



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:48 PM UTC

PDB ID : 2VPX / pdb_00002vpx
Title : Polysulfide reductase with bound quinone (UQ1)
Authors : Jormakka, M.; Yokoyama, K.; Yano, T.; Tamakoshi, M.; Akimoto, S.; Shimamura, T.; Curmi, P.; Iwata, S.
Deposited on : 2008-03-09
Resolution : 3.10 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

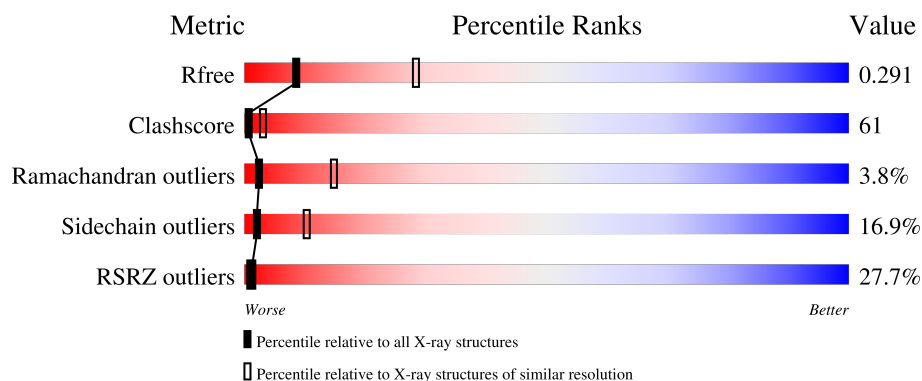
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	765	23% 27% 47% 18% 5% .
1	E	765	30% 29% 44% 17% 6% .
2	B	195	6% 35% 49% 12% ..
2	F	195	42% 33% 50% 13% ..
3	C	253	20% 46% 38% 14% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	253	42% 36% 45% 14%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	A	1764	-	-	X	-
4	SF4	B	1194	-	-	X	-
4	SF4	B	1195	-	-	X	-
4	SF4	B	1196	-	-	X	-
4	SF4	F	1194	-	-	X	-
4	SF4	F	1195	-	-	X	-
7	UQ1	C	1252	-	-	X	-
7	UQ1	G	1251	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20229 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 THIOSULFATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	0	0	1
			5896	3802	1032	1043	19			
1	E	735	Total	C	N	O	S	0	0	1
			5896	3802	1032	1043	19			

- Molecule 2 is a protein called NRFC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	194	Total	C	N	O	S	0	0	1
			1475	930	256	269	20			
2	F	194	Total	C	N	O	S	0	0	1
			1475	930	256	269	20			

- Molecule 3 is a protein called HYPOTHETICAL MEMBRANE SPANNING PROTEIN.

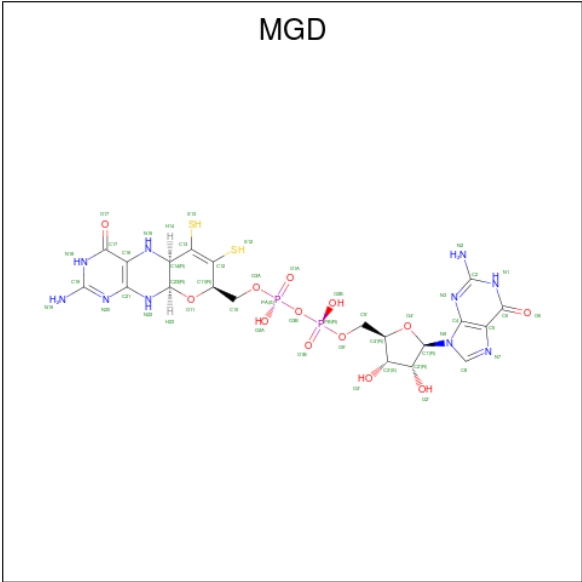
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	251	Total	C	N	O	S	0	0	1
			1948	1323	320	303	2			
3	G	251	Total	C	N	O	S	0	0	1
			1948	1323	320	303	2			

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).

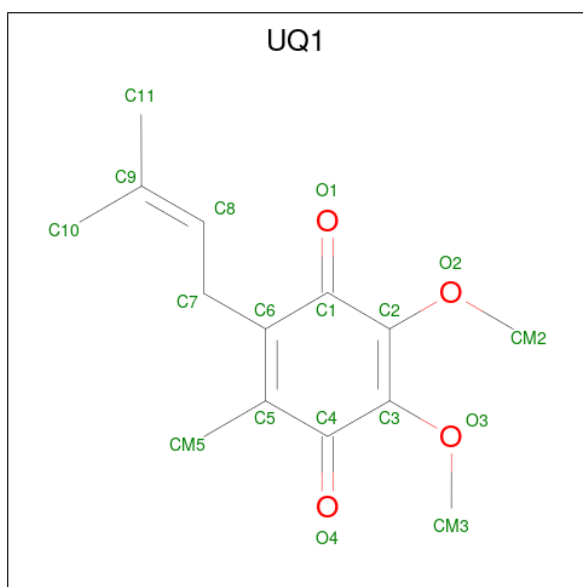


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 6 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mo	0	0
			1	1		
6	E	1	Total	Mo	0	0
			1	1		

- Molecule 7 is UBIQUINONE-1 (CCD ID: UQ1) (formula: C₁₄H₁₈O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			18	14	4		
7	G	1	Total	C	O	0	0
			18	14	4		

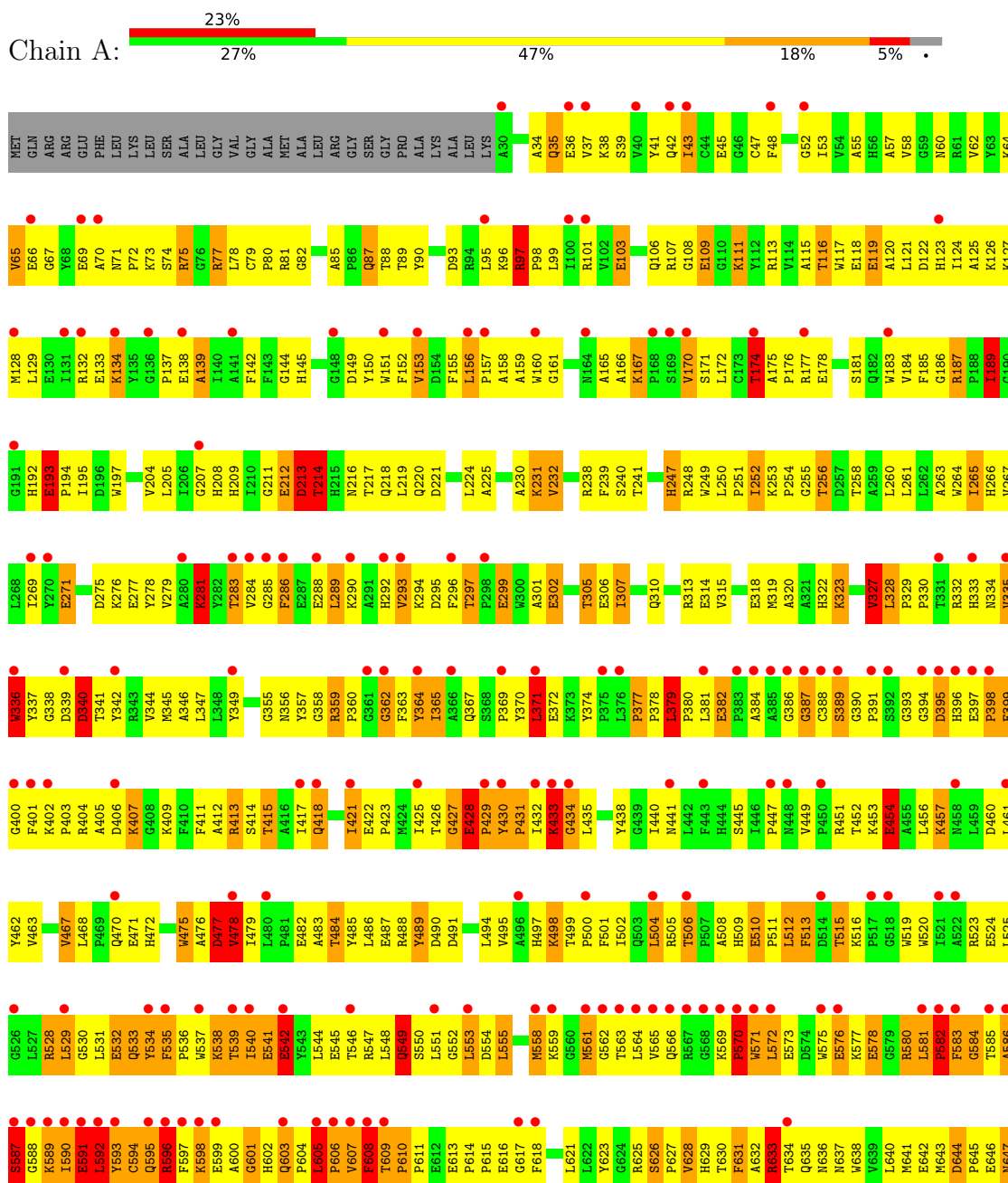
- Molecule 8 is water.

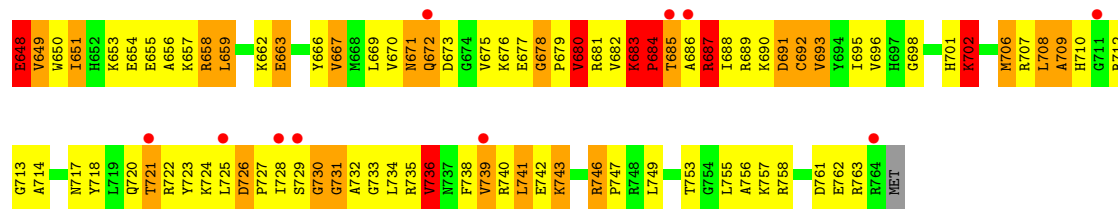
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	387	Total	O	0	0
			387	387		
8	B	149	Total	O	0	0
			149	149		
8	C	90	Total	O	0	0
			90	90		
8	E	452	Total	O	0	0
			452	452		
8	F	130	Total	O	0	0
			130	130		
8	G	77	Total	O	0	0
			77	77		

3 Residue-property plots

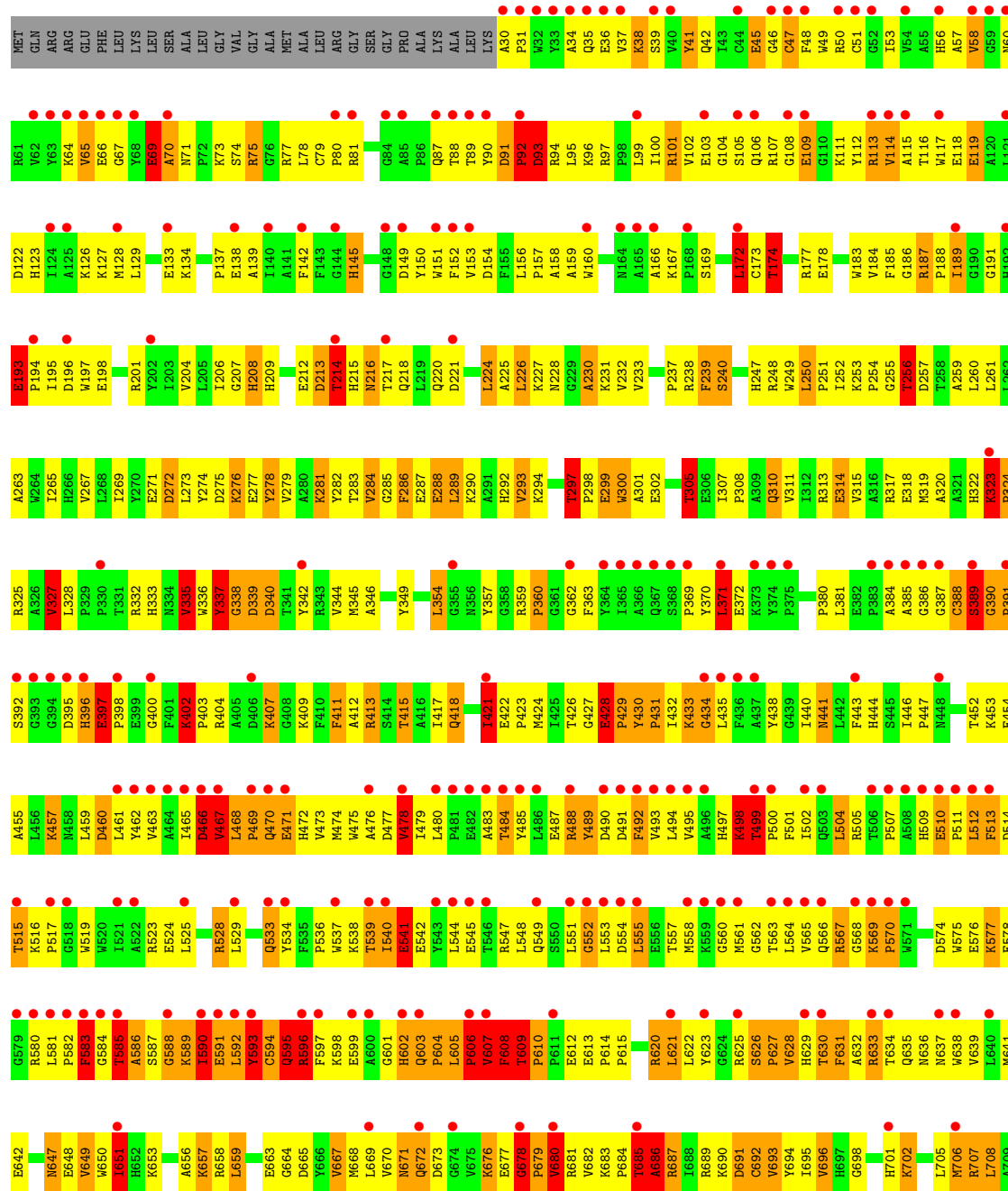
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



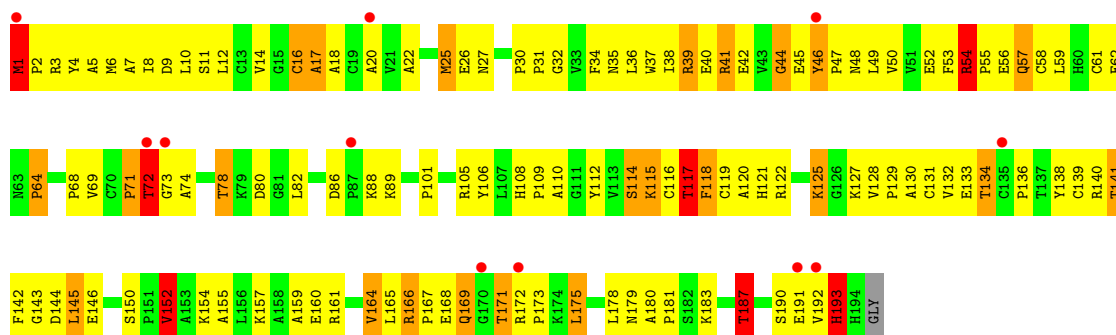


● Molecule 1: THIOSULFATE REDUCTASE

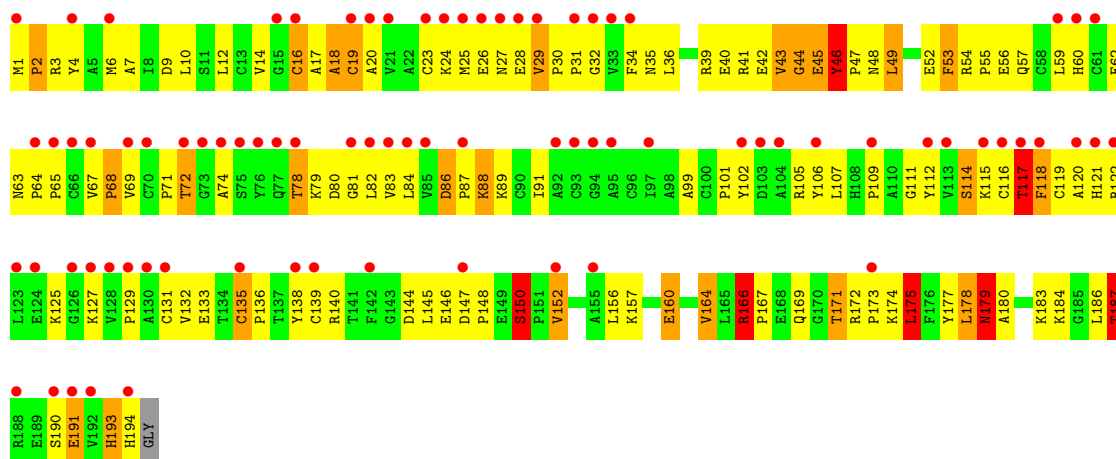




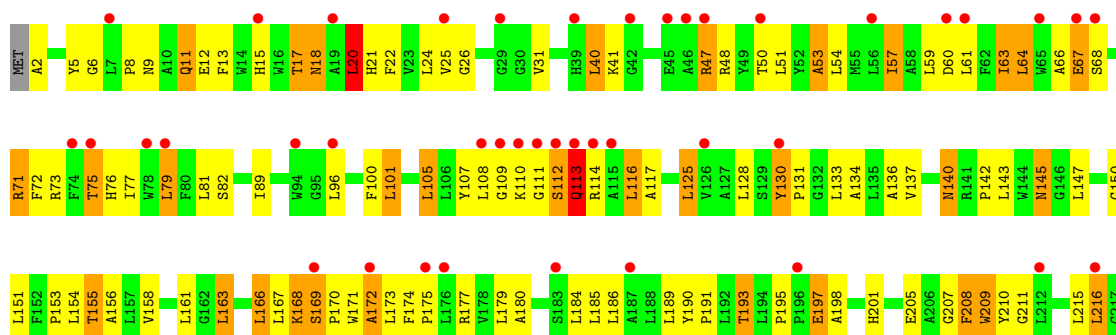
• Molecule 2: NRFC PROTEIN

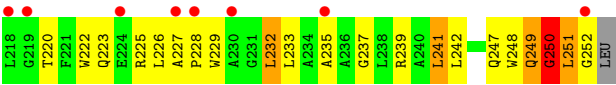


• Molecule 2: NRFC PROTEIN

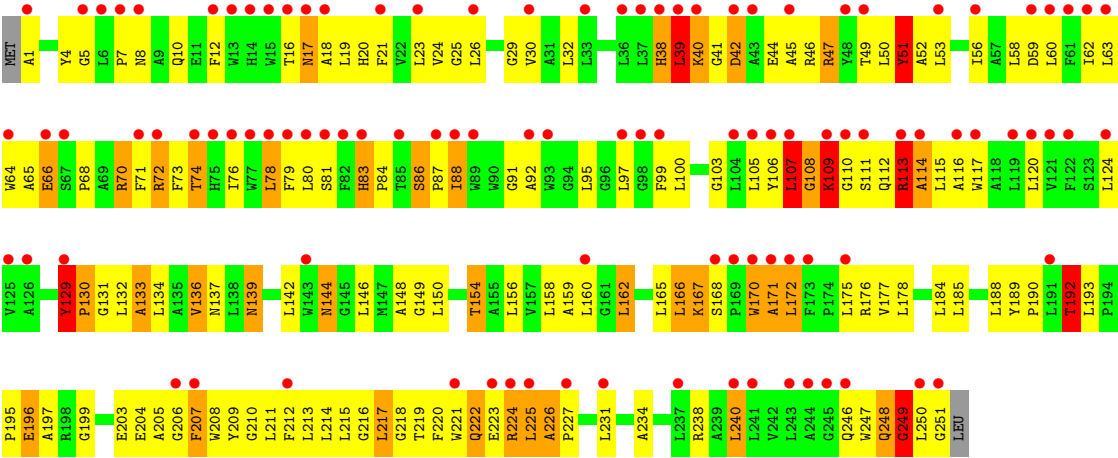


• Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN





● Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.59Å 161.16Å 239.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.10 40.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.00-3.10) 99.2 (40.00-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.301 , 0.314 0.293 , 0.291	Depositor DCC
R_{free} test set	1642 reflections (2.04%)	wwPDB-VP
Wilson B-factor (Å ²)	75.2	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 97.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	20229	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: MO, UQ1, MGD, SF4

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	1.01	3/6079 (0.0%)	1.58	128/8267 (1.5%)
1	E	1.16	17/6079 (0.3%)	1.73	167/8267 (2.0%)
2	B	1.18	1/1512 (0.1%)	1.63	29/2058 (1.4%)
2	F	1.18	5/1512 (0.3%)	1.75	43/2058 (2.1%)
3	C	0.93	4/2016 (0.2%)	1.33	26/2764 (0.9%)
3	G	0.97	1/2016 (0.0%)	1.55	45/2764 (1.6%)
All	All	1.08	31/19214 (0.2%)	1.62	438/26178 (1.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	592	LEU	CG-CD1	15.83	2.04	1.52
1	E	387	GLY	C-N	-11.44	1.17	1.33
3	C	114	ARG	NE-CZ	9.20	1.43	1.33
1	E	593	TYR	CA-C	-8.97	1.40	1.52
1	A	364	TYR	C-O	-8.82	1.12	1.24
1	E	323	LYS	CA-C	8.72	1.62	1.53
1	E	388	CYS	N-CA	-8.01	1.35	1.46
1	E	594	CYS	C-O	-7.71	1.14	1.24
1	E	685	THR	CA-C	7.63	1.62	1.52
1	E	586	ALA	CA-CB	-7.28	1.44	1.53
3	C	114	ARG	CZ-NH1	7.25	1.42	1.32
3	C	114	ARG	CD-NE	6.62	1.55	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	763	ARG	C-N	-6.45	1.24	1.33
1	E	230	ALA	C-O	-6.18	1.16	1.23
1	A	692	CYS	CA-C	-6.15	1.45	1.52
2	F	193	HIS	C-N	-6.14	1.24	1.33
3	C	251	LEU	C-N	-6.06	1.24	1.33
1	E	323	LYS	C-O	-6.03	1.17	1.24
2	F	43	VAL	CA-CB	-5.88	1.46	1.54
1	E	421	ILE	CA-CB	-5.65	1.46	1.54
2	B	193	HIS	C-N	-5.62	1.25	1.33
1	E	720	GLN	CA-C	-5.49	1.47	1.53
1	A	570	PRO	C-N	-5.45	1.28	1.33
1	E	388	CYS	CA-C	-5.43	1.45	1.52
1	E	323	LYS	C-N	5.30	1.44	1.34
2	F	177	TYR	CA-C	-5.24	1.46	1.52
3	G	109	LYS	C-O	5.19	1.31	1.24
2	F	44	GLY	CA-C	-5.17	1.46	1.52
2	F	135	CYS	CB-SG	5.08	1.98	1.81
1	E	594	CYS	N-CA	-5.08	1.40	1.46
1	E	240	SER	N-CA	-5.03	1.39	1.45

