0.56
1:M:444:LEU:O	1:M:448:LYS:HB2	2.05	0.56
2:D:17:ASN:HD22	2:D:17:ASN:N	2.02	0.56
2:B:184:MET:HE3	5:B:500:B13:H353	1.87	0.56
2:B:226:VAL:HG11	2:B:237:ILE:CD1	2.31	0.56
5:D:500:B13:H262	5:D:500:B13:H601	1.87	0.56
1:E:353:ARG:HA	1:E:356:MET:HE2	1.87	0.56
2:N:252:ARG:O	2:N:256:HIS:HB2	2.05	0.56
1:O:19:PHE:CE1	1:O:356:MET:HE1	2.40	0.56
2:D:37:ASP:O	2:D:39:LEU:N	2.29	0.56
1:E:109:MET:HE1	1:E:122:LEU:HD13	1.87	0.56
1:G:123:ARG:NH2	1:G:265:PRO:O	2.39	0.56
2:P:188:MET:HB3	2:P:218:PHE:CZ	2.41	0.56
1:E:448:LYS:HE3	1:E:456:PRO:HG2	1.86	0.56
1:A:132:ASN:ND2	1:A:135:PHE:H	2.03	0.56
1:A:265:PRO:HA	1:A:283:PRO:O	2.06	0.56
2:B:167:LEU:HB2	2:B:197:MET:CE	2.36	0.56
1:E:229:ILE:HD11	2:F:138:ILE:HD13	1.88	0.56
1:G:364:ASP:CG	1:G:365:PRO:HD2	2.31	0.56
1:K:132:ASN:ND2	1:K:135:PHE:H	2.03	0.56
2:J:37:ASP:C	2:J:39:LEU:H	2.14	0.56
1:E:353:ARG:HD3	1:E:372:TYR:CE1	2.40	0.56
2:N:131:ALA:HB1	2:N:190:ALA:HB3	1.86	0.56
1:O:444:LEU:O	1:O:448:LYS:HB2	2.06	0.56
2:B:45:LYS:HE3	2:B:49:GLU:OE2	2.05	0.56
1:C:293:CYS:HB3	1:C:329:TRP:CZ2	2.40	0.56
1:E:372:TYR:OH	2:F:1:MET:HE2	2.05	0.56
1:I:132:ASN:C	1:I:132:ASN:HD22	2.14	0.56
1:K:354:ASP:OD2	2:L:1:MET:HA	2.06	0.56
1:M:87:HIS:NE2	1:M:124:HIS:HD2	2.04	0.56
2:N:216:GLN:HE22	2:N:258:HIS:H	1.54	0.56
5:F:500:B13:H361	5:F:500:B13:H351	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:37:ASP:O	2:J:39:LEU:N	2.30	0.55
1:K:5:ARG:NH2	6:K:611:HOH:O	2.30	0.55
2:B:68:ASP:HB3	2:B:71:ASP:HB2	1.88	0.55
2:F:137:ASP:HB3	2:F:141:ASN:ND2	2.21	0.55
1:M:73:MET:HE2	1:M:81:ILE:HB	1.87	0.55
1:G:444:LEU:O	1:G:448:LYS:HB2	2.06	0.55
1:K:353:ARG:CA	1:K:356:MET:HE2	2.36	0.55
2:D:138:ILE:HG13	5:D:500:B13:O51	2.06	0.55
1:K:50:GLU:CD	1:K:50:GLU:H	2.14	0.55
1:O:312:ASN:HB3	1:O:333:LEU:HD11	1.88	0.55
1:I:123:ARG:NH2	1:I:265:PRO:O	2.40	0.55
2:J:218:PHE:O	2:J:221:GLN:HG2	2.07	0.55
1:A:47:PRO:HB3	1:A:61:GLU:HG2	1.88	0.55
2:F:176:ILE:HD13	2:F:242:ILE:HD11	1.87	0.55
1:G:353:ARG:HA	1:G:356:MET:HE3	1.88	0.55
6:I:562:HOH:O	2:J:96:PRO:HG2	2.07	0.55
1:K:361:ARG:HH22	1:K:373:ASP:CG	2.15	0.55
2:P:130:VAL:HG23	2:P:140:LYS:HD3	1.88	0.55
5:B:500:B13:H601	5:B:500:B13:H262	1.89	0.55
2:J:59:LEU:HD11	2:J:77:LEU:HD21	1.88	0.55
2:N:106:LEU:HD11	2:N:148:ARG:HD3	1.88	0.55
2:H:222:PHE:O	2:H:252:ARG:NH2	2.39	0.55
1:O:99:ALA:HB2	1:O:152:GLN:HB3	1.89	0.54
1:O:244:VAL:HG22	1:O:369:MET:HE3	1.89	0.54
1:O:265:PRO:HA	1:O:283:PRO:O	2.07	0.54
1:C:305:GLN:HA	1:C:356:MET:CE	2.35	0.54
2:H:87:LEU:HD22	2:H:92:VAL:HG21	1.89	0.54
2:H:131:ALA:HB1	2:H:190:ALA:HB3	1.89	0.54
2:H:136:HIS:HB3	2:H:183:LEU:HD13	1.89	0.54
1:C:72:ARG:NH2	6:C:515:HOH:O	2.39	0.54
1:E:342:THR:HG22	1:G:355:LEU:HD12	1.90	0.54
2:H:195:ASN:HD21	2:H:224:LEU:H	1.54	0.54
1:K:73:MET:HE3	1:K:78:PHE:HB2	1.90	0.54
1:C:361:ARG:HH22	1:C:373:ASP:CG	2.15	0.54
2:D:127:VAL:HG13	2:D:157:LEU:HD23	1.89	0.54
1:G:132:ASN:ND2	1:G:134:GLU:H	2.04	0.54
1:O:128:ASP:CG	1:O:166:MET:HE2	2.32	0.54
2:B:127:VAL:HG13	2:B:157:LEU:HD23	1.89	0.54
1:G:187:SER:HA	1:G:191:LEU:HD12	1.89	0.54
2:H:51:GLU:O	2:H:55:VAL:HG23	2.08	0.54
1:I:441:ASP:O	1:I:445:THR:HG23	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:69:VAL:O	1:K:73:MET:HG2	2.08	0.54
1:M:224:ASN:ND2	1:M:269:CYS:HB2	2.22	0.54
1:O:143:TYR:O	1:O:146:PHE:HB3	2.07	0.54
1:O:353:ARG:HD3	1:O:372:TYR:CE1	2.43	0.54
1:M:224:ASN:HD21	1:M:269:CYS:HB2	1.73	0.54
1:C:265:PRO:HA	1:C:283:PRO:O	2.07	0.54
1:K:444:LEU:O	1:K:448:LYS:HB2	2.08	0.54
1:M:43:ILE:HG22	1:M:81:ILE:HD11	1.90	0.54
1:E:354:ASP:HB3	2:F:2:LEU:HD12	1.90	0.53
2:L:134:ASP:OD1	2:L:136:HIS:ND1	2.32	0.53
2:L:166:VAL:O	2:L:170:VAL:HG23	2.08	0.53
1:O:132:ASN:HD22	1:O:134:GLU:N	2.05	0.53
2:P:218:PHE:O	2:P:221:GLN:HG2	2.08	0.53
2:F:192:LYS:HG2	2:F:222:PHE:CE2	2.42	0.53
2:D:179:THR:HG22	2:D:208:ALA:HB3	1.90	0.53
2:D:216:GLN:HE21	2:D:258:HIS:CD2	2.26	0.53
1:K:132:ASN:HD21	1:K:135:PHE:H	1.56	0.53
1:M:361:ARG:HH22	1:M:373:ASP:CG	2.16	0.53
2:P:195:ASN:ND2	2:P:224:LEU:H	2.06	0.53
1:K:373:ASP:HB3	2:L:1:MET:HE1	1.91	0.53
1:M:131:GLU:HB2	1:M:136:LEU:HA	1.91	0.53
1:A:302:LEU:HB2	1:A:360:ASP:HB2	1.91	0.53
2:D:206:PRO:HG2	2:D:241:ILE:HD12	1.91	0.53
1:G:19:PHE:CE1	1:G:356:MET:HE1	2.44	0.53
1:E:301:ASN:HD22	1:E:304:MET:HE2	1.74	0.53
1:G:132:ASN:HD21	1:G:134:GLU:HG2	1.74	0.53
1:M:89:GLN:NE2	1:M:90:GLN:HB3	2.24	0.53
2:D:17:ASN:H	2:D:17:ASN:ND2	2.03	0.52
2:L:219:VAL:CG2	2:L:227:TYR:HB2	2.35	0.52
2:F:135:VAL:O	2:F:135:VAL:CG1	2.57	0.52
2:H:206:PRO:HG2	2:H:241:ILE:HD12	1.90	0.52
2:H:230:GLU:HG3	2:H:232:ALA:H	1.74	0.52
5:J:500:B13:H363	5:J:500:B13:H401	1.73	0.52
1:A:3:ALA:HB2	6:A:675:HOH:O	2.09	0.52
1:C:132:ASN:C	1:C:132:ASN:HD22	2.18	0.52
1:E:19:PHE:CD1	1:E:356:MET:HE1	2.45	0.52
1:E:331:GLU:HB3	1:G:292:THR:HG21	1.90	0.52
1:M:435:ASP:OD2	1:M:438:LYS:HB2	2.09	0.52
1:E:372:TYR:CZ	2:F:1:MET:HE2	2.44	0.52
1:K:290:THR:O	1:K:290:THR:HG22	2.10	0.52
1:O:218:THR:HG23	1:O:270:GLY:N	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:215:ASN:ND2	2:D:217:ASP:H	2.08	0.52
2:H:136:HIS:CB	2:H:183:LEU:HD13	2.40	0.52
2:L:52:GLU:H	2:L:52:GLU:CD	2.17	0.52
1:M:64:ARG:NE	6:M:565:HOH:O	2.42	0.52
2:N:216:GLN:HE21	2:N:258:HIS:HD2	1.55	0.52
1:I:218:THR:HG23	1:I:270:GLY:CA	2.39	0.52
2:N:191:PHE:CE2	2:N:209:CYS:HB3	2.40	0.52
1:O:50:GLU:CD	1:O:50:GLU:H	2.18	0.52
1:O:132:ASN:HD21	1:O:135:PHE:H	1.58	0.52
1:E:324:THR:CG2	1:E:326:VAL:HG22	2.40	0.52
1:G:229:ILE:HD11	2:H:138:ILE:HD13	1.90	0.52
1:M:99:ALA:HB2	1:M:152:GLN:HB3	1.92	0.52
1:M:169:LYS:HD2	5:N:500:B13:H473	1.92	0.52
2:F:128:CYS:O	2:F:157:LEU:HB2	2.10	0.51
2:F:227:TYR:H	2:F:256:HIS:HE1	1.58	0.51
1:G:301:ASN:HA	1:G:304:MET:HE2	1.91	0.51
1:C:133:ARG:HD2	2:D:160:ASP:HB3	1.91	0.51
1:M:352:LEU:O	1:M:356:MET:HE2	2.10	0.51
2:B:116:SER:C	2:B:118:ALA:H	2.18	0.51
2:H:122:THR:HG21	2:H:153:ASN:HB2	1.92	0.51
1:K:352:LEU:C	1:K:356:MET:HE2	2.34	0.51
2:B:184:MET:HB2	2:B:187:THR:HB	1.92	0.51
2:H:95:LEU:HB3	2:H:96:PRO:HD3	1.93	0.51
1:I:218:THR:HG23	1:I:270:GLY:N	2.26	0.51
1:M:132:ASN:HD21	1:M:135:PHE:H	1.59	0.51
1:O:23:LYS:HD3	1:O:24:TYR:CZ	2.46	0.51
5:B:500:B13:H252	5:B:500:B13:C61	2.41	0.51
2:J:167:LEU:HG	2:J:197:MET:HG2	1.91	0.51
1:K:27:LYS:HG2	1:K:33:GLU:HG2	1.92	0.51
1:O:87:HIS:NE2	1:O:124:HIS:HD2	2.08	0.51
1:E:280:THR:HB	1:E:282:MET:CG	2.41	0.51
1:C:125:THR:HG21	1:C:267:LYS:HE2	1.93	0.51
1:E:132:ASN:C	1:E:132:ASN:HD22	2.19	0.51
1:O:248:ALA:HB2	1:O:369:MET:HE2	1.93	0.51
1:A:143:TYR:O	1:A:146:PHE:HB3	2.11	0.51
1:K:237:ASN:HA	2:L:95:LEU:HB2	1.92	0.50
2:L:159:ARG:O	2:L:161:VAL:N	2.44	0.50
1:M:137:GLN:HG2	6:M:612:HOH:O	2.11	0.50
1:I:237:ASN:HA	2:J:95:LEU:HB2	1.93	0.50
2:P:179:THR:HG22	2:P:208:ALA:HB3	1.93	0.50
1:A:353:ARG:HD3	1:A:372:TYR:CE1	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:ASP:O	1:E:119:LYS:HG2	2.10	0.50
1:E:293:CYS:HB3	1:E:329:TRP:CE2	2.47	0.50
2:F:94:PHE:H	2:F:97:ASN:ND2	2.09	0.50
2:L:135:VAL:HG22	2:L:159:ARG:HE	1.77	0.50
2:N:206:PRO:HG2	2:N:241:ILE:HD12	1.92	0.50
1:A:324:THR:CG2	1:A:326:VAL:HG22	2.42	0.50
2:B:162:PRO:O	2:B:163:ALA:HB3	2.12	0.50
1:E:293:CYS:HB3	1:E:329:TRP:CZ2	2.46	0.50
2:F:122:THR:HG21	2:F:153:ASN:HB2	1.94	0.50
2:D:184:MET:HG2	5:D:500:B13:H302	1.94	0.50
2:L:41:TYR:HB3	2:L:42:PRO:HD3	1.92	0.50
2:L:195:ASN:HD21	2:L:224:LEU:H	1.60	0.50
2:J:81:MET:HE2	2:J:149:ALA:HB1	1.94	0.50
2:B:234:ALA:HB3	2:B:235:PRO:HD3	1.93	0.50
2:F:195:ASN:ND2	2:F:224:LEU:HB2	2.27	0.50
1:C:28:ALA:HB2	1:C:213:ILE:CD1	2.41	0.50
1:C:59:ILE:O	1:C:63:GLU:HG3	2.12	0.50
2:P:230:GLU:O	2:P:233:ASP:HB2	2.11	0.50
1:E:400:CYS:O	1:E:404:ILE:HG12	2.12	0.49
1:G:352:LEU:O	1:G:356:MET:HE2	2.12	0.49
1:I:18:THR:CG2	1:I:21:VAL:HG13	2.42	0.49
1:K:353:ARG:HD3	1:K:372:TYR:CE1	2.47	0.49
2:J:134:ASP:OD2	2:J:187:THR:HG21	2.11	0.49
2:J:195:ASN:ND2	2:J:224:LEU:HB2	2.27	0.49
2:F:135:VAL:O	2:F:135:VAL:HG12	2.12	0.49
1:G:132:ASN:ND2	1:G:134:GLU:HG2	2.28	0.49
1:G:352:LEU:C	1:G:356:MET:HE2	2.37	0.49
1:K:361:ARG:NH2	1:K:373:ASP:OD1	2.45	0.49
2:H:223:ALA:O	2:H:248:VAL:HG11	2.13	0.49
2:P:31:GLU:HA	2:P:34:TYR:CD1	2.48	0.49
1:A:305:GLN:CA	1:A:356:MET:HE3	2.34	0.49
1:I:373:ASP:HB3	2:J:1:MET:HE1	1.95	0.49
1:O:133:ARG:NH2	2:P:165:GLU:OE2	2.46	0.49
2:F:127:VAL:HG13	2:F:157:LEU:HD23	1.93	0.49
2:N:138:ILE:HG13	5:N:500:B13:C50	2.43	0.49
1:O:132:ASN:HD21	1:O:134:GLU:HG2	1.76	0.49
2:N:31:GLU:HA	2:N:34:TYR:CD1	2.48	0.49
1:A:317:TYR:HA	1:A:325:THR:HG21	1.93	0.49
2:F:116:SER:OG	2:F:117:GLY:N	2.44	0.49
2:B:252:ARG:HG2	2:B:256:HIS:CE1	2.48	0.49
2:D:185:THR:HG23	5:D:500:B13:H332	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:42:GLU:OE2	1:K:123:ARG:HD2	2.12	0.49
1:M:218:THR:HG23	1:M:270:GLY:N	2.27	0.49
1:O:113:HIS:HD2	1:O:118:ILE:O	1.96	0.49
2:B:17:ASN:HD22	2:B:17:ASN:N	1.95	0.49
2:H:195:ASN:HD22	2:H:224:LEU:HB2	1.78	0.49
1:I:148:GLU:O	1:I:152:GLN:HG2	2.11	0.49
1:I:317:TYR:CE1	1:I:324:THR:HG21	2.44	0.49
1:E:317:TYR:HA	1:E:325:THR:CG2	2.43	0.48
1:K:60:LYS:HE3	1:K:64:ARG:HE	1.78	0.48
1:M:265:PRO:HA	1:M:283:PRO:O	2.12	0.48
1:I:81:ILE:HD13	1:I:82:ILE:O	2.13	0.48
1:G:133:ARG:HD2	2:H:160:ASP:HB3	1.95	0.48
1:E:136:LEU:HD21	1:E:169:LYS:HE3	1.96	0.48
1:E:258:TYR:CZ	1:E:284:MET:HE1	2.49	0.48
2:F:37:ASP:O	2:F:38:GLU:CB	2.54	0.48
5:H:500:B13:H363	5:H:500:B13:H401	1.79	0.48
1:M:237:ASN:HA	2:N:95:LEU:HB2	1.95	0.48
2:B:232:ALA:O	2:B:235:PRO:HD2	2.14	0.48
1:C:52:GLY:HA2	1:C:58:LEU:HD13	1.96	0.48
1:G:301:ASN:HD22	1:G:304:MET:HE1	1.77	0.48
1:M:352:LEU:C	1:M:356:MET:HE2	2.38	0.48
1:M:373:ASP:HB3	2:N:1:MET:HE1	1.96	0.48
1:A:181:ILE:HB	1:A:182:PRO:HD3	1.95	0.48
6:C:686:HOH:O	2:D:138:ILE:HG12	2.13	0.48
1:G:132:ASN:HD21	1:G:135:PHE:H	1.61	0.48
2:J:137:ASP:HB2	5:J:500:B13:H522	1.78	0.48
1:K:317:TYR:HA	1:K:325:THR:CG2	2.44	0.48
1:M:347:LYS:HE3	6:M:616:HOH:O	2.13	0.48
1:E:354:ASP:CB	2:F:2:LEU:HD12	2.44	0.48
1:G:22:SER:HB3	1:G:277:LYS:HE3	1.96	0.48
1:G:47:PRO:HB3	1:G:61:GLU:HG2	1.95	0.48
1:K:387:ASP:HB2	6:K:614:HOH:O	2.13	0.48
2:L:144:THR:HG22	6:L:518:HOH:O	2.13	0.48
2:L:163:ALA:C	2:L:197:MET:HE1	2.38	0.48
2:N:13:LEU:C	2:N:13:LEU:HD12	2.38	0.48
5:D:500:B13:H262	5:D:500:B13:H19	1.61	0.48
1:E:289:LYS:NZ	1:G:336:ASP:OD1	2.47	0.48
1:E:350:LYS:HG2	1:E:353:ARG:NH2	2.29	0.48
1:I:36:ALA:HA	6:I:568:HOH:O	2.14	0.48
1:I:265:PRO:HA	1:I:283:PRO:O	2.14	0.48
1:K:305:GLN:HA	1:K:356:MET:HE3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:ASP:OD1	1:K:27:LYS:NZ	2.32	0.47
2:F:130:VAL:HG12	2:F:134:ASP:HB3	1.96	0.47
1:G:324:THR:HG22	1:G:327:GLN:HG3	1.96	0.47
1:K:26:VAL:HG12	1:K:213:ILE:HD13	1.95	0.47
1:O:324:THR:CG2	1:O:326:VAL:HG22	2.44	0.47
2:P:195:ASN:ND2	2:P:224:LEU:HB2	2.29	0.47
1:A:19:PHE:CD1	1:A:356:MET:HE1	2.49	0.47
1:A:324:THR:HG23	1:A:326:VAL:HG22	1.96	0.47
1:A:331:GLU:HG2	1:C:292:THR:HG21	1.96	0.47
1:E:361:ARG:HH22	1:E:373:ASP:CG	2.22	0.47
1:I:128:ASP:CG	1:I:166:MET:HE2	2.39	0.47
2:N:20:LEU:HD11	1:O:116:TYR:CE1	2.49	0.47
1:A:317:TYR:HA	1:A:325:THR:CG2	2.44	0.47
2:H:105:MET:HE3	2:H:109:ILE:HD12	1.96	0.47
2:J:177:MET:HG2	2:J:178:LEU:N	2.29	0.47
2:N:85:ILE:HD11	2:N:149:ALA:O	2.15	0.47
1:E:361:ARG:NH2	1:E:373:ASP:OD1	2.47	0.47
1:I:301:ASN:HD22	1:I:304:MET:CE	2.27	0.47
2:J:127:VAL:HG23	2:J:175:PRO:HG3	1.96	0.47
2:L:189:TYR:HD2	2:L:192:LYS:HG3	1.79	0.47
1:O:364:ASP:CG	1:O:365:PRO:HD2	2.38	0.47
1:K:88:VAL:HG22	1:K:91:MET:SD	2.54	0.47
1:K:353:ARG:HA	1:K:356:MET:HE1	1.90	0.47
1:A:224:ASN:ND2	1:A:269:CYS:HB2	2.30	0.47
2:H:127:VAL:HG22	2:H:155:VAL:CG1	2.45	0.47
1:I:42:GLU:OE2	1:I:123:ARG:HD2	2.15	0.47
1:K:317:TYR:CE1	1:K:324:THR:CG2	2.97	0.47
2:L:37:ASP:O	2:L:39:LEU:N	2.43	0.47
2:L:189:TYR:O	2:L:192:LYS:HB2	2.15	0.47
1:A:28:ALA:HB2	1:A:213:ILE:HD13	1.97	0.47
1:C:218:THR:HG23	1:C:270:GLY:CA	2.45	0.47
2:D:163:ALA:C	2:D:197:MET:HE1	2.38	0.47
2:F:95:LEU:HB3	2:F:96:PRO:HD3	1.97	0.47
1:G:301:ASN:HD22	1:G:304:MET:HE2	1.79	0.47
2:H:138:ILE:O	2:H:142:ILE:HG13	2.14	0.47
1:I:228:PHE:CE2	5:J:500:B13:H543	2.49	0.47
1:K:411:LYS:HE3	2:L:4:PHE:O	2.14	0.47
2:L:227:TYR:CZ	2:L:229:GLU:HB3	2.49	0.47
1:M:128:ASP:HA	1:M:146:PHE:CE1	2.50	0.47
1:M:455:LYS:HB2	1:M:458:ASN:ND2	2.29	0.47
1:O:133:ARG:HD2	2:P:160:ASP:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ILE:HG23	1:A:326:VAL:HG11	1.97	0.47
1:E:203:ILE:O	1:E:206:ILE:HB	2.15	0.47
1:G:175:ALA:HB1	1:G:180:ASP:HB3	1.96	0.47
1:M:125:THR:HG21	1:M:267:LYS:HE2	1.96	0.47
1:G:224:ASN:HD21	1:G:269:CYS:HB2	1.79	0.47
2:H:185:THR:H	5:H:500:B13:H332	1.62	0.47
2:N:17:ASN:H	2:N:17:ASN:ND2	2.11	0.47
1:A:132:ASN:HD22	1:A:132:ASN:C	2.23	0.47
1:K:313:GLU:O	1:K:314:SER:HB2	2.15	0.47
1:C:169:LYS:HD2	5:D:500:B13:H473	1.96	0.46
2:D:68:ASP:HB3	2:D:71:ASP:HB2	1.96	0.46
1:C:19:PHE:CD1	1:C:356:MET:HE1	2.50	0.46
1:C:123:ARG:NH2	1:C:265:PRO:O	2.47	0.46
2:H:135:VAL:O	2:H:135:VAL:CG1	2.62	0.46
1:I:299:MET:HE1	1:I:366:GLN:HB3	1.97	0.46
1:K:248:ALA:HB2	1:K:369:MET:HE2	1.98	0.46
1:M:28:ALA:HB2	1:M:213:ILE:HD13	1.97	0.46
2:F:216:GLN:NE2	2:F:258:HIS:H	2.13	0.46
2:H:37:ASP:HB3	2:H:40:ILE:HB	1.98	0.46
2:H:127:VAL:HG23	2:H:175:PRO:HG3	1.96	0.46
1:I:324:THR:CG2	1:I:326:VAL:HG22	2.45	0.46
2:J:137:ASP:OD2	2:J:159:ARG:HD2	2.16	0.46
2:N:222:PHE:O	2:N:252:ARG:NH2	2.47	0.46
1:A:88:VAL:HG22	1:A:91:MET:SD	2.56	0.46
2:B:122:THR:HG21	2:B:153:ASN:HB2	1.98	0.46
2:B:219:VAL:HG21	2:B:227:TYR:HB2	1.96	0.46
1:C:73:MET:HE3	1:C:78:PHE:HB2	1.98	0.46
2:F:157:LEU:HD12	2:F:161:VAL:HG11	1.97	0.46
1:G:80:ALA:HA	1:G:119:LYS:O	2.16	0.46
1:G:176:VAL:HG13	1:G:177:LEU:HD13	1.97	0.46
1:I:353:ARG:HD3	1:I:372:TYR:CZ	2.50	0.46
2:L:105:MET:HE3	2:L:109:ILE:HD12	1.96	0.46
2:P:94:PHE:H	2:P:97:ASN:ND2	2.07	0.46
1:C:132:ASN:HD21	1:C:135:PHE:H	1.60	0.46
1:G:181:ILE:HB	1:G:182:PRO:HD3	1.98	0.46
1:K:293:CYS:HB3	1:K:329:TRP:CE2	2.49	0.46
1:E:147:LEU:HD22	1:E:206:ILE:HD11	1.97	0.46
1:K:317:TYR:HA	1:K:325:THR:HG21	1.98	0.46
1:O:79:PRO:HD2	6:O:595:HOH:O	2.16	0.46
2:D:159:ARG:O	2:D:161:VAL:HG23	2.15	0.46
2:J:116:SER:OG	2:J:117:GLY:N	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:192:LYS:HG2	2:L:222:PHE:HE2	1.80	0.46
2:L:206:PRO:HG2	2:L:241:ILE:HD12	1.96	0.46
2:H:135:VAL:O	2:H:135:VAL:HG13	2.15	0.46
5:N:500:B13:H262	5:N:500:B13:H19	1.69	0.46
2:B:185:THR:HG23	5:B:500:B13:H332	1.80	0.46
2:D:162:PRO:O	2:D:164:GLU:N	2.49	0.46
2:F:185:THR:HA	2:F:188:MET:HG3	1.98	0.46
1:M:133:ARG:HH11	1:M:133:ARG:HG2	1.80	0.46
1:M:305:GLN:HA	1:M:356:MET:HE3	1.98	0.46
1:O:237:ASN:HA	2:P:95:LEU:HB2	1.97	0.46
1:A:290:THR:O	1:A:290:THR:HG22	2.16	0.46
2:B:16:TYR:CD1	1:C:116:TYR:HB3	2.50	0.46
1:C:353:ARG:HD3	1:C:372:TYR:CE1	2.51	0.46
2:F:184:MET:HG2	5:F:500:B13:C30	2.38	0.46
2:F:184:MET:HB3	2:F:186:THR:HG22	1.98	0.46
5:H:500:B13:H362	5:H:500:B13:H411	1.75	0.46
1:O:73:MET:HE3	1:O:78:PHE:HB2	1.98	0.46
2:P:17:ASN:HD22	2:P:17:ASN:N	2.10	0.46
6:A:673:HOH:O	1:C:289:LYS:HE3	2.16	0.45
1:K:426:LYS:O	1:K:430:GLU:HG2	2.16	0.45
2:B:81:MET:O	2:B:85:ILE:HD12	2.16	0.45
1:I:142:LYS:HB2	6:I:540:HOH:O	2.16	0.45
2:J:206:PRO:HG2	2:J:241:ILE:HD12	1.98	0.45
2:L:118:ALA:O	2:L:119:THR:HB	2.16	0.45
1:M:132:ASN:C	1:M:132:ASN:HD22	2.24	0.45
1:O:325:THR:CG2	1:O:326:VAL:N	2.79	0.45
1:C:50:GLU:CD	1:C:50:GLU:H	2.24	0.45
2:D:59:LEU:O	2:D:63:ILE:HG12	2.17	0.45
2:H:252:ARG:O	2:H:256:HIS:HB2	2.17	0.45
2:N:219:VAL:HG21	2:N:227:TYR:CB	2.45	0.45
1:A:295:HIS:HD2	6:B:534:HOH:O	1.99	0.45
1:G:186:TYR:O	1:G:190:CYS:HB2	2.16	0.45
1:I:143:TYR:O	1:I:146:PHE:HB3	2.16	0.45
1:I:290:THR:HG22	1:I:290:THR:O	2.16	0.45
2:J:135:VAL:CG1	2:J:135:VAL:O	2.64	0.45
2:J:185:THR:O	2:J:188:MET:HE2	2.17	0.45
1:O:19:PHE:CD1	1:O:356:MET:HE1	2.52	0.45
1:O:132:ASN:ND2	1:O:132:ASN:C	2.75	0.45
2:P:137:ASP:HB2	5:P:500:B13:H522	1.81	0.45
2:B:161:VAL:HA	2:B:162:PRO:HD3	1.64	0.45
1:C:444:LEU:O	1:C:448:LYS:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:70:ILE:HD11	2:H:120:PRO:HA	1.98	0.45
1:A:116:TYR:HB3	2:D:16:TYR:CD1	2.52	0.45
1:G:292:THR:HA	1:G:295:HIS:O	2.17	0.45
5:J:500:B13:H19	5:J:500:B13:H262	1.66	0.45
2:P:204:LYS:HZ1	2:P:248:VAL:H	1.64	0.45
1:E:94:ASN:O	1:E:95:PRO:C	2.59	0.45
2:L:161:VAL:HA	2:L:162:PRO:HD3	1.78	0.45
2:N:163:ALA:O	2:N:166:VAL:HB	2.16	0.45
1:E:83:LEU:HD13	1:E:109:MET:CE	2.45	0.45
1:E:305:GLN:HA	1:E:356:MET:CE	2.44	0.45
1:G:361:ARG:NH2	1:G:373:ASP:OD1	2.49	0.45
1:I:411:LYS:HD3	2:J:6:GLU:HG2	1.98	0.45
2:J:59:LEU:O	2:J:63:ILE:HG12	2.16	0.45
1:K:137:GLN:NE2	1:K:142:LYS:HE2	2.31	0.45
2:F:136:HIS:CB	2:F:183:LEU:HD13	2.46	0.45
2:H:47:ILE:HD12	2:H:55:VAL:HG22	1.98	0.45
2:N:192:LYS:HG2	2:N:222:PHE:HE2	1.81	0.45
1:A:341:ASN:O	1:A:345:GLU:HG2	2.17	0.45
1:C:224:ASN:O	1:C:228:PHE:CD2	2.70	0.45
2:D:252:ARG:O	2:D:256:HIS:HB2	2.17	0.45
1:E:55:LYS:HG3	1:E:97:TRP:CD2	2.52	0.45
1:G:42:GLU:OE2	1:G:123:ARG:HD2	2.17	0.45
1:G:105:GLN:NE2	1:G:124:HIS:HE1	2.15	0.45
1:G:224:ASN:ND2	1:G:269:CYS:HB2	2.32	0.45
1:K:73:MET:HE2	1:K:81:ILE:HB	1.98	0.45
5:L:500:B13:H252	5:L:500:B13:C61	2.47	0.45
1:M:324:THR:CG2	1:M:326:VAL:HG22	2.47	0.45
1:O:83:LEU:HD13	1:O:109:MET:HE2	1.99	0.45
1:O:87:HIS:NE2	1:O:124:HIS:CD2	2.85	0.45
1:O:318:HIS:O	1:O:325:THR:HB	2.17	0.45
1:C:237:ASN:HA	2:D:95:LEU:HB2	1.99	0.44
2:F:222:PHE:O	2:F:252:ARG:NH2	2.50	0.44
1:I:126:ILE:N	1:I:126:ILE:HD12	2.32	0.44
2:D:248:VAL:HA	2:D:251:LEU:HD12	1.98	0.44
1:I:325:THR:CG2	1:I:326:VAL:N	2.81	0.44
2:L:130:VAL:CG1	2:L:134:ASP:HB3	2.46	0.44
2:N:130:VAL:CG1	2:N:134:ASP:HB3	2.47	0.44
1:I:289:LYS:NZ	1:I:301:ASN:HD21	2.15	0.44
2:J:63:ILE:HG23	2:J:72:LEU:HD12	1.99	0.44
1:M:224:ASN:O	1:M:228:PHE:HD2	2.01	0.44
1:C:105:GLN:HB3	1:C:109:MET:HE3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:227:TYR:CE2	2:D:229:GLU:HB3	2.52	0.44
1:G:325:THR:O	1:G:329:TRP:HD1	2.01	0.44
2:H:95:LEU:HD22	2:H:99:MET:HG2	2.00	0.44
2:H:197:MET:HE2	2:H:197:MET:HB3	1.88	0.44
5:J:500:B13:H362	5:J:500:B13:H411	1.81	0.44
1:O:81:ILE:HD13	1:O:82:ILE:N	2.33	0.44
1:C:87:HIS:NE2	1:C:124:HIS:HD2	2.14	0.44
1:E:302:LEU:HB2	1:E:360:ASP:HB2	1.98	0.44
2:L:130:VAL:HG23	2:L:140:LYS:HD3	1.99	0.44
2:L:234:ALA:O	2:L:237:ILE:HG22	2.18	0.44
1:M:133:ARG:CG	1:M:133:ARG:NH1	2.80	0.44
1:A:19:PHE:HD1	1:A:356:MET:HE1	1.82	0.44
1:A:317:TYR:HE1	1:A:324:THR:HG21	1.82	0.44
1:A:353:ARG:HA	1:A:356:MET:CE	2.36	0.44
2:B:59:LEU:HD23	2:B:72:LEU:HD13	2.00	0.44
1:K:228:PHE:HE1	1:K:295:HIS:HB2	1.82	0.44
2:N:162:PRO:O	2:N:163:ALA:HB3	2.18	0.44
2:P:82:GLY:HA2	2:P:85:ILE:HD12	2.00	0.44
1:A:132:ASN:HD22	1:A:134:GLU:H	1.66	0.44
2:B:197:MET:HB3	2:B:197:MET:HE2	1.63	0.44
1:C:218:THR:HG23	1:C:270:GLY:N	2.33	0.44
1:C:441:ASP:O	1:C:445:THR:HG23	2.18	0.44
1:M:132:ASN:ND2	1:M:135:PHE:H	2.14	0.44
2:N:185:THR:O	2:N:188:MET:HE2	2.17	0.44
2:N:218:PHE:O	2:N:221:GLN:HG2	2.18	0.44
5:P:500:B13:H363	5:P:500:B13:H401	1.83	0.44
1:C:237:ASN:O	2:D:96:PRO:HD3	2.18	0.44
2:F:188:MET:HB3	2:F:218:PHE:CZ	2.52	0.44
1:G:18:THR:CG2	1:G:21:VAL:HG13	2.47	0.44
1:I:196:MET:HE1	1:I:217:ASP:CB	2.48	0.44
1:M:64:ARG:CZ	2:P:258:HIS:OXT	2.66	0.44
1:M:218:THR:C	1:M:220:CYS:H	2.26	0.44
1:G:131:GLU:HB2	1:G:166:MET:HE1	2.00	0.44
1:G:138:LEU:HD12	1:G:458:ASN:HB3	1.98	0.44
2:H:216:GLN:NE2	2:H:258:HIS:H	2.15	0.44
2:J:130:VAL:HG23	2:J:140:LYS:HD3	2.00	0.44
1:K:105:GLN:O	1:K:109:MET:HG3	2.18	0.44
2:B:51:GLU:O	2:B:55:VAL:HG23	2.18	0.43
2:D:181:THR:OG1	5:D:500:B13:N3B	2.46	0.43
1:G:324:THR:CG2	1:G:326:VAL:HG22	2.48	0.43
1:G:325:THR:HG23	1:G:326:VAL:N	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:227:TYR:H	2:J:256:HIS:HE1	1.66	0.43
2:L:219:VAL:HG21	2:L:227:TYR:CB	2.38	0.43
2:N:138:ILE:O	2:N:142:ILE:HG13	2.18	0.43
1:C:73:MET:HE2	1:C:81:ILE:HB	2.00	0.43
1:C:293:CYS:HB3	1:C:329:TRP:CE2	2.53	0.43
1:C:355:LEU:HD13	2:D:2:LEU:CD1	2.48	0.43
2:B:131:ALA:HB1	2:B:190:ALA:HB3	1.99	0.43
2:B:181:THR:OG1	5:B:500:B13:N3B	2.44	0.43
1:C:47:PRO:HB3	1:C:61:GLU:HG2	2.00	0.43
1:C:56:GLU:CD	1:C:56:GLU:N	2.76	0.43
1:C:373:ASP:OD1	1:C:373:ASP:N	2.50	0.43
2:D:159:ARG:O	2:D:161:VAL:N	2.51	0.43
1:I:72:ARG:NH2	6:K:520:HOH:O	2.51	0.43
1:I:73:MET:HE1	1:I:334:ALA:CB	2.41	0.43
2:L:94:PHE:H	2:L:97:ASN:HD22	1.66	0.43
2:N:95:LEU:HB3	2:N:96:PRO:HD3	1.99	0.43
2:B:17:ASN:ND2	2:B:17:ASN:N	2.57	0.43
1:E:145:VAL:HA	1:E:148:GLU:OE1	2.18	0.43
2:H:68:ASP:HB3	2:H:71:ASP:HB2	2.00	0.43
2:J:130:VAL:HG12	2:J:134:ASP:HB3	1.99	0.43
1:K:113:HIS:HD2	1:K:118:ILE:O	2.02	0.43
1:K:196:MET:HE3	1:K:196:MET:HB3	1.94	0.43
5:N:500:B13:C61	5:N:500:B13:H252	2.48	0.43
1:A:43:ILE:HG22	1:A:81:ILE:HD11	2.01	0.43
1:A:237:ASN:O	2:B:96:PRO:HD3	2.18	0.43
2:B:95:LEU:HD22	2:B:99:MET:HG2	2.01	0.43
2:D:127:VAL:HG22	2:D:155:VAL:HG13	2.00	0.43
1:O:27:LYS:HE3	1:O:33:GLU:OE2	2.19	0.43
2:B:37:ASP:HB3	2:B:40:ILE:HB	2.01	0.43
2:D:95:LEU:HB3	2:D:96:PRO:HD3	2.01	0.43
1:G:132:ASN:ND2	1:G:135:PHE:H	2.15	0.43
1:G:356:MET:HE3	1:G:356:MET:HB2	1.91	0.43
2:N:87:LEU:HD22	2:N:92:VAL:HG21	2.01	0.43
2:N:167:LEU:HB2	2:N:197:MET:HE3	2.00	0.43
1:A:105:GLN:HB3	1:A:109:MET:HE3	2.00	0.43
2:F:87:LEU:HB3	2:F:92:VAL:HG22	1.99	0.43
2:H:199:LEU:C	2:H:201:ASN:N	2.75	0.43
2:H:216:GLN:HE21	2:H:258:HIS:HB2	1.83	0.43
2:J:127:VAL:HG22	2:J:155:VAL:CG1	2.49	0.43
1:K:218:THR:HG23	1:K:270:GLY:N	2.33	0.43
1:O:106:LYS:NZ	1:O:157:GLY:O	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:13:LEU:HD12	2:J:13:LEU:C	2.44	0.43
2:J:82:GLY:HA2	2:J:85:ILE:HD12	2.01	0.43
1:K:196:MET:HE1	1:K:257:ALA:HB2	2.00	0.43
2:B:229:GLU:O	5:B:500:B13:H2R	2.19	0.43
1:C:360:ASP:O	1:C:361:ARG:C	2.61	0.43
2:F:167:LEU:C	2:F:169:ALA:H	2.27	0.43
1:K:45:TYR:HB3	1:K:326:VAL:CG1	2.49	0.43
1:O:73:MET:HE3	1:O:78:PHE:CB	2.49	0.43
1:A:361:ARG:NH2	1:A:373:ASP:OD1	2.51	0.43
1:E:132:ASN:HD21	1:E:135:PHE:H	1.65	0.43
5:H:500:B13:H262	5:H:500:B13:H19	1.85	0.43
5:J:500:B13:H472	5:J:500:B13:H481	1.96	0.43
1:K:68:ASP:OD2	1:K:317:TYR:OH	2.35	0.43
2:L:206:PRO:HG2	2:L:241:ILE:CD1	2.49	0.43
2:N:82:GLY:HA2	2:N:85:ILE:HD12	2.00	0.43
1:O:26:VAL:CG1	1:O:213:ILE:HD13	2.49	0.43
1:O:105:GLN:NE2	1:O:124:HIS:HE1	2.17	0.43
1:A:287:GLU:OE1	1:A:313:GLU:OE2	2.36	0.42
1:C:73:MET:HE1	1:C:334:ALA:HB2	2.00	0.42
5:D:500:B13:H362	5:D:500:B13:H411	1.73	0.42
1:G:402:ASN:O	1:G:406:GLU:HG3	2.18	0.42
2:B:224:LEU:HA	2:B:248:VAL:HG21	2.00	0.42
1:E:317:TYR:HA	1:E:325:THR:HG22	2.01	0.42
2:H:242:ILE:HG22	2:H:242:ILE:O	2.19	0.42
1:I:285:THR:OG1	1:I:309:CYS:HB2	2.19	0.42
2:J:161:VAL:HA	2:J:162:PRO:HD3	1.95	0.42
2:J:233:ASP:O	2:J:237:ILE:HG22	2.19	0.42
1:M:301:ASN:HD22	1:M:304:MET:HE2	1.84	0.42
1:A:370:LEU:HD12	1:A:370:LEU:HA	1.93	0.42
2:D:95:LEU:HD11	2:D:142:ILE:HG12	2.01	0.42
1:E:417:PHE:HZ	2:F:97:ASN:HD21	1.67	0.42
1:G:43:ILE:HG22	1:G:81:ILE:HD11	2.01	0.42
2:H:224:LEU:HA	2:H:248:VAL:HG21	2.01	0.42
1:I:81:ILE:HD13	1:I:82:ILE:N	2.34	0.42
1:M:196:MET:HE1	1:M:257:ALA:HB2	2.01	0.42
2:B:63:ILE:H	2:B:63:ILE:HG12	1.73	0.42
1:C:64:ARG:HD2	6:C:533:HOH:O	2.19	0.42
2:F:220:SER:C	2:F:222:PHE:H	2.27	0.42
1:K:324:THR:CG2	1:K:326:VAL:HG22	2.49	0.42
1:M:361:ARG:NH2	1:M:373:ASP:CG	2.76	0.42
1:O:47:PRO:HB3	1:O:61:GLU:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ASP:O	1:A:445:THR:HG23	2.19	0.42
2:B:130:VAL:HG12	2:B:134:ASP:HB3	2.01	0.42
1:C:224:ASN:HB3	1:C:228:PHE:HE2	1.85	0.42
2:D:161:VAL:HA	2:D:162:PRO:HD3	1.70	0.42
1:E:109:MET:HE1	1:E:122:LEU:HB2	2.01	0.42
1:G:119:LYS:HE3	6:G:561:HOH:O	2.18	0.42
2:H:256:HIS:HB3	2:H:257:LYS:H	1.59	0.42
2:J:67:LYS:HB3	2:J:68:ASP:H	1.65	0.42
2:J:188:MET:O	2:J:191:PHE:HB2	2.18	0.42
1:K:436:MET:O	1:K:440:MET:HG2	2.19	0.42
5:N:500:B13:H401	5:N:500:B13:H8	1.84	0.42
1:O:426:LYS:O	1:O:430:GLU:HG3	2.19	0.42
2:D:256:HIS:HB3	2:D:257:LYS:H	1.57	0.42
2:F:161:VAL:HA	2:F:162:PRO:HD3	1.73	0.42
1:G:76:VAL:HG12	1:G:76:VAL:O	2.19	0.42
1:G:88:VAL:HG22	1:G:91:MET:SD	2.59	0.42
1:I:18:THR:HG23	1:I:21:VAL:HG13	2.02	0.42
1:I:196:MET:HE1	1:I:217:ASP:HB3	2.01	0.42
1:K:218:THR:HG23	1:K:270:GLY:CA	2.50	0.42
1:M:128:ASP:HA	1:M:146:PHE:HE1	1.84	0.42
2:B:37:ASP:O	2:B:39:LEU:N	2.49	0.42
2:B:59:LEU:O	2:B:63:ILE:HG12	2.19	0.42
1:E:364:ASP:CG	1:E:365:PRO:HD2	2.44	0.42
2:F:136:HIS:HB2	2:F:183:LEU:HD13	2.02	0.42
1:K:106:LYS:NZ	1:K:157:GLY:O	2.53	0.42
1:K:172:PHE:CD2	1:K:172:PHE:C	2.97	0.42
2:L:192:LYS:HG2	2:L:222:PHE:CE2	2.54	0.42
5:L:500:B13:H361	5:L:500:B13:H351	2.01	0.42
1:M:353:ARG:HD3	1:M:372:TYR:CZ	2.55	0.42
2:N:132:GLU:HB3	2:N:161:VAL:O	2.20	0.42
1:O:22:SER:HB3	1:O:277:LYS:HE3	2.02	0.42
1:A:22:SER:HB3	1:A:277:LYS:HE3	2.02	0.42
1:I:132:ASN:HD21	1:I:135:PHE:H	1.66	0.42
1:K:101:VAL:O	1:K:105:GLN:HG3	2.20	0.42
1:M:249:ILE:O	1:M:252:PRO:HD2	2.19	0.42
2:P:167:LEU:HB2	2:P:197:MET:CE	2.41	0.42
2:D:67:LYS:HB3	2:D:68:ASP:H	1.56	0.42
5:F:500:B13:H362	5:F:500:B13:H411	1.67	0.42
2:L:17:ASN:HD22	2:L:17:ASN:N	2.15	0.42
1:M:289:LYS:NZ	1:M:301:ASN:HD21	2.18	0.42
2:N:234:ALA:O	2:N:237:ILE:HG22	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:126:ILE:HD12	1:O:126:ILE:N	2.34	0.42
1:O:285:THR:OG1	1:O:309:CYS:HB2	2.20	0.42
2:D:110:GLU:HA	2:D:113:LYS:HB2	2.02	0.42
2:D:134:ASP:OD2	2:D:187:THR:HG21	2.20	0.42
1:E:187:SER:HA	1:E:191:LEU:HD12	2.01	0.42
1:E:203:ILE:HA	1:E:206:ILE:HD12	2.02	0.42
2:F:41:TYR:HB3	2:F:42:PRO:HD3	2.02	0.42
1:G:132:ASN:OD1	1:G:137:GLN:NE2	2.51	0.42
1:G:218:THR:HG23	1:G:270:GLY:N	2.35	0.42
2:L:135:VAL:O	2:L:135:VAL:HG13	2.19	0.42
2:N:43:ILE:HG21	2:N:76:ALA:HB1	2.01	0.42
2:N:130:VAL:HG12	2:N:134:ASP:HB3	2.02	0.42
1:E:132:ASN:OD1	1:E:137:GLN:NE2	2.53	0.41
2:D:130:VAL:HG23	2:D:140:LYS:HD3	2.02	0.41
1:M:360:ASP:O	1:M:361:ARG:C	2.62	0.41
2:N:161:VAL:HA	2:N:162:PRO:HD3	1.78	0.41
1:O:452:LYS:HD3	1:O:452:LYS:HA	1.95	0.41
1:A:87:HIS:NE2	1:A:124:HIS:CD2	2.89	0.41
1:A:361:ARG:HH22	1:A:373:ASP:CG	2.28	0.41
2:F:216:GLN:HE21	2:F:258:HIS:HD2	1.68	0.41
2:J:135:VAL:HB	5:J:500:B13:H421	2.02	0.41
2:J:159:ARG:O	2:J:161:VAL:HG23	2.20	0.41
2:J:234:ALA:HB3	2:J:235:PRO:HD3	2.01	0.41
5:J:500:B13:H363	5:J:500:B13:N40	2.35	0.41
5:B:500:B13:H411	5:B:500:B13:H362	1.80	0.41
2:D:70:ILE:HD11	2:D:120:PRO:HG3	2.01	0.41
2:D:195:ASN:HD22	2:D:224:LEU:HB2	1.86	0.41
1:E:266:GLY:HA3	1:E:284:MET:SD	2.60	0.41
1:K:106:LYS:HA	1:K:106:LYS:HD3	1.76	0.41
2:L:74:ASP:HA	2:L:78:MET:HB2	2.02	0.41
2:L:226:VAL:HG11	2:L:237:ILE:HD11	2.02	0.41
2:N:178:LEU:O	2:N:207:PHE:HA	2.21	0.41
2:P:147:LEU:HB3	2:P:154:VAL:HG21	2.01	0.41
2:B:95:LEU:HB3	2:B:96:PRO:HD3	2.03	0.41
2:B:216:GLN:NE2	2:B:258:HIS:H	2.15	0.41
1:C:143:TYR:O	1:C:146:PHE:HB3	2.21	0.41
1:C:354:ASP:OD2	2:D:1:MET:HA	2.20	0.41
1:E:287:GLU:OE1	1:E:313:GLU:OE2	2.38	0.41
1:I:317:TYR:HE1	1:I:324:THR:CG2	2.30	0.41
2:L:185:THR:HG23	5:L:500:B13:H332	1.86	0.41
1:M:452:LYS:HD3	1:M:452:LYS:HA	1.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:500:B13:H362	5:P:500:B13:H411	1.74	0.41
1:A:302:LEU:C	1:A:302:LEU:HD23	2.45	0.41
2:B:195:ASN:HD22	2:B:224:LEU:HB2	1.84	0.41
1:E:146:PHE:CZ	1:E:150:PHE:HE2	2.39	0.41
2:F:74:ASP:HA	2:F:78:MET:HB2	2.03	0.41
1:I:22:SER:HB3	1:I:277:LYS:HE3	2.02	0.41
2:L:256:HIS:HB3	2:L:257:LYS:H	1.57	0.41
2:N:159:ARG:O	2:N:161:VAL:N	2.52	0.41
2:D:60:GLN:O	2:D:64:GLU:HG3	2.21	0.41
2:F:214:VAL:HG12	2:F:227:TYR:CE1	2.55	0.41
5:H:500:B13:H472	5:H:500:B13:H481	1.88	0.41
2:J:252:ARG:O	2:J:256:HIS:HB2	2.21	0.41
2:N:136:HIS:CB	2:N:183:LEU:HD13	2.51	0.41
1:O:126:ILE:N	1:O:126:ILE:CD1	2.84	0.41
1:O:305:GLN:HA	1:O:356:MET:HE3	2.02	0.41
1:A:131:GLU:OE2	2:B:159:ARG:NH2	2.52	0.41
1:A:218:THR:HG23	1:A:270:GLY:CA	2.50	0.41
2:B:87:LEU:HB3	2:B:92:VAL:HG22	2.03	0.41
1:C:290:THR:O	1:C:290:THR:HG22	2.21	0.41
5:L:500:B13:H262	5:L:500:B13:H19	1.83	0.41
5:L:500:B13:H621	5:L:500:B13:H18	1.71	0.41
2:P:135:VAL:HB	5:P:500:B13:C43	2.50	0.41
1:A:123:ARG:NH2	1:A:265:PRO:O	2.53	0.41
2:D:95:LEU:O	2:D:96:PRO:C	2.64	0.41
1:E:116:TYR:HB3	2:H:16:TYR:CD1	2.55	0.41
2:H:167:LEU:HB2	2:H:197:MET:HE3	2.03	0.41
2:H:193:GLU:O	2:H:197:MET:HB3	2.20	0.41
1:I:47:PRO:HB3	1:I:61:GLU:HG2	2.02	0.41
1:I:317:TYR:CE1	1:I:324:THR:CG2	3.04	0.41
2:J:159:ARG:HB3	2:J:160:ASP:H	1.63	0.41
1:K:73:MET:HE3	1:K:78:PHE:CB	2.50	0.41
1:K:247:ARG:CZ	1:K:271:TYR:HB2	2.50	0.41
2:L:135:VAL:O	2:L:135:VAL:CG1	2.68	0.41
1:M:87:HIS:NE2	1:M:124:HIS:CD2	2.87	0.41
1:O:101:VAL:O	1:O:105:GLN:HG3	2.21	0.41
1:O:132:ASN:ND2	1:O:134:GLU:HG2	2.36	0.41
2:P:37:ASP:O	2:P:37:ASP:OD2	2.39	0.41
2:P:95:LEU:HB3	2:P:96:PRO:HD3	2.02	0.41
2:P:143:VAL:HG21	5:P:500:B13:C9B	2.50	0.41
2:P:169:ALA:O	2:P:173:GLU:HG2	2.21	0.41
2:P:256:HIS:HB3	2:P:257:LYS:H	1.76	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:ARG:O	2:B:161:VAL:HG23	2.21	0.41
2:B:247:ASP:HB3	2:B:250:GLU:HB2	2.01	0.41
1:C:196:MET:HE1	1:C:217:ASP:HB3	2.03	0.41
2:D:119:THR:HA	2:D:120:PRO:HD3	1.90	0.41
2:F:182:ALA:O	2:F:211:GLY:HA3	2.21	0.41
1:G:317:TYR:HA	1:G:325:THR:CG2	2.50	0.41
1:E:94:ASN:HB2	1:E:97:TRP:CD1	2.56	0.40
2:J:132:GLU:HB3	2:J:161:VAL:O	2.21	0.40
1:K:356:MET:HE3	1:K:356:MET:HB2	1.71	0.40
1:M:325:THR:CG2	1:M:326:VAL:N	2.83	0.40
2:N:63:ILE:H	2:N:63:ILE:HG12	1.74	0.40
1:O:88:VAL:HG22	1:O:91:MET:SD	2.62	0.40
1:O:289:LYS:HZ3	1:O:304:MET:HE1	1.85	0.40
2:B:218:PHE:O	2:B:221:GLN:HG2	2.21	0.40
1:C:224:ASN:HB3	1:C:228:PHE:CE2	2.56	0.40
1:E:76:VAL:O	1:E:76:VAL:HG12	2.22	0.40
2:F:173:GLU:O	2:F:174:LYS:C	2.63	0.40
2:F:206:PRO:HG2	2:F:241:ILE:CD1	2.51	0.40
1:K:131:GLU:OE2	2:L:159:ARG:NH2	2.54	0.40
1:K:325:THR:CG2	1:K:326:VAL:N	2.85	0.40
2:L:231:ALA:HB2	5:L:500:B13:O6R	2.21	0.40
5:N:500:B13:H362	5:N:500:B13:H411	1.79	0.40
1:C:357:MET:SD	1:C:357:MET:C	3.04	0.40
1:G:132:ASN:HD22	1:G:134:GLU:H	1.67	0.40
1:I:46:ALA:HA	1:I:47:PRO:HD3	1.88	0.40
1:M:285:THR:OG1	1:M:309:CYS:HB2	2.22	0.40
1:O:290:THR:HG22	1:O:290:THR:O	2.22	0.40
2:D:143:VAL:HG13	2:D:234:ALA:CB	2.52	0.40
1:G:265:PRO:HA	1:G:283:PRO:O	2.21	0.40
2:H:226:VAL:HG11	2:H:237:ILE:HG12	2.04	0.40
1:I:228:PHE:CE2	5:J:500:B13:C54	3.05	0.40
2:J:134:ASP:HB2	2:J:187:THR:HG21	2.03	0.40
2:J:229:GLU:HG3	2:J:230:GLU:H	1.86	0.40
2:N:37:ASP:C	2:N:39:LEU:H	2.29	0.40
1:O:179:ASN:HA	6:O:526:HOH:O	2.20	0.40
1:O:352:LEU:O	1:O:356:MET:HE2	2.21	0.40
1:C:252:PRO:HG3	1:C:393:ALA:HA	2.04	0.40
1:C:285:THR:OG1	1:C:309:CYS:HB2	2.20	0.40
2:D:138:ILE:HG13	5:D:500:B13:C50	2.52	0.40
1:E:123:ARG:NH2	1:E:265:PRO:O	2.54	0.40
1:E:348:ASN:O	1:E:351:VAL:HG12	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:362:TYR:HB2	2:J:9:LEU:HD21	2.03	0.40
2:N:87:LEU:HD22	2:N:92:VAL:CG2	2.52	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	457/461 (99%)	442 (97%)	15 (3%)	0	100	100
1	C	457/461 (99%)	440 (96%)	17 (4%)	0	100	100
1	E	457/461 (99%)	433 (95%)	21 (5%)	3 (1%)	18	34
1	G	457/461 (99%)	434 (95%)	22 (5%)	1 (0%)	43	63
1	I	457/461 (99%)	439 (96%)	17 (4%)	1 (0%)	43	63
1	K	457/461 (99%)	439 (96%)	18 (4%)	0	100	100
1	M	457/461 (99%)	439 (96%)	18 (4%)	0	100	100
1	O	457/461 (99%)	439 (96%)	18 (4%)	0	100	100
2	B	256/258 (99%)	239 (93%)	13 (5%)	4 (2%)	7	14
2	D	256/258 (99%)	224 (88%)	28 (11%)	4 (2%)	7	14
2	F	256/258 (99%)	227 (89%)	26 (10%)	3 (1%)	10	20
2	H	256/258 (99%)	235 (92%)	18 (7%)	3 (1%)	10	20
2	J	256/258 (99%)	237 (93%)	14 (6%)	5 (2%)	6	10
2	L	256/258 (99%)	235 (92%)	15 (6%)	6 (2%)	5	8
2	N	256/258 (99%)	229 (90%)	23 (9%)	4 (2%)	7	14
2	P	256/258 (99%)	240 (94%)	13 (5%)	3 (1%)	10	20
All	All	5704/5752 (99%)	5371 (94%)	296 (5%)	37 (1%)	21	38