All (438) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	PHE	N-CA-C	22.60	140.98	113.41
2	F	171	THR	N-CA-C	22.29	137.68	111.82
3	G	114	ALA	N-CA-C	-19.80	89.41	114.56
1	E	467	VAL	N-CA-C	17.70	128.94	110.36
1	A	189	ILE	N-CA-C	-17.26	96.96	111.81
2	F	44	GLY	N-CA-C	16.43	135.48	112.81
1	E	323	LYS	C-N-CD	-16.02	85.35	120.60
2	B	169	GLN	N-CA-C	-15.96	88.33	110.35
3	G	225	LEU	N-CA-C	-15.45	91.42	112.12
1	E	189	ILE	N-CA-C	-14.45	96.26	111.58
1	E	582	PRO	N-CA-C	13.90	132.02	113.40
3	C	114	ARG	N-CA-C	-13.24	95.57	113.18
1	E	594	CYS	N-CA-C	13.12	127.83	111.69
1	E	659	LEU	N-CA-C	-12.82	89.98	109.60
2	F	16	CYS	N-CA-C	-12.64	92.68	110.50
1	E	323	LYS	CA-C-N	12.55	157.13	127.00
1	E	323	LYS	C-N-CA	12.55	157.13	127.00
1	A	608	PHE	N-CA-C	-12.41	97.39	112.54
2	B	46	TYR	N-CA-C	11.82	135.93	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	GLU	N-CA-C	-11.81	94.89	110.24
1	E	595	GLN	N-CA-CB	-11.69	91.49	110.42
3	G	18	ALA	N-CA-C	-11.54	99.31	113.50
2	B	72	THR	N-CA-C	-11.40	92.19	109.86
1	E	185	PHE	N-CA-C	-11.35	86.62	110.80
3	G	249	GLY	N-CA-C	11.33	140.04	113.18
3	G	193	LEU	CA-C-N	-10.99	109.06	120.38
3	G	193	LEU	C-N-CA	-10.99	109.06	120.38
1	A	213	ASP	N-CA-C	-10.87	92.62	109.25
1	E	323	LYS	O-C-N	-10.81	110.79	121.27
1	E	585	THR	CB-CA-C	10.75	131.82	110.42
1	E	583	PHE	N-CA-C	10.68	133.54	110.80
2	B	1	MET	CA-C-N	-10.62	106.56	119.84
2	B	1	MET	C-N-CA	-10.62	106.56	119.84
1	E	213	ASP	N-CA-C	-10.59	93.05	109.25
1	E	608	PHE	N-CA-C	-10.50	99.64	111.82
1	A	433	LYS	N-CA-C	-10.50	94.92	110.46
1	E	240	SER	N-CA-CB	-10.50	93.61	110.51
1	A	592	LEU	N-CA-C	10.34	132.83	110.80
1	E	388	CYS	N-CA-C	10.30	132.74	110.80
1	E	665	ASP	N-CA-C	10.26	124.30	110.35
1	A	364	TYR	N-CA-C	10.20	124.99	112.54
1	E	323	LYS	CB-CA-C	10.07	126.07	109.56
1	E	680	VAL	CB-CA-C	-10.02	95.69	110.62
3	G	171	ALA	N-CA-C	9.83	123.01	111.71
1	A	477	ASP	N-CA-C	-9.82	93.35	108.96
1	E	324	PRO	N-CD-CG	-9.79	92.05	103.80
2	F	152	VAL	CB-CA-C	-9.79	99.19	112.02
1	E	421	ILE	N-CA-CB	-9.65	99.44	112.28
1	E	583	PHE	CA-C-N	9.64	128.84	122.18
1	E	583	PHE	C-N-CA	9.64	128.84	122.18
1	E	212	GLU	N-CA-C	-9.55	99.98	112.68
1	E	686	ALA	N-CA-C	9.45	130.93	110.80
1	E	590	ILE	CB-CA-C	-9.37	99.29	110.91
2	F	43	VAL	N-CA-C	-9.27	94.05	107.77
1	E	207	GLY	N-CA-C	-9.21	97.51	111.24
1	E	340	ASP	N-CA-C	9.18	122.27	111.71
2	B	152	VAL	CB-CA-C	-9.13	99.62	112.22
3	G	166	LEU	N-CA-C	-9.07	103.35	112.97
1	E	583	PHE	N-CA-CB	-9.06	95.17	110.49
1	E	685	THR	CA-C-N	9.06	138.85	121.54
1	E	685	THR	C-N-CA	9.06	138.85	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	683	LYS	CA-C-N	9.05	131.16	119.84
1	A	683	LYS	C-N-CA	9.05	131.16	119.84
1	A	736	VAL	N-CA-CB	-9.02	100.62	112.26
3	C	226	LEU	N-CA-C	-8.97	102.47	113.41
2	F	16	CYS	CA-C-N	-8.90	106.77	122.62
2	F	16	CYS	C-N-CA	-8.90	106.77	122.62
3	G	4	TYR	N-CA-C	-8.90	93.90	108.41
1	E	390	GLY	N-CA-C	-8.88	94.23	112.34
2	B	44	GLY	N-CA-C	8.87	122.22	112.29
1	E	736	VAL	N-CA-CB	-8.86	100.49	112.28
1	A	644	ASP	CA-C-N	8.84	129.58	120.04
1	A	644	ASP	C-N-CA	8.84	129.58	120.04
1	E	216	ASN	N-CA-C	8.79	121.75	111.02
2	F	64	PRO	N-CA-C	8.77	121.40	110.70
1	E	593	TYR	CB-CA-C	-8.76	92.99	110.42
3	C	195	PRO	N-CA-C	-8.67	101.31	110.58
1	E	184	VAL	N-CA-C	8.63	120.41	111.00
1	A	691	ASP	CB-CA-C	-8.59	92.36	110.31
1	E	327	VAL	CB-CA-C	-8.55	97.01	110.69
1	E	594	CYS	N-CA-CB	-8.49	97.54	110.20
1	E	288	GLU	N-CA-C	-8.47	102.76	113.43
1	A	591	GLU	N-CA-C	-8.45	102.06	111.28
3	G	248	GLN	N-CA-CB	-8.45	98.93	110.67
1	E	593	TYR	N-CA-C	-8.43	92.85	110.80
1	E	150	TYR	N-CA-C	-8.42	102.19	111.36
1	E	92	PRO	N-CA-C	-8.41	95.14	112.47
1	E	678	GLY	CA-C-N	-8.39	110.77	119.83
1	E	678	GLY	C-N-CA	-8.39	110.77	119.83
1	A	327	VAL	CB-CA-C	-8.38	97.59	110.50
1	E	174	THR	N-CA-C	8.35	123.59	113.23
1	A	193	GLU	CA-C-N	8.34	130.26	119.84
1	A	193	GLU	C-N-CA	8.34	130.26	119.84
2	B	46	TYR	CB-CA-C	-8.26	93.90	110.17
1	A	212	GLU	N-CA-C	-8.25	101.70	112.68
1	A	571	TRP	N-CA-CB	-8.22	98.85	108.96
2	F	43	VAL	CA-C-N	-8.21	114.15	122.69
2	F	43	VAL	C-N-CA	-8.21	114.15	122.69
1	E	278	TYR	N-CA-C	-8.21	102.27	111.14
2	F	29	VAL	CA-C-N	8.18	128.81	120.38
2	F	29	VAL	C-N-CA	8.18	128.81	120.38
3	G	207	PHE	CB-CA-C	-8.17	94.17	110.42
1	A	534	TYR	N-CA-C	-8.10	96.02	109.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	LEU	CA-C-N	-8.09	112.05	120.38
1	A	328	LEU	C-N-CA	-8.09	112.05	120.38
1	A	211	GLY	N-CA-C	-8.06	104.95	113.58
3	G	83	HIS	CA-C-N	8.06	129.92	119.84
3	G	83	HIS	C-N-CA	8.06	129.92	119.84
1	A	628	VAL	N-CA-CB	-8.06	103.34	112.21
1	E	231	LYS	N-CA-CB	-8.05	97.23	110.52
1	A	731	GLY	N-CA-C	8.05	120.78	111.36
1	E	323	LYS	CA-CB-CG	-8.01	98.09	114.10
1	E	409	LYS	N-CA-C	8.00	122.86	113.18
1	A	340	ASP	N-CA-C	7.95	127.73	110.80
2	F	46	TYR	N-CA-C	7.89	127.24	109.81
3	C	6	GLY	N-CA-C	-7.88	97.86	112.37
3	G	131	GLY	N-CA-C	-7.85	94.58	113.18
1	A	427	GLY	N-CA-C	-7.83	104.41	115.30
1	E	592	LEU	N-CA-C	7.82	120.94	109.69
3	G	130	PRO	N-CA-C	-7.80	96.40	112.47
1	E	603	GLN	N-CA-C	7.67	126.76	109.81
1	A	596	ARG	N-CA-C	-7.64	102.52	112.68
2	F	29	VAL	N-CA-C	-7.63	101.47	108.95
1	E	421	ILE	N-CA-C	-7.62	104.93	112.17
1	E	590	ILE	N-CA-CB	7.61	119.01	110.72
3	C	113	GLN	N-CA-C	7.54	126.86	110.80
1	E	606	PRO	N-CA-C	-7.52	96.99	112.47
1	A	467	VAL	CB-CA-C	-7.49	103.57	110.91
1	A	583	PHE	O-C-N	7.43	132.47	122.59
1	A	365	ILE	N-CA-CB	7.42	123.47	111.23
1	A	174	THR	N-CA-C	7.38	122.46	113.38
1	E	354	LEU	N-CA-C	-7.36	103.90	113.17
2	F	175	LEU	N-CA-C	-7.30	96.37	108.34
3	C	116	LEU	N-CA-C	-7.29	104.52	113.41
3	G	168	SER	N-CA-C	-7.28	99.07	109.62
1	A	659	LEU	N-CA-C	-7.27	95.32	110.80
1	A	508	ALA	N-CA-C	-7.25	104.23	113.23
1	E	588	GLY	CA-C-N	-7.23	112.53	122.30
1	E	588	GLY	C-N-CA	-7.23	112.53	122.30
1	A	601	GLY	CA-C-N	-7.21	111.49	122.81
1	A	601	GLY	C-N-CA	-7.21	111.49	122.81
1	E	38	LYS	N-CA-C	-7.21	95.50	108.48
1	E	710	HIS	N-CA-C	7.19	126.12	110.80
1	A	409	LYS	N-CA-C	7.17	121.78	112.89
1	E	281	LYS	N-CA-C	7.11	122.24	113.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	387	GLY	CA-C-N	-7.10	107.98	121.54
1	E	387	GLY	C-N-CA	-7.10	107.98	121.54
1	E	339	ASP	N-CA-C	-7.10	101.77	111.56
1	E	433	LYS	N-CA-C	-7.08	98.69	109.95
1	A	359	ARG	CA-C-N	-7.08	111.53	120.23
1	A	359	ARG	C-N-CA	-7.08	111.53	120.23
3	G	51	TYR	N-CA-C	-7.04	95.81	110.80
2	F	83	VAL	N-CA-C	-7.03	98.30	108.36
1	E	478	VAL	N-CA-C	-7.02	94.73	109.34
1	E	707	ARG	N-CA-C	7.01	119.78	111.71
1	E	335	VAL	N-CA-CB	-7.01	99.67	111.23
1	A	371	LEU	N-CA-C	-6.97	96.14	108.13
1	E	96	LYS	N-CA-C	6.96	122.33	113.55
2	F	160	GLU	N-CA-C	-6.96	103.46	112.23
1	E	214	THR	N-CA-CB	-6.96	99.76	111.17
1	E	402	LYS	CA-C-N	-6.92	113.53	120.31
1	E	402	LYS	C-N-CA	-6.92	113.53	120.31
2	F	14	VAL	N-CA-C	-6.91	106.26	112.90
1	E	466	ASP	CA-C-N	6.90	129.50	120.60
1	E	466	ASP	C-N-CA	6.90	129.50	120.60
1	A	648	GLU	N-CA-CB	-6.87	99.27	110.81
1	E	49	TRP	N-CA-C	-6.87	104.38	112.89
1	E	172	LEU	CA-CB-CG	-6.86	92.30	116.30
1	A	581	LEU	N-CA-C	-6.85	100.30	108.25
1	A	626	SER	N-CA-C	-6.85	99.69	109.62
1	A	219	LEU	N-CA-C	-6.83	103.76	111.14
1	E	297	THR	N-CA-CB	-6.82	101.78	110.03
1	E	400	GLY	N-CA-C	-6.79	97.09	113.18
3	C	8	PRO	N-CA-C	-6.78	101.26	111.57
2	B	16	CYS	N-CA-C	-6.78	96.05	107.99
1	E	385	ALA	N-CA-C	6.77	118.09	108.54
1	E	712	ARG	N-CA-C	6.77	119.97	109.07
2	B	180	ALA	CA-C-N	6.75	126.55	119.05
2	B	180	ALA	C-N-CA	6.75	126.55	119.05
1	E	174	THR	N-CA-CB	-6.74	99.93	110.44
1	E	187	ARG	CA-C-N	6.72	126.89	120.31
1	E	187	ARG	C-N-CA	6.72	126.89	120.31
1	E	731	GLY	N-CA-C	6.71	129.07	113.18
3	C	5	TYR	N-CA-C	-6.70	96.29	108.02
1	A	185	PHE	CA-C-N	-6.66	108.35	121.41
1	A	185	PHE	C-N-CA	-6.66	108.35	121.41
1	E	668	MET	N-CA-C	-6.66	99.36	109.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	324	PRO	CA-N-CD	-6.65	102.19	111.50
1	A	707	ARG	N-CA-C	6.63	119.34	111.71
3	C	136	ALA	N-CA-C	6.62	120.94	112.34
1	E	734	LEU	N-CA-C	6.59	121.07	112.89
2	F	18	ALA	N-CA-C	6.59	118.46	111.28
1	E	335	VAL	CB-CA-C	6.59	122.09	111.29
2	F	152	VAL	N-CA-CB	6.56	118.96	110.57
1	E	710	HIS	CA-C-N	-6.54	108.58	121.41
1	E	710	HIS	C-N-CA	-6.54	108.58	121.41
1	A	513	PHE	CB-CA-C	-6.51	109.07	116.63
2	B	72	THR	N-CA-CB	-6.51	100.04	110.39
3	G	78	LEU	N-CA-C	-6.51	104.27	111.82
1	E	337	TYR	N-CA-C	6.50	124.64	110.80
3	G	170	TRP	N-CA-C	6.50	119.18	111.71
1	A	491	ASP	N-CA-C	-6.48	101.53	110.35
1	E	596	ARG	N-CA-C	-6.48	104.06	112.68
1	A	454	GLU	N-CA-C	-6.44	104.19	111.14
1	A	498	LYS	N-CA-C	-6.43	103.39	111.11
1	E	338	GLY	N-CA-C	6.42	124.23	115.30
1	E	498	LYS	N-CA-C	-6.41	100.86	111.37
1	E	45	GLU	N-CA-C	-6.39	105.35	112.57
1	E	226	LEU	N-CA-C	-6.38	104.40	111.36
1	A	606	PRO	N-CA-C	-6.38	105.88	113.86
1	E	428	GLU	N-CA-C	6.37	123.88	109.81
1	A	271	GLU	N-CA-C	-6.36	105.16	113.17
3	G	72	ARG	N-CA-C	-6.34	105.31	114.12
1	E	593	TYR	N-CA-CB	6.33	121.19	110.49
1	E	47	CYS	N-CA-C	-6.33	99.88	108.24
2	F	187	THR	N-CA-CB	-6.33	100.27	109.83
1	E	492	PHE	N-CA-C	6.32	119.20	110.35
1	E	428	GLU	CA-C-N	-6.31	111.95	119.84
1	E	428	GLU	C-N-CA	-6.31	111.95	119.84
1	A	281	LYS	N-CA-C	6.28	120.94	113.28
1	A	649	VAL	CB-CA-C	-6.26	103.02	111.15
1	E	687	ARG	CB-CG-CD	-6.24	96.94	111.30
1	E	271	GLU	N-CA-C	-6.23	105.32	113.17
1	A	582	PRO	N-CA-C	6.21	125.25	112.47
3	G	107	LEU	N-CA-C	-6.21	104.28	112.72
1	E	34	ALA	CA-C-N	6.17	133.32	121.54
1	E	34	ALA	C-N-CA	6.17	133.32	121.54
1	E	411	PHE	N-CA-C	6.16	118.07	111.36
1	E	706	MET	N-CA-C	-6.15	95.64	107.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	499	THR	CB-CA-C	-6.14	102.85	109.85
1	E	692	CYS	N-CA-C	6.14	118.29	109.14
1	E	152	PHE	N-CA-C	6.13	120.62	113.20
3	G	129	TYR	CA-C-N	-6.13	112.17	119.84
3	G	129	TYR	C-N-CA	-6.13	112.17	119.84
1	A	684	PRO	CA-C-N	-6.12	114.28	122.72
1	A	684	PRO	C-N-CA	-6.12	114.28	122.72
1	A	583	PHE	CA-C-N	6.09	133.36	121.41
1	A	583	PHE	C-N-CA	6.09	133.36	121.41
1	E	324	PRO	N-CA-C	-6.08	96.29	112.10
1	E	276	LYS	N-CA-C	6.08	117.98	111.36
1	A	153	VAL	N-CA-C	6.07	118.02	111.58
1	E	69	GLU	N-CA-C	-6.06	101.95	110.50
1	A	663	GLU	N-CA-C	6.06	121.37	111.37
3	G	219	THR	N-CA-C	-6.05	105.39	112.89
2	F	166	ARG	CB-CA-C	-6.05	106.91	111.20
2	B	108	HIS	N-CA-C	-6.04	101.42	110.24
2	B	169	GLN	CA-C-N	-6.04	109.56	121.41
2	B	169	GLN	C-N-CA	-6.04	109.56	121.41
3	G	42	ASP	N-CA-C	6.04	119.12	110.24
2	F	156	LEU	N-CA-C	-6.02	104.63	111.07
3	C	53	ALA	N-CA-C	-6.02	104.84	111.82
1	E	154	ASP	N-CA-C	6.02	120.62	113.28
1	A	489	TYR	N-CA-C	-6.00	100.51	110.17
1	A	706	MET	N-CA-C	-6.00	96.71	107.98
3	G	177	VAL	N-CA-C	-5.99	105.88	111.45
1	A	265	ILE	N-CA-C	-5.98	104.68	110.42
3	G	70	ARG	N-CA-C	5.98	117.49	110.97
3	G	172	LEU	N-CA-C	5.98	117.47	111.07
3	C	20	LEU	N-CA-C	-5.97	104.69	111.14
1	E	256	THR	N-CA-CB	-5.96	101.62	110.61
1	E	478	VAL	CB-CA-C	5.94	121.04	111.29
1	A	374	TYR	N-CA-C	-5.94	102.17	109.65
1	A	35	GLN	N-CA-C	-5.93	102.54	110.55
3	C	169	SER	CA-C-N	5.91	125.61	119.05
3	C	169	SER	C-N-CA	5.91	125.61	119.05
1	A	150	TYR	N-CA-C	-5.89	104.77	111.07
1	A	583	PHE	N-CA-C	5.89	123.34	110.80
1	E	198	GLU	N-CA-C	5.88	118.48	111.71
1	A	232	VAL	N-CA-C	5.88	116.40	108.17
2	F	179	ASN	N-CA-C	5.87	123.30	110.80
1	E	193	GLU	CA-C-N	5.86	127.16	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	193	GLU	C-N-CA	5.86	127.16	119.84
3	G	162	LEU	N-CA-C	-5.86	104.59	110.97
1	E	214	THR	CB-CA-C	5.82	120.49	111.13
1	E	402	LYS	N-CA-C	5.81	117.21	109.83
1	A	407	LYS	CA-C-N	-5.80	113.48	122.30
1	A	407	LYS	C-N-CA	-5.80	113.48	122.30
1	E	749	LEU	CA-C-N	-5.79	114.30	120.03
1	E	749	LEU	C-N-CA	-5.79	114.30	120.03
1	A	97	ARG	CA-C-N	-5.79	114.30	120.03
1	A	97	ARG	C-N-CA	-5.79	114.30	120.03
3	G	5	GLY	N-CA-C	-5.79	102.35	112.53
2	F	117	THR	N-CA-CB	-5.78	101.68	111.27
3	G	47	ARG	N-CA-C	-5.76	104.90	111.07
2	F	86	ASP	N-CA-C	-5.76	98.32	108.69
3	C	41	LYS	N-CA-C	-5.72	106.06	113.16
3	G	109	LYS	N-CA-C	5.72	118.16	109.63
1	A	749	LEU	CA-C-N	-5.71	114.73	120.21
1	A	749	LEU	C-N-CA	-5.71	114.73	120.21
1	E	690	LYS	CA-C-N	5.71	131.13	121.14
1	E	690	LYS	C-N-CA	5.71	131.13	121.14
2	B	71	PRO	N-CA-C	5.71	121.05	113.40
1	E	460	ASP	N-CA-C	-5.70	105.43	112.90
1	A	98	PRO	CA-N-CD	-5.70	104.02	112.00
1	E	371	LEU	N-CA-C	-5.70	98.53	107.93
1	A	736	VAL	CB-CA-C	5.68	118.25	111.20
1	E	489	TYR	CB-CA-C	-5.68	100.37	109.75
2	F	2	PRO	N-CA-C	-5.68	100.77	112.47
1	A	45	GLU	N-CA-C	-5.68	106.25	112.72
3	G	224	ARG	N-CA-C	-5.66	105.69	113.56
1	E	93	ASP	N-CA-C	5.66	122.85	110.80
1	A	377	PRO	N-CA-C	-5.65	104.54	110.58
2	F	139	CYS	CA-C-N	-5.65	114.24	122.65
2	F	139	CYS	C-N-CA	-5.65	114.24	122.65
3	C	101	LEU	N-CA-C	-5.64	104.51	111.40
3	G	213	LEU	N-CA-C	-5.64	104.52	111.40
1	E	34	ALA	N-CA-C	-5.64	100.59	108.54
2	F	19	CYS	N-CA-C	-5.62	105.07	111.14
2	F	16	CYS	O-C-N	-5.62	116.23	122.86
1	A	364	TYR	CA-C-N	5.62	132.08	121.97
1	A	364	TYR	C-N-CA	5.62	132.08	121.97
1	A	680	VAL	CB-CA-C	-5.61	102.18	110.82
2	F	135	CYS	CA-C-N	5.59	125.25	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	135	CYS	C-N-CA	5.59	125.25	119.05
1	E	305	THR	N-CA-CB	-5.58	101.94	110.26
1	E	757	LYS	N-CA-C	5.56	119.79	112.89
2	F	64	PRO	CA-C-N	-5.56	114.09	119.87
2	F	64	PRO	C-N-CA	-5.56	114.09	119.87
1	A	633	ARG	N-CA-C	5.53	122.57	110.80
2	B	54	ARG	CA-C-N	-5.53	114.02	119.99
2	B	54	ARG	C-N-CA	-5.53	114.02	119.99
3	C	250	GLY	N-CA-C	5.53	126.28	113.18
3	C	168	LYS	N-CA-C	5.52	119.59	112.86
1	A	542	GLU	N-CA-C	-5.51	105.19	111.14
2	B	11	SER	N-CA-C	-5.51	106.06	112.89
1	A	617	GLY	N-CA-C	-5.51	107.76	114.92
1	A	356	ASN	N-CA-C	5.50	119.99	113.28
1	A	307	ILE	N-CA-C	-5.50	101.56	108.05
2	B	4	TYR	N-CA-C	5.49	118.41	110.28
1	A	709	ALA	N-CA-C	-5.49	106.94	113.97
3	G	248	GLN	CA-C-O	5.48	124.84	118.97
1	A	475	TRP	N-CA-C	-5.48	105.39	113.61
1	E	651	ILE	CB-CA-C	-5.48	100.91	110.71
3	C	64	LEU	N-CA-C	-5.47	105.47	111.82
1	A	648	GLU	CB-CA-C	5.45	119.19	109.65
1	E	41	TYR	N-CA-C	-5.45	101.59	110.20
2	B	46	TYR	CA-C-N	5.45	127.15	120.94
2	B	46	TYR	C-N-CA	5.45	127.15	120.94
1	A	476	ALA	N-CA-C	5.44	118.97	110.32
1	E	193	GLU	N-CA-C	5.42	117.29	109.48
1	A	570	PRO	N-CA-C	5.42	123.64	112.47
2	B	134	THR	CB-CA-C	-5.41	101.91	111.05
1	E	67	GLY	N-CA-C	-5.41	104.15	112.85
1	E	431	PRO	N-CA-C	5.40	118.95	110.80
1	E	300	TRP	N-CA-C	-5.40	105.31	111.14
2	B	64	PRO	N-CA-C	5.39	117.28	110.70
2	B	175	LEU	N-CA-C	-5.38	98.44	108.02
3	C	125	LEU	N-CA-C	-5.38	105.85	112.90
1	E	58	VAL	N-CA-C	-5.38	98.16	109.34
1	E	397	GLU	N-CA-C	5.38	121.69	109.81
1	E	446	ILE	CA-C-N	-5.37	115.06	120.21
1	E	446	ILE	C-N-CA	-5.37	115.06	120.21
1	A	479	ILE	N-CA-C	-5.37	100.60	108.11
1	E	191	GLY	N-CA-C	5.36	118.72	112.50
3	C	26	GLY	N-CA-C	-5.36	106.01	112.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	113	ARG	N-CA-C	5.35	122.20	110.80
1	E	739	VAL	N-CA-CB	-5.35	101.92	111.92
2	F	53	PHE	N-CA-C	-5.35	99.81	108.52
1	E	91	ASP	CA-C-N	-5.34	113.17	119.84
1	E	91	ASP	C-N-CA	-5.34	113.17	119.84
1	E	758	ARG	N-CA-C	-5.33	103.01	109.57
1	A	736	VAL	N-CA-C	-5.33	107.78	112.90
1	E	630	THR	CB-CA-C	-5.33	102.26	110.78
2	F	105	ARG	N-CA-C	5.33	118.49	109.76
3	G	133	ALA	N-CA-C	-5.32	106.05	112.54
2	F	4	TYR	N-CA-C	5.32	117.94	109.96
1	A	247	HIS	N-CA-C	-5.32	105.53	112.23
1	A	67	GLY	N-CA-C	-5.31	104.05	112.66
1	A	411	PHE	N-CA-C	5.31	116.87	111.14
1	E	239	PHE	CB-CA-C	-5.30	102.09	111.05
1	E	407	LYS	CA-C-N	-5.30	113.29	122.83
1	E	407	LYS	C-N-CA	-5.30	113.29	122.83
1	A	726	ASP	N-CA-C	-5.29	101.59	109.42
1	A	576	GLU	N-CA-C	5.28	117.03	111.28
3	C	237	GLY	N-CA-C	-5.27	106.40	112.73
1	E	75	ARG	CB-CG-CD	-5.27	99.18	111.30
1	E	185	PHE	CA-C-N	-5.27	111.08	121.41
1	E	185	PHE	C-N-CA	-5.27	111.08	121.41
1	A	590	ILE	N-CA-C	5.27	115.48	110.42
1	E	215	HIS	N-CA-C	-5.26	102.26	110.10
1	E	294	LYS	N-CA-C	5.26	117.69	111.33
1	A	149	ASP	N-CA-C	-5.25	106.83	113.18
1	E	685	THR	N-CA-CB	-5.24	101.63	110.49
1	A	572	LEU	N-CA-C	-5.24	107.02	113.41
3	G	248	GLN	O-C-N	5.24	128.82	122.48
1	E	467	VAL	N-CA-CB	-5.23	104.70	110.51
1	A	583	PHE	CB-CA-C	-5.23	100.01	110.42
1	A	75	ARG	CB-CA-C	-5.22	104.18	111.80
1	A	506	THR	CA-C-N	-5.20	114.42	119.78
1	A	506	THR	C-N-CA	-5.20	114.42	119.78
2	B	57	GLN	CA-CB-CG	-5.20	103.69	114.10
1	A	614	PRO	CA-C-N	-5.20	114.88	120.03
1	A	614	PRO	C-N-CA	-5.20	114.88	120.03
1	A	379	LEU	CA-C-N	-5.17	113.37	119.84
1	A	379	LEU	C-N-CA	-5.17	113.37	119.84
3	G	217	LEU	N-CA-C	-5.16	107.05	113.19
2	F	111	GLY	N-CA-C	5.16	123.53	114.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ASN	N-CA-C	5.16	119.11	112.41
3	G	25	GLY	N-CA-C	-5.15	100.97	113.18
1	A	34	ALA	N-CA-C	-5.15	107.16	113.50
3	C	47	ARG	N-CA-C	5.14	118.01	111.69
2	B	171	THR	N-CA-C	5.13	119.39	113.18
1	A	214	THR	N-CA-CB	-5.13	103.39	111.39
1	A	139	ALA	N-CA-C	-5.12	106.88	113.02
2	B	187	THR	N-CA-CB	-5.11	102.45	109.97
1	E	35	GLN	CA-C-N	5.10	128.01	120.82
1	E	35	GLN	C-N-CA	5.10	128.01	120.82
1	A	294	LYS	N-CA-C	5.10	117.23	111.11
1	A	549	GLN	N-CA-C	-5.10	105.41	110.97
1	A	336	TRP	N-CA-C	5.09	121.65	110.80
1	E	105	SER	CA-C-N	5.09	127.94	120.71
1	E	105	SER	C-N-CA	5.09	127.94	120.71
1	A	566	GLN	CA-C-N	-5.08	114.57	122.09
1	A	566	GLN	C-N-CA	-5.08	114.57	122.09
3	G	226	ALA	CA-C-N	-5.08	113.69	119.28
3	G	226	ALA	C-N-CA	-5.08	113.69	119.28
1	A	746	ARG	N-CA-C	-5.08	103.19	109.64
3	C	166	LEU	N-CA-C	-5.07	105.84	112.23
2	B	117	THR	N-CA-CB	-5.07	102.96	110.61
3	G	192	THR	N-CA-CB	-5.06	103.00	110.53
1	A	658	ARG	N-CA-C	-5.05	105.68	111.14
3	C	134	ALA	N-CA-C	-5.05	105.96	111.82
3	G	7	PRO	N-CA-C	-5.05	103.35	111.38
1	E	184	VAL	CB-CA-C	-5.05	105.47	112.24
3	G	86	SER	N-CA-C	5.04	118.48	108.59
1	E	541	GLU	N-CA-C	-5.04	105.86	111.36
1	A	692	CYS	N-CA-C	5.04	117.06	109.41
3	C	209	TRP	N-CA-C	-5.03	105.50	111.69
2	F	186	LEU	CA-C-N	5.03	127.85	120.71
2	F	186	LEU	C-N-CA	5.03	127.85	120.71
3	C	113	GLN	CB-CA-C	-5.02	100.42	110.42
1	E	679	PRO	N-CA-C	5.02	118.76	111.03
1	A	690	LYS	CA-C-N	5.02	129.10	120.72
1	A	690	LYS	C-N-CA	5.02	129.10	120.72
1	E	430	TYR	N-CA-C	-5.01	103.71	108.22
2	F	150	SER	CA-C-N	-5.01	113.87	119.19
2	F	150	SER	C-N-CA	-5.01	113.87	119.19
1	A	702	LYS	N-CA-C	-5.01	96.67	107.49

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	323	LYS	Mainchain

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	5896	0	5814	830	3
1	E	5896	0	5815	786	3
2	B	1475	0	1453	185	0
2	F	1475	0	1453	159	0
3	C	1948	0	2001	180	0
3	G	1948	0	2004	208	0
4	A	8	0	0	2	0
4	B	32	0	0	8	0
4	E	8	0	0	1	0
4	F	32	0	0	6	0
5	A	94	0	43	12	0
5	E	94	0	43	23	0
6	A	1	0	0	0	0
6	E	1	0	0	1	0
7	C	18	0	18	26	0
7	G	18	0	18	22	0
8	A	387	0	0	104	0
8	B	149	0	0	41	0
8	C	90	0	0	11	0
8	E	452	0	0	141	0
8	F	130	0	0	31	0
8	G	77	0	0	35	0
All	All	20229	0	18662	2296	3

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 61.