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	256	HIS
2	F	256	HIS
2	H	256	HIS
2	L	37	ASP
2	L	256	HIS
2	B	256	HIS
2	D	163	ALA
1	E	53	ALA
1	E	305	GLN
2	F	38	GLU
1	G	53	ALA
2	J	256	HIS
2	J	257	LYS
2	D	119	THR
2	D	160	ASP
2	H	119	THR
2	J	119	THR
2	L	119	THR
2	F	119	THR
2	J	37	ASP
2	L	160	ASP
2	L	163	ALA
2	N	69	PRO
2	P	38	GLU
2	P	119	THR
2	P	256	HIS
2	B	119	THR
2	H	201	ASN
2	J	69	PRO
2	L	68	ASP
2	N	68	ASP
2	N	186	THR
2	B	159	ARG
2	B	192	LYS
1	I	313	GLU
2	N	160	ASP
1	E	81	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	373/374 (100%)	347 (93%)	26 (7%)	14	29
1	C	373/374 (100%)	342 (92%)	31 (8%)	10	22
1	E	373/374 (100%)	339 (91%)	34 (9%)	9	19
1	G	373/374 (100%)	344 (92%)	29 (8%)	11	24
1	I	373/374 (100%)	347 (93%)	26 (7%)	14	29
1	K	373/374 (100%)	352 (94%)	21 (6%)	19	39
1	M	373/374 (100%)	342 (92%)	31 (8%)	10	22
1	O	373/374 (100%)	342 (92%)	31 (8%)	10	22
2	B	206/206 (100%)	186 (90%)	20 (10%)	8	17
2	D	206/206 (100%)	182 (88%)	24 (12%)	5	11
2	F	206/206 (100%)	185 (90%)	21 (10%)	7	15
2	H	206/206 (100%)	188 (91%)	18 (9%)	9	21
2	J	206/206 (100%)	183 (89%)	23 (11%)	6	12
2	L	206/206 (100%)	184 (89%)	22 (11%)	6	13
2	N	206/206 (100%)	186 (90%)	20 (10%)	8	17
2	P	206/206 (100%)	179 (87%)	27 (13%)	4	8
All	All	4632/4640 (100%)	4228 (91%)	404 (9%)	9	21

All (404) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	21	VAL
1	A	72	ARG
1	A	81	ILE
1	A	115	GLU
1	A	124	HIS
1	A	132	ASN
1	A	134	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	135	PHE
1	A	142	LYS
1	A	151	GLU
1	A	170	GLU
1	A	177	LEU
1	A	184	LEU
1	A	185	LEU
1	A	198	LEU
1	A	213	ILE
1	A	233	LEU
1	A	299	MET
1	A	324	THR
1	A	353	ARG
1	A	355	LEU
1	A	370	LEU
1	A	438	LYS
1	A	444	LEU
1	A	445	THR
2	B	9	LEU
2	B	17	ASN
2	B	24	LEU
2	B	39	LEU
2	B	47	ILE
2	B	63	ILE
2	B	92	VAL
2	B	95	LEU
2	B	123	LYS
2	B	147	LEU
2	B	155	VAL
2	B	167	LEU
2	B	183	LEU
2	B	186	THR
2	B	187	THR
2	B	197	MET
2	B	201	ASN
2	B	204	LYS
2	B	214	VAL
2	B	246	THR
1	C	5	ARG
1	C	21	VAL
1	C	81	ILE
1	C	124	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	132	ASN
1	C	133	ARG
1	C	134	GLU
1	C	135	PHE
1	C	142	LYS
1	C	151	GLU
1	C	170	GLU
1	C	177	LEU
1	C	184	LEU
1	C	185	LEU
1	C	198	LEU
1	C	205	LYS
1	C	213	ILE
1	C	233	LEU
1	C	267	LYS
1	C	299	MET
1	C	324	THR
1	C	325	THR
1	C	347	LYS
1	C	353	ARG
1	C	355	LEU
1	C	370	LEU
1	C	434	ASP
1	C	438	LYS
1	C	444	LEU
1	C	445	THR
1	C	448	LYS
2	D	9	LEU
2	D	17	ASN
2	D	24	LEU
2	D	36	LYS
2	D	38	GLU
2	D	47	ILE
2	D	83	VAL
2	D	92	VAL
2	D	95	LEU
2	D	113	LYS
2	D	146	LEU
2	D	147	LEU
2	D	155	VAL
2	D	167	LEU
2	D	183	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	186	THR
2	D	187	THR
2	D	188	MET
2	D	192	LYS
2	D	201	ASN
2	D	204	LYS
2	D	214	VAL
2	D	219	VAL
2	D	256	HIS
1	E	5	ARG
1	E	7	THR
1	E	21	VAL
1	E	23	LYS
1	E	72	ARG
1	E	81	ILE
1	E	124	HIS
1	E	132	ASN
1	E	137	GLN
1	E	141	ASP
1	E	142	LYS
1	E	144	SER
1	E	170	GLU
1	E	177	LEU
1	E	185	LEU
1	E	197	GLU
1	E	198	LEU
1	E	213	ILE
1	E	217	ASP
1	E	233	LEU
1	E	298	VAL
1	E	299	MET
1	E	324	THR
1	E	325	THR
1	E	347	LYS
1	E	353	ARG
1	E	355	LEU
1	E	370	LEU
1	E	395	ASN
1	E	405	GLU
1	E	438	LYS
1	E	444	LEU
1	E	449	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	453	VAL
2	F	1	MET
2	F	9	LEU
2	F	17	ASN
2	F	36	LYS
2	F	38	GLU
2	F	47	ILE
2	F	63	ILE
2	F	89	ASP
2	F	92	VAL
2	F	95	LEU
2	F	106	LEU
2	F	107	GLU
2	F	110	GLU
2	F	123	LYS
2	F	150	ASN
2	F	157	LEU
2	F	167	LEU
2	F	183	LEU
2	F	229	GLU
2	F	246	THR
2	F	256	HIS
1	G	5	ARG
1	G	21	VAL
1	G	72	ARG
1	G	81	ILE
1	G	115	GLU
1	G	124	HIS
1	G	132	ASN
1	G	134	GLU
1	G	141	ASP
1	G	142	LYS
1	G	151	GLU
1	G	170	GLU
1	G	177	LEU
1	G	184	LEU
1	G	185	LEU
1	G	198	LEU
1	G	213	ILE
1	G	233	LEU
1	G	241	THR
1	G	299	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	311	SER
1	G	324	THR
1	G	355	LEU
1	G	359	SER
1	G	370	LEU
1	G	413	GLU
1	G	434	ASP
1	G	441	ASP
1	G	444	LEU
2	H	9	LEU
2	H	17	ASN
2	H	36	LYS
2	H	47	ILE
2	H	63	ILE
2	H	95	LEU
2	H	135	VAL
2	H	146	LEU
2	H	150	ASN
2	H	161	VAL
2	H	167	LEU
2	H	183	LEU
2	H	186	THR
2	H	201	ASN
2	H	216	GLN
2	H	248	VAL
2	H	253	GLU
2	H	256	HIS
1	I	5	ARG
1	I	21	VAL
1	I	72	ARG
1	I	81	ILE
1	I	124	HIS
1	I	132	ASN
1	I	134	GLU
1	I	135	PHE
1	I	142	LYS
1	I	170	GLU
1	I	177	LEU
1	I	184	LEU
1	I	185	LEU
1	I	198	LEU
1	I	213	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	233	LEU
1	I	324	THR
1	I	325	THR
1	I	347	LYS
1	I	353	ARG
1	I	355	LEU
1	I	370	LEU
1	I	430	GLU
1	I	444	LEU
1	I	445	THR
1	I	448	LYS
2	J	1	MET
2	J	9	LEU
2	J	17	ASN
2	J	36	LYS
2	J	47	ILE
2	J	63	ILE
2	J	89	ASP
2	J	92	VAL
2	J	95	LEU
2	J	123	LYS
2	J	135	VAL
2	J	138	ILE
2	J	144	THR
2	J	146	LEU
2	J	147	LEU
2	J	159	ARG
2	J	167	LEU
2	J	183	LEU
2	J	186	THR
2	J	187	THR
2	J	192	LYS
2	J	219	VAL
2	J	236	LYS
1	K	5	ARG
1	K	21	VAL
1	K	81	ILE
1	K	106	LYS
1	K	124	HIS
1	K	132	ASN
1	K	134	GLU
1	K	142	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	170	GLU
1	K	177	LEU
1	K	184	LEU
1	K	185	LEU
1	K	198	LEU
1	K	233	LEU
1	K	298	VAL
1	K	324	THR
1	K	325	THR
1	K	355	LEU
1	K	370	LEU
1	K	405	GLU
1	K	444	LEU
2	L	1	MET
2	L	9	LEU
2	L	17	ASN
2	L	36	LYS
2	L	47	ILE
2	L	63	ILE
2	L	92	VAL
2	L	95	LEU
2	L	121	LYS
2	L	123	LYS
2	L	135	VAL
2	L	144	THR
2	L	147	LEU
2	L	157	LEU
2	L	164	GLU
2	L	167	LEU
2	L	183	LEU
2	L	186	THR
2	L	204	LYS
2	L	214	VAL
2	L	216	GLN
2	L	246	THR
1	M	5	ARG
1	M	21	VAL
1	M	22	SER
1	M	81	ILE
1	M	126	ILE
1	M	131	GLU
1	M	132	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	133	ARG
1	M	134	GLU
1	M	135	PHE
1	M	142	LYS
1	M	151	GLU
1	M	170	GLU
1	M	177	LEU
1	M	184	LEU
1	M	185	LEU
1	M	198	LEU
1	M	213	ILE
1	M	218	THR
1	M	233	LEU
1	M	298	VAL
1	M	299	MET
1	M	324	THR
1	M	325	THR
1	M	347	LYS
1	M	353	ARG
1	M	355	LEU
1	M	370	LEU
1	M	430	GLU
1	M	438	LYS
1	M	444	LEU
2	N	1	MET
2	N	9	LEU
2	N	17	ASN
2	N	36	LYS
2	N	38	GLU
2	N	47	ILE
2	N	63	ILE
2	N	92	VAL
2	N	95	LEU
2	N	109	ILE
2	N	121	LYS
2	N	155	VAL
2	N	167	LEU
2	N	183	LEU
2	N	188	MET
2	N	199	LEU
2	N	204	LYS
2	N	214	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	241	ILE
2	N	246	THR
1	O	5	ARG
1	O	21	VAL
1	O	22	SER
1	O	81	ILE
1	O	124	HIS
1	O	126	ILE
1	O	132	ASN
1	O	134	GLU
1	O	135	PHE
1	O	142	LYS
1	O	148	GLU
1	O	151	GLU
1	O	170	GLU
1	O	177	LEU
1	O	184	LEU
1	O	185	LEU
1	O	198	LEU
1	O	213	ILE
1	O	218	THR
1	O	233	LEU
1	O	298	VAL
1	O	299	MET
1	O	324	THR
1	O	325	THR
1	O	347	LYS
1	O	353	ARG
1	O	355	LEU
1	O	370	LEU
1	O	434	ASP
1	O	438	LYS
1	O	444	LEU
2	P	1	MET
2	P	9	LEU
2	P	17	ASN
2	P	20	LEU
2	P	24	LEU
2	P	36	LYS
2	P	39	LEU
2	P	47	ILE
2	P	63	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	92	VAL
2	P	95	LEU
2	P	119	THR
2	P	123	LYS
2	P	135	VAL
2	P	144	THR
2	P	146	LEU
2	P	147	LEU
2	P	157	LEU
2	P	167	LEU
2	P	183	LEU
2	P	186	THR
2	P	192	LYS
2	P	204	LYS
2	P	219	VAL
2	P	241	ILE
2	P	249	THR
2	P	250	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	113	HIS
1	A	124	HIS
1	A	132	ASN
1	A	137	GLN
1	A	235	ASN
1	A	295	HIS
1	A	301	ASN
2	B	17	ASN
2	B	60	GLN
2	B	97	ASN
2	B	171	GLN
2	B	195	ASN
2	B	201	ASN
2	B	216	GLN
2	B	258	HIS
1	C	113	HIS
1	C	124	HIS
1	C	132	ASN
1	C	156	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	301	ASN
2	D	17	ASN
2	D	97	ASN
2	D	150	ASN
2	D	195	ASN
2	D	215	ASN
2	D	216	GLN
2	D	258	HIS
1	E	93	ASN
1	E	105	GLN
1	E	124	HIS
1	E	132	ASN
1	E	137	GLN
1	E	301	ASN
1	E	348	ASN
2	F	17	ASN
2	F	97	ASN
2	F	150	ASN
2	F	153	ASN
2	F	195	ASN
2	F	215	ASN
2	F	216	GLN
1	G	89	GLN
1	G	105	GLN
1	G	113	HIS
1	G	124	HIS
1	G	132	ASN
1	G	137	GLN
1	G	156	ASN
1	G	179	ASN
1	G	235	ASN
1	G	295	HIS
1	G	301	ASN
1	G	348	ASN
2	H	17	ASN
2	H	97	ASN
2	H	195	ASN
2	H	201	ASN
2	H	216	GLN
2	H	256	HIS
1	I	93	ASN
1	I	113	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	124	HIS
1	I	132	ASN
1	I	137	GLN
1	I	156	ASN
1	I	295	HIS
1	I	301	ASN
1	I	366	GLN
2	J	17	ASN
2	J	150	ASN
2	J	153	ASN
2	J	195	ASN
2	J	201	ASN
2	J	256	HIS
2	J	258	HIS
1	K	13	ASN
1	K	93	ASN
1	K	105	GLN
1	K	113	HIS
1	K	124	HIS
1	K	132	ASN
1	K	137	GLN
1	K	156	ASN
1	K	295	HIS
1	K	301	ASN
1	K	348	ASN
2	L	17	ASN
2	L	97	ASN
2	L	195	ASN
2	L	215	ASN
1	M	89	GLN
1	M	93	ASN
1	M	105	GLN
1	M	113	HIS
1	M	124	HIS
1	M	132	ASN
1	M	295	HIS
1	M	301	ASN
1	M	348	ASN
2	N	17	ASN
2	N	97	ASN
2	N	141	ASN
2	N	195	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	201	ASN
2	N	215	ASN
2	N	216	GLN
1	O	103	HIS
1	O	105	GLN
1	O	113	HIS
1	O	124	HIS
1	O	132	ASN
1	O	137	GLN
1	O	235	ASN
1	O	295	HIS
1	O	301	ASN
1	O	348	ASN
2	P	17	ASN
2	P	97	ASN
2	P	115	ASN
2	P	195	ASN
2	P	216	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 20 are 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	$\# Z > 2$
5	B13	J	500	6,2	83,100,100	2.07	18 (21%)	106,164,164	1.99	22 (20%)
5	B13	B	500	2	83,100,100	2.08	17 (20%)	106,164,164	2.01	28 (26%)
5	B13	L	500	6,2	83,100,100	2.08	18 (21%)	106,164,164	1.98	26 (24%)
5	B13	N	500	2	83,100,100	2.09	18 (21%)	106,164,164	2.05	27 (25%)
5	B13	H	500	2	83,100,100	2.12	19 (22%)	106,164,164	2.08	23 (21%)
5	B13	P	500	2	83,100,100	2.02	17 (20%)	106,164,164	2.11	33 (31%)
5	B13	F	500	2	83,100,100	2.09	17 (20%)	106,164,164	2.04	28 (26%)
5	B13	D	500	2	83,100,100	2.12	19 (22%)	106,164,164	2.02	27 (25%)