All (2296) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:HIS:CE1	1:A:606:PRO:HG3	1.48	1.46
3:G:78:LEU:HD21	7:G:1251:UQ1:C7	1.49	1.43
1:E:592:LEU:HA	1:E:603:GLN:NE2	1.19	1.41
1:A:186:GLY:HA3	1:A:583:PHE:C	1.40	1.41
1:E:605:LEU:H	1:E:605:LEU:CD2	1.30	1.39
1:A:591:GLU:OE2	1:A:604:PRO:HG3	1.22	1.36
1:A:184:VAL:CG2	1:A:592:LEU:HD23	1.58	1.33
1:E:388:CYS:HB2	1:E:593:TYR:OH	1.30	1.27
2:B:41:ARG:HH11	2:B:187:THR:CG2	1.47	1.27
1:A:582:PRO:HB2	8:A:2093:HOH:O	1.27	1.27
2:B:46:TYR:HB2	8:B:2034:HOH:O	1.34	1.27
1:A:604:PRO:O	1:A:606:PRO:HD2	1.33	1.25
1:E:602:HIS:CE1	1:E:606:PRO:HG3	1.70	1.24
2:F:57:GLN:NE2	2:F:140:ARG:HH22	1.34	1.23
3:G:207:PHE:CE2	3:G:211:LEU:HD13	1.71	1.23
1:A:97:ARG:HH21	1:A:763:ARG:NH2	1.36	1.23
1:A:601:GLY:HA2	8:A:2281:HOH:O	1.06	1.23
1:E:591:GLU:OE1	1:E:604:PRO:HB3	1.30	1.22
1:E:592:LEU:CA	1:E:603:GLN:HE21	1.49	1.22
3:C:171:TRP:O	3:C:171:TRP:CE3	1.95	1.20
1:E:605:LEU:HD23	1:E:605:LEU:N	1.40	1.19
1:A:583:PHE:CE2	1:A:588:GLY:N	2.10	1.19
1:A:337:TYR:O	1:A:340:ASP:OD2	1.57	1.19
1:A:395:ASP:O	1:A:399:GLU:HB2	1.39	1.19
1:E:477:ASP:O	1:E:478:VAL:HG23	1.35	1.18
1:E:116:THR:HG22	1:E:119:GLU:HB3	1.19	1.17
1:E:36:GLU:O	1:E:58:VAL:CG2	1.93	1.17
1:A:288:GLU:HB3	1:A:591:GLU:HG3	1.27	1.17
1:A:395:ASP:HA	1:A:399:GLU:CG	1.74	1.16
1:E:602:HIS:CD2	1:E:604:PRO:HD2	1.78	1.16
1:A:42:GLN:O	1:A:53:ILE:HG13	1.45	1.15
2:F:57:GLN:HE22	2:F:140:ARG:NH2	1.43	1.15
1:A:77:ARG:NH1	2:B:138:TYR:HE2	1.43	1.14
1:A:284:VAL:O	1:A:590:ILE:HG22	1.44	1.14
1:E:36:GLU:O	1:E:58:VAL:HG22	0.98	1.14
1:E:323:LYS:HD3	1:E:354:LEU:CA	1.77	1.14
1:A:584:GLY:HA2	8:A:2274:HOH:O	0.98	1.14
1:A:428:GLU:HB3	1:A:429:PRO:HD2	1.29	1.14
1:A:97:ARG:NH2	1:A:763:ARG:HH22	1.44	1.13
3:G:1:ALA:HB1	8:G:2001:HOH:O	1.48	1.13
1:E:477:ASP:O	1:E:478:VAL:CG2	1.96	1.13
1:E:511:PRO:HB3	1:E:515:THR:HG22	1.30	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:78:LEU:HD21	7:G:1251:UQ1:C8	1.79	1.12
1:A:184:VAL:HG23	1:A:592:LEU:CD2	1.80	1.12
1:E:339:ASP:HB2	1:E:607:VAL:HG11	1.30	1.11
1:E:602:HIS:NE2	1:E:604:PRO:HD2	1.65	1.11
1:E:607:VAL:O	1:E:607:VAL:HG12	1.45	1.11
3:G:78:LEU:HD21	7:G:1251:UQ1:H71	1.28	1.11
1:E:591:GLU:CD	1:E:604:PRO:HB3	1.76	1.10
1:E:592:LEU:CA	1:E:603:GLN:NE2	2.11	1.10
1:A:604:PRO:O	1:A:606:PRO:CD	2.00	1.10
1:E:97:ARG:HG3	8:E:2028:HOH:O	1.50	1.09
1:A:397:GLU:HB3	1:A:398:PRO:HD3	1.12	1.09
2:B:134:THR:O	2:B:134:THR:HG23	1.51	1.09
1:E:562:GLY:O	8:E:2314:HOH:O	1.66	1.09
3:G:154:THR:CG2	3:G:238:ARG:HE	1.66	1.09
1:A:69:GLU:O	8:A:2032:HOH:O	1.69	1.09
1:E:607:VAL:O	1:E:607:VAL:CG1	1.98	1.08
1:E:592:LEU:HD23	1:E:603:GLN:HE22	1.19	1.08
1:E:763:ARG:HG2	8:E:2441:HOH:O	1.53	1.08
1:E:116:THR:CG2	1:E:119:GLU:H	1.66	1.08
1:A:632:ALA:O	1:A:635:GLN:HG2	1.54	1.08
2:B:41:ARG:HD2	2:B:187:THR:CG2	1.83	1.08
1:E:602:HIS:HE1	1:E:606:PRO:CG	1.67	1.08
1:A:395:ASP:CA	1:A:399:GLU:HG3	1.81	1.07
1:E:591:GLU:OE1	1:E:604:PRO:CB	2.02	1.07
1:A:279:VAL:HG13	1:A:283:THR:HG21	1.33	1.07
3:C:22:PHE:O	3:C:239:ARG:NH1	1.86	1.07
1:E:47:CYS:HB2	8:E:2450:HOH:O	1.52	1.07
1:A:467:VAL:HB	8:A:2226:HOH:O	1.54	1.07
1:A:591:GLU:OE2	1:A:604:PRO:CG	2.02	1.07
2:F:57:GLN:NE2	2:F:140:ARG:NH2	2.01	1.07
1:A:43:ILE:HG13	1:A:505:ARG:HB3	1.14	1.06
1:E:95:LEU:HD12	1:E:466:ASP:O	1.53	1.06
1:E:626:SER:HB2	8:E:2347:HOH:O	1.54	1.06
1:A:592:LEU:O	1:A:593:TYR:HB2	1.52	1.06
1:E:605:LEU:CD2	1:E:605:LEU:N	1.92	1.06
1:E:230:ALA:O	8:E:2138:HOH:O	1.71	1.06
1:E:653:LYS:HD2	1:E:686:ALA:HB2	1.34	1.06
1:A:685:THR:HB	2:B:42:GLU:OE2	1.56	1.05
2:B:134:THR:O	2:B:134:THR:CG2	1.99	1.05
3:C:17:THR:CG2	3:C:67:GLU:HG3	1.85	1.05
1:A:172:LEU:HD13	1:A:445:SER:O	1.56	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLY:HA3	1:A:583:PHE:O	1.57	1.05
1:E:342:TYR:CD1	1:E:607:VAL:HB	1.91	1.05
1:E:413:ARG:HD3	8:E:2248:HOH:O	1.57	1.05
1:E:429:PRO:HD2	8:E:2257:HOH:O	1.54	1.05
3:G:38:HIS:HD2	3:G:45:ALA:HB1	1.15	1.05
1:A:186:GLY:CA	1:A:583:PHE:C	2.29	1.04
1:A:165:ALA:O	1:A:415:THR:HG21	1.55	1.04
1:A:651:ILE:HD11	1:A:682:VAL:HG13	1.39	1.04
1:A:602:HIS:CE1	1:A:606:PRO:CG	2.40	1.04
2:B:41:ARG:HH11	2:B:187:THR:HG22	1.17	1.04
1:E:224:LEU:HD12	8:E:2132:HOH:O	1.56	1.04
1:A:170:VAL:O	1:A:175:ALA:HB2	1.56	1.03
2:B:46:TYR:CD1	8:B:2034:HOH:O	2.10	1.03
2:B:41:ARG:HD2	2:B:187:THR:HG21	1.32	1.03
1:E:598:LYS:HD2	8:E:2330:HOH:O	1.58	1.03
2:F:41:ARG:HD2	2:F:187:THR:CG2	1.89	1.02
2:B:25:MET:HE2	2:B:25:MET:HA	1.41	1.02
1:A:116:THR:HG22	1:A:119:GLU:H	1.17	1.02
3:G:221:TRP:HE3	3:G:225:LEU:HD22	1.19	1.01
3:C:155:THR:HG22	3:C:239:ARG:HE	1.24	1.01
3:C:171:TRP:O	3:C:171:TRP:CD2	2.14	1.01
1:E:424:MET:HE2	1:E:455:ALA:HB1	1.43	1.01
1:A:583:PHE:HE2	1:A:588:GLY:N	1.53	1.00
1:A:763:ARG:HG2	8:A:2379:HOH:O	1.58	1.00
1:A:632:ALA:O	1:A:635:GLN:CG	2.09	1.00
1:A:591:GLU:HB3	1:A:603:GLN:NE2	1.77	0.99
1:E:533:GLN:HE21	1:E:533:GLN:H	1.07	0.99
1:A:591:GLU:CD	1:A:604:PRO:HG3	1.87	0.99
1:A:603:GLN:HB3	1:A:604:PRO:HD3	1.38	0.99
3:G:221:TRP:CE3	3:G:225:LEU:HD22	1.98	0.99
3:G:38:HIS:CD2	3:G:45:ALA:HB1	1.97	0.99
2:B:192:VAL:HG21	8:B:2017:HOH:O	1.63	0.99
1:A:116:THR:CG2	1:A:119:GLU:H	1.74	0.99
1:A:531:LEU:O	1:A:534:TYR:O	1.80	0.98
1:A:580:ARG:CB	1:A:580:ARG:HH11	1.77	0.98
1:A:729:SER:O	1:A:731:GLY:N	1.96	0.98
1:A:42:GLN:O	1:A:53:ILE:CG1	2.11	0.98
2:B:72:THR:HG22	2:B:74:ALA:H	1.22	0.98
1:E:764:ARG:N	8:E:2445:HOH:O	1.96	0.98
1:A:434:GLY:HA2	1:A:461:LEU:O	1.62	0.98
1:E:349:TYR:OH	1:E:591:GLU:HA	1.63	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:41:ARG:HD2	2:F:187:THR:HG23	1.41	0.98
1:E:92:PRO:O	1:E:94:ARG:N	1.95	0.98
1:A:569:LYS:O	8:A:2269:HOH:O	1.82	0.98
1:E:635:GLN:O	1:E:641:MET:HG3	1.64	0.97
1:A:335:VAL:O	1:A:733:GLY:HA2	1.64	0.97
3:G:111:SER:HB3	8:G:2032:HOH:O	1.62	0.97
1:A:585:THR:O	1:A:586:ALA:HB3	1.64	0.97
3:G:207:PHE:HE2	3:G:211:LEU:HD13	1.09	0.97
2:B:46:TYR:CE2	8:B:2031:HOH:O	2.17	0.97
3:C:207:GLY:O	3:C:210:TYR:N	1.97	0.97
1:A:360:PRO:HD3	1:A:571:TRP:CE3	1.99	0.96
1:A:680:VAL:HG11	8:A:2311:HOH:O	1.64	0.96
2:B:160:GLU:H	2:B:179:ASN:HD21	1.06	0.96
1:E:323:LYS:CD	1:E:354:LEU:HA	1.94	0.96
1:E:551:LEU:O	1:E:553:LEU:N	1.98	0.96
1:E:608:PHE:O	8:E:2335:HOH:O	1.82	0.96
1:A:284:VAL:HG23	1:A:587:SER:HB3	1.47	0.96
1:E:323:LYS:HD3	1:E:354:LEU:HA	0.97	0.96
2:F:41:ARG:HH11	2:F:187:THR:CG2	1.79	0.96
2:F:46:TYR:HB3	8:F:2034:HOH:O	1.64	0.96
1:E:428:GLU:O	1:E:430:TYR:N	1.97	0.96
1:E:209:HIS:HE1	1:E:625:ARG:H	1.12	0.96
1:E:635:GLN:O	1:E:641:MET:CG	2.13	0.96
1:A:314:GLU:O	1:A:318:GLU:HG3	1.65	0.95
1:E:112:TYR:OH	1:E:474:MET:O	1.84	0.95
1:E:397:GLU:HB3	1:E:398:PRO:HD3	1.48	0.95
1:E:606:PRO:O	1:E:608:PHE:N	1.98	0.95
3:G:206:GLY:O	3:G:209:TYR:N	1.99	0.95
1:E:116:THR:HG23	1:E:119:GLU:H	1.30	0.95
2:F:2:PRO:HD2	2:F:80:ASP:OD2	1.67	0.94
1:A:345:MET:HE2	1:A:605:LEU:HD22	1.46	0.94
1:A:599:GLU:O	8:A:2280:HOH:O	1.85	0.94
1:E:324:PRO:HD3	8:E:2167:HOH:O	1.66	0.94
1:A:763:ARG:HB2	8:A:2382:HOH:O	1.66	0.94
1:E:297:THR:HG22	1:E:300:TRP:H	1.31	0.94
1:A:349:TYR:OH	1:A:591:GLU:O	1.86	0.93
1:A:183:TRP:CH2	1:A:596:ARG:HD3	2.01	0.93
3:C:140:ASN:HD22	3:C:140:ASN:H	1.16	0.93
1:A:276:LYS:HA	8:A:2148:HOH:O	1.68	0.93
1:E:569:LYS:HD2	8:E:2320:HOH:O	1.66	0.93
1:A:629:HIS:ND1	1:A:634:THR:HG23	1.82	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:LEU:CD1	1:E:466:ASP:O	2.16	0.93
3:C:17:THR:HG21	3:C:67:GLU:HG3	1.49	0.93
1:A:395:ASP:HA	1:A:399:GLU:HG3	0.93	0.93
1:A:397:GLU:HB3	1:A:398:PRO:CD	1.99	0.93
3:G:20:HIS:ND1	3:G:59:ASP:OD2	2.00	0.93
1:A:42:GLN:NE2	1:A:505:ARG:HD3	1.83	0.92
1:E:493:VAL:HG13	8:E:2013:HOH:O	1.68	0.92
2:B:25:MET:HA	2:B:25:MET:CE	2.00	0.92
2:B:41:ARG:NH1	2:B:187:THR:CG2	2.32	0.92
2:B:16:CYS:O	2:B:16:CYS:SG	2.27	0.92
1:A:604:PRO:C	1:A:606:PRO:CD	2.43	0.92
3:C:108:LEU:O	3:C:110:LYS:HG2	1.68	0.92
1:A:42:GLN:NE2	1:A:485:TYR:O	2.03	0.92
1:A:335:VAL:CG1	1:A:732:ALA:O	2.18	0.92
1:A:519:TRP:CE2	1:A:540:ILE:HG12	2.05	0.92
2:B:159:ALA:O	2:F:183:LYS:HE2	1.70	0.92
3:G:129:TYR:OH	7:G:1251:UQ1:O4	1.88	0.92
3:G:139:ASN:H	3:G:139:ASN:HD22	1.17	0.92
1:E:604:PRO:O	1:E:606:PRO:HD3	1.69	0.91
3:G:206:GLY:O	3:G:210:GLY:N	2.01	0.91
1:A:97:ARG:NH2	1:A:763:ARG:NH2	2.08	0.91
1:E:301:ALA:O	1:E:305:THR:HB	1.71	0.91
3:C:128:LEU:HB3	8:C:2063:HOH:O	1.68	0.91
1:E:428:GLU:O	1:E:429:PRO:C	2.08	0.91
1:E:602:HIS:HE1	1:E:606:PRO:HG3	0.78	0.91
1:E:614:PRO:HG2	8:E:2341:HOH:O	1.70	0.91
1:A:608:PHE:CD1	1:A:608:PHE:O	2.23	0.91
3:C:53:ALA:O	3:C:57:ILE:HG13	1.70	0.91
1:E:305:THR:HG22	1:E:307:ILE:H	1.35	0.91
1:A:607:VAL:HG12	1:A:607:VAL:O	1.71	0.90
2:F:47:PRO:HD2	8:F:2034:HOH:O	1.69	0.90
1:E:494:LEU:HD22	1:E:502:ILE:HG12	1.54	0.90
1:E:116:THR:CG2	1:E:119:GLU:HB3	2.01	0.90
1:E:388:CYS:SG	1:E:413:ARG:NE	2.44	0.90
1:A:397:GLU:CB	1:A:398:PRO:HD3	2.02	0.90
1:A:602:HIS:ND1	1:A:606:PRO:HG3	1.86	0.90
1:E:590:ILE:HG13	8:E:2178:HOH:O	1.72	0.90
1:A:653:LYS:HG3	1:A:684:PRO:O	1.72	0.90
1:A:186:GLY:HA3	1:A:584:GLY:N	1.87	0.90
2:F:65:PRO:HD2	4:F:1196:SF4:S4	2.11	0.90
2:F:160:GLU:H	2:F:179:ASN:HD21	1.10	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:ALA:HA	3:C:175:PRO:HG2	1.54	0.89
3:G:154:THR:HG22	3:G:238:ARG:HE	1.35	0.89
1:A:413:ARG:CD	1:A:413:ARG:H	1.86	0.89
1:E:305:THR:CG2	1:E:307:ILE:H	1.85	0.89
1:E:648:GLU:HG2	1:E:681:ARG:HH12	1.36	0.89
2:F:72:THR:HG22	2:F:74:ALA:H	1.36	0.89
1:A:97:ARG:HH21	1:A:763:ARG:HH22	0.93	0.89
1:E:510:GLU:HG3	8:E:2299:HOH:O	1.71	0.89
1:A:93:ASP:OD1	1:A:758:ARG:NH2	2.04	0.89
1:A:256:THR:HG21	1:A:305:THR:HA	1.55	0.89
1:A:400:GLY:HA3	8:A:2192:HOH:O	1.73	0.89
1:E:116:THR:HG22	1:E:119:GLU:CB	2.01	0.89
1:E:608:PHE:O	1:E:608:PHE:CD1	2.26	0.89
2:B:146:GLU:HG2	8:B:2110:HOH:O	1.73	0.88
1:A:607:VAL:HG13	1:A:609:THR:OG1	1.72	0.88
1:E:81:ARG:HG2	1:E:628:VAL:O	1.73	0.88
1:A:207:GLY:O	5:A:1766:MGD:O5'	1.92	0.88
3:C:168:LYS:HE2	8:C:2065:HOH:O	1.72	0.88
7:C:1252:UQ1:HM32	7:C:1252:UQ1:O2	1.74	0.88
3:G:78:LEU:CD2	7:G:1251:UQ1:C8	2.52	0.88
1:A:602:HIS:HE1	1:A:606:PRO:HG3	1.07	0.88
1:A:183:TRP:HE1	1:A:413:ARG:HH22	1.22	0.88
1:A:183:TRP:HH2	1:A:596:ARG:HD3	1.36	0.87
3:C:64:LEU:HB3	7:C:1252:UQ1:H113	1.53	0.87
2:B:117:THR:HG21	8:B:2095:HOH:O	1.75	0.87
1:A:672:GLN:NE2	1:A:738:PHE:H	1.73	0.87
1:E:256:THR:HG21	1:E:305:THR:HA	1.55	0.87
1:E:488:ARG:HD3	1:E:490:ASP:OD2	1.74	0.87
2:B:41:ARG:NH1	2:B:187:THR:HG22	1.89	0.87
1:A:116:THR:HG22	1:A:119:GLU:HB3	1.54	0.87
1:A:209:HIS:HE1	1:A:625:ARG:H	1.23	0.87
1:E:685:THR:HG22	2:F:42:GLU:CD	1.99	0.87
3:C:155:THR:CG2	3:C:239:ARG:HE	1.88	0.87
3:G:78:LEU:CD2	7:G:1251:UQ1:C7	2.46	0.87
1:A:580:ARG:HH11	1:A:580:ARG:HB3	1.38	0.86
2:F:146:GLU:HG2	8:F:2003:HOH:O	1.73	0.86
1:A:153:VAL:HG11	1:A:167:LYS:HE2	1.57	0.86
3:G:196:GLU:HG2	8:G:2055:HOH:O	1.72	0.86
1:A:75:ARG:HD2	1:A:220:GLN:HE22	1.37	0.86
1:A:335:VAL:HG11	1:A:732:ALA:O	1.73	0.86
7:G:1251:UQ1:O2	7:G:1251:UQ1:HM32	1.74	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:THR:HG22	8:E:2179:HOH:O	1.73	0.86
1:A:591:GLU:HB3	1:A:603:GLN:HE22	1.37	0.86
1:E:629:HIS:ND1	1:E:634:THR:HG23	1.90	0.86
1:A:591:GLU:O	1:A:592:LEU:HD12	1.75	0.86
2:B:46:TYR:HD1	8:B:2034:HOH:O	1.48	0.86
2:B:57:GLN:HE22	2:B:140:ARG:HH22	1.21	0.86
1:A:77:ARG:NH1	2:B:138:TYR:CE2	2.28	0.86
1:E:498:LYS:HE2	8:E:2119:HOH:O	1.76	0.86
1:E:342:TYR:HD1	1:E:607:VAL:HB	1.36	0.86
2:B:160:GLU:H	2:B:179:ASN:ND2	1.72	0.86
1:A:651:ILE:HD11	1:A:682:VAL:CG1	2.06	0.85
1:A:601:GLY:CA	8:A:2281:HOH:O	1.73	0.85
1:E:592:LEU:CD2	1:E:603:GLN:HE22	1.89	0.85
1:A:393:GLY:HA3	1:A:407:LYS:CE	2.07	0.85
1:E:562:GLY:C	8:E:2314:HOH:O	2.09	0.85
2:F:117:THR:HG23	2:F:120:ALA:H	1.41	0.85
3:G:111:SER:O	3:G:115:LEU:HD12	1.76	0.85
1:A:184:VAL:HG23	1:A:592:LEU:HD23	0.86	0.85
1:A:629:HIS:HA	1:A:634:THR:HG21	1.58	0.85
8:B:2145:HOH:O	3:C:251:LEU:HD11	1.75	0.85
1:E:89:THR:OG1	1:E:484:THR:HG21	1.77	0.85
1:E:308:PRO:HB2	8:E:2195:HOH:O	1.77	0.85
1:A:604:PRO:C	1:A:606:PRO:HD3	2.01	0.85
1:A:48:PHE:CE1	1:A:145:HIS:CE1	2.65	0.84
1:A:605:LEU:H	1:A:605:LEU:CD2	1.90	0.84
1:E:277:GLU:O	1:E:281:LYS:HG2	1.76	0.84
1:A:342:TYR:CD1	1:A:607:VAL:HB	2.13	0.84
1:A:647:ASN:C	1:A:648:GLU:HG3	2.00	0.84
1:A:186:GLY:CA	1:A:583:PHE:O	2.26	0.84
1:A:390:GLY:H	1:A:595:GLN:HE22	1.26	0.84
1:E:511:PRO:HB3	1:E:515:THR:CG2	2.08	0.84
1:A:345:MET:HE3	1:A:592:LEU:HD11	1.59	0.84
3:G:234:ALA:O	3:G:238:ARG:HG3	1.76	0.84
1:A:75:ARG:HH11	1:A:220:GLN:NE2	1.76	0.83
1:A:686:ALA:HB3	8:A:2331:HOH:O	1.77	0.83
1:A:320:ALA:O	1:A:323:LYS:HG2	1.78	0.83
3:C:235:ALA:O	3:C:239:ARG:HG3	1.78	0.83
1:A:138:GLU:OE2	1:A:402:LYS:HB2	1.78	0.83
2:F:1:MET:HA	8:F:2058:HOH:O	1.78	0.83
1:A:42:GLN:HE22	1:A:505:ARG:HD3	1.42	0.83
1:A:231:LYS:HA	1:A:247:HIS:CD2	2.13	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:THR:HG22	1:A:722:ARG:HG3	1.60	0.83
3:G:206:GLY:O	3:G:207:PHE:C	2.21	0.83
1:E:109:GLU:HG3	8:E:2067:HOH:O	1.77	0.83
1:E:297:THR:CG2	1:E:299:GLU:H	1.90	0.83
1:A:336:TRP:CD1	1:A:336:TRP:H	1.93	0.83
3:C:64:LEU:HD21	7:C:1252:UQ1:C3	2.08	0.83
1:E:473:VAL:HG11	8:E:2276:HOH:O	1.79	0.83
1:E:592:LEU:HD23	1:E:603:GLN:NE2	1.92	0.83
1:A:740:ARG:NH1	8:A:2361:HOH:O	2.09	0.83
1:E:539:THR:HG23	1:E:542:GLU:H	1.44	0.83
1:E:590:ILE:CG1	8:E:2178:HOH:O	2.25	0.83
1:E:608:PHE:CD1	1:E:608:PHE:C	2.52	0.83
1:A:377:PRO:HG2	1:A:533:GLN:HG3	1.61	0.82
1:A:429:PRO:O	1:A:430:TYR:CD2	2.31	0.82
1:A:279:VAL:HG13	1:A:283:THR:CG2	2.07	0.82
3:G:222:GLN:OE1	3:G:222:GLN:HA	1.80	0.82
1:A:633:ARG:HD2	5:A:1765:MGD:O2B	1.78	0.82
3:C:155:THR:HG21	3:C:239:ARG:HG2	1.62	0.82
2:F:72:THR:HG23	2:F:89:LYS:HB3	1.62	0.82
2:B:46:TYR:CB	8:B:2034:HOH:O	2.04	0.82
1:A:393:GLY:HA3	1:A:407:LYS:HE3	1.59	0.82
2:F:67:VAL:HB	2:F:68:PRO:HD3	1.60	0.82
3:C:241:LEU:C	3:C:241:LEU:HD12	2.04	0.81
1:E:239:PHE:HB3	1:E:687:ARG:HB3	1.62	0.81
1:A:388:CYS:HA	1:A:593:TYR:OH	1.79	0.81
1:E:88:THR:HG23	1:E:468:LEU:HD21	1.61	0.81
1:E:232:VAL:H	1:E:247:HIS:CD2	1.98	0.81
3:G:76:ILE:O	3:G:80:LEU:HG	1.80	0.81
1:A:428:GLU:O	1:A:429:PRO:C	2.20	0.81
2:B:46:TYR:HE2	8:B:2031:HOH:O	1.58	0.81
1:E:339:ASP:CB	1:E:607:VAL:HG11	2.10	0.81
1:E:635:GLN:NE2	1:E:635:GLN:H	1.79	0.81
2:F:57:GLN:HE22	2:F:140:ARG:HH22	1.03	0.81
3:C:173:LEU:HG	3:C:173:LEU:O	1.80	0.81
1:E:453:LYS:HG2	1:E:475:TRP:CH2	2.15	0.81
3:G:21:PHE:O	3:G:238:ARG:NH1	2.14	0.81
2:B:6:MET:HE3	8:B:2046:HOH:O	1.80	0.81
1:E:75:ARG:HH11	1:E:220:GLN:NE2	1.77	0.81
1:E:469:PRO:O	1:E:706:MET:HG3	1.80	0.81
3:C:140:ASN:H	3:C:140:ASN:ND2	1.73	0.81
1:A:605:LEU:H	1:A:605:LEU:HD23	1.44	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:671:ASN:C	1:E:671:ASN:HD22	1.89	0.81
1:A:393:GLY:HA3	1:A:407:LYS:NZ	1.95	0.81
1:A:585:THR:O	1:A:586:ALA:CB	2.28	0.81
1:E:297:THR:HG23	1:E:299:GLU:H	1.43	0.81
1:E:438:TYR:HD2	8:E:2092:HOH:O	1.63	0.81
3:C:207:GLY:O	3:C:209:TRP:N	2.14	0.80
1:E:209:HIS:HE1	1:E:625:ARG:N	1.79	0.80
1:A:677:GLU:O	1:A:678:GLY:O	1.99	0.80
1:E:397:GLU:HB3	1:E:398:PRO:CD	2.11	0.80
1:E:604:PRO:O	1:E:606:PRO:CD	2.29	0.80
3:G:107:LEU:O	3:G:109:LYS:N	2.13	0.80
1:A:390:GLY:N	1:A:595:GLN:HE22	1.79	0.80
1:E:75:ARG:HH11	1:E:220:GLN:HE21	1.27	0.80