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
5	B13	J	500	6,2	-	22/56/223/223	0/3/11/11
5	B13	B	500	2	-	18/56/223/223	0/3/11/11
5	B13	L	500	6,2	-	21/56/223/223	0/3/11/11
5	B13	N	500	2	-	25/56/223/223	0/3/11/11
5	B13	H	500	2	-	20/56/223/223	0/3/11/11
5	B13	P	500	2	-	20/56/223/223	0/3/11/11
5	B13	F	500	2	-	19/56/223/223	0/3/11/11
5	B13	D	500	2	-	19/56/223/223	0/3/11/11

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	500	B13	C5R-C4R	-8.91	1.21	1.51
5	D	500	B13	C5R-C4R	-8.88	1.22	1.51
5	P	500	B13	C5R-C4R	-8.77	1.22	1.51
5	J	500	B13	C5R-C4R	-8.77	1.22	1.51
5	L	500	B13	C5R-C4R	-8.76	1.22	1.51
5	H	500	B13	C5R-C4R	-8.68	1.22	1.51
5	F	500	B13	C5R-C4R	-8.67	1.22	1.51
5	N	500	B13	C5R-C4R	-8.63	1.22	1.51
5	B	500	B13	O5B-C5B	6.48	1.51	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	500	B13	C6-N22	6.40	1.43	1.35
5	N	500	B13	C6-N22	6.34	1.43	1.35
5	L	500	B13	O5B-C5B	6.32	1.51	1.37
5	H	500	B13	O5B-C5B	6.31	1.51	1.37
5	N	500	B13	O5B-C5B	6.25	1.51	1.37
5	F	500	B13	O5B-C5B	6.20	1.50	1.37
5	H	500	B13	C6-N22	6.16	1.43	1.35
5	D	500	B13	O5B-C5B	6.01	1.50	1.37
5	L	500	B13	C6-N22	5.98	1.43	1.35
5	F	500	B13	C6-N22	5.94	1.43	1.35
5	J	500	B13	C11-C10	-5.92	1.36	1.50
5	B	500	B13	C11-C10	-5.92	1.36	1.50
5	H	500	B13	C11-C10	-5.89	1.37	1.50
5	J	500	B13	C6-N22	5.84	1.42	1.35
5	F	500	B13	C11-C10	-5.80	1.37	1.50
5	J	500	B13	O5B-C5B	5.72	1.49	1.37
5	P	500	B13	C6-N22	5.64	1.42	1.35
5	P	500	B13	O5B-C5B	5.64	1.49	1.37
5	L	500	B13	C11-C10	-5.60	1.37	1.50
5	D	500	B13	C11-C10	-5.57	1.37	1.50
5	P	500	B13	C11-C10	-5.57	1.37	1.50
5	N	500	B13	C11-C10	-5.50	1.37	1.50
5	B	500	B13	C6-N22	5.14	1.41	1.35
5	H	500	B13	C6B-C5B	4.27	1.47	1.39
5	N	500	B13	C6B-C5B	4.00	1.46	1.39
5	D	500	B13	C35-C5	3.98	1.56	1.50
5	D	500	B13	C6B-C5B	3.98	1.46	1.39
5	L	500	B13	C6B-C5B	3.96	1.46	1.39
5	F	500	B13	C6B-C5B	3.95	1.46	1.39
5	L	500	B13	C35-C5	3.88	1.56	1.50
5	J	500	B13	C6B-C5B	3.80	1.46	1.39
5	J	500	B13	C35-C5	3.78	1.56	1.50
5	B	500	B13	C6B-C5B	3.72	1.46	1.39
5	B	500	B13	C20-C1	3.71	1.61	1.52
5	B	500	B13	C35-C5	3.63	1.56	1.50
5	F	500	B13	C20-C1	3.63	1.61	1.52
5	J	500	B13	O8R-C5R	3.58	1.57	1.42
5	J	500	B13	C20-C1	3.58	1.61	1.52
5	P	500	B13	C20-C1	3.56	1.61	1.52
5	H	500	B13	O8R-C5R	3.54	1.57	1.42
5	H	500	B13	C36-C7	3.53	1.60	1.54
5	N	500	B13	C20-C1	3.53	1.61	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	500	B13	C35-C5	3.52	1.56	1.50
5	F	500	B13	O8R-C5R	3.50	1.57	1.42
5	H	500	B13	C20-C1	3.49	1.61	1.52
5	N	500	B13	O8R-C5R	3.49	1.57	1.42
5	D	500	B13	C25-C2	3.48	1.60	1.54
5	P	500	B13	C6B-C5B	3.45	1.45	1.39
5	D	500	B13	O8R-C5R	3.44	1.56	1.42
5	L	500	B13	O8R-C5R	3.44	1.56	1.42
5	P	500	B13	O8R-C5R	3.43	1.56	1.42
5	L	500	B13	C20-C1	3.43	1.61	1.52
5	B	500	B13	O8R-C5R	3.42	1.56	1.42
5	H	500	B13	C35-C5	3.42	1.55	1.50
5	P	500	B13	C35-C5	3.32	1.55	1.50
5	F	500	B13	C35-C5	3.32	1.55	1.50
5	B	500	B13	C55-C17	3.31	1.60	1.55
5	J	500	B13	C25-C2	3.30	1.60	1.54
5	F	500	B13	C36-C7	3.27	1.59	1.54
5	N	500	B13	C36-C7	3.22	1.59	1.54
5	J	500	B13	C36-C7	3.22	1.59	1.54
5	D	500	B13	C20-C1	3.10	1.60	1.52
5	L	500	B13	C55-C17	3.07	1.59	1.55
5	P	500	B13	C55-C17	3.04	1.59	1.55
5	J	500	B13	C2B-N1B	2.98	1.42	1.37
5	F	500	B13	C2B-N1B	2.97	1.42	1.37
5	N	500	B13	C55-C17	2.97	1.59	1.55
5	P	500	B13	C25-C2	2.97	1.59	1.54
5	H	500	B13	C2B-N1B	2.93	1.42	1.37
5	F	500	B13	C7-C6	2.93	1.60	1.54
5	H	500	B13	C55-C17	2.93	1.59	1.55
5	B	500	B13	C25-C2	2.90	1.59	1.54
5	N	500	B13	C7-C6	2.89	1.60	1.54
5	F	500	B13	C25-C2	2.89	1.59	1.54
5	D	500	B13	C36-C7	2.89	1.59	1.54
5	L	500	B13	C36-C7	2.88	1.59	1.54
5	D	500	B13	C2B-N1B	2.86	1.42	1.37
5	J	500	B13	C55-C17	2.85	1.59	1.55
5	P	500	B13	C36-C7	2.83	1.59	1.54
5	D	500	B13	C55-C17	2.80	1.59	1.55
5	F	500	B13	C55-C17	2.78	1.59	1.55
5	N	500	B13	C25-C2	2.74	1.59	1.54
5	H	500	B13	C1R-N1B	2.71	1.53	1.46
5	D	500	B13	C2R-C3R	-2.71	1.47	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	500	B13	C2B-N1B	2.71	1.42	1.37
5	F	500	B13	C1R-N1B	2.67	1.53	1.46
5	P	500	B13	C2B-N1B	2.61	1.42	1.37
5	L	500	B13	C25-C2	2.59	1.59	1.54
5	L	500	B13	C2R-C3R	-2.59	1.47	1.53
5	B	500	B13	C36-C7	2.59	1.58	1.54
5	D	500	B13	C60-C61	-2.57	1.45	1.51
5	H	500	B13	C25-C2	2.54	1.59	1.54
5	J	500	B13	C1R-N1B	2.54	1.53	1.46
5	L	500	B13	C2B-N1B	2.48	1.41	1.37
5	D	500	B13	C7-C6	2.46	1.59	1.54
5	N	500	B13	C2B-N1B	2.45	1.41	1.37
5	H	500	B13	C7-C6	2.45	1.59	1.54
5	B	500	B13	C30-C3	2.42	1.57	1.53
5	L	500	B13	C7-C6	2.41	1.59	1.54
5	B	500	B13	C1R-N1B	2.41	1.53	1.46
5	N	500	B13	C1R-N1B	2.40	1.53	1.46
5	D	500	B13	C7B-C8B	2.37	1.43	1.39
5	J	500	B13	C2R-C3R	-2.36	1.47	1.53
5	P	500	B13	C1R-N1B	2.35	1.52	1.46
5	D	500	B13	C53-C15	2.30	1.54	1.50
5	F	500	B13	C13-C14	2.28	1.56	1.52
5	H	500	B13	C2R-C3R	-2.27	1.48	1.53
5	N	500	B13	C2R-C3R	-2.27	1.48	1.53
5	L	500	B13	C13-C14	2.26	1.56	1.52
5	P	500	B13	C48-C13	2.23	1.59	1.54
5	H	500	B13	C7B-C8B	2.22	1.43	1.39
5	N	500	B13	P-O4	-2.22	1.45	1.55
5	D	500	B13	P-O4	-2.21	1.45	1.55
5	H	500	B13	P-O4	-2.21	1.45	1.55
5	L	500	B13	C1R-N1B	2.20	1.52	1.46
5	L	500	B13	P-O4	-2.19	1.45	1.55
5	P	500	B13	P-O4	-2.17	1.45	1.55
5	J	500	B13	C30-C3	2.16	1.57	1.53
5	J	500	B13	P-O4	-2.14	1.45	1.55
5	D	500	B13	C1R-N1B	2.14	1.52	1.46
5	B	500	B13	P-O4	-2.13	1.45	1.55
5	P	500	B13	C7-C6	2.13	1.59	1.54
5	H	500	B13	C13-C14	2.13	1.56	1.52
5	F	500	B13	P-O4	-2.11	1.45	1.55
5	B	500	B13	C2R-C3R	-2.10	1.48	1.53
5	P	500	B13	C30-C3	2.09	1.57	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	500	B13	C60-C61	-2.08	1.46	1.51
5	F	500	B13	C2R-C3R	-2.06	1.48	1.53
5	B	500	B13	C46-C12	2.06	1.58	1.53
5	N	500	B13	C60-C61	-2.06	1.46	1.51
5	H	500	B13	C60-C61	-2.05	1.46	1.51
5	L	500	B13	C30-C3	2.05	1.57	1.53
5	J	500	B13	C7B-C8B	2.04	1.42	1.39
5	N	500	B13	C30-C3	2.02	1.57	1.53

All (214) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	500	B13	O6R-C4R-C5R	8.13	126.41	109.22
5	N	500	B13	O6R-C4R-C5R	8.12	126.38	109.22
5	B	500	B13	O6R-C4R-C5R	8.08	126.29	109.22
5	N	500	B13	C1R-N1B-C2B	-7.94	109.48	127.09
5	J	500	B13	O6R-C4R-C5R	7.74	125.58	109.22
5	P	500	B13	O6R-C4R-C5R	7.69	125.48	109.22
5	L	500	B13	O6R-C4R-C5R	7.64	125.36	109.22
5	D	500	B13	O6R-C4R-C5R	7.62	125.33	109.22
5	H	500	B13	O6R-C4R-C5R	7.36	124.78	109.22
5	H	500	B13	C1R-N1B-C2B	-7.25	111.01	127.09
5	J	500	B13	C1R-N1B-C2B	-6.98	111.59	127.09
5	L	500	B13	C1R-N1B-C2B	-6.83	111.93	127.09
5	B	500	B13	C1R-N1B-C2B	-6.38	112.94	127.09
5	P	500	B13	C1R-N1B-C2B	-6.27	113.17	127.09
5	F	500	B13	C1R-N1B-C2B	-6.22	113.29	127.09
5	H	500	B13	C8B-N1B-C1R	6.04	135.62	125.41
5	D	500	B13	C1R-N1B-C2B	-5.92	113.97	127.09
5	H	500	B13	C5R-C4R-C3R	5.46	132.03	114.84
5	J	500	B13	C5R-C4R-C3R	5.37	131.76	114.84
5	D	500	B13	C8B-N1B-C1R	5.35	134.46	125.41
5	L	500	B13	C8B-N1B-C1R	5.35	134.46	125.41
5	J	500	B13	C8B-N1B-C1R	5.30	134.38	125.41
5	L	500	B13	C5R-C4R-C3R	5.11	130.92	114.84
5	P	500	B13	C5R-C4R-C3R	5.11	130.92	114.84
5	F	500	B13	C5R-C4R-C3R	5.07	130.81	114.84
5	F	500	B13	C8B-N1B-C1R	5.01	133.89	125.41
5	B	500	B13	O7R-C2R-C3R	4.90	124.90	111.19
5	B	500	B13	C8B-N1B-C1R	4.86	133.62	125.41
5	N	500	B13	C8B-N1B-C1R	4.85	133.61	125.41
5	D	500	B13	C5R-C4R-C3R	4.79	129.93	114.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	500	B13	C5R-C4R-C3R	4.79	129.92	114.84
5	N	500	B13	O7R-C2R-C3R	4.70	124.36	111.19
5	H	500	B13	C60-C18-C17	4.69	122.74	114.63
5	P	500	B13	O7R-C2R-C3R	4.68	124.30	111.19
5	N	500	B13	C5R-C4R-C3R	4.64	129.47	114.84
5	P	500	B13	C8B-N1B-C1R	4.60	133.20	125.41
5	H	500	B13	O7R-C2R-C3R	4.57	123.99	111.19
5	H	500	B13	O34-C32-C31	-4.39	107.80	121.04
5	F	500	B13	O7R-C2R-C3R	4.26	123.12	111.19
5	P	500	B13	C7-C37-C38	4.26	126.89	114.28
5	F	500	B13	O34-C32-C31	-4.21	108.33	121.04
5	J	500	B13	O7R-C2R-C3R	4.20	122.94	111.19
5	L	500	B13	O7R-C2R-C3R	4.16	122.83	111.19
5	J	500	B13	C18-C60-C61	4.09	124.44	114.04
5	P	500	B13	C18-C60-C61	4.05	124.33	114.04
5	D	500	B13	O34-C32-C31	-4.03	108.87	121.04
5	H	500	B13	C7-C37-C38	4.02	126.19	114.28
5	B	500	B13	O34-C32-C31	-4.00	108.95	121.04
5	L	500	B13	O34-C32-C31	-3.99	108.98	121.04
5	D	500	B13	O7R-C2R-C3R	3.95	122.25	111.19
5	P	500	B13	O34-C32-C31	-3.95	109.11	121.04
5	J	500	B13	C7-C37-C38	3.94	125.95	114.28
5	N	500	B13	O34-C32-C31	-3.86	109.38	121.04
5	H	500	B13	C55-C17-C16	3.85	122.78	111.93
5	J	500	B13	O34-C32-C31	-3.76	109.69	121.04
5	B	500	B13	O6R-C1R-N1B	3.73	115.25	108.09
5	N	500	B13	C55-C17-C16	3.73	122.44	111.93
5	F	500	B13	C60-C18-C17	3.67	120.98	114.63
5	P	500	B13	C60-C18-C17	3.64	120.93	114.63
5	H	500	B13	C54-C17-C55	-3.64	102.62	109.36
5	F	500	B13	C9B-C8B-N1B	3.59	106.90	105.30
5	P	500	B13	C9B-C8B-N1B	3.59	106.90	105.30
5	B	500	B13	C9B-C8B-N1B	3.55	106.88	105.30
5	F	500	B13	O6R-C1R-N1B	3.52	114.85	108.09
5	D	500	B13	O6R-C1R-N1B	3.52	114.84	108.09
5	N	500	B13	C7-C37-C38	3.50	124.62	114.28
5	L	500	B13	O6R-C1R-N1B	3.48	114.77	108.09
5	P	500	B13	C42-C41-C8	3.45	124.43	114.65
5	F	500	B13	C55-C17-C16	3.45	121.66	111.93
5	D	500	B13	C41-C42-C43	-3.41	100.96	112.55
5	F	500	B13	C36-C7-C6	3.38	127.01	109.79
5	B	500	B13	C36-C7-C6	3.34	126.82	109.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	500	B13	O8R-C5R-C4R	3.32	122.64	111.33
5	N	500	B13	C36-C7-C6	3.31	126.64	109.79
5	D	500	B13	C42-C41-C8	3.29	123.97	114.65
5	N	500	B13	C47-C12-C13	3.29	122.32	111.55
5	N	500	B13	C60-C18-C17	3.29	120.31	114.63
5	B	500	B13	C55-C17-C16	3.27	121.15	111.93
5	J	500	B13	C55-C17-C16	3.26	121.13	111.93
5	D	500	B13	C41-C8-C7	-3.26	105.22	114.19
5	F	500	B13	O8R-C5R-C4R	3.25	122.41	111.33
5	H	500	B13	C18-C60-C61	3.22	122.22	114.04
5	F	500	B13	C18-C60-C61	3.20	122.17	114.04
5	B	500	B13	C18-C60-C61	3.20	122.17	114.04
5	H	500	B13	O6R-C1R-N1B	3.18	114.20	108.09
5	N	500	B13	O8R-C5R-C4R	3.16	122.10	111.33
5	P	500	B13	C36-C7-C6	3.16	125.89	109.79
5	D	500	B13	C60-C18-C17	3.15	120.07	114.63
5	H	500	B13	C42-C41-C8	3.13	123.53	114.65
5	B	500	B13	C17-C16-N24	3.10	112.58	109.22
5	F	500	B13	C42-C41-C8	3.08	123.37	114.65
5	N	500	B13	O6R-C1R-N1B	3.07	113.99	108.09
5	L	500	B13	C18-C60-C61	3.06	121.83	114.04
5	D	500	B13	C55-C17-C16	3.06	120.56	111.93
5	D	500	B13	O2-C3R-C4R	-3.06	99.24	110.03
5	N	500	B13	O2-C3R-C4R	-3.06	99.25	110.03
5	J	500	B13	O6R-C1R-N1B	3.05	113.94	108.09
5	H	500	B13	C36-C7-C6	3.04	125.26	109.79
5	L	500	B13	C60-C18-C17	3.02	119.84	114.63
5	L	500	B13	C55-C17-C16	2.99	120.36	111.93
5	L	500	B13	C36-C7-C6	2.97	124.94	109.79
5	J	500	B13	C36-C7-C6	2.96	124.87	109.79
5	D	500	B13	C7-C37-C38	2.95	123.02	114.28
5	D	500	B13	C36-C7-C6	2.95	124.83	109.79
5	B	500	B13	C4R-O6R-C1R	-2.95	102.95	109.47
5	D	500	B13	C47-C12-C13	2.94	121.19	111.55
5	L	500	B13	C42-C41-C8	2.93	122.95	114.65
5	P	500	B13	O6R-C1R-N1B	2.90	113.66	108.09
5	N	500	B13	C18-C60-C61	2.89	121.40	114.04
5	P	500	B13	C55-C17-C16	2.89	120.06	111.93
5	J	500	B13	C41-C42-C43	-2.84	102.91	112.55
5	N	500	B13	C36-C7-C37	-2.84	105.92	110.74
5	P	500	B13	C54-C17-C55	-2.83	104.13	109.36
5	D	500	B13	C36-C7-C37	-2.82	105.94	110.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	500	B13	C18-C60-C61	2.82	121.21	114.04
5	L	500	B13	C47-C12-C13	2.81	120.77	111.55
5	L	500	B13	C7-C37-C38	2.81	122.58	114.28
5	N	500	B13	C54-C17-C55	-2.80	104.17	109.36
5	L	500	B13	C36-C7-C37	-2.78	106.01	110.74
5	H	500	B13	C9B-C8B-N1B	2.77	106.53	105.30
5	N	500	B13	P-O3-C2P	2.73	130.44	121.10
5	F	500	B13	C41-C8-C7	-2.72	106.70	114.19
5	B	500	B13	C12-C13-C14	2.69	105.61	100.78
5	L	500	B13	C31-C30-C3	-2.68	107.48	114.08
5	N	500	B13	C9B-C8B-N1B	2.68	106.49	105.30
5	J	500	B13	C47-C12-C13	2.65	120.24	111.55
5	F	500	B13	P-O3-C2P	2.65	130.15	121.10
5	P	500	B13	C3P-C2P-C1P	-2.63	106.34	111.42
5	N	500	B13	C42-C41-C8	2.62	122.08	114.65
5	J	500	B13	C3P-C2P-C1P	-2.62	106.37	111.42
5	L	500	B13	O2-C3R-C4R	-2.62	100.81	110.03
5	J	500	B13	C4R-O6R-C1R	-2.61	103.70	109.47
5	L	500	B13	O8R-C5R-C4R	2.60	120.20	111.33
5	L	500	B13	C4R-O6R-C1R	-2.60	103.73	109.47
5	P	500	B13	C4R-O6R-C1R	-2.59	103.75	109.47
5	L	500	B13	C31-C32-N33	2.58	124.76	116.49
5	F	500	B13	C36-C7-C37	-2.56	106.39	110.74
5	H	500	B13	O2-C3R-C4R	-2.56	101.01	110.03
5	D	500	B13	C2P-C1P-N59	-2.56	109.16	112.92
5	D	500	B13	C4R-O6R-C1R	-2.55	103.84	109.47
5	B	500	B13	N1B-C2B-N3B	-2.53	110.34	113.94
5	P	500	B13	N1B-C2B-N3B	-2.53	110.34	113.94
5	H	500	B13	C47-C12-C13	2.52	119.80	111.55
5	D	500	B13	O8R-C5R-C4R	2.52	119.90	111.33
5	P	500	B13	P-O3-C2P	2.50	129.64	121.10
5	B	500	B13	C47-C12-C13	2.49	119.70	111.55
5	F	500	B13	C47-C12-C13	2.48	119.68	111.55
5	J	500	B13	O8R-C5R-C4R	2.48	119.77	111.33
5	F	500	B13	C7-C37-C38	2.47	121.58	114.28
5	F	500	B13	O2-C3R-C4R	-2.47	101.33	110.03
5	P	500	B13	C31-C32-N33	2.46	124.37	116.49
5	F	500	B13	C3P-C2P-C1P	-2.45	106.69	111.42
5	P	500	B13	C5B-C4B-C9B	-2.45	116.41	118.74
5	F	500	B13	C25-C2-C3	2.43	116.42	111.72
5	H	500	B13	C31-C32-N33	2.43	124.27	116.49
5	P	500	B13	C37-C38-N40	2.41	123.95	116.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	500	B13	N1B-C2B-N3B	-2.40	110.53	113.94
5	D	500	B13	C31-C32-N33	2.39	124.14	116.49
5	B	500	B13	C36-C7-C37	-2.38	106.69	110.74
5	H	500	B13	C37-C7-C8	-2.37	102.11	108.37
5	B	500	B13	C60-C18-C17	2.35	118.70	114.63
5	H	500	B13	C12-C13-C14	2.35	105.00	100.78
5	L	500	B13	C2-C26-C27	2.35	121.72	115.19
5	N	500	B13	C47-C12-C46	-2.34	102.67	108.26
5	B	500	B13	C42-C41-C8	2.33	121.24	114.65
5	P	500	B13	O8R-C5R-C4R	2.31	119.21	111.33
5	P	500	B13	C1P-N59-C57	-2.31	117.73	122.69
5	F	500	B13	C41-C42-C43	-2.28	104.80	112.55
5	B	500	B13	C7-C37-C38	2.28	121.02	114.28
5	B	500	B13	C9B-N3B-C2B	2.26	107.18	104.40
5	D	500	B13	C3P-C2P-C1P	-2.25	107.07	111.42
5	P	500	B13	O7R-C2R-C1R	2.25	117.84	110.10
5	J	500	B13	C60-C18-C17	2.24	118.51	114.63
5	F	500	B13	C31-C32-N33	2.24	123.67	116.49
5	J	500	B13	C42-C41-C8	2.23	120.98	114.65
5	D	500	B13	C6B-C5B-C4B	2.23	122.63	120.19
5	N	500	B13	C31-C32-N33	2.22	123.62	116.49
5	P	500	B13	C7B-C8B-C9B	2.22	124.79	122.23
5	P	500	B13	C47-C12-C13	2.22	118.83	111.55
5	B	500	B13	C31-C32-N33	2.20	123.55	116.49
5	P	500	B13	C25-C2-C3	2.19	115.95	111.72
5	J	500	B13	C9B-C8B-N1B	2.19	106.27	105.30
5	L	500	B13	C41-C42-C43	-2.17	105.18	112.55
5	B	500	B13	O2-C3R-C4R	-2.17	102.39	110.03
5	L	500	B13	P-O3-C2P	2.16	128.47	121.10
5	L	500	B13	C11-N23-C14	-2.15	108.43	111.89
5	N	500	B13	C47-C12-C11	2.15	117.21	111.58
5	N	500	B13	C4R-O6R-C1R	-2.15	104.73	109.47
5	D	500	B13	C1P-N59-C57	-2.14	118.09	122.69
5	J	500	B13	C31-C32-N33	2.14	123.36	116.49
5	J	500	B13	C6B-C5B-C4B	2.14	122.54	120.19
5	B	500	B13	C12-C11-N23	2.14	113.99	103.63
5	B	500	B13	C25-C2-C3	2.14	115.85	111.72
5	N	500	B13	O7R-C2R-C1R	2.12	117.41	110.10
5	F	500	B13	C31-C30-C3	-2.12	108.87	114.08
5	P	500	B13	C36-C7-C37	-2.12	107.14	110.74
5	P	500	B13	C9B-N3B-C2B	2.10	106.98	104.40
5	F	500	B13	C12-C13-C14	2.10	104.54	100.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	500	B13	C46-C12-C13	-2.10	104.69	111.55
5	P	500	B13	C41-C8-C7	-2.09	108.44	114.19
5	D	500	B13	C7B-C8B-C9B	2.09	124.64	122.23
5	N	500	B13	C11-N23-C14	-2.07	108.56	111.89
5	N	500	B13	C37-C38-N40	2.05	122.84	116.49
5	F	500	B13	O34-C32-N33	2.04	128.00	122.53
5	P	500	B13	C17-C16-N24	2.04	111.44	109.22
5	H	500	B13	C12-C11-N23	2.04	113.50	103.63
5	P	500	B13	C6B-C7B-C8B	-2.03	115.02	119.10
5	J	500	B13	N1B-C2B-N3B	-2.03	111.06	113.94
5	H	500	B13	O34-C32-N33	2.02	127.94	122.53
5	B	500	B13	C7B-C6B-C5B	2.02	122.01	119.88
5	B	500	B13	C41-C8-C7	-2.01	108.64	114.19
5	F	500	B13	C12-C11-N23	2.00	113.34	103.63
5	D	500	B13	C37-C38-N40	2.00	122.69	116.49
5	B	500	B13	O7R-C2R-C1R	2.00	116.99	110.10