1:E:113:ARG:NH1	1:E:114:VAL:HG13	1.96	0.80
1:E:232:VAL:H	1:E:247:HIS:HD2	1.30	0.80
3:G:139:ASN:H	3:G:139:ASN:ND2	1.80	0.80
1:A:457:LYS:HA	8:A:2221:HOH:O	1.80	0.80
1:A:170:VAL:O	1:A:175:ALA:CB	2.30	0.80
1:E:431:PRO:HD2	8:E:2260:HOH:O	1.82	0.80
1:A:232:VAL:H	1:A:247:HIS:HD2	1.25	0.80
1:A:395:ASP:O	1:A:399:GLU:CB	2.25	0.80
3:C:155:THR:HG21	3:C:239:ARG:CG	2.12	0.80
1:E:183:TRP:CH2	1:E:596:ARG:HD3	2.17	0.80
1:A:561:MET:O	1:A:563:THR:N	2.14	0.80
1:E:539:THR:HG22	1:E:542:GLU:CB	2.12	0.80
1:A:342:TYR:HD1	1:A:607:VAL:HB	1.47	0.79
1:E:71:ASN:HD22	1:E:74:SER:H	1.29	0.79
1:E:183:TRP:HH2	1:E:596:ARG:HD3	1.45	0.79
1:E:311:VAL:HB	8:E:2195:HOH:O	1.80	0.79
1:E:95:LEU:HD21	8:E:2276:HOH:O	1.82	0.79
1:E:109:GLU:CG	8:E:2067:HOH:O	2.29	0.79
1:E:100:ILE:HG12	1:E:478:VAL:HG22	1.63	0.79
3:G:78:LEU:HD21	7:G:1251:UQ1:H72	1.62	0.79
2:B:16:CYS:O	2:B:18:ALA:N	2.14	0.79
1:E:95:LEU:HD11	8:E:2276:HOH:O	1.80	0.79
1:E:605:LEU:N	1:E:605:LEU:HD22	1.94	0.79
1:E:648:GLU:HG2	1:E:681:ARG:NH1	1.97	0.79
1:E:717:ASN:HD22	5:E:1765:MGD:H192	1.30	0.79
1:E:97:ARG:NH2	1:E:763:ARG:HD2	1.97	0.79
1:A:519:TRP:NE1	1:A:540:ILE:HG12	1.96	0.79
1:A:625:ARG:HH22	5:A:1765:MGD:H15	1.31	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:171:TRP:O	3:C:172:ALA:HB2	1.82	0.79
1:A:285:GLY:O	1:A:590:ILE:HG23	1.83	0.79
1:A:605:LEU:HD23	1:A:605:LEU:N	1.97	0.79
1:A:583:PHE:HE2	1:A:588:GLY:H	1.25	0.78
1:E:297:THR:CG2	1:E:299:GLU:HG2	2.13	0.78
1:A:629:HIS:CA	1:A:634:THR:HG21	2.13	0.78
1:E:139:ALA:O	1:E:433:LYS:O	2.02	0.78
1:E:746:ARG:HH11	1:E:746:ARG:HG3	1.48	0.78
1:A:673:ASP:OD2	1:A:721:THR:HG21	1.84	0.78
1:E:673:ASP:OD2	1:E:721:THR:CG2	2.32	0.78
1:A:651:ILE:HD13	1:A:656:ALA:HB2	1.63	0.78
2:B:41:ARG:HH11	2:B:187:THR:HG23	1.48	0.78
1:A:604:PRO:C	1:A:606:PRO:HD2	2.06	0.78
1:E:589:LYS:HB3	1:E:592:LEU:HB2	1.65	0.78
1:A:209:HIS:O	1:A:213:ASP:HB3	1.83	0.78
1:A:510:GLU:HG3	8:A:2022:HOH:O	1.84	0.78
2:F:41:ARG:HH11	2:F:187:THR:HG23	1.48	0.78
1:A:36:GLU:O	1:A:58:VAL:HG22	1.84	0.78
1:E:397:GLU:CB	1:E:398:PRO:HD3	2.14	0.78
1:A:301:ALA:O	1:A:305:THR:HB	1.84	0.78
1:A:367:GLN:HG3	8:A:2268:HOH:O	1.83	0.78
3:G:12:PHE:CZ	3:G:246:GLN:HG2	2.18	0.78
1:A:70:ALA:O	8:A:2035:HOH:O	1.99	0.77
1:A:174:THR:HG23	1:A:178:GLU:HG2	1.66	0.77
1:E:339:ASP:HB2	1:E:607:VAL:CG1	2.13	0.77
2:F:55:PRO:HG2	4:F:1194:SF4:S2	2.23	0.77
1:A:483:ALA:HA	1:A:515:THR:CG2	2.14	0.77
3:C:145:ASN:C	3:C:145:ASN:HD22	1.89	0.77
1:E:38:LYS:HG3	8:E:2019:HOH:O	1.84	0.77
1:A:339:ASP:HB3	1:A:607:VAL:HG11	1.65	0.77
1:A:428:GLU:HB3	1:A:429:PRO:CD	2.10	0.77
2:F:3:ARG:HD2	2:F:62:GLU:OE2	1.84	0.77
1:A:382:GLU:HA	8:A:2184:HOH:O	1.83	0.77
1:A:395:ASP:C	1:A:399:GLU:HB2	2.09	0.77
1:E:424:MET:HG2	1:E:459:LEU:HD21	1.67	0.77
2:F:40:GLU:HB2	8:F:2020:HOH:O	1.85	0.77
1:A:396:HIS:HB3	1:A:403:PRO:HB3	1.66	0.77
1:E:116:THR:HG21	8:E:2072:HOH:O	1.84	0.77
1:E:602:HIS:CD2	1:E:604:PRO:CD	2.62	0.77
2:F:57:GLN:HE21	2:F:140:ARG:HH22	1.33	0.77
1:A:345:MET:HE2	1:A:605:LEU:CD2	2.15	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:SER:HB3	3:C:252:GLY:N	1.98	0.77
1:E:386:GLY:O	1:E:388:CYS:SG	2.40	0.77
1:A:116:THR:HG22	1:A:119:GLU:N	1.97	0.77
1:E:483:ALA:N	1:E:516:LYS:O	2.16	0.77
3:G:88:ILE:CD1	7:G:1251:UQ1:HM33	2.14	0.77
1:A:647:ASN:HD22	1:A:647:ASN:H	1.33	0.76
1:E:762:GLU:HB2	8:E:2444:HOH:O	1.84	0.76
2:F:160:GLU:H	2:F:179:ASN:ND2	1.83	0.76
1:E:259:ALA:HB3	8:E:2193:HOH:O	1.85	0.76
2:B:41:ARG:HD2	2:B:187:THR:HG23	1.68	0.76
1:E:639:VAL:HG11	2:F:25:MET:HE3	1.67	0.76
1:A:578:GLU:HB3	1:A:580:ARG:HD3	1.66	0.76
3:C:108:LEU:O	3:C:110:LYS:CG	2.34	0.76
1:E:100:ILE:HG23	1:E:478:VAL:HG22	1.67	0.76
1:E:651:ILE:HD11	1:E:682:VAL:CG1	2.16	0.76
1:A:422:GLU:HB3	1:A:423:PRO:HD3	1.68	0.76
1:E:153:VAL:HG11	1:E:167:LYS:HE2	1.68	0.76
1:E:642:GLU:OE2	2:F:32:GLY:N	2.15	0.76
3:G:150:LEU:O	3:G:154:THR:HB	1.86	0.76
1:A:595:GLN:O	1:A:595:GLN:CG	2.34	0.76
2:F:3:ARG:HG2	8:F:2002:HOH:O	1.85	0.76
3:G:206:GLY:HA2	3:G:209:TYR:HB3	1.67	0.76
1:A:152:PHE:O	1:A:157:PRO:HD3	1.85	0.76
1:A:284:VAL:O	1:A:590:ILE:CG2	2.31	0.76
1:E:434:GLY:HA2	1:E:461:LEU:O	1.85	0.76
1:A:73:LYS:NZ	1:A:192:HIS:HD2	1.83	0.75
1:A:139:ALA:O	1:A:433:LYS:O	2.03	0.75
1:A:184:VAL:CG2	1:A:592:LEU:CD2	2.49	0.75
1:A:286:PHE:HA	1:A:590:ILE:HG21	1.68	0.75
1:A:305:THR:HG22	1:A:307:ILE:H	1.51	0.75
1:A:653:LYS:HD2	1:A:686:ALA:H	1.48	0.75
1:E:577:LYS:HE2	8:E:2321:HOH:O	1.85	0.75
1:A:467:VAL:HG13	8:A:2047:HOH:O	1.86	0.75
1:A:606:PRO:O	1:A:608:PHE:N	2.18	0.75
1:E:488:ARG:HB2	1:E:517:PRO:HB3	1.67	0.75
1:E:673:ASP:OD2	1:E:721:THR:HG21	1.86	0.75
3:G:225:LEU:HB3	8:G:2068:HOH:O	1.85	0.75
1:A:232:VAL:H	1:A:247:HIS:CD2	2.04	0.75
2:B:17:ALA:HB1	2:B:20:ALA:HB3	1.68	0.75
1:E:69:GLU:O	1:E:70:ALA:HB3	1.84	0.75
1:E:118:GLU:HG3	8:E:2305:HOH:O	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:GLY:O	1:A:428:GLU:O	2.03	0.75
1:A:642:GLU:HG2	2:B:34:PHE:HZ	1.52	0.75
1:A:511:PRO:HB3	1:A:515:THR:HG22	1.67	0.75
1:A:611:PRO:HB3	8:A:2136:HOH:O	1.85	0.75
1:E:253:LYS:O	1:E:256:THR:HB	1.86	0.75
1:A:346:ALA:HB2	1:A:605:LEU:CD1	2.15	0.75
1:E:174:THR:HG23	1:E:178:GLU:HG2	1.68	0.75
3:C:101:LEU:O	3:C:105:LEU:HD12	1.86	0.75
1:E:318:GLU:O	1:E:322:HIS:HD2	1.70	0.75
1:A:595:GLN:O	1:A:595:GLN:HG3	1.85	0.75
3:C:61:LEU:HD22	7:C:1252:UQ1:H101	1.68	0.75
3:C:197:GLU:HG2	8:C:2075:HOH:O	1.85	0.75
1:E:305:THR:HG23	1:E:307:ILE:HG12	1.68	0.75
1:E:421:ILE:CG2	1:E:421:ILE:O	2.33	0.75
2:F:169:GLN:NE2	8:F:2107:HOH:O	2.19	0.74
1:E:116:THR:CG2	1:E:119:GLU:N	2.48	0.74
1:E:591:GLU:OE2	1:E:604:PRO:HG3	1.87	0.74
3:G:154:THR:CG2	3:G:238:ARG:NE	2.46	0.74
1:A:89:THR:OG1	1:A:484:THR:HG21	1.88	0.74
1:A:99:LEU:O	1:A:478:VAL:HA	1.88	0.74
1:A:349:TYR:HE1	1:A:605:LEU:HD21	1.52	0.74
3:C:64:LEU:HD22	7:C:1252:UQ1:C1	2.17	0.74
1:A:330:PRO:HD2	8:A:2164:HOH:O	1.86	0.74
1:A:484:THR:HG22	1:A:487:GLU:HG3	1.69	0.74
1:E:209:HIS:CE1	1:E:625:ARG:H	2.02	0.74
1:A:336:TRP:H	1:A:336:TRP:HD1	1.34	0.74
1:A:672:GLN:HE22	1:A:738:PHE:H	1.32	0.74
1:E:315:VAL:HG12	1:E:319:MET:HE3	1.69	0.74
1:E:575:TRP:O	1:E:578:GLU:HB2	1.86	0.74
1:E:75:ARG:HD2	1:E:220:GLN:HE22	1.53	0.74
3:G:129:TYR:CD2	3:G:130:PRO:HD3	2.22	0.74
1:A:75:ARG:HH11	1:A:220:GLN:HE21	1.35	0.74
1:A:592:LEU:O	1:A:593:TYR:CB	2.33	0.74
1:A:687:ARG:NH2	2:B:40:GLU:OE2	2.20	0.74
1:E:597:PHE:HB3	8:E:2325:HOH:O	1.86	0.74
1:E:720:GLN:HB3	8:E:2418:HOH:O	1.88	0.74
1:E:391:PRO:O	1:E:413:ARG:HG2	1.87	0.73
1:A:186:GLY:H	1:A:583:PHE:HA	1.53	0.73
1:A:349:TYR:CE2	1:A:590:ILE:O	2.41	0.73
1:A:685:THR:HB	2:B:42:GLU:CD	2.13	0.73
2:F:117:THR:HG21	8:F:2077:HOH:O	1.86	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:PRO:O	2:B:48:ASN:OD1	2.07	0.73
1:E:69:GLU:O	1:E:70:ALA:CB	2.36	0.73
2:F:78:THR:HG21	8:F:2059:HOH:O	1.88	0.73
1:A:195:ILE:HA	1:A:362:GLY:O	1.88	0.73
1:A:488:ARG:NH2	5:A:1765:MGD:O6	2.21	0.73
2:B:46:TYR:O	8:B:2033:HOH:O	2.06	0.73
1:A:519:TRP:CE2	1:A:540:ILE:CG1	2.71	0.73
2:B:121:HIS:O	2:B:125:LYS:HE2	1.89	0.73
3:G:78:LEU:CD2	7:G:1251:UQ1:H71	2.14	0.73
3:C:21:HIS:CE1	3:C:64:LEU:HD11	2.24	0.73
1:E:284:VAL:HG12	1:E:592:LEU:CD1	2.19	0.73
2:F:78:THR:HG22	2:F:80:ASP:H	1.52	0.73
1:A:153:VAL:CG1	1:A:167:LYS:HE2	2.19	0.73
1:A:400:GLY:CA	8:A:2192:HOH:O	2.31	0.73
1:A:631:PHE:O	1:A:698:GLY:HA3	1.88	0.73
1:E:424:MET:HE2	1:E:455:ALA:CB	2.17	0.73
1:E:91:ASP:O	1:E:92:PRO:O	2.07	0.73
1:E:346:ALA:N	1:E:605:LEU:HD12	2.04	0.73
1:E:477:ASP:C	1:E:478:VAL:HG23	2.14	0.73
1:E:708:LEU:HA	8:E:2406:HOH:O	1.89	0.73
1:A:71:ASN:HD22	1:A:74:SER:H	1.33	0.73
1:A:413:ARG:H	1:A:413:ARG:HD2	1.52	0.73
1:A:608:PHE:CD1	1:A:608:PHE:C	2.62	0.73
1:E:421:ILE:O	1:E:421:ILE:HG23	1.87	0.72
1:E:511:PRO:CB	1:E:515:THR:HG22	2.14	0.72
1:E:438:TYR:CD2	8:E:2092:HOH:O	2.40	0.72
1:E:551:LEU:O	1:E:553:LEU:HB2	1.89	0.72
1:E:734:LEU:HD22	8:E:2418:HOH:O	1.89	0.72
1:A:391:PRO:O	1:A:413:ARG:HB3	1.89	0.72
2:B:47:PRO:HD3	8:B:2036:HOH:O	1.89	0.72
1:E:470:GLN:HG2	1:E:706:MET:SD	2.29	0.72
3:G:51:TYR:N	8:G:2015:HOH:O	2.23	0.72
3:G:115:LEU:HD13	8:G:2031:HOH:O	1.89	0.72
3:G:154:THR:HG21	3:G:238:ARG:HG2	1.72	0.72
1:E:672:GLN:NE2	1:E:738:PHE:H	1.87	0.72
1:E:465:ILE:O	1:E:466:ASP:HB3	1.88	0.72
1:E:622:LEU:HD22	5:E:1766:MGD:H8	1.70	0.72
1:A:95:LEU:HD12	1:A:467:VAL:C	2.15	0.72
8:A:2013:HOH:O	2:B:25:MET:HE1	1.88	0.72
3:C:222:TRP:CG	3:C:223:GLN:N	2.54	0.72
1:E:553:LEU:HD21	1:E:557:THR:HG21	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:605:LEU:H	1:E:605:LEU:HD23	0.58	0.72
1:A:166:ALA:HB2	1:A:415:THR:HG23	1.70	0.72
1:A:413:ARG:H	1:A:413:ARG:NE	1.86	0.72
2:F:47:PRO:CD	8:F:2034:HOH:O	2.32	0.72
3:G:221:TRP:HZ3	3:G:225:LEU:HD13	1.54	0.72
1:A:299:GLU:OE2	1:A:313:ARG:NH2	2.17	0.71
1:A:601:GLY:N	8:A:2281:HOH:O	2.00	0.71
1:A:632:ALA:O	1:A:635:GLN:HG3	1.89	0.71
1:A:338:GLY:O	1:A:726:ASP:HA	1.90	0.71
1:A:561:MET:HE1	1:A:564:LEU:HD12	1.71	0.71
1:E:299:GLU:OE2	1:E:313:ARG:NH2	2.15	0.71
1:E:589:LYS:HG2	1:E:592:LEU:HD12	1.72	0.71
1:E:708:LEU:O	1:E:712:ARG:HD2	1.91	0.71
2:F:45:GLU:HB2	8:F:2027:HOH:O	1.89	0.71
1:A:79:CYS:HB2	1:A:80:PRO:HD2	1.72	0.71
1:A:305:THR:O	1:A:306:GLU:HB2	1.89	0.71
2:B:72:THR:HG21	2:B:89:LYS:O	1.90	0.71
2:B:117:THR:HG22	2:B:119:CYS:N	2.04	0.71
1:E:100:ILE:HG23	1:E:478:VAL:CG2	2.20	0.71
1:A:183:TRP:CB	1:A:592:LEU:HD22	2.20	0.71
2:B:27:ASN:HD21	2:B:121:HIS:CE1	2.08	0.71
3:C:47:ARG:NH1	3:C:107:TYR:O	2.24	0.71
2:F:43:VAL:HG23	8:F:2122:HOH:O	1.91	0.71
1:A:349:TYR:CE1	1:A:605:LEU:HD21	2.26	0.71
1:A:387:GLY:O	1:A:593:TYR:CE1	2.44	0.71
2:B:78:THR:HG21	8:B:2068:HOH:O	1.91	0.71
1:E:589:LYS:NZ	8:E:2324:HOH:O	2.23	0.71
2:F:117:THR:HG22	2:F:119:CYS:H	1.55	0.71
1:A:121:LEU:HD13	1:A:524:GLU:HB3	1.72	0.71
1:A:152:PHE:O	1:A:157:PRO:CD	2.39	0.71
2:F:88:LYS:O	3:G:74:THR:HG22	1.91	0.71
1:A:539:THR:CG2	1:A:541:GLU:HG2	2.21	0.71
1:A:729:SER:O	1:A:729:SER:OG	2.00	0.71
1:E:585:THR:OG1	1:E:589:LYS:HE3	1.90	0.71
3:G:196:GLU:CD	3:G:196:GLU:H	1.97	0.71
3:G:206:GLY:HA2	3:G:209:TYR:CB	2.21	0.71
1:A:635:GLN:HG3	1:A:701:HIS:NE2	2.06	0.70
3:G:105:LEU:HG	8:G:2031:HOH:O	1.89	0.70
1:A:95:LEU:HD11	1:A:468:LEU:O	1.90	0.70
1:A:642:GLU:HG2	2:B:34:PHE:CZ	2.25	0.70
1:A:495:VAL:HG13	8:A:2018:HOH:O	1.90	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:VAL:CB	8:E:2195:HOH:O	2.38	0.70
1:A:314:GLU:HG2	8:A:2161:HOH:O	1.91	0.70
2:B:46:TYR:CE2	8:B:2035:HOH:O	2.45	0.70
3:C:197:GLU:CD	3:C:197:GLU:H	1.99	0.70
1:A:37:VAL:HG12	1:A:38:LYS:N	2.05	0.70
1:E:97:ARG:HH21	1:E:763:ARG:NH1	1.88	0.70
1:A:388:CYS:HA	1:A:593:TYR:CE1	2.26	0.70
1:A:594:CYS:O	1:A:598:LYS:HG3	1.91	0.70
1:A:583:PHE:CE2	1:A:587:SER:C	2.69	0.70
2:B:117:THR:CG2	2:B:120:ALA:H	2.04	0.70
3:C:61:LEU:HD22	7:C:1252:UQ1:C10	2.21	0.70
1:E:670:VAL:HG22	1:E:676:LYS:HG3	1.73	0.70
1:A:231:LYS:HA	1:A:247:HIS:NE2	2.06	0.70
1:A:580:ARG:CB	1:A:580:ARG:NH1	2.52	0.70
2:F:41:ARG:HD2	2:F:187:THR:HG21	1.70	0.70
7:G:1251:UQ1:H8	7:G:1251:UQ1:HM51	1.74	0.70
1:E:539:THR:CG2	1:E:542:GLU:H	2.04	0.70
1:E:647:ASN:H	1:E:647:ASN:HD22	1.38	0.70
2:F:41:ARG:HH11	2:F:187:THR:HG22	1.57	0.70
1:A:755:LEU:O	1:A:758:ARG:HD3	1.92	0.69
1:E:418:GLN:NE2	1:E:418:GLN:H	1.89	0.69
1:E:465:ILE:O	1:E:466:ASP:CB	2.40	0.69
1:E:490:ASP:O	8:E:2288:HOH:O	2.10	0.69
1:E:588:GLY:HA3	8:E:2174:HOH:O	1.90	0.69
2:F:72:THR:HG21	2:F:89:LYS:O	1.91	0.69
1:A:73:LYS:HZ1	1:A:192:HIS:HD2	1.39	0.69
3:C:59:LEU:O	3:C:63:ILE:HG23	1.92	0.69
1:E:282:TYR:O	1:E:587:SER:HB3	1.92	0.69
1:A:335:VAL:HG13	1:A:732:ALA:C	2.17	0.69
2:B:22:ALA:HB2	2:B:134:THR:HG21	1.75	0.69
2:B:72:THR:HG23	2:B:89:LYS:HB3	1.75	0.69
1:E:342:TYR:HD1	1:E:607:VAL:CB	2.06	0.69
1:A:238:ARG:HG3	1:A:688:ILE:HD12	1.73	0.69
1:A:293:VAL:HG13	1:A:293:VAL:O	1.91	0.69
2:B:2:PRO:HB3	2:B:144:ASP:CG	2.17	0.69
1:E:606:PRO:CD	1:E:607:VAL:H	2.04	0.69
1:E:669:LEU:CD2	1:E:741:LEU:HD22	2.22	0.69
3:C:241:LEU:C	3:C:241:LEU:CD1	2.64	0.69
7:C:1252:UQ1:HM51	7:C:1252:UQ1:H8	1.74	0.69
1:A:708:LEU:HD22	1:A:755:LEU:HB3	1.74	0.69
3:G:105:LEU:HB3	8:G:2011:HOH:O	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:HE2	8:A:2223:HOH:O	1.93	0.69
1:A:602:HIS:ND1	1:A:606:PRO:CG	2.51	0.69
1:E:639:VAL:HG21	2:F:25:MET:HE1	1.74	0.69
2:B:44:GLY:O	2:B:49:LEU:HD13	1.93	0.69
1:E:90:TYR:OH	1:E:509:HIS:HE1	1.76	0.69
1:E:591:GLU:HG3	1:E:591:GLU:O	1.90	0.69
2:B:44:GLY:O	2:B:49:LEU:CD1	2.40	0.68
1:E:116:THR:HG22	1:E:119:GLU:H	1.49	0.68
1:E:474:MET:HE3	8:E:2069:HOH:O	1.93	0.68
1:A:642:GLU:OE2	2:B:31:PRO:O	2.11	0.68
1:E:649:VAL:HG13	1:E:695:ILE:CG2	2.23	0.68
1:A:134:LYS:HE2	8:A:2075:HOH:O	1.92	0.68
2:F:164:VAL:HG22	2:F:173:PRO:HB2	1.75	0.68
1:A:109:GLU:OE2	1:A:111:LYS:HE2	1.93	0.68
1:A:710:HIS:O	8:A:2345:HOH:O	2.12	0.68
1:E:687:ARG:NH2	2:F:40:GLU:OE2	2.27	0.68
2:B:142:PHE:C	2:B:152:VAL:HG22	2.18	0.68
3:G:207:PHE:HE2	3:G:211:LEU:CD1	1.97	0.68
1:A:429:PRO:O	1:A:430:TYR:CG	2.46	0.68
1:E:539:THR:HG22	1:E:542:GLU:HB2	1.76	0.68
1:E:740:ARG:NH1	8:E:2426:HOH:O	2.26	0.68
1:E:391:PRO:HG3	1:E:411:PHE:CZ	2.29	0.68
1:A:603:GLN:HB3	1:A:604:PRO:CD	2.20	0.68
1:E:30:ALA:HB3	8:E:2002:HOH:O	1.92	0.68
1:E:284:VAL:HG12	1:E:592:LEU:HD12	1.74	0.68
1:E:671:ASN:ND2	1:E:673:ASP:H	1.91	0.68
1:A:53:ILE:HD12	1:A:65:VAL:HG22	1.76	0.67
1:A:609:THR:O	1:A:610:PRO:C	2.37	0.67
1:A:256:THR:CG2	1:A:305:THR:HA	2.23	0.67
2:B:57:GLN:HE22	2:B:140:ARG:NH2	1.90	0.67
1:E:632:ALA:O	1:E:635:GLN:NE2	2.27	0.67
8:E:2383:HOH:O	2:F:49:LEU:HD11	1.94	0.67
3:C:239:ARG:NH2	8:C:2084:HOH:O	2.26	0.67
1:E:479:ILE:O	1:E:480:LEU:HD23	1.95	0.67
1:E:633:ARG:HD2	5:E:1765:MGD:O2B	1.94	0.67
1:A:380:PRO:HD3	1:A:534:TYR:OH	1.94	0.67
1:A:653:LYS:CG	1:A:684:PRO:O	2.42	0.67
3:C:18:ASN:OD1	3:C:67:GLU:OE2	2.11	0.67
1:E:686:ALA:HB1	8:E:2383:HOH:O	1.94	0.67
1:A:183:TRP:HB2	1:A:592:LEU:HD22	1.77	0.67
1:E:81:ARG:NH1	1:E:630:THR:OG1	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:HIS:HE1	1:E:218:GLN:NE2	1.92	0.67
1:E:267:VAL:HG22	8:E:2197:HOH:O	1.94	0.67
1:E:297:THR:HG21	8:E:2189:HOH:O	1.94	0.67
1:A:204:VAL:HB	1:A:328:LEU:HG	1.76	0.67
3:C:21:HIS:HE1	3:C:64:LEU:HD11	1.59	0.67
3:C:207:GLY:O	3:C:208:PHE:C	2.35	0.67
1:E:310:GLN:NE2	1:E:314:GLU:OE2	2.27	0.67
1:A:382:GLU:HB3	8:A:2185:HOH:O	1.94	0.67
2:B:57:GLN:O	2:B:58:CYS:C	2.37	0.67
3:C:112:SER:O	3:C:113:GLN:HG2	1.95	0.67
1:A:558:MET:HE2	1:A:558:MET:HA	1.75	0.67
3:G:208:TRP:HA	3:G:208:TRP:CE3	2.30	0.67
1:A:120:ALA:HB3	8:A:2065:HOH:O	1.94	0.67
1:A:292:HIS:NE2	1:A:604:PRO:HB2	2.10	0.67
1:A:428:GLU:O	1:A:430:TYR:N	2.28	0.67
2:B:88:LYS:O	3:C:75:THR:HG22	1.94	0.67
3:C:222:TRP:CG	3:C:223:GLN:H	2.11	0.67
1:E:108:GLY:HA3	8:E:2065:HOH:O	1.95	0.67
1:E:129:LEU:O	1:E:133:GLU:HG2	1.95	0.67
1:E:478:VAL:HG23	8:E:2281:HOH:O	1.94	0.67
1:A:630:THR:H	1:A:634:THR:HG21	1.59	0.66
1:E:604:PRO:C	1:E:606:PRO:HD3	2.20	0.66
1:A:166:ALA:HB2	1:A:415:THR:CG2	2.24	0.66
2:B:47:PRO:CD	8:B:2036:HOH:O	2.42	0.66
1:E:204:VAL:HB	1:E:328:LEU:HG	1.77	0.66
3:C:155:THR:CG2	3:C:239:ARG:NE	2.58	0.66
1:E:589:LYS:HG2	1:E:592:LEU:CD1	2.25	0.66
2:F:193:HIS:HB2	8:F:2130:HOH:O	1.94	0.66
1:A:239:PHE:HB3	1:A:687:ARG:HB3	1.78	0.66