There are no chirality outliers.

All (164) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	500	B13	C18-C60-C61-N62
5	B	500	B13	C18-C60-C61-O63
5	B	500	B13	C2-C3-C30-C31
5	B	500	B13	C4-C3-C30-C31
5	B	500	B13	C14-C13-C48-C49
5	B	500	B13	C38-C37-C7-C36
5	B	500	B13	C7-C37-C38-O39
5	D	500	B13	C1P-C2P-O3-P
5	D	500	B13	C18-C60-C61-N62
5	D	500	B13	C18-C60-C61-O63
5	D	500	B13	C2-C3-C30-C31
5	D	500	B13	C4-C3-C30-C31
5	D	500	B13	C7-C37-C38-O39
5	D	500	B13	C7-C37-C38-N40
5	F	500	B13	C1P-C2P-O3-P
5	F	500	B13	C18-C60-C61-N62
5	F	500	B13	C18-C60-C61-O63
5	F	500	B13	C2-C3-C30-C31
5	F	500	B13	C4-C3-C30-C31
5	F	500	B13	C38-C37-C7-C8
5	F	500	B13	C38-C37-C7-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	F	500	B13	C38-C37-C7-C36
5	H	500	B13	N59-C1P-C2P-O3
5	H	500	B13	N59-C1P-C2P-C3P
5	H	500	B13	C18-C60-C61-N62
5	H	500	B13	C18-C60-C61-O63
5	H	500	B13	C2-C3-C30-C31
5	H	500	B13	C4-C3-C30-C31
5	H	500	B13	C14-C13-C48-C49
5	H	500	B13	C38-C37-C7-C8
5	H	500	B13	C38-C37-C7-C6
5	H	500	B13	C38-C37-C7-C36
5	H	500	B13	C7-C37-C38-N40
5	J	500	B13	N59-C1P-C2P-O3
5	J	500	B13	C18-C60-C61-N62
5	J	500	B13	C18-C60-C61-O63
5	J	500	B13	C2-C3-C30-C31
5	J	500	B13	C4-C3-C30-C31
5	J	500	B13	C14-C13-C48-C49
5	J	500	B13	C12-C13-C48-C49
5	J	500	B13	C38-C37-C7-C36
5	J	500	B13	C7-C37-C38-O39
5	L	500	B13	C2P-O3-P-O2
5	L	500	B13	N59-C1P-C2P-O3
5	L	500	B13	N59-C1P-C2P-C3P
5	L	500	B13	C18-C60-C61-N62
5	L	500	B13	C18-C60-C61-O63
5	N	500	B13	C3P-C2P-O3-P
5	N	500	B13	C1P-C2P-O3-P
5	N	500	B13	N59-C1P-C2P-C3P
5	N	500	B13	C18-C60-C61-N62
5	N	500	B13	C18-C60-C61-O63
5	N	500	B13	C3-C2-C26-C27
5	N	500	B13	C2-C3-C30-C31
5	N	500	B13	C4-C3-C30-C31
5	N	500	B13	C7-C37-C38-N40
5	P	500	B13	C3P-C2P-O3-P
5	P	500	B13	C1P-C2P-O3-P
5	P	500	B13	N59-C1P-C2P-O3
5	P	500	B13	N59-C1P-C2P-C3P
5	P	500	B13	C18-C60-C61-N62
5	P	500	B13	C18-C60-C61-O63
5	P	500	B13	C7-C37-C38-O39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	P	500	B13	C7-C37-C38-N40
5	H	500	B13	C3R-C4R-C5R-O8R
5	J	500	B13	C42-C41-C8-C9
5	N	500	B13	C14-C13-C48-C49
5	B	500	B13	C7-C37-C38-N40
5	H	500	B13	C7-C37-C38-O39
5	J	500	B13	C7-C37-C38-N40
5	L	500	B13	C7-C37-C38-N40
5	B	500	B13	C12-C13-C48-C49
5	H	500	B13	C12-C13-C48-C49
5	N	500	B13	C12-C13-C48-C49
5	N	500	B13	C42-C41-C8-C9
5	F	500	B13	O6R-C4R-C5R-O8R
5	J	500	B13	O6R-C4R-C5R-O8R
5	N	500	B13	O6R-C4R-C5R-O8R
5	P	500	B13	C3R-C4R-C5R-O8R
5	B	500	B13	C42-C41-C8-C9
5	H	500	B13	C42-C41-C8-C9
5	N	500	B13	C25-C2-C26-C27
5	L	500	B13	C7-C37-C38-O39
5	N	500	B13	C7-C37-C38-O39
5	B	500	B13	C2R-C1R-N1B-C8B
5	D	500	B13	C2R-C1R-N1B-C8B
5	F	500	B13	C2R-C1R-N1B-C8B
5	H	500	B13	C2R-C1R-N1B-C8B
5	J	500	B13	C2R-C1R-N1B-C8B
5	L	500	B13	C2R-C1R-N1B-C8B
5	P	500	B13	C2R-C1R-N1B-C8B
5	D	500	B13	O6R-C4R-C5R-O8R
5	N	500	B13	N59-C1P-C2P-O3
5	H	500	B13	C17-C55-C56-C57
5	F	500	B13	C14-C13-C48-C49
5	P	500	B13	C14-C13-C48-C49
5	D	500	B13	C3P-C2P-O3-P
5	F	500	B13	C3P-C2P-O3-P
5	P	500	B13	C42-C41-C8-C9
5	L	500	B13	O6R-C4R-C5R-O8R
5	J	500	B13	C8-C41-C42-C43
5	B	500	B13	O6R-C4R-C5R-O8R
5	J	500	B13	N59-C1P-C2P-C3P
5	F	500	B13	C12-C13-C48-C49
5	P	500	B13	C12-C13-C48-C49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	F	500	B13	C8-C41-C42-C43
5	J	500	B13	C17-C55-C56-C57
5	N	500	B13	C17-C55-C56-C57
5	F	500	B13	C42-C41-C8-C9
5	D	500	B13	C12-C13-C48-C49
5	P	500	B13	C30-C31-C32-O34
5	B	500	B13	C1P-C2P-O3-P
5	D	500	B13	C14-C13-C48-C49
5	J	500	B13	C3-C2-C26-C27
5	D	500	B13	O6R-C1R-N1B-C8B
5	L	500	B13	O6R-C1R-N1B-C8B
5	N	500	B13	C2R-C1R-N1B-C8B
5	P	500	B13	C30-C31-C32-N33
5	J	500	B13	C38-C37-C7-C8
5	J	500	B13	C42-C41-C8-C7
5	H	500	B13	C30-C31-C32-O34
5	N	500	B13	C30-C31-C32-O34
5	N	500	B13	C42-C41-C8-C7
5	L	500	B13	C3-C30-C31-C32
5	B	500	B13	C30-C31-C32-O34
5	L	500	B13	C17-C55-C56-C57
5	L	500	B13	C4-C3-C30-C31
5	P	500	B13	C4-C3-C30-C31
5	D	500	B13	C42-C41-C8-C9
5	L	500	B13	C42-C41-C8-C9
5	J	500	B13	C17-C18-C60-C61
5	F	500	B13	C4R-C3R-O2-P
5	B	500	B13	O6R-C1R-N1B-C8B
5	F	500	B13	O6R-C1R-N1B-C8B
5	H	500	B13	O6R-C1R-N1B-C8B
5	J	500	B13	O6R-C1R-N1B-C8B
5	N	500	B13	O6R-C1R-N1B-C8B
5	P	500	B13	O6R-C1R-N1B-C8B
5	H	500	B13	C30-C31-C32-N33
5	N	500	B13	C30-C31-C32-N33
5	L	500	B13	C30-C31-C32-O34
5	B	500	B13	C38-C37-C7-C8
5	L	500	B13	C3R-C4R-C5R-O8R
5	L	500	B13	C30-C31-C32-N33
5	F	500	B13	C2R-C3R-O2-P
5	D	500	B13	C19-C18-C60-C61
5	J	500	B13	C19-C18-C60-C61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	P	500	B13	C17-C18-C60-C61
5	P	500	B13	C19-C18-C60-C61
5	B	500	B13	C30-C31-C32-N33
5	B	500	B13	C3P-C2P-O3-P
5	L	500	B13	C2-C3-C30-C31
5	P	500	B13	C2-C3-C30-C31
5	D	500	B13	C30-C31-C32-N33
5	D	500	B13	C17-C18-C60-C61
5	L	500	B13	C4R-C3R-O2-P
5	F	500	B13	C17-C55-C56-C57
5	L	500	B13	C38-C37-C7-C36
5	D	500	B13	C3R-C4R-C5R-O8R
5	N	500	B13	C3R-C4R-C5R-O8R
5	N	500	B13	C17-C18-C60-C61
5	L	500	B13	C2R-C3R-O2-P
5	N	500	B13	C13-C48-C49-C50
5	D	500	B13	C30-C31-C32-O34

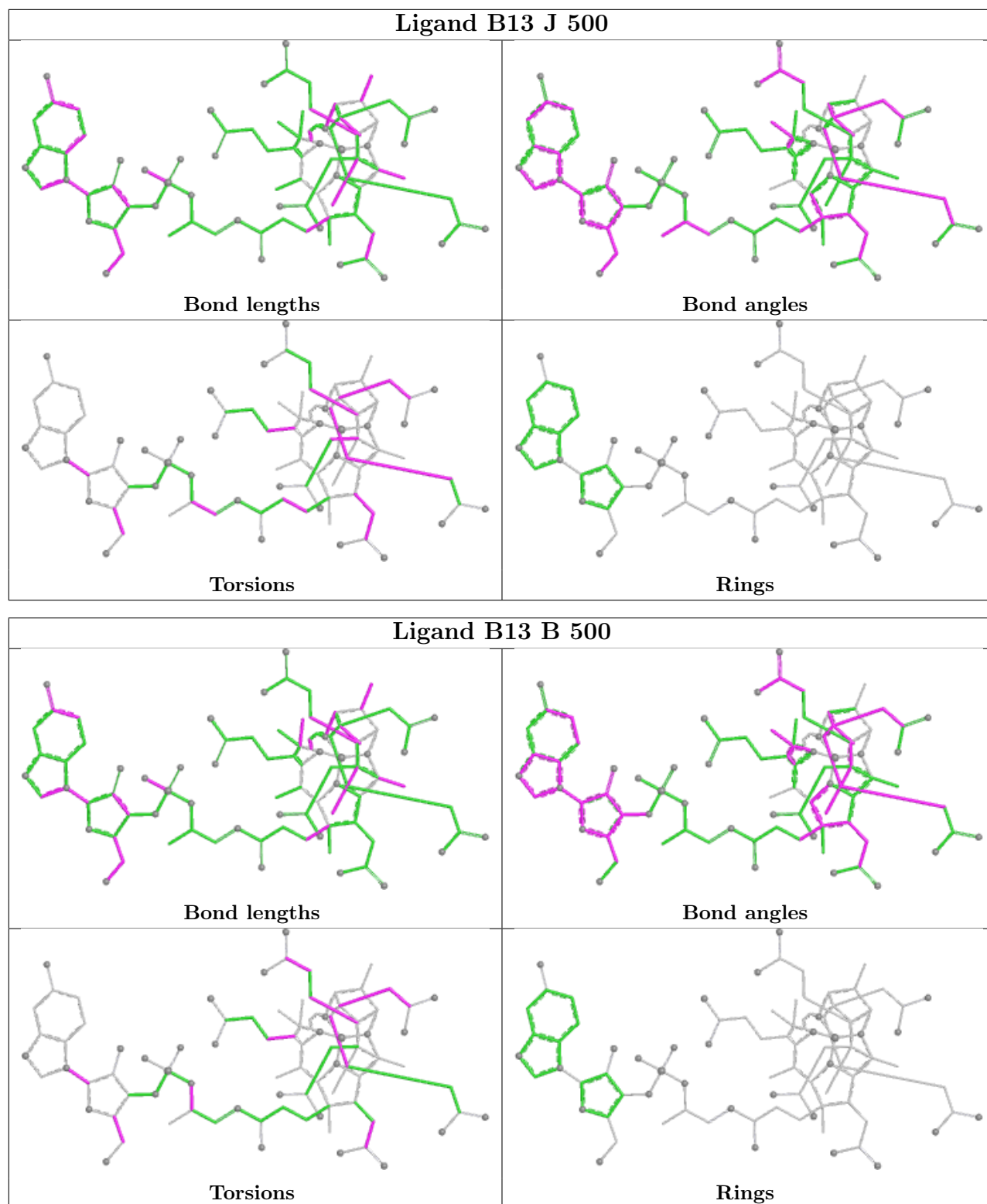
There are no ring outliers.