2:B:3:ARG:HG2	8:B:2001:HOH:O	1.95	0.66
1:E:297:THR:HG23	1:E:299:GLU:HG2	1.77	0.66
1:A:345:MET:HG2	1:A:592:LEU:HD21	1.78	0.66
1:A:428:GLU:CB	1:A:429:PRO:HD2	2.17	0.66
1:E:635:GLN:NE2	1:E:635:GLN:N	2.43	0.66
1:A:252:ILE:CD1	1:A:256:THR:HG22	2.25	0.66
3:C:171:TRP:O	3:C:172:ALA:CB	2.42	0.66
1:E:396:HIS:CE1	1:E:404:ARG:H	2.14	0.66
1:E:539:THR:HG23	1:E:541:GLU:HG2	1.78	0.66
1:E:679:PRO:HG2	1:E:747:PRO:HB3	1.77	0.66
1:A:602:HIS:CD2	1:A:604:PRO:HD2	2.31	0.66
1:E:539:THR:HG22	1:E:542:GLU:HB3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:166:ARG:HH22	3:G:248:GLN:HE21	1.44	0.66
1:A:357:TYR:HA	1:A:363:PHE:HB2	1.77	0.66
1:A:580:ARG:HH11	1:A:580:ARG:HB2	1.58	0.66
1:A:483:ALA:HA	1:A:515:THR:HG21	1.78	0.66
1:A:583:PHE:HE2	1:A:588:GLY:CA	2.08	0.65
2:B:192:VAL:HG12	2:B:193:HIS:N	2.12	0.65
1:E:93:ASP:OD1	1:E:758:ARG:NH2	2.29	0.65
1:A:293:VAL:O	1:A:293:VAL:CG1	2.43	0.65
2:F:2:PRO:HB3	2:F:144:ASP:CG	2.21	0.65
3:G:206:GLY:O	3:G:209:TYR:CA	2.43	0.65
1:A:319:MET:CE	1:A:328:LEU:HD11	2.25	0.65
2:B:57:GLN:NE2	2:B:140:ARG:HH22	1.91	0.65
3:C:17:THR:CG2	3:C:67:GLU:CG	2.69	0.65
1:E:495:VAL:CG2	8:E:2296:HOH:O	2.45	0.65
3:G:39:LEU:HD13	3:G:116:ALA:HB3	1.79	0.65
1:A:428:GLU:O	1:A:430:TYR:O	2.14	0.65
2:B:166:ARG:NH2	3:C:249:GLN:NE2	2.43	0.65
2:B:117:THR:HB	8:B:2010:HOH:O	1.96	0.65
1:E:647:ASN:HD21	1:E:714:ALA:H	1.45	0.65
3:G:20:HIS:CE1	3:G:63:LEU:HD21	2.31	0.65
3:G:156:LEU:HD12	3:G:178:LEU:HD13	1.79	0.65
1:A:42:GLN:CD	1:A:505:ARG:HB2	2.21	0.65
3:G:189:TYR:O	3:G:192:THR:HB	1.97	0.65
1:E:116:THR:HG23	1:E:119:GLU:N	2.09	0.65
1:A:75:ARG:NH1	1:A:220:GLN:NE2	2.44	0.65
1:A:122:ASP:OD1	1:A:528:ARG:NH1	2.29	0.65
1:A:107:ARG:HG2	1:A:475:TRP:O	1.97	0.65
1:A:346:ALA:HB2	1:A:605:LEU:HD13	1.78	0.65
1:A:187:ARG:NH2	1:A:367:GLN:NE2	2.45	0.64
1:A:345:MET:HE3	1:A:592:LEU:CD1	2.26	0.64
1:E:608:PHE:C	8:E:2335:HOH:O	2.30	0.64
1:A:591:GLU:CB	1:A:603:GLN:HE22	2.10	0.64
1:A:604:PRO:O	1:A:606:PRO:HD3	1.94	0.64
1:E:79:CYS:HB2	1:E:80:PRO:HD2	1.79	0.64
1:E:279:VAL:O	1:E:283:THR:HB	1.96	0.64
1:E:590:ILE:O	1:E:592:LEU:HG	1.97	0.64
2:F:194:HIS:N	8:F:2129:HOH:O	2.29	0.64
3:G:38:HIS:CE1	8:G:2011:HOH:O	2.50	0.64
1:A:73:LYS:HZ1	1:A:192:HIS:CD2	2.15	0.64
1:A:540:ILE:O	1:A:544:LEU:HG	1.97	0.64
3:C:130:TYR:CD2	3:C:131:PRO:HD3	2.32	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:TYR:HB2	1:A:570:PRO:HB3	1.78	0.64
1:A:471:GLU:O	1:A:471:GLU:HG2	1.98	0.64
1:A:525:LEU:O	1:A:529:LEU:HG	1.98	0.64
1:A:581:LEU:HD11	8:A:2272:HOH:O	1.97	0.64
1:A:658:ARG:C	1:A:659:LEU:O	2.34	0.64
1:A:671:ASN:HD21	1:A:675:VAL:H	1.46	0.64
3:G:206:GLY:C	3:G:209:TYR:H	2.04	0.64
1:E:256:THR:CG2	1:E:305:THR:HA	2.28	0.64
1:E:388:CYS:HB2	1:E:593:TYR:HH	1.55	0.64
1:A:39:SER:HB2	8:A:2005:HOH:O	1.97	0.64
1:A:427:GLY:O	1:A:430:TYR:O	2.15	0.64
1:A:581:LEU:CD1	8:A:2272:HOH:O	2.45	0.64
1:A:689:ARG:NH2	1:A:691:ASP:OD2	2.31	0.64
2:B:72:THR:CG2	2:B:74:ALA:H	2.05	0.64
2:B:166:ARG:HH22	3:C:249:GLN:NE2	1.94	0.64
1:E:591:GLU:CD	1:E:604:PRO:CB	2.60	0.64
3:G:207:PHE:O	3:G:211:LEU:N	2.31	0.64
1:A:558:MET:CE	1:A:561:MET:SD	2.86	0.64
1:E:77:ARG:NE	8:E:2044:HOH:O	2.30	0.64
3:G:30:VAL:HG12	3:G:52:ALA:HB2	1.80	0.64
3:G:76:ILE:HG12	3:G:80:LEU:HD11	1.80	0.64
1:A:519:TRP:CZ2	1:A:540:ILE:HG13	2.33	0.64
3:C:140:ASN:HD22	3:C:140:ASN:N	1.93	0.64
1:E:467:VAL:HG12	1:E:468:LEU:HG	1.80	0.64
2:F:43:VAL:CG2	8:F:2122:HOH:O	2.46	0.64
1:A:364:TYR:HB2	1:A:570:PRO:CB	2.28	0.64
1:A:388:CYS:HA	1:A:593:TYR:CZ	2.33	0.64
1:E:396:HIS:HB3	1:E:407:LYS:HE3	1.80	0.64
1:E:474:MET:HE2	1:E:705:LEU:CD1	2.28	0.64
1:E:569:LYS:CD	8:E:2320:HOH:O	2.35	0.64
1:E:642:GLU:HG3	8:E:2435:HOH:O	1.97	0.64
1:E:81:ARG:HE	1:E:214:THR:HG22	1.62	0.63
1:A:349:TYR:HH	1:A:591:GLU:C	2.00	0.63
2:B:36:LEU:HD11	8:B:2105:HOH:O	1.98	0.63
3:C:21:HIS:CE1	3:C:64:LEU:HG	2.33	0.63
1:E:549:GLN:HG3	8:E:2311:HOH:O	1.98	0.63
2:F:72:THR:HG22	2:F:74:ALA:N	2.09	0.63
1:A:367:GLN:O	1:A:500:PRO:HG3	1.96	0.63
1:E:519:TRP:CE2	1:E:540:ILE:CG1	2.81	0.63
3:G:49:THR:HG21	8:G:2011:HOH:O	1.97	0.63
1:A:633:ARG:CD	5:A:1765:MGD:O2B	2.46	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:651:ILE:HD13	1:E:656:ALA:HB2	1.80	0.63
1:A:186:GLY:C	1:A:583:PHE:O	2.41	0.63
1:A:195:ILE:HG12	1:A:329:PRO:HB3	1.81	0.63
8:B:2029:HOH:O	3:C:2:ALA:HB1	1.98	0.63
1:E:88:THR:HG21	1:E:467:VAL:HG11	1.79	0.63
1:E:658:ARG:C	1:E:659:LEU:O	2.30	0.63
3:G:220:PHE:HD1	8:G:2063:HOH:O	1.81	0.63
1:A:151:TRP:O	1:A:156:LEU:HB2	1.99	0.63
3:C:21:HIS:ND1	3:C:64:LEU:HG	2.13	0.63
1:E:551:LEU:O	1:E:552:GLY:C	2.42	0.63
7:G:1251:UQ1:O2	7:G:1251:UQ1:CM3	2.46	0.63
1:A:73:LYS:NZ	1:A:192:HIS:CD2	2.67	0.63
1:E:186:GLY:HA3	1:E:584:GLY:N	2.14	0.63
1:E:621:LEU:HD22	1:E:622:LEU:O	1.98	0.63
1:A:286:PHE:CA	1:A:590:ILE:HG21	2.29	0.62
1:A:360:PRO:HD3	1:A:571:TRP:CZ3	2.34	0.62
1:A:603:GLN:CB	1:A:604:PRO:HD3	2.22	0.62
1:E:591:GLU:O	1:E:603:GLN:NE2	2.32	0.62
1:A:80:PRO:HD3	2:B:18:ALA:HB2	1.81	0.62
1:A:426:THR:HG23	8:A:2049:HOH:O	1.98	0.62
2:B:140:ARG:NH2	8:B:2046:HOH:O	2.32	0.62
3:C:64:LEU:HD22	7:C:1252:UQ1:C6	2.29	0.62
1:A:93:ASP:CG	1:A:758:ARG:HH22	2.06	0.62
1:A:96:LYS:HB3	1:A:513:PHE:HB3	1.81	0.62
1:E:553:LEU:CD2	1:E:557:THR:HG21	2.29	0.62
1:E:635:GLN:H	1:E:635:GLN:HE21	1.46	0.62
1:A:607:VAL:HG13	1:A:609:THR:CB	2.29	0.62
1:E:186:GLY:H	1:E:583:PHE:HA	1.63	0.62
1:E:418:GLN:H	1:E:418:GLN:HE21	1.44	0.62
1:E:470:GLN:NE2	8:E:2277:HOH:O	2.32	0.62
1:E:632:ALA:C	1:E:635:GLN:NE2	2.57	0.62
2:F:115:LYS:HG3	2:F:116:CYS:O	2.00	0.62
1:A:71:ASN:HD21	1:A:73:LYS:HB2	1.64	0.62
1:A:319:MET:HE1	1:A:328:LEU:HD11	1.79	0.62
1:A:379:LEU:O	1:A:380:PRO:C	2.42	0.62
7:C:1252:UQ1:HM51	7:C:1252:UQ1:C8	2.30	0.62
1:E:512:LEU:O	1:E:515:THR:HB	2.00	0.62
2:F:91:ILE:HD12	7:G:1251:UQ1:O1	1.99	0.62
1:A:536:PRO:HG2	1:A:537:TRP:H	1.65	0.62
2:B:134:THR:O	2:B:134:THR:HG22	1.93	0.62
1:E:607:VAL:HG23	8:E:2145:HOH:O	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ILE:HD12	1:A:65:VAL:CG2	2.29	0.62
1:A:630:THR:N	1:A:634:THR:HG21	2.15	0.62
1:A:635:GLN:O	1:A:709:ALA:HB2	1.98	0.62
2:B:25:MET:HE2	2:B:25:MET:CA	2.24	0.62
7:C:1252:UQ1:O2	7:C:1252:UQ1:CM3	2.46	0.62
1:E:204:VAL:HG21	1:E:319:MET:HE2	1.80	0.62
2:F:41:ARG:CD	2:F:187:THR:HG23	2.23	0.62
3:G:172:LEU:O	3:G:176:ARG:HG3	2.00	0.62
7:G:1251:UQ1:C8	7:G:1251:UQ1:HM51	2.30	0.62
2:B:2:PRO:HB3	2:B:144:ASP:HB2	1.82	0.62
1:A:483:ALA:CA	1:A:515:THR:HG23	2.29	0.62
1:A:523:ARG:HG3	1:A:535:PHE:HB3	1.81	0.62
1:A:646:GLU:O	1:A:648:GLU:OE2	2.18	0.62
1:E:297:THR:HG22	1:E:300:TRP:N	2.10	0.62
3:G:139:ASN:HD22	3:G:139:ASN:N	1.95	0.62
1:A:37:VAL:HG13	1:A:57:ALA:O	2.00	0.62
1:A:335:VAL:HG13	1:A:732:ALA:O	1.97	0.62
1:E:311:VAL:CG2	8:E:2195:HOH:O	2.48	0.62
1:E:701:HIS:O	1:E:710:HIS:O	2.16	0.62
1:A:580:ARG:NH1	1:A:580:ARG:HB2	2.14	0.61
3:C:171:TRP:O	3:C:171:TRP:CG	2.53	0.61
3:C:172:ALA:CA	3:C:175:PRO:HG2	2.29	0.61
1:E:359:ARG:HD3	8:E:2222:HOH:O	1.98	0.61
1:E:533:GLN:HE21	1:E:533:GLN:N	1.89	0.61
3:G:240:LEU:C	3:G:240:LEU:HD12	2.24	0.61
1:A:152:PHE:O	1:A:157:PRO:CG	2.48	0.61
3:G:20:HIS:NE2	3:G:63:LEU:HD21	2.14	0.61
1:A:42:GLN:O	1:A:53:ILE:HG12	2.00	0.61
1:A:118:GLU:H	1:A:118:GLU:CD	2.07	0.61
1:A:284:VAL:CG2	1:A:587:SER:HB3	2.25	0.61
1:A:535:PHE:N	1:A:536:PRO:CD	2.62	0.61
3:C:128:LEU:HD22	8:C:2063:HOH:O	2.00	0.61
1:E:591:GLU:OE1	1:E:604:PRO:CA	2.48	0.61
1:E:627:PRO:HB2	2:F:16:CYS:HA	1.83	0.61
1:E:724:LYS:HG2	8:E:2423:HOH:O	2.00	0.61
3:C:207:GLY:HA2	3:C:210:TYR:HB3	1.83	0.61
3:C:248:TRP:CE2	3:C:250:GLY:HA3	2.35	0.61
3:G:207:PHE:C	3:G:207:PHE:CD2	2.77	0.61
3:G:226:ALA:HB3	3:G:227:PRO:HD3	1.82	0.61
1:A:335:VAL:HG13	1:A:733:GLY:HA2	1.82	0.61
1:A:627:PRO:HB2	2:B:16:CYS:HA	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:LEU:O	1:E:478:VAL:HA	2.01	0.61
1:E:345:MET:HB2	1:E:605:LEU:HD13	1.82	0.61
1:E:519:TRP:CE2	1:E:540:ILE:HG13	2.35	0.61
1:E:598:LYS:HB3	1:E:599:GLU:OE1	2.01	0.61
1:A:39:SER:OG	8:A:2004:HOH:O	2.16	0.61
1:A:388:CYS:O	1:A:391:PRO:HD3	2.01	0.61
1:A:427:GLY:C	1:A:428:GLU:O	2.44	0.61
1:A:534:TYR:O	1:A:535:PHE:HB2	1.99	0.61
3:C:207:GLY:C	3:C:209:TRP:N	2.58	0.61
1:A:320:ALA:O	1:A:323:LYS:CG	2.48	0.61
1:E:281:LYS:HG3	1:E:282:TYR:CE1	2.36	0.61
1:A:336:TRP:O	1:A:735:ARG:HB2	2.00	0.61
1:A:346:ALA:HB2	1:A:605:LEU:HD12	1.83	0.61
7:C:1252:UQ1:C8	7:C:1252:UQ1:CM5	2.78	0.61
1:E:286:PHE:C	1:E:288:GLU:H	2.07	0.61
3:G:115:LEU:HB3	8:G:2031:HOH:O	2.00	0.61
7:G:1251:UQ1:C8	7:G:1251:UQ1:CM5	2.78	0.61
1:A:358:GLY:O	1:A:571:TRP:HA	2.00	0.61
2:B:2:PRO:HD2	2:B:80:ASP:OD2	2.01	0.61
2:B:114:SER:O	2:B:115:LYS:HB3	2.00	0.61
1:E:81:ARG:HE	1:E:214:THR:CG2	2.14	0.61
1:E:286:PHE:CB	8:E:2178:HOH:O	2.49	0.61
1:E:686:ALA:CB	8:E:2383:HOH:O	2.48	0.61
1:E:689:ARG:NH2	1:E:691:ASP:OD2	2.21	0.61
1:A:572:LEU:HD22	8:A:2272:HOH:O	2.01	0.61
1:E:336:TRP:O	1:E:340:ASP:OD1	2.19	0.61
2:F:44:GLY:O	2:F:45:GLU:HB2	2.00	0.61
3:G:70:ARG:HG2	3:G:71:PHE:H	1.65	0.61
1:A:239:PHE:O	1:A:687:ARG:HD2	2.01	0.60
2:B:121:HIS:O	2:B:125:LYS:CE	2.48	0.60
3:C:64:LEU:CD2	7:C:1252:UQ1:C2	2.79	0.60
3:G:144:ASN:OD1	3:G:192:THR:CG2	2.49	0.60
2:B:122:ARG:HB3	2:B:127:LYS:HB2	1.82	0.60
8:E:2165:HOH:O	2:F:46:TYR:HB2	2.00	0.60
1:A:396:HIS:CB	1:A:403:PRO:HB3	2.30	0.60
1:A:721:THR:OG1	8:A:2353:HOH:O	2.16	0.60
1:E:81:ARG:NE	1:E:214:THR:HG22	2.15	0.60
1:E:209:HIS:CG	5:E:1766:MGD:H5'1	2.36	0.60
3:G:38:HIS:CE1	3:G:105:LEU:HD22	2.35	0.60
3:G:227:PRO:O	3:G:231:LEU:HB2	2.01	0.60
1:A:295:ASP:HB2	8:A:2156:HOH:O	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ALA:N	8:A:2186:HOH:O	2.25	0.60
3:C:140:ASN:O	3:C:142:PRO:HD3	2.01	0.60
3:C:145:ASN:C	3:C:145:ASN:ND2	2.55	0.60
2:B:27:ASN:HD21	2:B:121:HIS:HE1	1.48	0.60
3:C:21:HIS:ND1	3:C:60:ASP:OD1	2.34	0.60
3:C:67:GLU:HG2	3:C:67:GLU:O	2.01	0.60
3:C:77:ILE:HG12	3:C:81:LEU:HD11	1.83	0.60
2:F:39:ARG:HD2	2:F:56:GLU:OE2	2.00	0.60
2:B:2:PRO:HB3	2:B:144:ASP:CB	2.31	0.60
1:E:81:ARG:HD2	1:E:630:THR:OG1	2.02	0.60
1:E:391:PRO:HG2	1:E:392:SER:H	1.65	0.60
1:E:684:PRO:O	1:E:685:THR:C	2.43	0.60
1:A:636:ASN:HB2	1:A:706:MET:HE2	1.84	0.60
1:E:93:ASP:O	1:E:469:PRO:HD3	2.01	0.60
1:A:36:GLU:O	1:A:36:GLU:HG2	2.02	0.60
1:A:81:ARG:HE	1:A:214:THR:HG22	1.66	0.60
1:A:101:ARG:HB2	1:A:477:ASP:HA	1.84	0.60
1:A:582:PRO:C	8:A:2093:HOH:O	2.44	0.60
2:B:183:LYS:HE3	8:B:2142:HOH:O	2.02	0.60
1:E:342:TYR:CE1	1:E:607:VAL:HB	2.34	0.60
1:A:305:THR:HG23	1:A:307:ILE:HD12	1.83	0.60
3:C:64:LEU:HD21	7:C:1252:UQ1:C4	2.32	0.60
3:C:151:LEU:O	3:C:155:THR:HB	2.02	0.60
1:E:371:LEU:HD13	1:E:547:ARG:CZ	2.31	0.60
1:E:606:PRO:HG2	1:E:607:VAL:N	2.17	0.60
1:A:708:LEU:N	1:A:708:LEU:HD23	2.17	0.59
1:E:519:TRP:NE1	1:E:540:ILE:HG12	2.17	0.59
3:G:249:GLY:O	8:G:2075:HOH:O	2.16	0.59
1:A:209:HIS:CE1	1:A:625:ARG:H	2.11	0.59
1:A:336:TRP:CD1	1:A:336:TRP:N	2.60	0.59
3:C:20:LEU:HD13	3:C:63:ILE:HD13	1.83	0.59
1:A:81:ARG:HE	1:A:214:THR:CG2	2.15	0.59
1:A:558:MET:HE2	1:A:561:MET:SD	2.43	0.59
3:G:225:LEU:CB	8:G:2068:HOH:O	2.48	0.59
1:A:285:GLY:C	1:A:590:ILE:HG23	2.27	0.59
1:A:583:PHE:CE2	1:A:588:GLY:CA	2.83	0.59
1:A:595:GLN:HA	1:A:598:LYS:HD2	1.85	0.59
1:E:313:ARG:HD3	1:E:317:ARG:NH2	2.18	0.59
1:E:497:HIS:O	1:E:498:LYS:C	2.45	0.59
1:A:193:GLU:HG2	8:A:2118:HOH:O	2.03	0.59
1:E:97:ARG:HH22	1:E:763:ARG:HD2	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:466:ASP:HA	5:E:1765:MGD:N2	2.17	0.59
3:G:66:GLU:O	3:G:66:GLU:HG2	2.03	0.59
1:A:345:MET:CE	1:A:592:LEU:HD11	2.30	0.59
1:A:429:PRO:C	1:A:430:TYR:CD2	2.79	0.59
1:A:519:TRP:CD1	1:A:540:ILE:HG21	2.37	0.59
1:E:252:ILE:HG12	1:E:256:THR:HG22	1.85	0.59
1:A:413:ARG:HD2	1:A:413:ARG:N	2.16	0.59
1:A:421:ILE:HG22	1:A:421:ILE:O	2.01	0.59
1:E:346:ALA:H	1:E:605:LEU:HD12	1.67	0.59
3:G:221:TRP:HD1	8:G:2065:HOH:O	1.86	0.59
1:A:183:TRP:HB3	1:A:592:LEU:O	2.02	0.59
8:B:2075:HOH:O	3:C:82:SER:HB3	2.02	0.59
1:E:273:LEU:O	1:E:323:LYS:NZ	2.24	0.59
1:E:635:GLN:O	1:E:641:MET:HG2	1.99	0.59
1:E:755:LEU:O	1:E:758:ARG:HD3	2.02	0.59
1:A:284:VAL:HG23	1:A:587:SER:CB	2.30	0.59
1:A:415:THR:HG22	8:A:2200:HOH:O	2.03	0.59
1:A:483:ALA:HA	1:A:515:THR:HG23	1.82	0.59
1:E:37:VAL:HA	1:E:57:ALA:O	2.03	0.59
1:E:197:TRP:CG	1:E:221:ASP:HB3	2.38	0.59
1:E:568:GLY:O	1:E:570:PRO:HD3	2.03	0.59
1:A:554:ASP:OD2	1:A:554:ASP:N	2.36	0.59
1:A:673:ASP:OD2	1:A:721:THR:CG2	2.49	0.59
3:C:79:LEU:HD21	7:C:1252:UQ1:C8	2.33	0.59
1:E:41:TYR:HE1	1:E:560:GLY:O	1.86	0.59
1:E:397:GLU:CG	1:E:398:PRO:HD3	2.33	0.59
1:E:623:TYR:HA	1:E:695:ILE:O	2.02	0.59
1:A:422:GLU:HB2	8:A:2202:HOH:O	2.02	0.58
3:C:64:LEU:HD13	7:C:1252:UQ1:HM52	1.84	0.58
1:E:590:ILE:HB	8:E:2178:HOH:O	2.03	0.58
3:G:60:LEU:HD22	7:G:1251:UQ1:H101	1.84	0.58
1:A:454:GLU:HG2	8:A:2099:HOH:O	2.03	0.58
2:B:117:THR:HG22	2:B:119:CYS:H	1.68	0.58
1:E:606:PRO:CG	1:E:607:VAL:N	2.66	0.58
3:G:132:LEU:O	3:G:136:VAL:HB	2.03	0.58
1:A:231:LYS:CA	1:A:247:HIS:CD2	2.85	0.58
1:A:232:VAL:N	1:A:247:HIS:HD2	1.96	0.58
1:A:519:TRP:CZ2	1:A:540:ILE:CG1	2.87	0.58
1:A:599:GLU:HB2	8:A:2277:HOH:O	2.04	0.58
2:B:78:THR:HG22	2:B:80:ASP:H	1.69	0.58
1:E:263:ALA:HB2	1:E:301:ALA:HB2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LEU:HD13	1:A:706:MET:HE3	1.84	0.58
3:C:174:PHE:H	3:C:175:PRO:HD2	1.68	0.58
1:E:380:PRO:HD3	1:E:534:TYR:OH	2.03	0.58
1:E:630:THR:HG23	8:E:2450:HOH:O	2.02	0.58
2:F:46:TYR:C	2:F:46:TYR:CD1	2.79	0.58
1:A:289:LEU:HD12	1:A:590:ILE:HD11	1.86	0.58
1:A:519:TRP:CG	1:A:540:ILE:HG21	2.38	0.58
3:C:68:SER:O	3:C:71:ARG:HB3	2.03	0.58
1:E:173:CYS:SG	5:E:1766:MGD:S12	3.01	0.58
2:F:35:ASN:ND2	2:F:106:TYR:HE2	2.02	0.58
3:G:160:LEU:HB3	3:G:175:LEU:HB2	1.84	0.58
1:A:64:LYS:HE2	2:B:26:GLU:HB2	1.85	0.58
1:A:183:TRP:HB3	1:A:592:LEU:HD22	1.84	0.58
1:A:548:LEU:HD13	1:A:558:MET:HB2	1.86	0.58
1:E:239:PHE:O	1:E:687:ARG:HD2	2.03	0.58
1:E:647:ASN:HD22	1:E:647:ASN:N	1.95	0.58
3:G:189:TYR:HB3	3:G:190:PRO:HD3	1.86	0.58
8:A:2039:HOH:O	2:B:133:GLU:HG3	2.04	0.58
2:B:86:ASP:OD1	2:B:88:LYS:HB2	2.03	0.58
3:C:57:ILE:HG21	3:C:100:PHE:HB2	1.85	0.58
1:E:647:ASN:H	1:E:647:ASN:ND2	2.02	0.58
2:B:57:GLN:NE2	8:B:2046:HOH:O	2.36	0.58
1:E:142:PHE:CG	1:E:157:PRO:HG3	2.38	0.58
1:A:75:ARG:HD2	1:A:220:GLN:NE2	2.13	0.58
1:A:558:MET:HE1	1:A:561:MET:SD	2.44	0.58
1:A:583:PHE:CZ	1:A:587:SER:HA	2.39	0.58
2:B:32:GLY:N	8:B:2011:HOH:O	2.35	0.58
1:E:45:GLU:HG3	8:E:2011:HOH:O	2.03	0.58
1:E:335:VAL:HG13	1:E:732:ALA:O	2.04	0.58
1:E:412:ALA:HB1	1:E:413:ARG:NH1	2.19	0.58
1:E:651:ILE:HD11	1:E:682:VAL:HG12	1.86	0.58
3:G:16:THR:HG21	3:G:66:GLU:HB2	1.86	0.58
3:G:88:ILE:HD13	7:G:1251:UQ1:HM33	1.85	0.58
1:A:187:ARG:HH22	1:A:367:GLN:NE2	2.02	0.57
1:A:629:HIS:NE2	1:A:644:ASP:O	2.31	0.57
3:C:89:ILE:HD11	7:C:1252:UQ1:HM33	1.85	0.57
1:E:474:MET:HE2	1:E:705:LEU:HD11	1.86	0.57
2:F:190:SER:O	2:F:194:HIS:N	2.36	0.57
1:A:647:ASN:HD22	1:A:647:ASN:N	1.95	0.57
3:G:247:TRP:CE2	3:G:249:GLY:HA3	2.39	0.57
1:A:183:TRP:HH2	1:A:596:ARG:CD	2.14	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:345:MET:CB	1:E:605:LEU:HD13	2.34	0.57
2:F:19:CYS:HB2	2:F:131:CYS:HB2	1.86	0.57
1:A:81:ARG:HH21	1:A:214:THR:HG22	1.69	0.57
2:B:160:GLU:N	2:B:179:ASN:HD21	1.89	0.57
1:E:36:GLU:HB3	8:E:2005:HOH:O	2.04	0.57
1:E:265:ILE:HD11	1:E:349:TYR:HB2	1.86	0.57
3:G:46:ARG:HG3	8:G:2014:HOH:O	2.02	0.57
1:A:214:THR:HG23	1:A:214:THR:O	2.04	0.57
1:A:231:LYS:HB2	1:A:247:HIS:CD2	2.40	0.57
1:A:285:GLY:C	1:A:590:ILE:CG2	2.78	0.57
1:A:671:ASN:ND2	1:A:675:VAL:H	2.02	0.57
2:B:139:CYS:SG	4:B:1194:SF4:S3	3.02	0.57
1:E:574:ASP:HA	1:E:577:LYS:HD3	1.85	0.57
1:A:277:GLU:HB3	1:A:281:LYS:HZ3	1.70	0.57
1:A:623:TYR:HA	1:A:695:ILE:O	2.04	0.57
1:E:100:ILE:HG12	1:E:478:VAL:HG13	1.86	0.57
1:E:109:GLU:HG2	8:E:2067:HOH:O	1.99	0.57
1:E:519:TRP:CE2	1:E:540:ILE:HG12	2.39	0.57
1:E:632:ALA:C	1:E:635:GLN:HE22	2.13	0.57
2:F:35:ASN:HD22	2:F:106:TYR:HE2	1.52	0.57
2:F:166:ARG:HH22	3:G:248:GLN:NE2	2.01	0.57
3:G:206:GLY:CA	3:G:209:TYR:CB	2.82	0.57
1:A:647:ASN:C	1:A:648:GLU:CG	2.75	0.57
1:A:647:ASN:HD21	1:A:714:ALA:H	1.52	0.57
2:B:155:ALA:HB1	8:B:2114:HOH:O	2.04	0.57
1:E:100:ILE:HG12	1:E:478:VAL:CG2	2.33	0.57
1:A:124:ILE:HD11	1:A:478:VAL:HG11	1.87	0.57
1:A:134:LYS:CE	8:A:2075:HOH:O	2.50	0.57
3:C:50:THR:O	3:C:54:LEU:HG	2.05	0.57
1:E:602:HIS:NE2	1:E:604:PRO:CD	2.56	0.57
1:E:607:VAL:O	1:E:607:VAL:HG13	2.00	0.57
1:E:651:ILE:HD11	1:E:682:VAL:HG13	1.86	0.57
1:A:64:LYS:CE	2:B:26:GLU:HB2	2.34	0.57
1:E:153:VAL:CG1	1:E:167:LYS:HE2	2.35	0.57
2:F:147:ASP:O	2:F:150:SER:HB2	2.04	0.57
3:G:70:ARG:HG2	3:G:71:PHE:N	2.19	0.57
1:A:457:LYS:HD3	8:A:2220:HOH:O	2.05	0.56
3:C:79:LEU:HD21	7:C:1252:UQ1:H71	1.87	0.56
3:G:222:GLN:C	8:G:2068:HOH:O	2.47	0.56
1:A:184:VAL:HG22	1:A:592:LEU:HD23	1.73	0.56
1:A:483:ALA:CA	1:A:515:THR:CG2	2.81	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:HIS:CE1	3:C:64:LEU:CD1	2.88	0.56
1:E:81:ARG:HB2	4:E:1764:SF4:S3	2.44	0.56
1:E:601:GLY:HA2	8:E:2332:HOH:O	2.04	0.56
3:G:40:LYS:HG3	3:G:40:LYS:O	2.05	0.56
3:G:70:ARG:CG	3:G:71:PHE:N	2.67	0.56
1:A:231:LYS:HB2	1:A:247:HIS:CG	2.40	0.56
1:A:512:LEU:O	1:A:515:THR:HB	2.04	0.56
1:A:519:TRP:CD2	1:A:540:ILE:HG23	2.39	0.56
1:A:585:THR:O	1:A:585:THR:HG22	2.03	0.56
1:A:678:GLY:HA3	8:A:2329:HOH:O	2.06	0.56
2:B:129:PRO:HB3	4:B:1195:SF4:S3	2.46	0.56
2:B:191:GLU:HG3	8:B:2144:HOH:O	2.05	0.56
3:C:89:ILE:CD1	7:C:1252:UQ1:HM33	2.35	0.56
1:E:209:HIS:CD2	5:E:1766:MGD:H5'1	2.41	0.56
1:E:323:LYS:CD	1:E:354:LEU:CA	2.69	0.56
1:E:422:GLU:H	1:E:423:PRO:HD2	1.70	0.56
1:E:586:ALA:HB3	8:E:2324:HOH:O	2.04	0.56
1:E:247:HIS:CE1	8:E:2146:HOH:O	2.58	0.56
1:A:284:VAL:HB	1:A:589:LYS:HA	1.87	0.56
1:A:369:PRO:HG2	1:A:494:LEU:HB3	1.86	0.56
1:A:655:GLU:CD	1:A:658:ARG:HH22	2.13	0.56
1:E:275:ASP:N	1:E:323:LYS:HE3	2.20	0.56
1:E:590:ILE:CB	8:E:2178:HOH:O	2.53	0.56
1:A:635:GLN:C	1:A:709:ALA:HB2	2.30	0.56
1:A:647:ASN:H	1:A:647:ASN:ND2	1.99	0.56
3:C:17:THR:HG22	3:C:18:ASN:N	2.21	0.56
3:C:172:ALA:HA	3:C:175:PRO:CG	2.33	0.56
3:G:144:ASN:C	3:G:144:ASN:HD22	2.12	0.56
1:A:391:PRO:O	1:A:413:ARG:CB	2.54	0.56
1:A:592:LEU:C	1:A:592:LEU:HD13	2.30	0.56
2:B:112:TYR:HB3	3:C:73:ARG:NH2	2.20	0.56
2:B:192:VAL:HG12	2:B:193:HIS:H	1.70	0.56
1:E:433:LYS:HB3	1:E:460:ASP:HB2	1.87	0.56
1:E:454:GLU:HG2	8:E:2272:HOH:O	2.05	0.56
1:E:651:ILE:HD12	1:E:684:PRO:HA	1.87	0.56
2:F:57:GLN:HE22	2:F:140:ARG:HH21	1.47	0.56
1:A:159:ALA:HA	1:A:380:PRO:HD2	1.88	0.56
1:A:183:TRP:HE1	1:A:413:ARG:NH2	1.98	0.56
1:A:337:TYR:O	1:A:340:ASP:CG	2.41	0.56
3:C:108:LEU:HB3	3:C:110:LYS:HG3	1.88	0.56
1:E:91:ASP:C	1:E:92:PRO:O	2.49	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:ASP:OD2	1:E:276:LYS:NZ	2.20	0.56
1:A:103:GLU:OE1	1:A:103:GLU:HA	2.06	0.56
1:A:116:THR:HG23	1:A:118:GLU:N	2.21	0.56
1:A:390:GLY:H	1:A:595:GLN:NE2	1.99	0.56
1:A:555:LEU:O	1:A:559:LYS:HG3	2.05	0.56
1:E:214:THR:HG21	1:E:627:PRO:O	2.04	0.56
1:A:75:ARG:NH1	1:A:220:GLN:HE21	2.00	0.56
1:E:622:LEU:HD22	8:E:2425:HOH:O	2.05	0.56
3:G:107:LEU:C	3:G:109:LYS:H	2.13	0.56
1:A:305:THR:CG2	1:A:307:ILE:HB	2.36	0.55
1:A:342:TYR:CD2	1:A:605:LEU:HA	2.41	0.55
3:C:185:LEU:O	3:C:189:LEU:HG	2.06	0.55
1:E:428:GLU:OE1	1:E:428:GLU:HA	2.05	0.55
1:A:195:ILE:HD12	1:A:195:ILE:N	2.20	0.55
1:A:404:ARG:HG3	1:A:406:ASP:OD2	2.07	0.55
1:E:93:ASP:CG	1:E:758:ARG:HH22	2.14	0.55
1:E:173:CYS:SG	5:E:1765:MGD:S13	3.03	0.55
1:E:305:THR:HG23	1:E:307:ILE:H	1.69	0.55
1:E:315:VAL:HG12	1:E:319:MET:CE	2.37	0.55
1:E:620:ARG:HB3	8:E:2389:HOH:O	2.06	0.55
1:A:107:ARG:HB2	8:A:2221:HOH:O	2.05	0.55
1:A:124:ILE:O	1:A:128:MET:HG3	2.06	0.55
1:A:519:TRP:CG	1:A:540:ILE:CG2	2.89	0.55
2:B:36:LEU:CD1	8:B:2105:HOH:O	2.54	0.55
3:C:229:TRP:O	3:C:233:LEU:HG	2.06	0.55
1:A:548:LEU:C	1:A:553:LEU:O	2.50	0.55
1:E:297:THR:HG22	1:E:299:GLU:H	1.70	0.55
2:F:117:THR:HG22	2:F:119:CYS:N	2.21	0.55
2:F:172:ARG:N	2:F:173:PRO:HD3	2.22	0.55
1:E:519:TRP:CZ2	1:E:540:ILE:HG13	2.42	0.55
2:F:27:ASN:HD21	2:F:121:HIS:HE1	1.55	0.55
2:F:67:VAL:CB	2:F:68:PRO:HD3	2.33	0.55
1:A:449:VAL:O	1:A:453:LYS:HG3	2.06	0.55
1:A:467:VAL:CG2	8:A:2226:HOH:O	2.54	0.55
1:E:166:ALA:HB2	1:E:415:THR:CG2	2.36	0.55
1:A:254:PRO:HG2	1:A:692:CYS:SG	2.46	0.55
1:A:422:GLU:HB3	1:A:423:PRO:CD	2.36	0.55
3:C:21:HIS:CE1	3:C:64:LEU:CG	2.90	0.55
1:E:97:ARG:NH2	1:E:763:ARG:NH1	2.55	0.55
1:E:97:ARG:HH21	1:E:763:ARG:CZ	2.20	0.55
1:E:327:VAL:HG13	1:E:362:GLY:HA2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:345:MET:HB3	1:E:605:LEU:CD1	2.37	0.55
1:E:412:ALA:HB1	1:E:413:ARG:HH12	1.71	0.55
1:A:575:TRP:O	1:A:580:ARG:HG2	2.07	0.55
3:C:190:TYR:HB3	3:C:191:PRO:HD3	1.89	0.55
1:E:169:SER:O	1:E:174:THR:HB	2.06	0.55
1:E:287:GLU:N	1:E:287:GLU:OE1	2.40	0.55
1:E:320:ALA:O	1:E:323:LYS:HB2	2.06	0.55
1:A:654:GLU:HG3	8:A:2316:HOH:O	2.06	0.55
3:C:186:LEU:HD22	3:G:149:GLY:HA2	1.89	0.55
1:E:553:LEU:HD21	1:E:557:THR:CG2	2.37	0.55
1:A:79:CYS:CB	1:A:80:PRO:HD2	2.37	0.55
1:A:113:ARG:NH2	8:A:2063:HOH:O	2.40	0.55
1:E:336:TRP:O	1:E:338:GLY:N	2.40	0.55
1:E:672:GLN:NE2	1:E:672:GLN:H	2.05	0.55
3:G:60:LEU:HD23	3:G:63:LEU:HD12	1.88	0.55
1:A:501:PHE:HA	1:A:564:LEU:O	2.07	0.54
1:E:499:THR:HA	1:E:567:ARG:O	2.08	0.54
1:E:671:ASN:C	1:E:671:ASN:ND2	2.58	0.54
1:E:677:GLU:O	1:E:678:GLY:O	2.24	0.54
3:G:91:GLY:O	3:G:95:LEU:HD12	2.07	0.54
1:A:186:GLY:N	1:A:583:PHE:HA	2.23	0.54
1:E:609:THR:HG23	8:E:2336:HOH:O	2.07	0.54
3:G:139:ASN:ND2	8:G:2039:HOH:O	2.40	0.54
1:A:305:THR:CG2	1:A:307:ILE:H	2.18	0.54
1:A:488:ARG:HD3	1:A:490:ASP:OD2	2.07	0.54
1:E:75:ARG:NH1	1:E:220:GLN:HE21	2.00	0.54
1:E:158:ALA:HB1	1:E:381:LEU:O	2.06	0.54
1:E:297:THR:HG21	1:E:299:GLU:HG2	1.88	0.54
2:F:88:LYS:O	3:G:74:THR:CG2	2.54	0.54
1:A:310:GLN:HG3	8:A:2160:HOH:O	2.08	0.54
1:A:596:ARG:O	1:A:600:ALA:N	2.33	0.54
1:A:602:HIS:HE1	1:A:606:PRO:CG	1.99	0.54
2:B:55:PRO:HB2	8:B:2105:HOH:O	2.06	0.54
1:E:421:ILE:HD11	1:E:452:THR:HG23	1.90	0.54
2:F:91:ILE:CD1	7:G:1251:UQ1:O1	2.56	0.54
3:G:205:ALA:HB1	3:G:240:LEU:CD2	2.37	0.54
1:A:48:PHE:HE1	1:A:145:HIS:CE1	2.25	0.54
1:A:341:THR:OG1	1:A:729:SER:HB3	2.07	0.54
1:A:530:GLY:HA2	1:A:532:GLU:OE2	2.07	0.54
1:E:248:ARG:NH1	1:E:318:GLU:OE2	2.41	0.54
1:E:311:VAL:HG23	8:E:2195:HOH:O	2.05	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:100:LEU:HB3	8:G:2030:HOH:O	2.07	0.54
1:A:212:GLU:OE1	1:A:240:SER:HB2	2.08	0.54
1:A:255:GLY:HA2	1:A:337:TYR:CE1	2.42	0.54
1:E:53:ILE:HD12	1:E:65:VAL:HG22	1.90	0.54
1:E:492:PHE:HZ	1:E:548:LEU:HG	1.73	0.54
2:F:129:PRO:HB3	4:F:1195:SF4:S2	2.48	0.54
1:A:428:GLU:CB	1:A:429:PRO:CD	2.82	0.54
3:C:133:LEU:O	3:C:137:VAL:HG22	2.07	0.54
1:E:391:PRO:HD3	1:E:595:GLN:CD	2.32	0.54
1:E:536:PRO:O	8:E:2308:HOH:O	2.19	0.54
1:A:194:PRO:O	1:A:363:PHE:HA	2.08	0.54
1:A:533:GLN:HG2	1:A:534:TYR:N	2.22	0.54
2:B:106:TYR:CE1	2:B:114:SER:HB3	2.42	0.54
3:C:222:TRP:C	3:C:222:TRP:CD1	2.85	0.54
1:E:250:LEU:HD13	1:E:307:ILE:HG21	1.90	0.54
1:E:606:PRO:CG	1:E:607:VAL:H	2.21	0.54
1:E:627:PRO:CB	2:F:16:CYS:HA	2.38	0.54
1:E:708:LEU:HD22	1:E:755:LEU:HB3	1.90	0.54
2:F:78:THR:CG2	2:F:79:LYS:N	2.71	0.54
1:A:116:THR:HG22	1:A:119:GLU:CB	2.32	0.54
1:A:541:GLU:O	1:A:545:GLU:HG2	2.07	0.54
1:E:48:PHE:CZ	1:E:145:HIS:CE1	2.96	0.54
1:E:524:GLU:OE1	1:E:528:ARG:NH2	2.41	0.54
1:E:576:GLU:C	1:E:578:GLU:H	2.16	0.54
3:G:52:ALA:O	3:G:56:ILE:HG13	2.08	0.54
1:A:490:ASP:OD2	1:A:505:ARG:NH1	2.40	0.54
1:A:592:LEU:O	1:A:592:LEU:HD13	2.08	0.54
2:B:190:SER:CB	3:C:252:GLY:N	2.70	0.54
3:C:64:LEU:CD2	7:C:1252:UQ1:C3	2.82	0.54
1:E:39:SER:OG	1:E:56:HIS:ND1	2.31	0.54
1:E:186:GLY:HA3	1:E:583:PHE:C	2.33	0.54
1:E:606:PRO:CD	1:E:607:VAL:N	2.70	0.54
2:B:57:GLN:CD	8:B:2046:HOH:O	2.51	0.53
1:E:453:LYS:HG2	1:E:475:TRP:CZ2	2.43	0.53
2:F:16:CYS:O	4:F:1194:SF4:S3	2.66	0.53
1:A:115:ALA:HB1	1:A:119:GLU:HG2	1.89	0.53
1:E:69:GLU:HA	8:E:2038:HOH:O	2.07	0.53
1:E:227:LYS:HE2	2:F:12:LEU:HD11	1.89	0.53
1:E:345:MET:CB	1:E:605:LEU:CD1	2.86	0.53
2:F:107:LEU:HD21	3:G:68:PRO:HG2	1.90	0.53
1:A:138:GLU:CD	1:A:402:LYS:HB2	2.33	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:THR:CG2	1:A:757:LYS:HE2	2.38	0.53
1:A:761:ASP:C	1:A:763:ARG:H	2.16	0.53
3:C:64:LEU:CB	7:C:1252:UQ1:H113	2.32	0.53
1:E:48:PHE:CE1	1:E:145:HIS:CE1	2.96	0.53
2:F:9:ASP:HA	2:F:178:LEU:HB2	1.89	0.53
1:A:286:PHE:HA	1:A:590:ILE:CG2	2.36	0.53
1:A:596:ARG:NH1	1:A:600:ALA:CB	2.71	0.53
1:E:138:GLU:CD	1:E:402:LYS:HB2	2.33	0.53
1:E:201:ARG:HD3	8:E:2123:HOH:O	2.08	0.53
1:E:239:PHE:CB	1:E:687:ARG:HB3	2.36	0.53
1:E:717:ASN:ND2	5:E:1765:MGD:H192	2.02	0.53
2:F:190:SER:N	3:G:251:GLY:N	2.56	0.53
1:A:37:VAL:CG1	1:A:38:LYS:N	2.70	0.53
1:A:288:GLU:HB3	1:A:591:GLU:CG	2.19	0.53
1:A:689:ARG:NE	1:A:691:ASP:OD2	2.40	0.53
2:B:46:TYR:CD2	8:B:2035:HOH:O	2.61	0.53
2:B:47:PRO:CG	8:B:2036:HOH:O	2.57	0.53
1:E:346:ALA:N	1:E:605:LEU:CD1	2.70	0.53
1:E:724:LYS:CG	8:E:2423:HOH:O	2.56	0.53
3:G:206:GLY:CA	3:G:209:TYR:HB3	2.38	0.53
1:A:193:GLU:CG	8:A:2118:HOH:O	2.55	0.53
1:A:682:VAL:HG12	1:A:684:PRO:HD3	1.90	0.53
3:C:155:THR:CG2	3:C:239:ARG:CG	2.86	0.53
1:E:107:ARG:O	1:E:108:GLY:C	2.52	0.53
1:E:388:CYS:CB	1:E:593:TYR:OH	2.26	0.53
1:E:575:TRP:HB3	1:E:580:ARG:O	2.08	0.53
2:F:35:ASN:ND2	2:F:106:TYR:CE2	2.75	0.53
1:A:276:LYS:CA	8:A:2148:HOH:O	2.42	0.53
1:E:225:ALA:O	1:E:230:ALA:HB3	2.09	0.53
1:E:539:THR:CG2	1:E:541:GLU:HG2	2.38	0.53
1:E:592:LEU:HA	1:E:603:GLN:HE22	1.55	0.53
2:F:122:ARG:HG2	2:F:127:LYS:HE3	1.91	0.53
1:A:96:LYS:HB3	1:A:513:PHE:CB	2.38	0.53
1:A:158:ALA:HB1	1:A:381:LEU:O	2.09	0.53
1:A:589:LYS:O	1:A:592:LEU:CA	2.57	0.53
1:E:638:TRP:O	1:E:642:GLU:HB2	2.09	0.53
1:A:43:ILE:HB	1:A:505:ARG:HH21	1.74	0.53
2:B:5:ALA:HB3	2:B:145:LEU:HD13	1.91	0.53
2:B:117:THR:HG23	2:B:117:THR:O	2.09	0.53
3:G:208:TRP:HA	3:G:208:TRP:HE3	1.74	0.53
1:A:175:ALA:HB3	1:A:176:PRO:HD3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:HIS:HD2	5:A:1766:MGD:O2A	1.91	0.52
1:A:335:VAL:HG13	1:A:733:GLY:CA	2.38	0.52
1:A:482:GLU:HG2	1:A:483:ALA:H	1.75	0.52
1:E:397:GLU:HB3	8:E:2239:HOH:O	2.09	0.52
1:E:428:GLU:O	1:E:430:TYR:CA	2.57	0.52
1:E:622:LEU:HB2	1:E:693:VAL:O	2.09	0.52
1:E:669:LEU:HD23	1:E:741:LEU:HD22	1.90	0.52
1:A:295:ASP:O	1:A:297:THR:HG22	2.09	0.52
1:A:651:ILE:HG23	1:A:693:VAL:HG23	1.90	0.52
3:C:208:PHE:C	3:C:208:PHE:CD2	2.86	0.52
1:E:112:TYR:OH	1:E:476:ALA:O	2.27	0.52
1:E:112:TYR:CZ	1:E:474:MET:O	2.61	0.52
3:G:17:ASN:O	3:G:21:PHE:HD1	1.91	0.52
3:G:165:LEU:C	3:G:167:LYS:H	2.17	0.52
1:A:241:THR:HG21	2:B:14:VAL:HB	1.91	0.52
2:B:50:VAL:HG13	2:B:181:PRO:HB2	1.90	0.52
2:B:71:PRO:HB2	3:C:79:LEU:CD1	2.39	0.52
2:B:117:THR:CG2	2:B:117:THR:O	2.55	0.52
1:E:88:THR:CG2	1:E:467:VAL:HG11	2.39	0.52
1:E:283:THR:HG23	1:E:590:ILE:HG13	1.92	0.52
1:E:397:GLU:CB	1:E:398:PRO:CD	2.80	0.52
1:E:484:THR:HB	1:E:487:GLU:OE1	2.09	0.52
2:F:55:PRO:CG	4:F:1194:SF4:S2	2.96	0.52
1:A:85:ALA:HA	8:A:2041:HOH:O	2.09	0.52
1:E:160:TRP:CG	1:E:160:TRP:O	2.63	0.52
2:F:16:CYS:O	2:F:16:CYS:SG	2.67	0.52
2:F:67:VAL:HB	2:F:68:PRO:CD	2.37	0.52
1:A:81:ARG:HH21	1:A:214:THR:CG2	2.23	0.52
1:A:116:THR:HG23	1:A:118:GLU:H	1.73	0.52
1:A:370:TYR:CD2	1:A:551:LEU:HD21	2.45	0.52
2:B:132:VAL:HA	2:B:140:ARG:HG3	1.92	0.52
1:E:95:LEU:CD2	8:E:2276:HOH:O	2.50	0.52
1:E:469:PRO:O	1:E:706:MET:CG	2.55	0.52
2:F:44:GLY:HA3	8:F:2024:HOH:O	2.09	0.52
2:F:125:LYS:HE2	8:F:2078:HOH:O	2.10	0.52
3:G:195:PRO:HD2	3:G:196:GLU:OE2	2.09	0.52
1:A:591:GLU:O	1:A:592:LEU:CD1	2.53	0.52
2:B:88:LYS:O	3:C:75:THR:CG2	2.57	0.52
1:E:53:ILE:HD12	1:E:65:VAL:CG2	2.39	0.52
1:E:116:THR:HG22	1:E:119:GLU:N	2.19	0.52
1:E:149:ASP:CB	8:E:2092:HOH:O	2.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:THR:HG23	1:E:307:ILE:CG1	2.40	0.52
1:E:324:PRO:HD2	8:E:2210:HOH:O	2.08	0.52
1:E:492:PHE:CZ	1:E:548:LEU:HG	2.45	0.52
1:A:676:LYS:NZ	1:A:742:GLU:OE1	2.42	0.52
1:A:702:LYS:HG3	8:A:2229:HOH:O	2.09	0.52
2:B:3:ARG:HD2	2:B:62:GLU:OE2	2.09	0.52
3:C:155:THR:HG22	3:C:239:ARG:NE	2.08	0.52
1:E:204:VAL:HG21	1:E:319:MET:CE	2.39	0.52
1:A:87:GLN:HG3	1:A:637:ASN:CG	2.35	0.52
1:A:132:ARG:CD	8:A:2073:HOH:O	2.56	0.52
1:A:430:TYR:HB2	1:A:431:PRO:HD3	1.92	0.52
2:B:164:VAL:HG22	2:B:173:PRO:HB2	1.91	0.52
3:C:12:GLU:OE1	3:C:15:HIS:ND1	2.39	0.52
1:E:497:HIS:HB3	1:E:499:THR:O	2.10	0.52
2:F:72:THR:HG21	2:F:89:LYS:C	2.34	0.52
3:G:44:GLU:OE1	3:G:47:ARG:NH1	2.42	0.52
1:A:583:PHE:CZ	1:A:587:SER:CA	2.93	0.52
1:A:587:SER:O	1:A:589:LYS:HE2	2.09	0.52
1:E:71:ASN:HD21	1:E:73:LYS:HB2	1.75	0.52
1:E:101:ARG:HB2	1:E:477:ASP:HA	1.92	0.52
1:E:323:LYS:HD3	1:E:354:LEU:C	2.35	0.52
1:E:391:PRO:HD2	1:E:595:GLN:OE1	2.10	0.52
1:E:494:LEU:HD23	1:E:502:ILE:HG23	1.91	0.52
1:E:495:VAL:HG21	8:E:2296:HOH:O	2.08	0.52
1:A:43:ILE:HB	1:A:505:ARG:NH2	2.25	0.51
1:E:142:PHE:CD1	1:E:157:PRO:HB3	2.45	0.51
1:E:447:PRO:HB3	8:E:2418:HOH:O	2.09	0.51
3:G:148:ALA:HA	8:G:2045:HOH:O	2.10	0.51
3:G:205:ALA:HB1	3:G:240:LEU:HD22	1.91	0.51
1:A:386:GLY:HA3	1:A:391:PRO:HB2	1.90	0.51
2:B:72:THR:CG2	2:B:73:GLY:N	2.73	0.51
3:C:222:TRP:CD1	3:C:223:GLN:N	2.78	0.51
1:E:149:ASP:HA	8:E:2092:HOH:O	2.10	0.51
1:E:322:HIS:O	1:E:323:LYS:C	2.53	0.51
1:E:504:LEU:HD22	1:E:505:ARG:N	2.26	0.51
8:E:2132:HOH:O	2:F:138:TYR:CD1	2.54	0.51
2:F:63:ASN:HB2	8:F:2110:HOH:O	2.09	0.51
3:G:20:HIS:CE1	3:G:59:ASP:OD1	2.64	0.51
3:G:240:LEU:C	3:G:240:LEU:CD1	2.83	0.51
1:A:258:THR:HB	1:A:608:PHE:HA	1.92	0.51
1:E:548:LEU:CD1	1:E:555:LEU:HA	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:730:GLY:HA3	8:E:2250:HOH:O	2.10	0.51
3:G:39:LEU:HD13	3:G:116:ALA:CB	2.40	0.51
3:G:42:ASP:OD1	3:G:44:GLU:HG3	2.10	0.51
1:E:197:TRP:CB	1:E:221:ASP:HB3	2.40	0.51
1:E:488:ARG:HG3	8:E:2287:HOH:O	2.09	0.51
1:E:620:ARG:HA	1:E:738:PHE:HD2	1.75	0.51
2:F:164:VAL:CG2	2:F:173:PRO:HB2	2.40	0.51
3:G:20:HIS:HE1	3:G:59:ASP:OD1	1.92	0.51
1:A:43:ILE:CG1	1:A:505:ARG:HB3	2.10	0.51
1:A:680:VAL:HG22	1:A:714:ALA:HB2	1.92	0.51
3:C:145:ASN:OD1	3:C:193:THR:CG2	2.57	0.51
1:E:650:TRP:HB2	1:E:694:TYR:HB3	1.92	0.51
1:E:683:LYS:HE2	1:E:685:THR:HB	1.90	0.51
1:A:65:VAL:HG13	1:A:78:LEU:HD21	1.92	0.51
1:A:284:VAL:HG12	1:A:285:GLY:N	2.25	0.51
1:A:499:THR:HB	1:A:565:VAL:CG1	2.40	0.51
2:B:64:PRO:HB3	4:B:1196:SF4:S3	2.51	0.51
3:C:143:LEU:CD2	3:C:198:ALA:HB1	2.41	0.51
1:E:342:TYR:CD1	1:E:607:VAL:CB	2.77	0.51