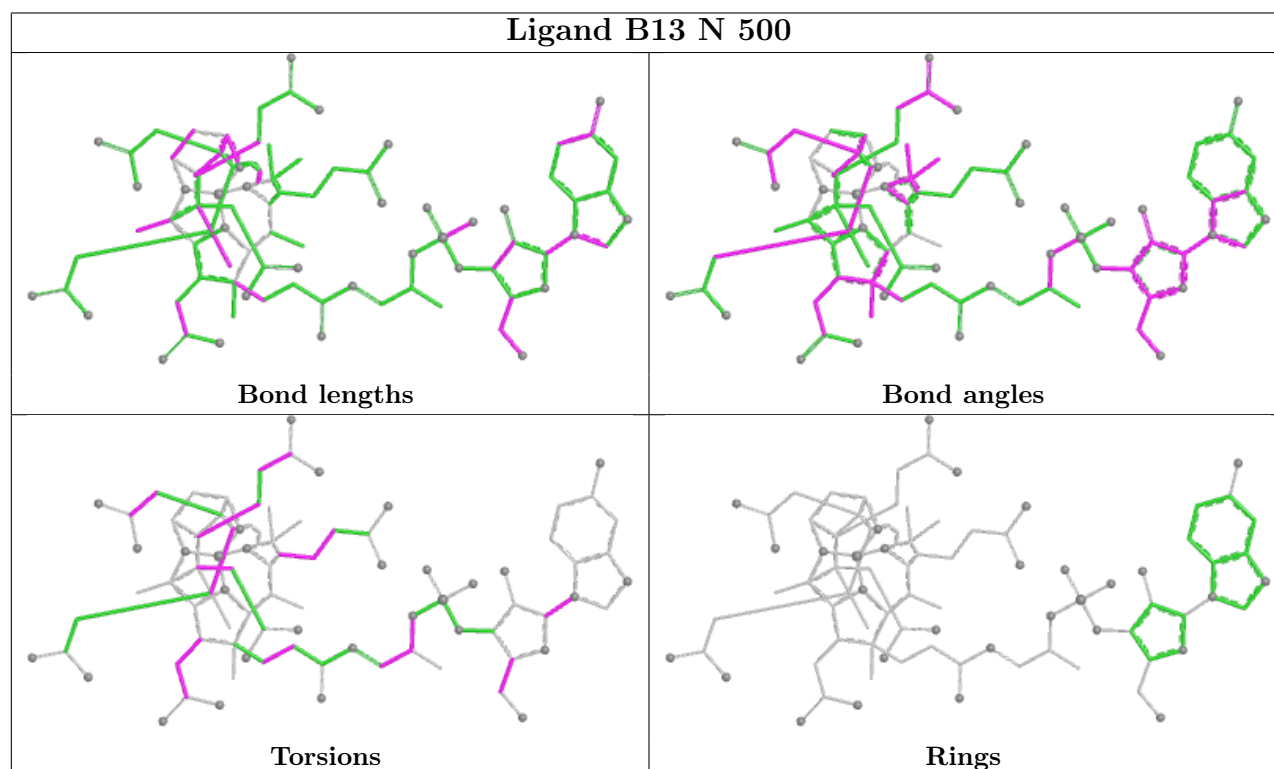
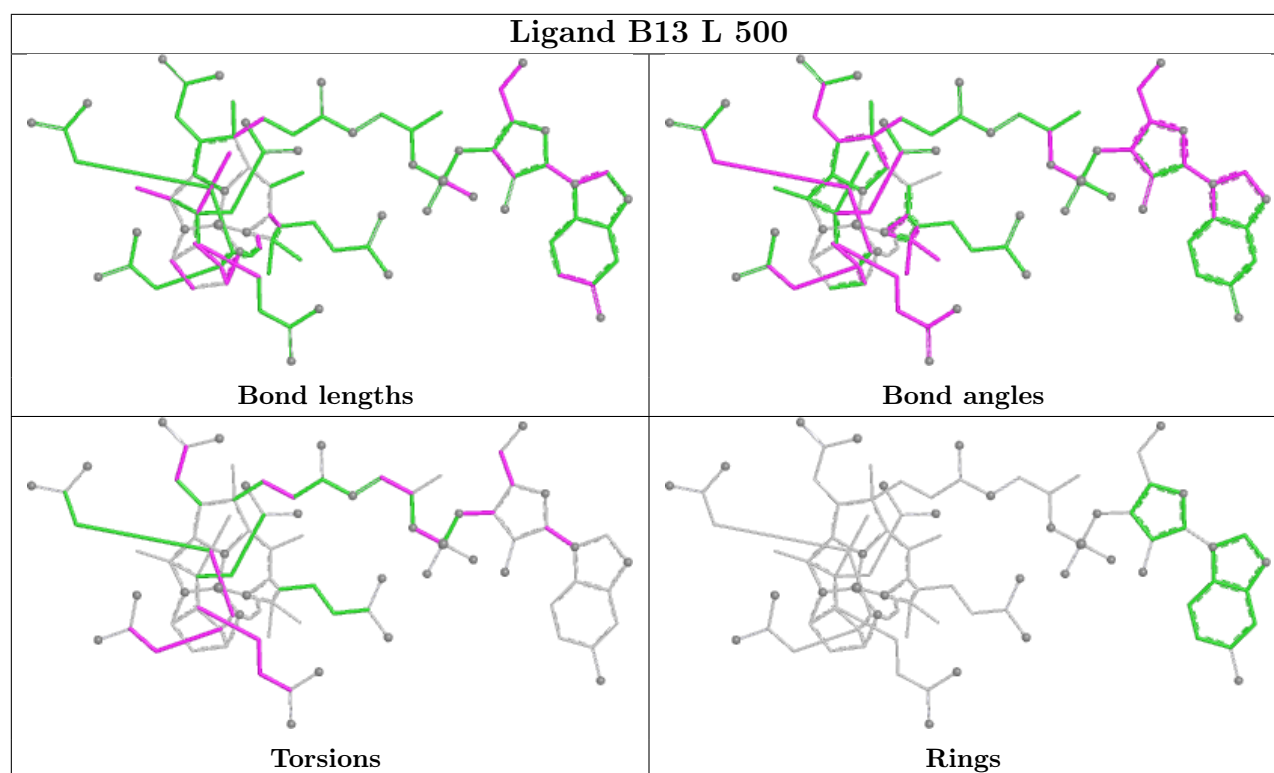
8 monomers are involved in 87 short contacts:

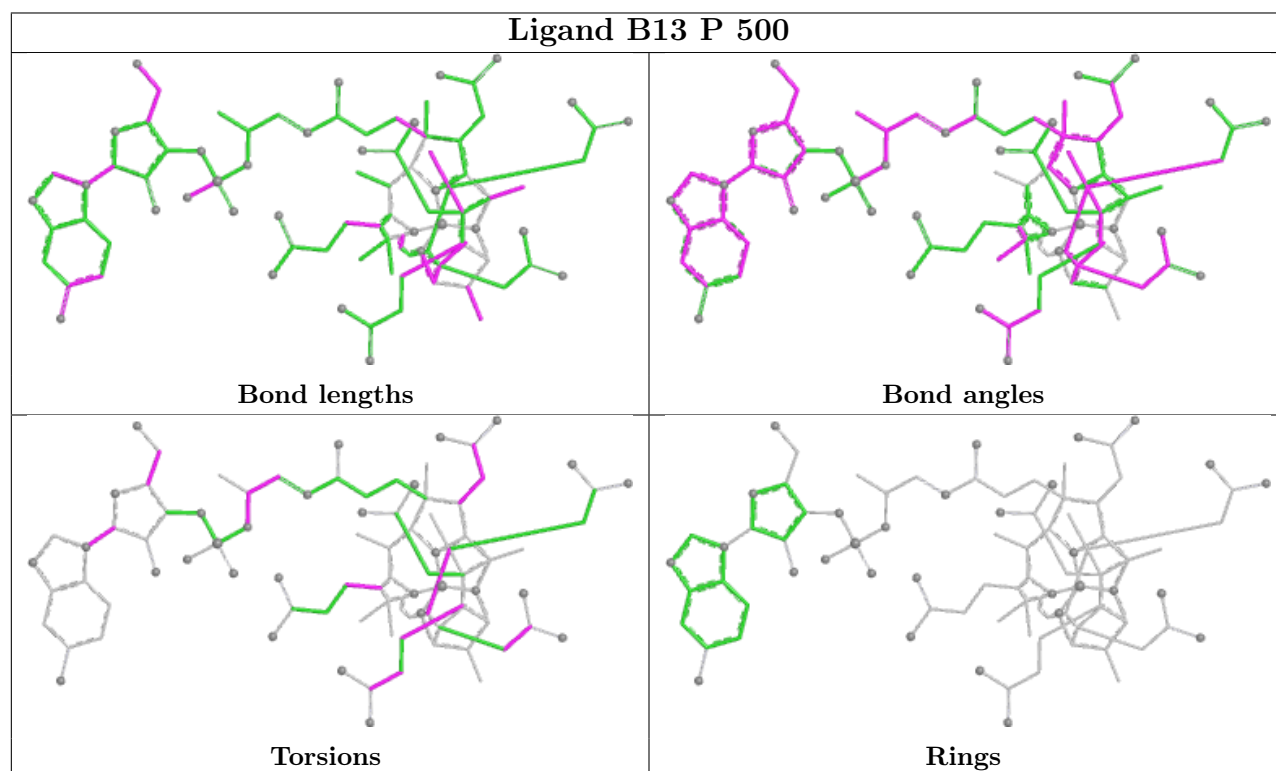
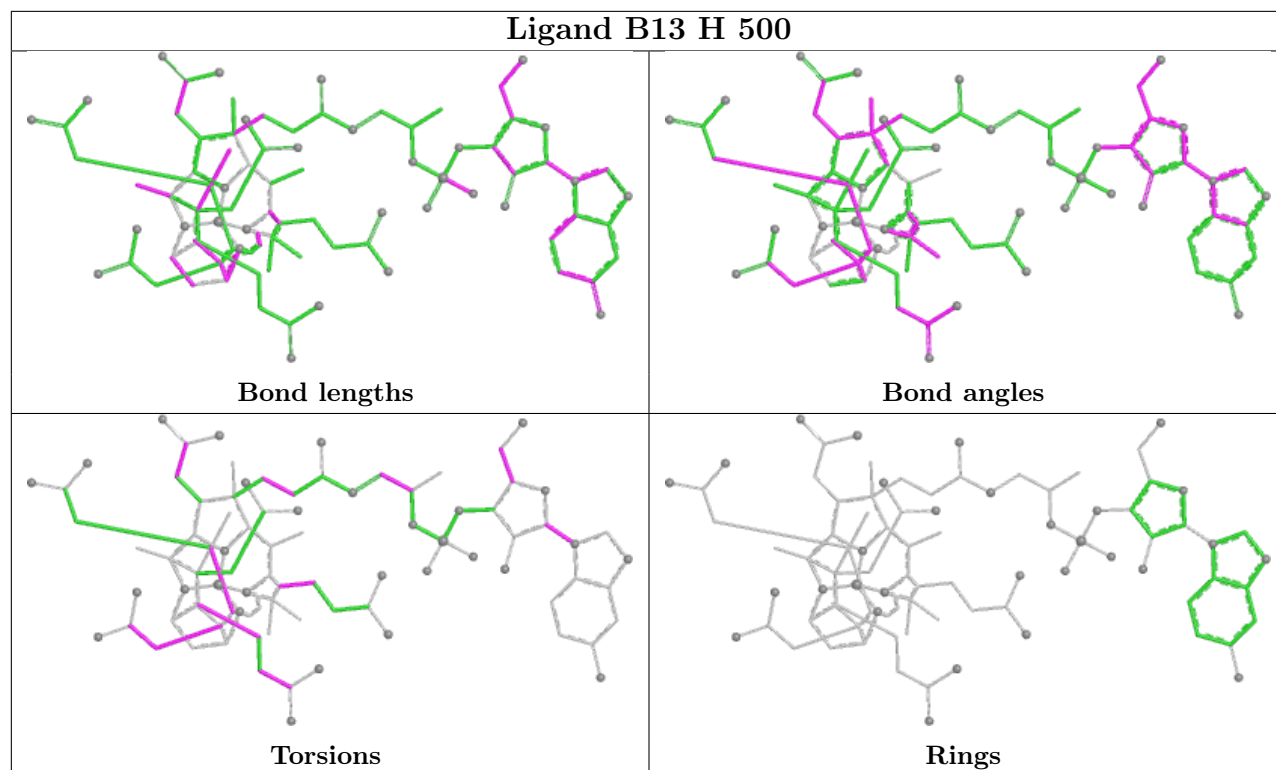
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	500	B13	14	0
5	B	500	B13	11	0
5	L	500	B13	10	0
5	N	500	B13	11	0
5	H	500	B13	10	0
5	P	500	B13	9	0
5	F	500	B13	7	0
5	D	500	B13	15	0

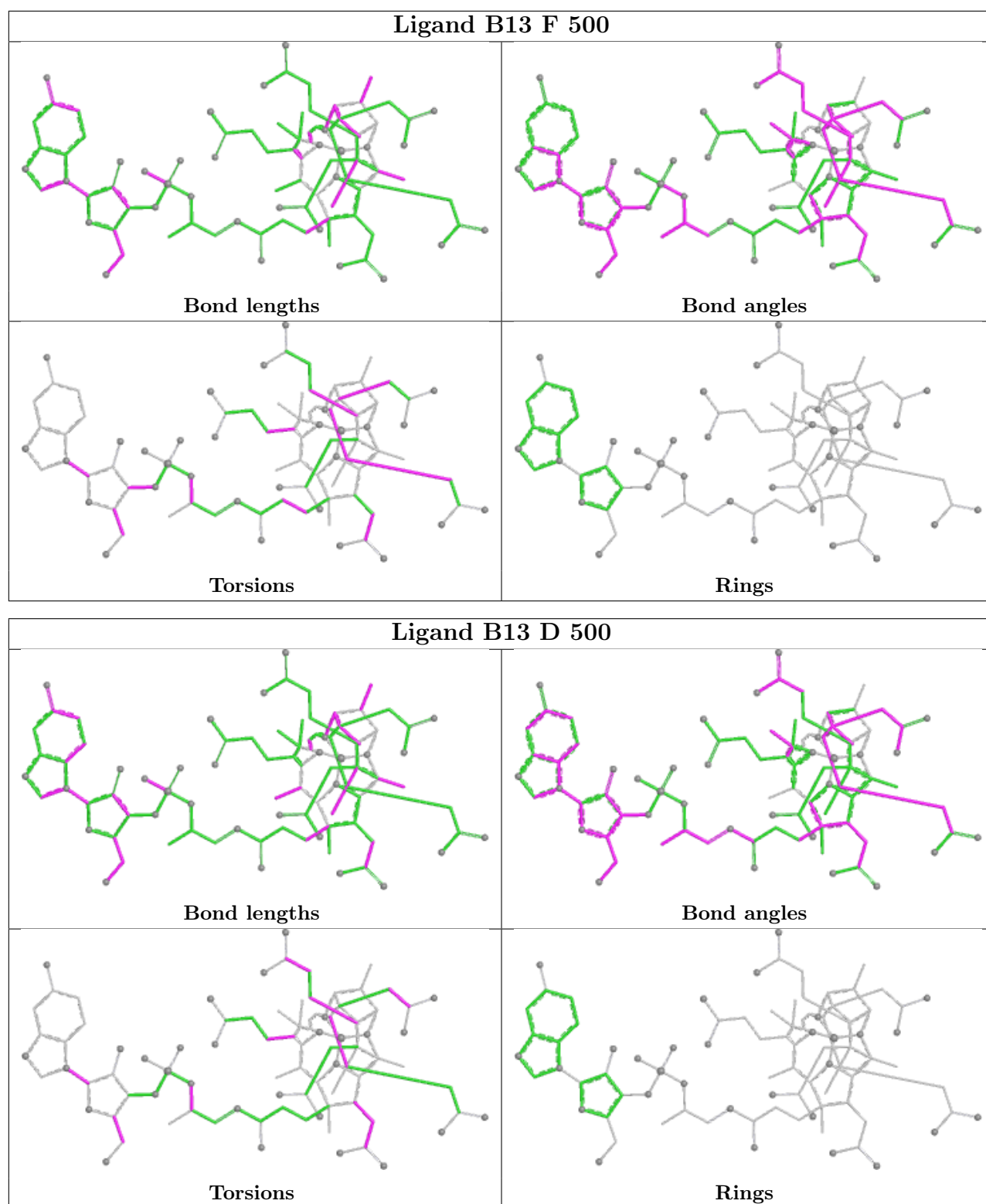
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	459/461 (99%)	-0.87	0	100	100	3, 11, 26, 38	0
1	C	459/461 (99%)	-0.88	0	100	100	3, 10, 23, 39	0
1	E	459/461 (99%)	-0.07	1 (0%)	91	89	25, 33, 42, 49	0
1	G	459/461 (99%)	-0.28	2 (0%)	88	86	18, 29, 40, 49	0
1	I	459/461 (99%)	-0.70	0	100	100	9, 20, 34, 50	0
1	K	459/461 (99%)	-0.66	0	100	100	12, 20, 33, 46	0
1	M	459/461 (99%)	-0.64	0	100	100	10, 20, 34, 48	0
1	O	459/461 (99%)	-0.75	0	100	100	7, 18, 32, 45	0
2	B	258/258 (100%)	1.01	37 (14%)	6	5	4, 66, 100, 107	0
2	D	258/258 (100%)	1.04	38 (14%)	6	4	5, 66, 100, 110	0
2	F	258/258 (100%)	0.80	19 (7%)	20	18	18, 72, 102, 112	0
2	H	258/258 (100%)	0.67	11 (4%)	40	35	28, 73, 104, 110	0
2	J	258/258 (100%)	0.61	17 (6%)	24	21	17, 64, 97, 107	0
2	L	258/258 (100%)	0.80	15 (5%)	29	25	12, 71, 102, 113	0
2	N	258/258 (100%)	1.04	37 (14%)	6	5	12, 73, 103, 110	0
2	P	258/258 (100%)	0.83	29 (11%)	10	8	17, 67, 98, 108	0
All	All	5736/5752 (99%)	-0.08	206 (3%)	46	41	3, 29, 92, 113	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	68	ASP	4.2
2	B	69	PRO	4.1
2	L	257	LYS	3.9
2	D	255	PHE	3.9
2	P	255	PHE	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	70	ILE	3.8
2	D	219	VAL	3.7
2	B	63	ILE	3.7
2	J	69	PRO	3.7
2	B	119	THR	3.5
2	D	251	LEU	3.5
2	B	73	ILE	3.5
2	P	253	GLU	3.4
2	N	72	LEU	3.4
2	D	237	ILE	3.4
2	B	12	VAL	3.3
2	D	224	LEU	3.3
2	J	237	ILE	3.2
2	B	116	SER	3.2
2	B	76	ALA	3.2
2	N	257	LYS	3.1
2	P	69	PRO	3.1
2	B	61	ALA	3.1
2	D	65	ALA	3.1
2	P	228	GLY	3.1
2	B	56	VAL	3.1
2	D	246	THR	3.0
2	B	71	ASP	3.0
2	B	112	CYS	3.0
2	J	248	VAL	3.0
2	P	242	ILE	3.0
2	D	149	ALA	3.0
2	J	257	LYS	3.0
2	N	76	ALA	2.9
2	J	251	LEU	2.9
2	N	56	VAL	2.9
2	D	69	PRO	2.9
2	B	243	ALA	2.8
2	J	240	ALA	2.8
2	L	242	ILE	2.8
2	N	223	ALA	2.8
2	P	223	ALA	2.8
2	N	258	HIS	2.8
2	D	248	VAL	2.8
2	F	65	ALA	2.8
2	B	242	ILE	2.7
2	F	69	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	3	ALA	2.7
2	P	155	VAL	2.7
2	H	61	ALA	2.7
2	D	225	GLY	2.7
2	L	117	GLY	2.7
2	B	109	ILE	2.7
2	P	257	LYS	2.7
2	F	66	GLY	2.6
2	P	237	ILE	2.6
2	N	199	LEU	2.6
2	F	149	ALA	2.6
2	L	61	ALA	2.6
2	N	73	ILE	2.6
2	P	241	ILE	2.6
2	N	8	SER	2.6
2	B	5	THR	2.6
2	D	240	ALA	2.6
2	L	258	HIS	2.6
2	D	112	CYS	2.6
2	B	55	VAL	2.6
2	P	254	LYS	2.6
2	F	167	LEU	2.6
2	F	257	LYS	2.6
2	P	236	LYS	2.6
2	D	242	ILE	2.5
2	J	110	GLU	2.5
2	H	79	VAL	2.5
2	B	257	LYS	2.5
2	D	116	SER	2.5
2	N	61	ALA	2.5
2	B	113	LYS	2.5
2	P	226	VAL	2.5
2	P	232	ALA	2.5
2	P	158	GLY	2.5
2	D	199	LEU	2.5
2	P	163	ALA	2.5
2	B	67	LYS	2.5
2	J	254	LYS	2.5
2	N	2	LEU	2.5
2	D	258	HIS	2.5
2	N	12	VAL	2.5
2	P	118	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	8	SER	2.5
2	D	186	THR	2.5
2	F	237	ILE	2.4
2	D	232	ALA	2.4
2	B	39	LEU	2.4
2	B	251	LEU	2.4
2	H	255	PHE	2.4
2	D	141	ASN	2.4
2	D	226	VAL	2.4
1	G	56	GLU	2.4
2	N	227	TYR	2.4
2	B	1	MET	2.4
2	H	223	ALA	2.4
2	J	243	ALA	2.4
2	B	43	ILE	2.4
2	J	241	ILE	2.4
2	N	77	LEU	2.4
2	J	255	PHE	2.4
2	N	255	PHE	2.4
2	P	219	VAL	2.4
2	D	223	ALA	2.4
2	L	118	ALA	2.4
2	D	142	ILE	2.3
2	F	63	ILE	2.3
2	F	67	LYS	2.3
1	G	3	ALA	2.3
2	J	245	THR	2.3
2	B	77	LEU	2.3
2	L	59	LEU	2.3
2	P	256	HIS	2.3
2	P	160	ASP	2.3
2	F	123	LYS	2.3
2	L	56	VAL	2.3
2	D	213	ALA	2.3
2	H	240	ALA	2.3
2	L	65	ALA	2.3
2	P	139	GLY	2.3
2	H	242	ILE	2.3
2	F	68	ASP	2.3
2	P	222	PHE	2.3
2	F	258	HIS	2.3
2	J	258	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	59	LEU	2.3
2	P	248	VAL	2.3
2	D	118	ALA	2.2
2	F	62	ALA	2.2
2	J	246	THR	2.2
2	B	117	GLY	2.2
2	J	256	HIS	2.2
2	N	151	GLY	2.2
2	F	242	ILE	2.2
2	L	73	ILE	2.2
2	L	109	ILE	2.2
2	N	254	LYS	2.2
2	D	190	ALA	2.2
2	N	65	ALA	2.2
2	N	232	ALA	2.2
2	H	246	THR	2.2
2	N	5	THR	2.2
2	P	258	HIS	2.2
2	D	205	ILE	2.2
2	F	70	ILE	2.2
2	L	120	PRO	2.2
2	N	248	VAL	2.2
2	F	249	THR	2.2
2	N	119	THR	2.2
2	N	176	ILE	2.2
2	D	137	ASP	2.2
2	B	255	PHE	2.2
2	N	243	ALA	2.2
2	D	58	GLY	2.2
2	H	251	LEU	2.2
2	L	39	LEU	2.2
2	P	157	LEU	2.2
2	D	126	VAL	2.1
2	D	136	HIS	2.1
2	P	65	ALA	2.1
2	P	243	ALA	2.1
2	F	246	THR	2.1
2	D	67	LYS	2.1
2	N	121	LYS	2.1
2	N	206	PRO	2.1
2	L	255	PHE	2.1
2	N	214	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	65	ALA	2.1
2	H	149	ALA	2.1
2	H	243	ALA	2.1
2	N	44	ALA	2.1
2	B	58	GLY	2.1
2	N	14	THR	2.1
2	N	157	LEU	2.1
2	D	109	ILE	2.1
2	J	70	ILE	2.1
2	L	237	ILE	2.1
2	N	63	ILE	2.1
2	D	256	HIS	2.1
2	D	163	ALA	2.1
2	N	59	LEU	2.1
2	P	117	GLY	2.1
2	J	137	ASP	2.1
2	B	120	PRO	2.1
2	F	190	ALA	2.1
2	B	199	LEU	2.1
2	D	157	LEU	2.1
2	D	227	TYR	2.1
2	B	118	ALA	2.0
2	B	13	LEU	2.0
2	D	147	LEU	2.0
2	P	251	LEU	2.0
2	N	219	VAL	2.0
2	N	146	LEU	2.0
2	B	151	GLY	2.0
2	N	186	THR	2.0
2	N	245	THR	2.0
2	N	246	THR	2.0
2	B	3	ASP	2.0
2	F	111	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