1:E:397:GLU:CB	8:E:2239:HOH:O	2.58	0.51
1:E:636:ASN:HA	1:E:708:LEU:HB2	1.91	0.51
1:E:648:GLU:CG	1:E:681:ARG:NH1	2.71	0.51
1:E:308:PRO:CB	8:E:2195:HOH:O	2.46	0.51
1:E:591:GLU:O	1:E:591:GLU:CG	2.57	0.51
2:F:27:ASN:O	2:F:28:GLU:C	2.53	0.51
1:A:72:PRO:HG2	1:A:501:PHE:CD2	2.45	0.51
2:B:117:THR:HG23	2:B:120:ALA:H	1.74	0.51
1:E:39:SER:HG	1:E:56:HIS:HD1	1.57	0.51
1:E:100:ILE:CG1	1:E:478:VAL:HG22	2.38	0.51
1:E:166:ALA:HB2	1:E:415:THR:HG21	1.93	0.51
1:E:369:PRO:HG2	1:E:494:LEU:HB3	1.93	0.51
1:A:69:GLU:C	8:A:2032:HOH:O	2.37	0.51
1:A:193:GLU:HB2	1:A:195:ILE:CD1	2.41	0.51
1:A:418:GLN:NE2	1:A:730:GLY:O	2.43	0.51
1:A:462:TYR:OH	1:A:472:HIS:O	2.22	0.51
2:B:166:ARG:HG2	8:B:2145:HOH:O	2.11	0.51
1:E:591:GLU:O	1:E:603:GLN:CD	2.53	0.51
1:A:42:GLN:NE2	1:A:505:ARG:CD	2.66	0.51
1:A:488:ARG:CD	1:A:490:ASP:OD2	2.59	0.51
1:A:607:VAL:O	1:A:607:VAL:CG1	2.44	0.51
2:F:36:LEU:HD22	4:F:1195:SF4:S4	2.51	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:VAL:HA	1:A:283:THR:HB	1.94	0.50
1:A:423:PRO:HB2	1:A:432:ILE:HD12	1.92	0.50
2:B:41:ARG:CD	2:B:187:THR:HG23	2.39	0.50
8:B:2025:HOH:O	3:C:251:LEU:HD11	2.11	0.50
1:E:553:LEU:CD2	1:E:557:THR:CG2	2.89	0.50
1:E:625:ARG:HD2	5:E:1766:MGD:C17	2.41	0.50
1:E:671:ASN:ND2	1:E:673:ASP:N	2.59	0.50
1:E:746:ARG:HH11	1:E:746:ARG:CG	2.22	0.50
3:G:86:SER:O	3:G:87:PRO:C	2.51	0.50
1:A:81:ARG:NE	1:A:214:THR:HG22	2.25	0.50
1:A:336:TRP:HA	1:A:735:ARG:HG3	1.93	0.50
1:A:494:LEU:HD22	1:A:502:ILE:HG12	1.91	0.50
1:A:666:TYR:CZ	1:A:681:ARG:HG3	2.46	0.50
3:C:228:PRO:O	3:C:232:LEU:HD12	2.12	0.50
1:E:60:ASN:ND2	8:E:2022:HOH:O	2.43	0.50
1:E:119:GLU:HG2	8:E:2075:HOH:O	2.11	0.50
1:E:193:GLU:H	1:E:193:GLU:CD	2.20	0.50
1:E:302:GLU:O	1:E:302:GLU:HG2	2.11	0.50
8:E:2132:HOH:O	2:F:138:TYR:CE1	2.64	0.50
1:A:90:TYR:OH	1:A:509:HIS:HE1	1.94	0.50
1:A:252:ILE:HG13	1:A:307:ILE:HD11	1.92	0.50
1:A:548:LEU:O	1:A:553:LEU:O	2.29	0.50
1:A:581:LEU:HD23	1:A:583:PHE:HE1	1.76	0.50
1:E:233:VAL:HG13	1:E:248:ARG:HB2	1.93	0.50
3:G:206:GLY:CA	3:G:209:TYR:HB2	2.42	0.50
1:A:605:LEU:N	1:A:606:PRO:CD	2.70	0.50
1:E:591:GLU:OE2	1:E:604:PRO:CG	2.58	0.50
1:E:685:THR:HG22	2:F:42:GLU:OE2	2.11	0.50
1:A:561:MET:O	1:A:563:THR:O	2.29	0.50
2:B:168:GLU:C	2:B:169:GLN:O	2.44	0.50
1:E:113:ARG:HB3	8:E:2042:HOH:O	2.12	0.50
1:E:123:HIS:CE1	8:E:2080:HOH:O	2.65	0.50
1:E:247:HIS:CD2	1:E:247:HIS:N	2.78	0.50
1:E:391:PRO:C	1:E:413:ARG:CG	2.85	0.50
1:E:435:LEU:HB3	1:E:459:LEU:CD1	2.42	0.50
3:G:208:TRP:O	3:G:212:PHE:CD2	2.64	0.50
1:A:65:VAL:CG1	1:A:78:LEU:HD21	2.42	0.50
1:A:339:ASP:HB3	1:A:607:VAL:CG1	2.38	0.50
1:A:477:ASP:C	1:A:478:VAL:HG23	2.37	0.50
3:C:150:GLY:HA2	3:G:185:LEU:HD22	1.93	0.50
1:E:256:THR:HG23	8:E:2193:HOH:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:470:GLN:O	1:E:471:GLU:C	2.53	0.50
1:E:591:GLU:OE2	1:E:604:PRO:HB3	2.09	0.50
1:E:620:ARG:O	1:E:620:ARG:CG	2.59	0.50
1:A:129:LEU:O	1:A:133:GLU:HG2	2.12	0.50
1:A:435:LEU:O	1:A:462:TYR:HA	2.12	0.50
1:A:596:ARG:CZ	1:A:600:ALA:HB1	2.42	0.50
1:A:647:ASN:ND2	1:A:713:GLY:HA3	2.26	0.50
1:E:634:THR:H	1:E:635:GLN:NE2	2.09	0.50
2:F:166:ARG:HD2	8:F:2105:HOH:O	2.11	0.50
3:G:65:ALA:O	3:G:70:ARG:NH1	2.45	0.50
1:A:628:VAL:HG13	1:A:640:LEU:HD22	1.94	0.50
3:C:108:LEU:O	3:C:109:GLY:C	2.55	0.50
1:E:79:CYS:CB	1:E:80:PRO:HD2	2.42	0.50
1:E:370:TYR:OH	1:E:372:GLU:HG3	2.11	0.50
1:E:462:TYR:CE1	1:E:463:VAL:O	2.65	0.50
2:F:117:THR:HG23	2:F:117:THR:O	2.10	0.50
1:A:77:ARG:NH2	8:A:2039:HOH:O	2.33	0.50
1:A:174:THR:HG23	1:A:178:GLU:CG	2.39	0.50
1:A:422:GLU:N	1:A:423:PRO:HD2	2.27	0.50
2:F:106:TYR:CE1	2:F:114:SER:HB3	2.47	0.50
1:A:66:GLU:HG3	8:A:2038:HOH:O	2.12	0.49
1:E:100:ILE:CG2	1:E:478:VAL:HG22	2.40	0.49
1:E:501:PHE:HB3	1:E:565:VAL:HG13	1.92	0.49
1:E:625:ARG:HH22	5:E:1765:MGD:H15	1.59	0.49
1:E:371:LEU:HD12	1:E:494:LEU:HD21	1.94	0.49
1:E:390:GLY:H	1:E:391:PRO:HD3	1.77	0.49
1:E:630:THR:H	1:E:634:THR:HG21	1.76	0.49
1:E:753:THR:HG22	1:E:757:LYS:HE3	1.93	0.49
2:F:160:GLU:N	2:F:179:ASN:HD21	1.94	0.49
3:G:92:ALA:CB	7:G:1251:UQ1:H8	2.42	0.49
1:A:95:LEU:N	1:A:467:VAL:O	2.36	0.49
1:A:430:TYR:HB2	1:A:431:PRO:CD	2.42	0.49
1:A:626:SER:HB2	1:A:696:VAL:HG11	1.94	0.49
3:C:161:LEU:CD1	3:C:179:LEU:HD12	2.42	0.49
1:E:626:SER:HB3	1:E:696:VAL:HG11	1.94	0.49
1:A:81:ARG:NH2	1:A:214:THR:HG22	2.26	0.49
1:A:393:GLY:HA3	1:A:407:LYS:HZ1	1.72	0.49
1:A:534:TYR:O	1:A:535:PHE:CB	2.61	0.49
2:B:159:ALA:O	2:F:183:LYS:CE	2.53	0.49
2:B:166:ARG:HH22	3:C:249:GLN:HE21	1.59	0.49
3:C:25:VAL:HG23	3:C:96:LEU:HD21	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:THR:HG23	1:A:256:THR:O	2.11	0.49
1:E:252:ILE:CG1	1:E:256:THR:HG22	2.41	0.49
3:G:206:GLY:O	3:G:209:TYR:CB	2.61	0.49
1:A:166:ALA:CB	1:A:415:THR:CG2	2.90	0.49
1:A:371:LEU:HD23	1:A:551:LEU:CD1	2.43	0.49
3:C:207:GLY:HA2	3:C:210:TYR:CB	2.42	0.49
2:F:166:ARG:NH2	3:G:248:GLN:HG3	2.27	0.49
1:A:122:ASP:HB2	8:A:2068:HOH:O	2.11	0.49
1:A:207:GLY:O	5:A:1766:MGD:PB	2.71	0.49
1:A:253:LYS:O	1:A:256:THR:HB	2.13	0.49
1:A:433:LYS:HD3	1:A:460:ASP:OD2	2.13	0.49
1:A:489:TYR:CD1	1:A:540:ILE:HD13	2.47	0.49
2:B:52:GLU:OE2	2:B:187:THR:HB	2.13	0.49
2:B:61:CYS:HB2	4:B:1196:SF4:S3	2.53	0.49
1:E:391:PRO:C	1:E:413:ARG:HG2	2.37	0.49
1:E:591:GLU:O	1:E:603:GLN:HG2	2.11	0.49
1:E:647:ASN:N	1:E:647:ASN:ND2	2.61	0.49
3:G:170:TRP:CE3	3:G:171:ALA:N	2.80	0.49
1:A:121:LEU:HD22	1:A:525:LEU:HG	1.94	0.49
1:A:338:GLY:HA3	1:A:724:LYS:HG2	1.93	0.49
1:A:349:TYR:OH	1:A:592:LEU:HG	2.12	0.49
1:A:405:ALA:HB2	1:A:430:TYR:CZ	2.48	0.49
1:E:614:PRO:HB3	1:E:738:PHE:CD2	2.47	0.49
1:A:267:VAL:O	1:A:271:GLU:HB2	2.12	0.49
1:A:588:GLY:HA3	8:A:2152:HOH:O	2.13	0.49
1:E:117:TRP:CE2	1:E:516:LYS:HG3	2.48	0.49
1:E:297:THR:HG22	1:E:299:GLU:N	2.27	0.49
1:E:630:THR:HA	5:E:1766:MGD:C17	2.42	0.49
2:F:23:CYS:SG	2:F:35:ASN:HB2	2.52	0.49
1:A:335:VAL:CG1	1:A:732:ALA:C	2.80	0.49
1:A:434:GLY:CA	1:A:461:LEU:O	2.50	0.49
3:C:227:ALA:HB3	3:C:228:PRO:HD3	1.95	0.49
1:E:292:HIS:HD2	8:E:2084:HOH:O	1.94	0.49
1:A:483:ALA:HB2	1:A:515:THR:CG2	2.43	0.48
2:B:190:SER:CA	3:C:252:GLY:N	2.76	0.48
1:E:80:PRO:HD3	2:F:18:ALA:HB2	1.95	0.48
1:E:90:TYR:OH	1:E:509:HIS:CE1	2.62	0.48
1:E:369:PRO:CG	1:E:494:LEU:HB3	2.43	0.48
1:E:474:MET:HE2	1:E:705:LEU:HD12	1.95	0.48
1:E:708:LEU:HD22	8:E:2406:HOH:O	2.12	0.48
2:F:146:GLU:O	2:F:148:PRO:HD3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:SER:C	8:A:2005:HOH:O	2.56	0.48
3:C:13:PHE:CZ	3:C:247:GLN:HG2	2.48	0.48
1:E:293:VAL:O	1:E:293:VAL:HG13	2.12	0.48
1:E:314:GLU:HG3	8:E:2199:HOH:O	2.12	0.48
1:E:423:PRO:HB2	1:E:432:ILE:HG13	1.94	0.48
1:E:672:GLN:HE22	1:E:738:PHE:H	1.62	0.48
2:F:117:THR:CG2	2:F:119:CYS:N	2.75	0.48
3:G:32:LEU:HD12	3:G:120:LEU:HD12	1.95	0.48
3:G:73:PHE:HA	8:G:2021:HOH:O	2.13	0.48
1:A:88:THR:HG23	1:A:468:LEU:HD21	1.95	0.48
1:A:170:VAL:HG12	1:A:171:SER:N	2.28	0.48
1:A:184:VAL:HG22	1:A:592:LEU:CB	2.43	0.48
1:A:266:HIS:C	1:A:266:HIS:CD2	2.91	0.48
1:A:389:SER:CA	1:A:595:GLN:HE22	2.27	0.48
1:A:618:PHE:CZ	1:A:740:ARG:HD3	2.48	0.48
2:B:39:ARG:HD2	2:B:56:GLU:OE2	2.14	0.48
2:B:150:SER:O	2:B:154:LYS:HG2	2.14	0.48
3:C:143:LEU:HD23	3:C:198:ALA:HB1	1.96	0.48
1:E:53:ILE:HG22	1:E:78:LEU:HD11	1.95	0.48
3:G:134:LEU:HG	8:G:2034:HOH:O	2.13	0.48
1:A:113:ARG:NE	8:A:2063:HOH:O	2.47	0.48
1:A:506:THR:CG2	8:A:2244:HOH:O	2.61	0.48
1:A:753:THR:HG22	1:A:757:LYS:HE2	1.94	0.48
3:C:71:ARG:HG2	3:C:72:PHE:N	2.28	0.48
1:E:172:LEU:HB3	5:E:1765:MGD:H23	1.95	0.48
1:E:186:GLY:HA3	1:E:584:GLY:CA	2.43	0.48
1:E:468:LEU:HB3	1:E:469:PRO:HD2	1.94	0.48
1:A:355:GLY:O	1:A:359:ARG:HG3	2.13	0.48
1:A:573:GLU:O	1:A:577:LYS:HG3	2.13	0.48
1:A:586:ALA:O	1:A:587:SER:CB	2.61	0.48
3:C:173:LEU:O	3:C:173:LEU:CG	2.58	0.48
3:C:174:PHE:N	3:C:175:PRO:HD2	2.29	0.48
1:A:483:ALA:CB	1:A:515:THR:CG2	2.92	0.48
2:B:57:GLN:O	2:B:59:LEU:HD23	2.14	0.48
1:E:596:ARG:CZ	1:E:601:GLY:HA3	2.44	0.48
1:E:669:LEU:HD21	1:E:741:LEU:HD22	1.93	0.48
1:A:449:VAL:CG1	1:A:453:LYS:HE3	2.44	0.48
1:A:629:HIS:ND1	1:A:634:THR:CG2	2.66	0.48
1:A:642:GLU:OE2	2:B:31:PRO:C	2.57	0.48
1:A:667:VAL:HG11	1:A:741:LEU:HB3	1.95	0.48
1:E:195:ILE:CD1	1:E:363:PHE:CE2	2.97	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:ASP:O	1:E:344:VAL:HG23	2.13	0.48
1:E:589:LYS:CB	1:E:592:LEU:HB2	2.40	0.48
2:F:72:THR:CG2	2:F:89:LYS:HB3	2.39	0.48
1:A:388:CYS:HA	1:A:593:TYR:HE1	1.74	0.48
1:E:174:THR:HG23	1:E:178:GLU:CG	2.41	0.48
1:E:422:GLU:HG3	8:E:2104:HOH:O	2.12	0.48
1:E:494:LEU:CD2	1:E:502:ILE:HG23	2.44	0.48
2:F:59:LEU:O	2:F:60:HIS:C	2.57	0.48
2:F:99:ALA:HB2	3:G:137:ASN:ND2	2.28	0.48
1:A:232:VAL:N	1:A:247:HIS:CD2	2.76	0.48
1:A:248:ARG:HB3	8:A:2133:HOH:O	2.13	0.48
1:A:263:ALA:O	1:A:267:VAL:HG23	2.14	0.48
1:A:712:ARG:NH2	8:A:2347:HOH:O	2.46	0.48
1:E:30:ALA:N	1:E:31:PRO:CD	2.77	0.48
1:E:595:GLN:O	1:E:595:GLN:HG3	2.10	0.48
1:A:249:TRP:O	1:A:251:PRO:HD3	2.14	0.47
3:C:63:ILE:O	3:C:67:GLU:HB3	2.13	0.47
1:E:500:PRO:O	1:E:566:GLN:N	2.33	0.47
1:E:540:ILE:O	1:E:544:LEU:HG	2.14	0.47
1:E:630:THR:HA	5:E:1766:MGD:N18	2.29	0.47
3:G:38:HIS:O	3:G:41:GLY:N	2.25	0.47
1:A:156:LEU:HB3	1:A:157:PRO:HD3	1.96	0.47
1:A:184:VAL:HG22	1:A:592:LEU:CG	2.43	0.47
1:A:277:GLU:HB3	1:A:281:LYS:NZ	2.28	0.47
1:A:319:MET:CE	1:A:328:LEU:CD1	2.92	0.47
1:A:393:GLY:CA	1:A:407:LYS:HE3	2.39	0.47
1:A:488:ARG:HG2	1:A:489:TYR:O	2.14	0.47
1:A:743:LYS:HG3	8:A:2365:HOH:O	2.14	0.47
2:B:117:THR:HG22	2:B:119:CYS:CA	2.43	0.47
1:E:77:ARG:NH1	2:F:135:CYS:O	2.47	0.47
1:E:159:ALA:HA	1:E:380:PRO:HD2	1.96	0.47
1:E:208:HIS:HE1	1:E:218:GLN:HE22	1.62	0.47
1:E:325:ARG:NH1	8:E:2211:HOH:O	2.28	0.47
1:E:622:LEU:HD22	5:E:1766:MGD:C8	2.43	0.47
1:E:734:LEU:CD2	8:E:2418:HOH:O	2.56	0.47
2:F:166:ARG:NH2	3:G:248:GLN:NE2	2.61	0.47
3:G:47:ARG:HH21	3:G:166:LEU:HB3	1.77	0.47
3:G:142:LEU:O	3:G:189:TYR:OH	2.30	0.47
3:G:207:PHE:HB3	3:G:208:TRP:H	1.37	0.47
1:A:71:ASN:ND2	1:A:73:LYS:HB2	2.29	0.47
1:A:457:LYS:HD2	8:A:2221:HOH:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:ALA:O	1:A:687:ARG:HG2	2.14	0.47
1:E:285:GLY:HA3	1:E:592:LEU:HD11	1.96	0.47
1:E:634:THR:H	1:E:635:GLN:HE22	1.62	0.47
1:E:650:TRP:O	1:E:693:VAL:HG22	2.14	0.47
1:A:578:GLU:HB3	1:A:580:ARG:CD	2.42	0.47
1:A:647:ASN:HD21	1:A:713:GLY:CA	2.27	0.47
1:A:722:ARG:NE	8:A:2356:HOH:O	2.48	0.47
2:B:36:LEU:HD12	2:B:37:TRP:N	2.30	0.47
2:B:71:PRO:HB2	3:C:79:LEU:HD11	1.95	0.47
1:E:288:GLU:HG3	8:E:2183:HOH:O	2.14	0.47
1:E:339:ASP:CB	1:E:607:VAL:CG1	2.85	0.47
1:E:426:THR:C	1:E:428:GLU:N	2.67	0.47
1:A:318:GLU:O	1:A:322:HIS:HD2	1.97	0.47
2:B:192:VAL:CG1	2:B:193:HIS:N	2.77	0.47
1:E:384:ALA:HB1	8:E:2237:HOH:O	2.15	0.47
1:E:502:ILE:O	1:E:563:THR:HA	2.13	0.47
1:A:42:GLN:OE1	1:A:506:THR:N	2.47	0.47
1:A:183:TRP:CH2	1:A:596:ARG:CD	2.85	0.47
1:A:471:GLU:OE2	1:A:718:TYR:OH	2.31	0.47
1:A:628:VAL:HG11	1:A:643:MET:HB2	1.96	0.47
1:A:651:ILE:HG23	1:A:693:VAL:CG2	2.44	0.47
2:B:161:ARG:HG2	2:B:179:ASN:HA	1.94	0.47
1:E:177:ARG:HA	1:E:344:VAL:HG11	1.96	0.47
1:E:238:ARG:NH2	1:E:240:SER:HB2	2.29	0.47
1:E:289:LEU:HD12	1:E:590:ILE:HG21	1.95	0.47
1:E:583:PHE:CD2	1:E:583:PHE:N	2.75	0.47
1:E:647:ASN:C	1:E:648:GLU:HG3	2.40	0.47
3:G:47:ARG:O	3:G:50:LEU:O	2.31	0.47
3:G:206:GLY:H	3:G:209:TYR:HB2	1.79	0.47
3:G:216:GLY:C	3:G:218:GLY:H	2.23	0.47
1:A:193:GLU:OE2	1:A:332:ARG:NH1	2.47	0.47
1:A:509:HIS:HD2	1:A:510:GLU:O	1.97	0.47
1:A:548:LEU:HD22	1:A:553:LEU:HD12	1.97	0.47
1:A:587:SER:O	1:A:589:LYS:CE	2.62	0.47
1:A:615:PRO:O	1:A:618:PHE:HB2	2.15	0.47
1:A:630:THR:H	1:A:634:THR:CG2	2.26	0.47
1:A:677:GLU:C	1:A:678:GLY:O	2.58	0.47
2:B:157:LYS:HD3	8:F:2038:HOH:O	2.15	0.47
1:E:48:PHE:CE1	1:E:631:PHE:CE1	3.03	0.47
1:E:201:ARG:CD	8:E:2123:HOH:O	2.62	0.47
1:E:302:GLU:HG3	1:E:307:ILE:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:500:PRO:HD3	1:E:567:ARG:O	2.14	0.47
1:E:602:HIS:CE1	1:E:606:PRO:CG	2.58	0.47
1:E:648:GLU:CG	1:E:681:ARG:HH12	2.16	0.47
1:E:649:VAL:HG13	1:E:695:ILE:HG23	1.95	0.47
1:E:669:LEU:CD2	1:E:741:LEU:CD2	2.91	0.47
1:E:670:VAL:HB	1:E:740:ARG:HG3	1.96	0.47
2:F:6:MET:HG2	2:F:175:LEU:HD22	1.97	0.47
2:F:174:LYS:HE2	8:F:2046:HOH:O	2.14	0.47
3:G:26:LEU:HG	3:G:158:LEU:HB3	1.97	0.47
3:G:53:LEU:O	3:G:99:PHE:HE1	1.97	0.47
3:G:112:GLN:N	8:G:2032:HOH:O	2.47	0.47
3:G:206:GLY:O	3:G:209:TYR:C	2.58	0.47
3:G:206:GLY:HA2	3:G:209:TYR:HB2	1.95	0.47
3:G:247:TRP:CZ2	3:G:249:GLY:HA3	2.49	0.47
1:A:132:ARG:HG2	1:A:132:ARG:O	2.14	0.47
1:A:671:ASN:C	1:A:671:ASN:HD22	2.22	0.47
1:A:686:ALA:CB	8:A:2331:HOH:O	2.49	0.47
3:C:166:LEU:C	3:C:168:LYS:H	2.22	0.47
3:C:201:HIS:CE1	3:C:205:GLU:HG3	2.50	0.47
1:E:428:GLU:C	1:E:430:TYR:N	2.69	0.47
2:F:175:LEU:HD12	2:F:175:LEU:C	2.39	0.47
1:A:422:GLU:N	1:A:423:PRO:CD	2.78	0.47
1:A:653:LYS:HD3	8:B:2026:HOH:O	2.15	0.47
1:E:95:LEU:CD1	8:E:2276:HOH:O	2.53	0.47
8:F:2075:HOH:O	3:G:72:ARG:HD3	2.15	0.47
3:G:20:HIS:CE1	3:G:59:ASP:OD2	2.67	0.47
1:E:523:ARG:HG2	1:E:523:ARG:HH11	1.80	0.47
1:E:680:VAL:HG22	1:E:714:ALA:HB2	1.97	0.47
2:F:87:PRO:HB3	2:F:112:TYR:CD1	2.50	0.47
1:A:647:ASN:HD21	1:A:713:GLY:HA3	1.80	0.46
3:C:76:HIS:O	3:C:79:LEU:HB2	2.15	0.46
1:E:196:ASP:OD1	1:E:360:PRO:HA	2.14	0.46
1:E:462:TYR:CD2	1:E:476:ALA:HA	2.50	0.46
3:G:142:LEU:HD21	3:G:197:ALA:O	2.14	0.46
1:A:263:ALA:HB2	1:A:301:ALA:HB2	1.96	0.46
1:A:358:GLY:N	1:A:363:PHE:O	2.46	0.46
1:A:717:ASN:HA	1:A:720:GLN:OE1	2.15	0.46
3:C:128:LEU:HA	8:C:2049:HOH:O	2.15	0.46
1:E:606:PRO:HG2	1:E:607:VAL:H	1.79	0.46
1:E:621:LEU:HD22	1:E:622:LEU:N	2.30	0.46
1:A:117:TRP:CE2	1:A:516:LYS:HG3	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLU:CD	1:A:118:GLU:N	2.72	0.46
1:A:209:HIS:CD2	1:A:209:HIS:H	2.33	0.46
1:A:396:HIS:CD2	1:A:403:PRO:CB	2.98	0.46
3:C:79:LEU:HD21	7:C:1252:UQ1:C7	2.45	0.46
1:E:106:GLN:NE2	8:E:2062:HOH:O	2.49	0.46
1:E:491:ASP:OD1	1:E:492:PHE:N	2.48	0.46
8:E:2383:HOH:O	2:F:49:LEU:CD1	2.60	0.46
1:A:482:GLU:HG2	1:A:483:ALA:N	2.30	0.46
1:A:555:LEU:HD23	1:A:555:LEU:HA	1.72	0.46
3:C:145:ASN:OD1	3:C:193:THR:HG23	2.16	0.46
1:E:113:ARG:CB	8:E:2042:HOH:O	2.63	0.46
1:E:500:PRO:CD	1:E:567:ARG:O	2.64	0.46
8:F:2028:HOH:O	3:G:250:LEU:HD12	2.14	0.46
1:A:107:ARG:O	1:A:457:LYS:HE3	2.16	0.46
1:A:264:TRP:CZ2	1:A:315:VAL:HG11	2.50	0.46
1:A:389:SER:HA	1:A:595:GLN:NE2	2.30	0.46
2:B:117:THR:HG22	2:B:120:ALA:H	1.77	0.46
3:C:166:LEU:HD21	3:C:228:PRO:HB2	1.98	0.46
1:E:708:LEU:O	1:E:712:ARG:CD	2.62	0.46
2:F:54:ARG:NH1	2:F:56:GLU:OE2	2.41	0.46
3:G:16:THR:CG2	3:G:66:GLU:HB2	2.45	0.46
1:A:225:ALA:C	1:A:230:ALA:HB3	2.41	0.46
1:A:666:TYR:CE1	1:A:681:ARG:HG3	2.51	0.46
1:A:712:ARG:NH1	8:A:2346:HOH:O	2.47	0.46
1:E:333:HIS:HB2	5:E:1766:MGD:S12	2.55	0.46
1:E:346:ALA:HB2	1:E:605:LEU:HD12	1.97	0.46
1:E:423:PRO:O	1:E:427:GLY:HA2	2.16	0.46
1:E:761:ASP:C	1:E:763:ARG:H	2.21	0.46
3:G:19:LEU:HD23	3:G:19:LEU:O	2.15	0.46
3:G:50:LEU:O	3:G:51:TYR:CD2	2.69	0.46
1:A:502:ILE:N	1:A:564:LEU:O	2.44	0.46
1:A:602:HIS:CE1	1:A:606:PRO:CD	2.97	0.46
1:E:64:LYS:HD2	8:E:2046:HOH:O	2.15	0.46
1:E:525:LEU:O	1:E:529:LEU:HG	2.16	0.46
1:E:537:TRP:CD1	1:E:537:TRP:H	2.34	0.46
1:A:122:ASP:CB	8:A:2068:HOH:O	2.63	0.46