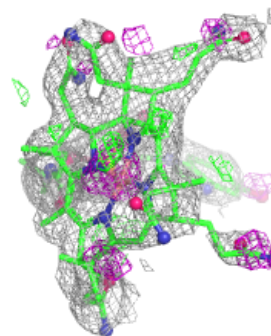
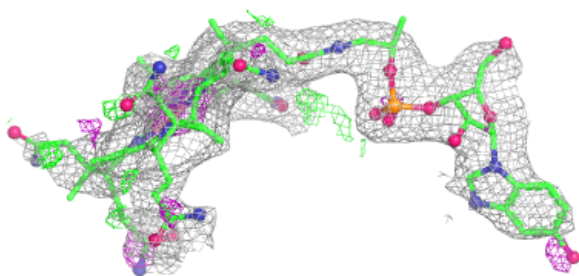
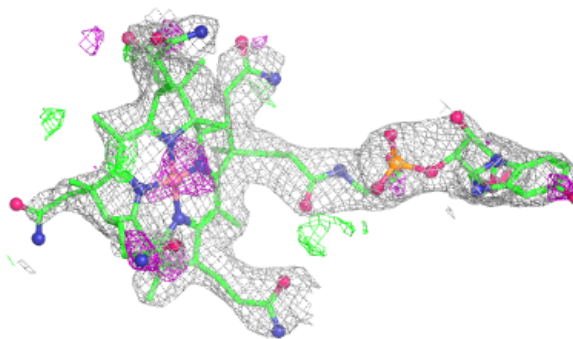
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	K	G	514	1/1	0.76	0.14	39,39,39,39	1
4	K	E	513	1/1	0.82	0.09	33,33,33,33	1
4	K	O	518	1/1	0.85	0.10	35,35,35,35	1
4	K	I	515	1/1	0.86	0.08	28,28,28,28	1
4	K	C	512	1/1	0.87	0.11	22,22,22,22	1
5	B13	N	500	90/90	0.87	0.12	60,66,72,73	0
5	B13	F	500	90/90	0.88	0.12	53,63,71,72	0
4	K	M	517	1/1	0.89	0.06	33,33,33,33	1
5	B13	L	500	90/90	0.90	0.11	41,47,58,59	0
4	K	A	511	1/1	0.92	0.10	23,23,23,23	1
5	B13	H	500	90/90	0.92	0.10	45,58,68,69	0
5	B13	P	500	90/90	0.92	0.10	31,40,45,52	0
5	B13	J	500	90/90	0.93	0.10	32,37,50,57	0
5	B13	D	500	90/90	0.93	0.10	20,30,40,42	0
4	K	K	516	1/1	0.94	0.08	31,31,31,31	1
5	B13	B	500	90/90	0.94	0.09	9,24,48,49	0
3	ZN	E	503	1/1	0.94	0.12	36,36,36,36	1
3	ZN	G	504	1/1	0.96	0.11	33,33,33,33	1
3	ZN	M	507	1/1	0.98	0.15	33,33,33,33	0
3	ZN	O	508	1/1	0.98	0.13	33,33,33,33	0
3	ZN	K	506	1/1	0.99	0.12	33,33,33,33	0
3	ZN	A	501	1/1	0.99	0.16	20,20,20,20	0
3	ZN	M	523	1/1	0.99	0.15	21,21,21,21	0
3	ZN	C	502	1/1	0.99	0.16	19,19,19,19	0
3	ZN	I	505	1/1	0.99	0.13	30,30,30,30	0
3	ZN	I	521	1/1	1.00	0.14	16,16,16,16	0
3	ZN	A	524	1/1	1.00	0.15	9,9,9,9	0
3	ZN	E	522	1/1	1.00	0.11	37,37,37,37	0

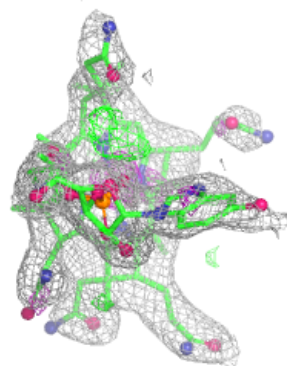
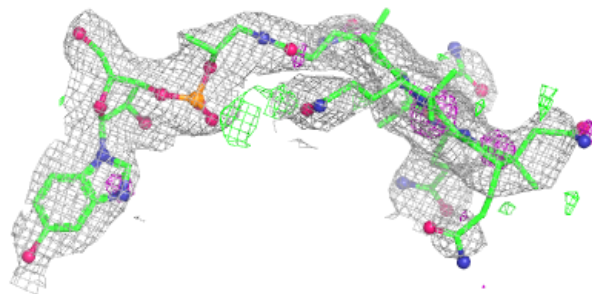
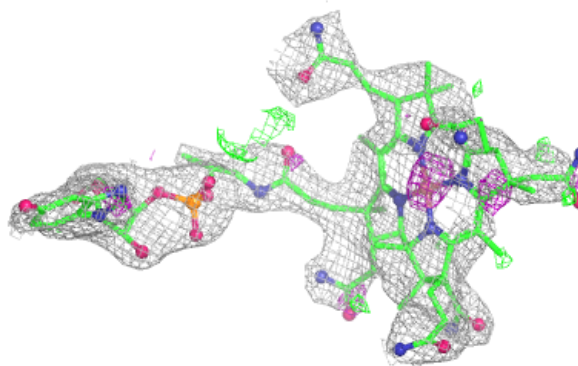
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B13 N 500:

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

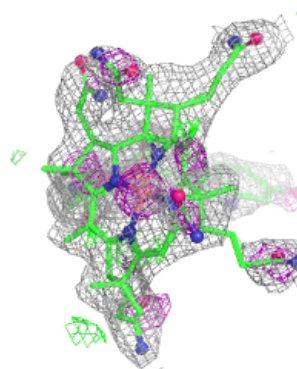
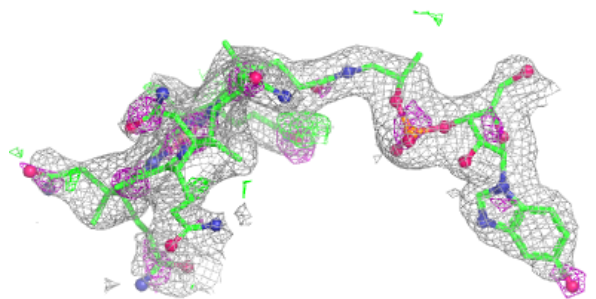
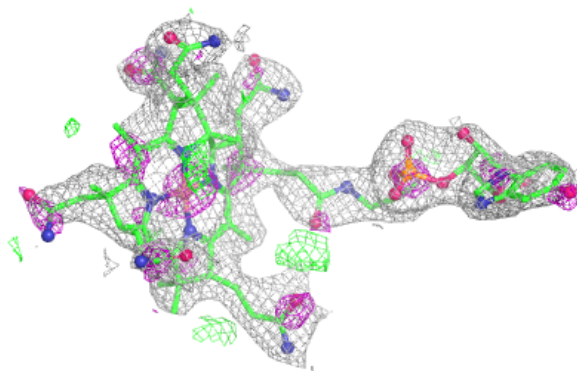
**Electron density around B13 F 500:**

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

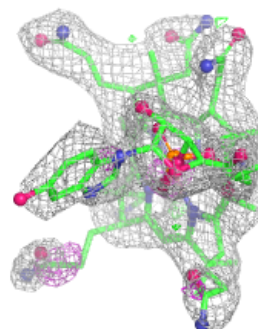
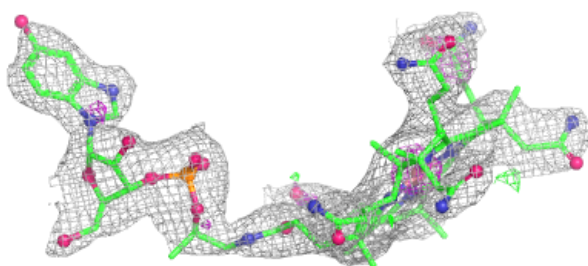
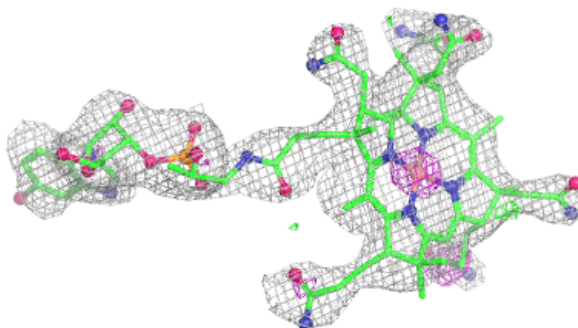


Electron density around B13 L 500:

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

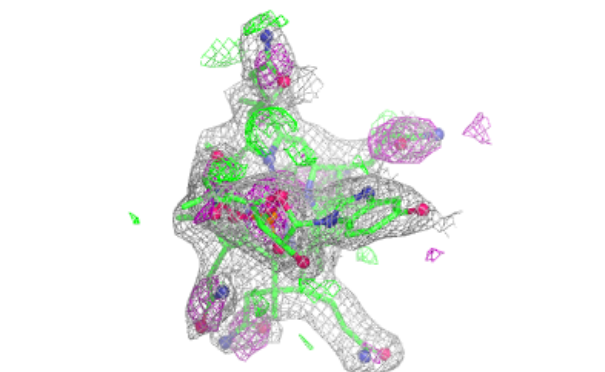
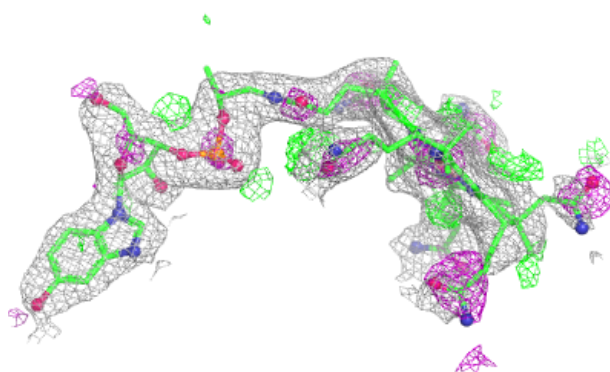
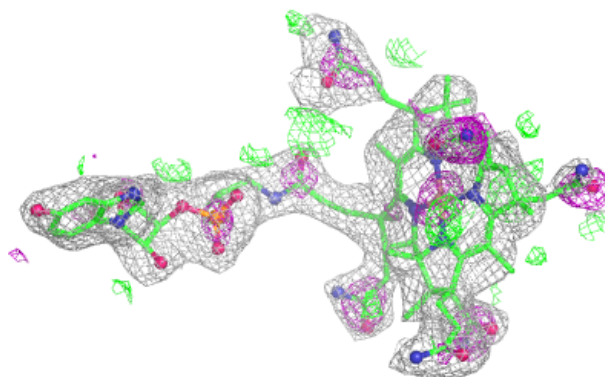
**Electron density around B13 H 500:**

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

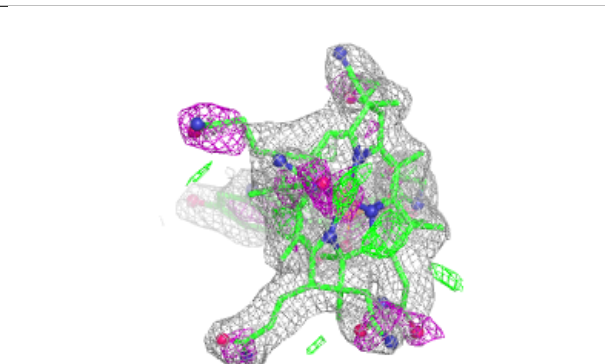
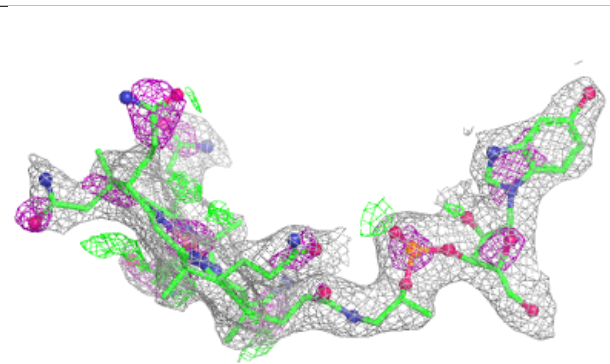
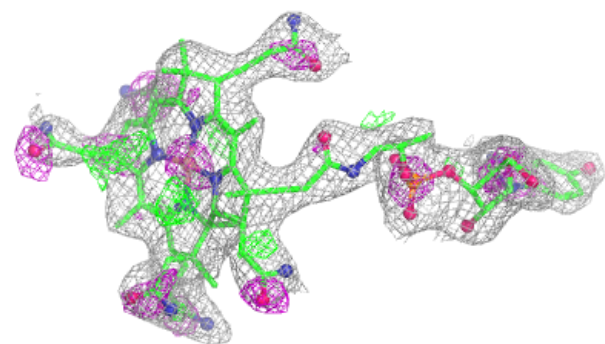


Electron density around B13 P 500:

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

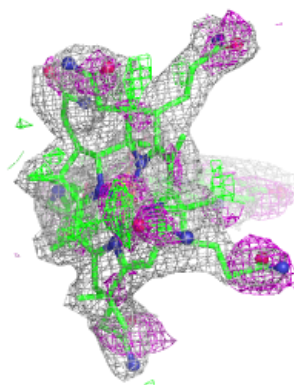
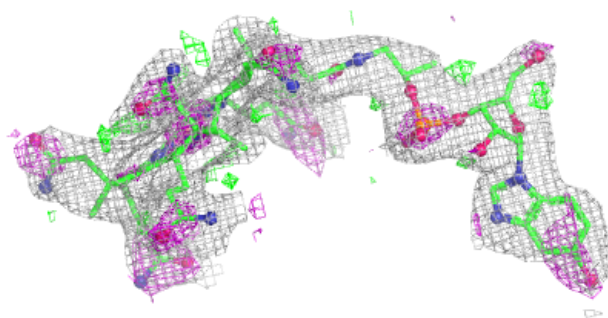
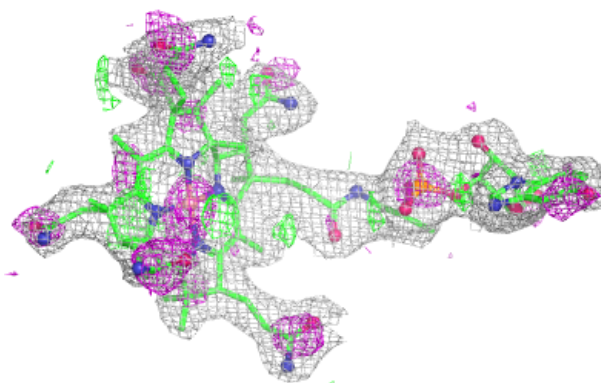
**Electron density around B13 J 500:**

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

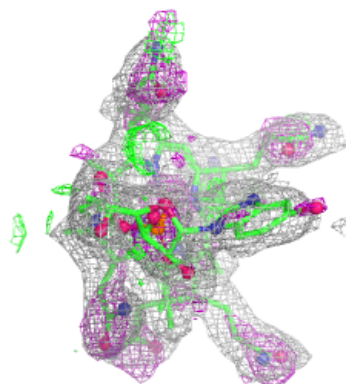
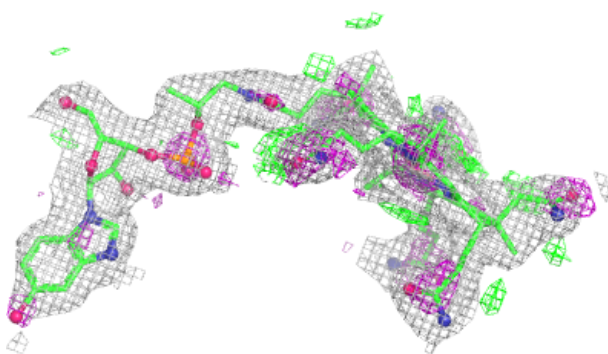
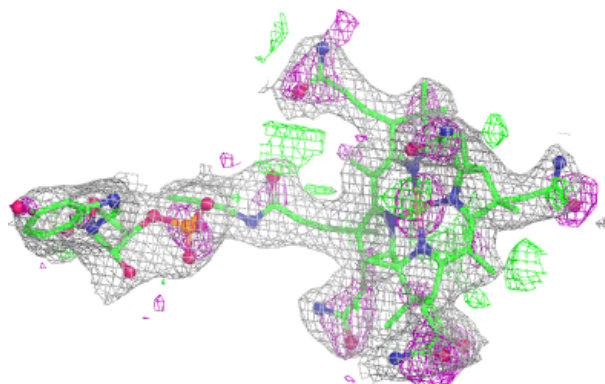


Electron density around B13 D 500:

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

**Electron density around B13 B 500:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.