1:A:523:ARG:HG2	1:A:523:ARG:HH11	1.80	0.46
1:A:650:TRP:O	1:A:693:VAL:HA	2.15	0.46
2:B:35:ASN:ND2	2:B:106:TYR:OH	2.49	0.46
3:C:31:VAL:HG12	3:C:53:ALA:HB2	1.98	0.46
3:C:193:THR:HG23	3:C:193:THR:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:ARG:HD2	1:E:220:GLN:NE2	2.24	0.46
1:E:201:ARG:NH2	1:E:228:ASN:O	2.37	0.46
1:E:249:TRP:CZ2	1:E:251:PRO:HB3	2.50	0.46
1:E:604:PRO:C	1:E:605:LEU:HD23	2.28	0.46
2:F:52:GLU:CD	2:F:187:THR:HB	2.40	0.46
3:G:23:LEU:HD22	3:G:62:ILE:HD12	1.98	0.46
3:G:46:ARG:CG	8:G:2014:HOH:O	2.59	0.46
3:G:92:ALA:HB2	7:G:1251:UQ1:H8	1.98	0.46
3:G:134:LEU:N	8:G:2034:HOH:O	2.48	0.46
1:A:231:LYS:HB3	1:A:231:LYS:HE3	1.60	0.46
1:A:284:VAL:N	1:A:588:GLY:O	2.32	0.46
1:A:339:ASP:CB	1:A:607:VAL:HG11	2.38	0.46
1:A:538:LYS:HE2	1:A:538:LYS:N	2.30	0.46
3:C:153:PRO:HB3	8:C:2063:HOH:O	2.14	0.46
3:C:215:LEU:O	3:C:216:LEU:C	2.58	0.46
1:E:282:TYR:C	1:E:587:SER:HB3	2.40	0.46
1:E:413:ARG:NH1	1:E:413:ARG:H	2.14	0.46
1:E:466:ASP:OD1	1:E:473:VAL:HG21	2.16	0.46
1:E:576:GLU:C	1:E:578:GLU:N	2.72	0.46
1:E:604:PRO:O	1:E:606:PRO:HD2	2.13	0.46
3:G:223:GLU:N	8:G:2068:HOH:O	2.47	0.46
1:A:42:GLN:OE1	1:A:506:THR:O	2.34	0.46
1:A:189:ILE:O	1:A:194:PRO:HD3	2.16	0.46
1:A:275:ASP:C	1:A:275:ASP:OD1	2.59	0.46
1:A:504:LEU:HD22	1:A:505:ARG:N	2.30	0.46
1:A:536:PRO:HG2	1:A:537:TRP:N	2.29	0.46
1:A:647:ASN:O	1:A:648:GLU:HG3	2.16	0.46
3:C:130:TYR:CZ	7:C:1252:UQ1:O4	2.63	0.46
3:C:220:THR:HA	3:C:227:ALA:HA	1.97	0.46
1:E:45:GLU:HB2	1:E:485:TYR:HB3	1.96	0.46
1:E:209:HIS:CE1	1:E:625:ARG:N	2.71	0.46
1:E:237:PRO:CB	1:E:689:ARG:HD3	2.46	0.46
1:A:113:ARG:CZ	8:A:2063:HOH:O	2.65	0.45
1:A:116:THR:HG23	1:A:118:GLU:OE1	2.16	0.45
1:A:252:ILE:HD11	1:A:256:THR:HG22	1.94	0.45
1:A:253:LYS:NZ	1:A:613:GLU:OE2	2.34	0.45
1:A:753:THR:HG22	1:A:757:LYS:CE	2.46	0.45
3:C:155:THR:CG2	3:C:239:ARG:CD	2.94	0.45
2:F:117:THR:HB	8:F:2011:HOH:O	2.14	0.45
3:G:100:LEU:O	3:G:103:GLY:N	2.47	0.45
3:G:144:ASN:C	3:G:144:ASN:ND2	2.74	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLY:HA2	1:A:438:TYR:O	2.16	0.45
1:A:224:LEU:HB3	8:A:2124:HOH:O	2.16	0.45
1:A:266:HIS:HB2	1:A:293:VAL:HG13	1.97	0.45
2:B:54:ARG:NH2	2:B:187:THR:O	2.46	0.45
1:E:335:VAL:CG1	1:E:335:VAL:O	2.64	0.45
1:E:533:GLN:O	1:E:536:PRO:HD3	2.17	0.45
1:A:453:LYS:HB3	1:A:475:TRP:CH2	2.51	0.45
3:C:173:LEU:O	3:C:177:ARG:HG3	2.16	0.45
1:E:45:GLU:HB2	1:E:485:TYR:CB	2.47	0.45
1:E:51:CYS:SG	1:E:216:ASN:HB3	2.57	0.45
1:E:255:GLY:HA2	1:E:337:TYR:CE1	2.52	0.45
1:E:594:CYS:O	1:E:598:LYS:HB2	2.16	0.45
2:F:1:MET:HE2	2:F:1:MET:HB2	1.87	0.45
2:F:178:LEU:O	2:F:180:ALA:N	2.48	0.45
1:A:412:ALA:HB2	1:A:728:ILE:O	2.15	0.45
1:A:569:LYS:HA	1:A:570:PRO:HD3	1.71	0.45
1:A:630:THR:O	1:A:631:PHE:C	2.60	0.45
1:A:734:LEU:C	1:A:736:VAL:H	2.24	0.45
2:B:143:GLY:N	2:B:152:VAL:CG2	2.79	0.45
1:E:50:ARG:HD2	8:E:2013:HOH:O	2.16	0.45
1:E:97:ARG:HH21	1:E:763:ARG:HD2	1.77	0.45
1:E:183:TRP:CD1	1:E:593:TYR:CE1	3.04	0.45
1:E:422:GLU:HB2	8:E:2253:HOH:O	2.16	0.45
1:E:702:LYS:HE3	1:E:718:TYR:CE2	2.51	0.45
1:A:66:GLU:HB3	8:A:2016:HOH:O	2.16	0.45
1:A:265:ILE:CG2	1:A:293:VAL:HG21	2.46	0.45
1:A:349:TYR:CZ	1:A:590:ILE:O	2.69	0.45
1:A:604:PRO:HA	1:A:605:LEU:HD23	1.98	0.45
2:B:50:VAL:CG1	2:B:181:PRO:HB2	2.47	0.45
1:E:75:ARG:NH1	1:E:220:GLN:NE2	2.55	0.45
1:E:422:GLU:N	1:E:423:PRO:CD	2.79	0.45
1:E:636:ASN:HB2	1:E:706:MET:HE2	1.98	0.45
1:A:390:GLY:N	1:A:391:PRO:HD3	2.31	0.45
1:A:596:ARG:NH1	1:A:600:ALA:HB1	2.30	0.45
1:E:187:ARG:NH1	8:E:2108:HOH:O	2.46	0.45
1:E:275:ASP:C	1:E:275:ASP:OD1	2.56	0.45
1:A:532:GLU:HB3	8:A:2253:HOH:O	2.16	0.45
1:A:533:GLN:HE21	1:A:533:GLN:H	1.65	0.45
1:A:602:HIS:CD2	1:A:603:GLN:H	2.35	0.45
2:B:160:GLU:N	2:B:179:ASN:ND2	2.52	0.45
3:C:128:LEU:CD2	3:C:156:ALA:HB3	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:345:MET:HB3	1:E:605:LEU:HD11	1.98	0.45
1:E:604:PRO:CA	1:E:605:LEU:HD23	2.47	0.45
1:E:633:ARG:HB2	5:E:1765:MGD:H2'	1.99	0.45
2:F:10:LEU:HD22	2:F:53:PHE:O	2.16	0.45
3:G:53:LEU:HB2	8:G:2015:HOH:O	2.17	0.45
1:A:142:PHE:O	1:A:165:ALA:HA	2.17	0.45
3:C:128:LEU:HD23	3:C:156:ALA:CB	2.47	0.45
1:E:315:VAL:O	1:E:319:MET:HG2	2.17	0.45
1:E:588:GLY:HA3	8:E:2107:HOH:O	2.17	0.45
1:E:604:PRO:C	1:E:605:LEU:CD2	2.79	0.45
2:F:191:GLU:HB2	8:F:2123:HOH:O	2.17	0.45
3:G:46:ARG:NH1	3:G:106:TYR:O	2.50	0.45
1:A:41:TYR:HD1	1:A:559:LYS:O	1.98	0.45
1:A:220:GLN:HA	2:B:136:PRO:O	2.16	0.45
1:A:319:MET:HE1	1:A:328:LEU:CD1	2.45	0.45
1:A:523:ARG:HG2	1:A:523:ARG:NH1	2.31	0.45
2:B:166:ARG:HD2	8:B:2124:HOH:O	2.16	0.45
2:B:192:VAL:CG1	2:B:193:HIS:H	2.30	0.45
1:E:115:ALA:HB1	1:E:119:GLU:HG2	1.98	0.45
1:E:183:TRP:CG	1:E:593:TYR:CD1	3.05	0.45
1:E:257:ASP:OD2	5:E:1766:MGD:N1	2.41	0.45
1:E:278:TYR:OH	1:E:357:TYR:HB3	2.17	0.45
1:E:590:ILE:HG22	1:E:591:GLU:N	2.31	0.45
1:E:726:ASP:O	1:E:729:SER:O	2.34	0.45
2:F:101:PRO:HD2	2:F:102:TYR:CD1	2.52	0.45
3:G:214:LEU:O	3:G:217:LEU:HB2	2.17	0.45
1:A:60:ASN:HB2	8:A:2021:HOH:O	2.16	0.45
1:A:80:PRO:HG2	1:A:627:PRO:O	2.16	0.45
1:A:197:TRP:HB2	1:A:221:ASP:HB3	1.98	0.45
1:A:683:LYS:HA	1:A:684:PRO:HD2	1.63	0.45
8:B:2025:HOH:O	3:C:251:LEU:CD1	2.63	0.45
1:E:388:CYS:O	1:E:389:SER:C	2.59	0.45
1:E:427:GLY:O	1:E:428:GLU:O	2.35	0.45
1:E:606:PRO:HD2	1:E:607:VAL:H	1.80	0.45
3:G:206:GLY:O	3:G:209:TYR:HB3	2.16	0.45
1:A:65:VAL:CG1	1:A:78:LEU:CD2	2.94	0.44
1:A:327:VAL:HG13	1:A:362:GLY:HA3	1.99	0.44
1:A:428:GLU:OE2	1:A:428:GLU:HA	1.94	0.44
1:A:655:GLU:OE2	1:A:658:ARG:NH2	2.49	0.44
1:A:657:LYS:O	1:A:659:LEU:O	2.34	0.44
3:C:17:THR:HG21	8:C:2014:HOH:O	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:LEU:HD22	7:C:1252:UQ1:H102	1.99	0.44
1:E:127:LYS:HD3	8:E:2083:HOH:O	2.17	0.44
1:E:707:ARG:NE	8:E:2403:HOH:O	2.48	0.44
1:A:73:LYS:HG3	1:A:501:PHE:HZ	1.81	0.44
1:A:183:TRP:NE1	1:A:413:ARG:HH22	2.04	0.44
1:A:648:GLU:HG2	1:A:681:ARG:NH1	2.33	0.44
2:B:130:ALA:HB3	4:B:1195:SF4:S2	2.57	0.44
2:B:167:PRO:O	2:B:169:GLN:O	2.36	0.44
2:B:183:LYS:NZ	2:F:157:LYS:O	2.50	0.44
3:C:108:LEU:HB3	3:C:110:LYS:CG	2.47	0.44
1:E:47:CYS:HB3	1:E:81:ARG:HH12	1.81	0.44
3:G:223:GLU:C	3:G:225:LEU:H	2.25	0.44
1:A:192:HIS:O	1:A:193:GLU:C	2.60	0.44
1:A:371:LEU:HG	1:A:502:ILE:HD13	1.98	0.44
1:A:541:GLU:HB2	1:A:555:LEU:HD12	1.99	0.44
1:A:638:TRP:HB2	1:A:756:ALA:HB2	2.00	0.44
1:A:727:PRO:HA	8:A:2197:HOH:O	2.16	0.44
1:E:114:VAL:HG21	8:E:2054:HOH:O	2.17	0.44
1:E:128:MET:HE1	1:E:529:LEU:HD11	1.98	0.44
1:E:138:GLU:OE2	1:E:402:LYS:HB2	2.16	0.44
1:E:403:PRO:O	1:E:430:TYR:OH	2.33	0.44
1:E:664:GLY:N	8:E:2372:HOH:O	2.46	0.44
2:F:82:LEU:HD12	2:F:84:LEU:HD11	1.98	0.44
2:F:132:VAL:HA	2:F:140:ARG:HG3	2.00	0.44
1:A:133:GLU:HG3	8:A:2074:HOH:O	2.17	0.44
1:E:74:SER:HB2	1:E:77:ARG:O	2.18	0.44
1:E:252:ILE:CD1	1:E:256:THR:HG22	2.48	0.44
1:E:730:GLY:N	8:E:2251:HOH:O	2.43	0.44
2:F:79:LYS:HD2	2:F:79:LYS:HA	1.72	0.44
1:A:394:GLY:CA	8:A:2188:HOH:O	2.65	0.44
1:A:418:GLN:H	1:A:418:GLN:HG3	1.39	0.44
1:A:447:PRO:HD3	8:A:2212:HOH:O	2.17	0.44
1:A:471:GLU:HB2	1:A:702:LYS:O	2.17	0.44
2:B:9:ASP:HA	2:B:178:LEU:HB2	1.99	0.44
2:B:172:ARG:HD3	8:F:2127:HOH:O	2.18	0.44
1:E:159:ALA:O	1:E:380:PRO:HG2	2.17	0.44
1:E:274:TYR:HA	1:E:323:LYS:NZ	2.33	0.44
1:E:336:TRP:HB3	1:E:735:ARG:HD2	2.00	0.44
1:E:642:GLU:OE2	2:F:31:PRO:HA	2.17	0.44
2:F:46:TYR:HB2	8:F:2033:HOH:O	2.17	0.44
1:A:252:ILE:HG13	1:A:307:ILE:CD1	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:ARG:NH1	2:B:187:THR:HG23	2.16	0.44
2:B:46:TYR:HE2	8:B:2035:HOH:O	1.91	0.44
2:B:78:THR:CG2	2:B:80:ASP:H	2.29	0.44
3:C:128:LEU:HD23	3:C:156:ALA:HB3	1.99	0.44
3:C:161:LEU:HD12	3:C:179:LEU:HD12	1.99	0.44
3:C:207:GLY:O	3:C:211:GLY:N	2.50	0.44
1:E:103:GLU:HG2	1:E:104:GLY:N	2.33	0.44
1:E:510:GLU:O	1:E:511:PRO:C	2.60	0.44
1:E:647:ASN:C	1:E:648:GLU:CG	2.91	0.44
3:G:23:LEU:CD2	3:G:62:ILE:HD12	2.48	0.44
3:G:199:GLY:O	3:G:203:GLU:HG3	2.18	0.44
1:A:38:LYS:HG2	8:A:2020:HOH:O	2.17	0.44
1:A:214:THR:HG21	1:A:627:PRO:O	2.18	0.44
1:A:596:ARG:CZ	1:A:600:ALA:CB	2.95	0.44
1:A:638:TRP:HB2	1:A:756:ALA:CB	2.47	0.44
2:B:61:CYS:HB3	2:B:171:THR:O	2.17	0.44
1:E:349:TYR:CE1	1:E:605:LEU:HD11	2.52	0.44
1:E:512:LEU:O	1:E:513:PHE:HB2	2.18	0.44
1:E:557:THR:O	1:E:561:MET:HG3	2.18	0.44
1:E:569:LYS:HB2	1:E:575:TRP:HE1	1.83	0.44
1:E:630:THR:O	1:E:631:PHE:O	2.34	0.44
1:E:757:LYS:O	1:E:758:ARG:C	2.61	0.44
3:G:81:SER:HB2	3:G:83:HIS:CD2	2.53	0.44
1:A:638:TRP:HB3	1:A:708:LEU:HD11	1.99	0.44
1:A:655:GLU:CD	1:A:658:ARG:NH2	2.75	0.44
2:B:116:CYS:HA	4:B:1195:SF4:S1	2.57	0.44
3:C:111:GLY:O	3:C:116:LEU:HD11	2.17	0.44
1:E:371:LEU:HD11	1:E:492:PHE:CD1	2.53	0.44
1:E:569:LYS:HB2	1:E:575:TRP:NE1	2.33	0.44
1:E:607:VAL:HG22	1:E:609:THR:OG1	2.18	0.44
2:F:106:TYR:CZ	2:F:114:SER:HB3	2.53	0.44
3:G:29:GLY:HA3	3:G:159:ALA:HB2	1.99	0.44
1:A:142:PHE:CG	1:A:157:PRO:HG3	2.53	0.44
1:A:339:ASP:CB	1:A:607:VAL:CG1	2.95	0.44
1:A:371:LEU:HD13	1:A:547:ARG:CZ	2.47	0.44
1:A:403:PRO:O	1:A:404:ARG:C	2.60	0.44
1:A:548:LEU:HD23	1:A:548:LEU:HA	1.72	0.44
1:A:669:LEU:HB3	1:A:739:VAL:HG21	2.00	0.44
2:B:7:ALA:HB3	2:B:141:THR:OG1	2.18	0.44
2:B:169:GLN:NE2	8:B:2128:HOH:O	2.33	0.44
3:C:171:TRP:O	3:C:171:TRP:HE3	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:HIS:HE1	1:E:605:LEU:O	2.01	0.44
1:E:510:GLU:HG3	1:E:510:GLU:H	1.46	0.44
1:E:512:LEU:HD12	1:E:512:LEU:HA	1.71	0.44
1:E:630:THR:HA	5:E:1766:MGD:O17	2.17	0.44
2:F:78:THR:HG23	2:F:79:LYS:N	2.32	0.44
1:A:302:GLU:O	1:A:302:GLU:HG3	2.17	0.43
1:A:607:VAL:C	1:A:609:THR:N	2.71	0.43
1:A:625:ARG:HD2	5:A:1766:MGD:C17	2.48	0.43
1:A:632:ALA:HB3	5:A:1765:MGD:O1B	2.17	0.43
1:E:412:ALA:CB	1:E:413:ARG:HH12	2.30	0.43
1:E:683:LYS:O	1:E:683:LYS:HG2	2.16	0.43
2:F:44:GLY:O	2:F:45:GLU:CB	2.66	0.43
1:A:278:TYR:OH	1:A:357:TYR:HB3	2.18	0.43
1:A:648:GLU:HG2	1:A:681:ARG:HH12	1.82	0.43
1:A:693:VAL:HG21	1:A:741:LEU:HD21	1.99	0.43
1:A:717:ASN:HD22	5:A:1765:MGD:H192	1.65	0.43
2:B:8:ILE:HD13	2:B:55:PRO:HG2	1.99	0.43
2:B:18:ALA:HB3	4:B:1194:SF4:S2	2.58	0.43
2:B:35:ASN:HB3	2:B:116:CYS:HB2	2.00	0.43
2:B:106:TYR:CZ	2:B:114:SER:HB3	2.53	0.43
2:B:142:PHE:C	2:B:152:VAL:CG2	2.90	0.43
5:E:1766:MGD:H8	8:E:2425:HOH:O	2.18	0.43
2:F:46:TYR:CG	2:F:47:PRO:N	2.83	0.43
3:G:133:ALA:HB3	8:G:2034:HOH:O	2.19	0.43
1:A:220:GLN:HG2	2:B:136:PRO:O	2.17	0.43
2:B:38:ILE:HD12	4:B:1194:SF4:S1	2.58	0.43
3:C:20:LEU:HD13	3:C:63:ILE:CD1	2.48	0.43
3:C:145:ASN:HD21	3:C:147:LEU:HB2	1.83	0.43
1:E:278:TYR:O	1:E:279:VAL:C	2.61	0.43
1:E:553:LEU:HA	1:E:553:LEU:HD23	1.72	0.43
2:F:184:LYS:HE2	8:F:2121:HOH:O	2.19	0.43
3:G:79:PHE:CZ	7:G:1251:UQ1:H103	2.52	0.43
1:A:116:THR:CG2	1:A:119:GLU:N	2.60	0.43
1:A:137:PRO:HD2	1:A:138:GLU:OE1	2.18	0.43
1:A:501:PHE:CA	1:A:564:LEU:O	2.67	0.43
1:A:597:PHE:HB3	1:A:598:LYS:H	1.61	0.43
2:B:1:MET:O	2:B:146:GLU:OE1	2.36	0.43
1:E:187:ARG:HB3	1:E:188:PRO:CD	2.48	0.43
1:E:613:GLU:HB3	1:E:614:PRO:HD2	2.00	0.43
3:G:222:GLN:CB	8:G:2068:HOH:O	2.67	0.43
1:A:65:VAL:HG13	1:A:78:LEU:CD2	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:LEU:O	2:B:166:ARG:C	2.61	0.43
3:C:25:VAL:HB	3:C:60:ASP:OD2	2.19	0.43
3:C:77:ILE:HG12	3:C:81:LEU:CD1	2.47	0.43
3:C:209:TRP:CD1	8:C:2082:HOH:O	2.71	0.43
1:E:115:ALA:HB1	1:E:119:GLU:CG	2.49	0.43
1:E:457:LYS:CD	8:E:2064:HOH:O	2.66	0.43
1:E:457:LYS:HD3	8:E:2064:HOH:O	2.17	0.43
1:E:717:ASN:ND2	8:E:2414:HOH:O	2.51	0.43
2:F:175:LEU:C	2:F:175:LEU:CD1	2.91	0.43
3:G:178:LEU:HD23	3:G:178:LEU:HA	1.81	0.43
1:A:39:SER:CB	8:A:2005:HOH:O	2.63	0.43
1:A:161:GLY:C	1:A:381:LEU:HD11	2.43	0.43
1:A:181:SER:HB2	1:A:189:ILE:HD12	2.01	0.43
1:A:335:VAL:O	1:A:337:TYR:N	2.51	0.43
1:A:539:THR:HG21	1:A:541:GLU:HG2	2.00	0.43
1:A:717:ASN:ND2	5:A:1765:MGD:H192	2.17	0.43
1:E:69:GLU:HA	1:E:75:ARG:HA	1.99	0.43
1:E:133:GLU:HB2	8:E:2087:HOH:O	2.18	0.43
1:E:252:ILE:HD11	1:E:256:THR:HG22	1.99	0.43
1:E:281:LYS:HG3	1:E:282:TYR:CD1	2.54	0.43
1:E:422:GLU:N	1:E:423:PRO:HD2	2.33	0.43
1:E:494:LEU:CD2	1:E:502:ILE:HG12	2.38	0.43
3:G:206:GLY:N	3:G:209:TYR:HB2	2.34	0.43
1:A:435:LEU:N	1:A:461:LEU:O	2.51	0.43
2:B:41:ARG:CD	2:B:187:THR:CG2	2.75	0.43
3:C:51:LEU:O	3:C:54:LEU:HB2	2.19	0.43
3:C:79:LEU:HD12	3:C:79:LEU:HA	1.84	0.43
1:E:100:ILE:HA	1:E:478:VAL:HG22	2.00	0.43
1:E:472:HIS:HE1	8:E:2262:HOH:O	2.02	0.43
1:E:534:TYR:C	1:E:536:PRO:HD3	2.43	0.43
1:E:598:LYS:N	8:E:2325:HOH:O	2.51	0.43
1:E:609:THR:O	1:E:610:PRO:C	2.60	0.43
1:E:633:ARG:CD	5:E:1765:MGD:O2B	2.66	0.43
3:G:38:HIS:CE1	3:G:105:LEU:HD13	2.53	0.43
3:G:63:LEU:HD22	7:G:1251:UQ1:C3	2.49	0.43
1:A:137:PRO:HB2	1:A:160:TRP:NE1	2.34	0.43
1:A:394:GLY:HA2	8:A:2189:HOH:O	2.18	0.43
1:A:395:ASP:CA	1:A:399:GLU:CG	2.63	0.43
1:A:635:GLN:HG2	1:A:635:GLN:H	1.32	0.43
3:C:241:LEU:HD12	3:C:242:LEU:N	2.33	0.43
1:E:466:ASP:OD1	1:E:473:VAL:CG2	2.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:29:VAL:HA	2:F:30:PRO:HD3	1.64	0.43
3:G:176:ARG:O	3:G:220:PHE:HE2	2.02	0.43
1:A:573:GLU:HG2	8:A:2271:HOH:O	2.18	0.43
1:A:592:LEU:CD1	1:A:592:LEU:C	2.92	0.43
3:C:207:GLY:C	3:C:209:TRP:H	2.26	0.43
1:E:274:TYR:H	1:E:274:TYR:HD2	1.64	0.43
1:E:346:ALA:CA	1:E:605:LEU:HD12	2.49	0.43
1:E:569:LYS:H	1:E:569:LYS:HG2	1.45	0.43
1:E:620:ARG:HD3	1:E:735:ARG:O	2.18	0.43
2:F:71:PRO:HB2	3:G:78:LEU:HD12	2.00	0.43
1:A:118:GLU:HG3	8:A:2252:HOH:O	2.18	0.43
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.88	0.43
1:A:523:ARG:HA	1:A:535:PHE:CD2	2.54	0.43
1:A:572:LEU:O	1:A:576:GLU:HB2	2.18	0.43
1:A:581:LEU:HD23	1:A:583:PHE:CE1	2.54	0.43
1:A:642:GLU:CD	2:B:31:PRO:O	2.62	0.43
3:C:40:LEU:HD13	3:C:117:ALA:CB	2.48	0.43
1:E:64:LYS:HE3	2:F:26:GLU:HB2	2.01	0.43
1:E:226:LEU:HD23	1:E:226:LEU:HA	1.86	0.43
1:E:286:PHE:C	1:E:288:GLU:N	2.76	0.43
1:E:305:THR:CG2	1:E:307:ILE:HB	2.49	0.43
1:E:630:THR:HA	5:E:1766:MGD:H18	1.84	0.43
2:B:25:MET:CE	2:B:25:MET:CA	2.81	0.42
2:B:64:PRO:O	2:B:68:PRO:HD2	2.18	0.42
1:E:206:ILE:CD1	1:E:261:LEU:HD21	2.48	0.42
1:E:548:LEU:HD12	1:E:555:LEU:HA	2.00	0.42
1:E:630:THR:C	1:E:631:PHE:O	2.62	0.42
1:A:87:GLN:HG3	1:A:637:ASN:ND2	2.34	0.42
1:A:394:GLY:N	8:A:2188:HOH:O	2.53	0.42
1:E:195:ILE:HD13	1:E:363:PHE:CE2	2.54	0.42
1:E:495:VAL:HG13	8:E:2018:HOH:O	2.18	0.42
1:E:622:LEU:O	1:E:623:TYR:HB3	2.19	0.42
2:F:46:TYR:CD2	2:F:47:PRO:HD3	2.54	0.42
2:F:59:LEU:HD13	2:F:173:PRO:HB3	2.01	0.42
1:A:108:GLY:C	1:A:109:GLU:O	2.57	0.42
1:A:519:TRP:CG	1:A:540:ILE:HG23	2.54	0.42
1:E:117:TRP:CE2	1:E:516:LYS:CG	3.02	0.42
1:E:391:PRO:C	1:E:413:ARG:HG3	2.44	0.42
1:E:441:ASN:HD21	1:E:444:HIS:HD2	1.68	0.42
1:E:604:PRO:CA	1:E:605:LEU:CD2	2.97	0.42
2:F:35:ASN:ND2	2:F:106:TYR:OH	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:221:TRP:CZ3	3:G:225:LEU:HD13	2.44	0.42
1:A:327:VAL:CG1	1:A:362:GLY:HA3	2.49	0.42
3:C:11:GLN:NE2	3:C:11:GLN:H	2.18	0.42
1:E:614:PRO:HA	1:E:615:PRO:HD3	1.89	0.42
1:E:658:ARG:HB3	1:E:658:ARG:NH1	2.34	0.42
1:E:734:LEU:C	1:E:736:VAL:H	2.27	0.42
3:G:217:LEU:CD2	8:G:2063:HOH:O	2.67	0.42
1:A:499:THR:O	1:A:499:THR:OG1	2.37	0.42
1:A:535:PHE:N	1:A:536:PRO:HD3	2.34	0.42
1:A:743:LYS:CG	8:A:2365:HOH:O	2.68	0.42
1:E:173:CYS:HG	6:E:1767:MO:MO	1.56	0.42
1:E:297:THR:CG2	1:E:299:GLU:N	2.69	0.42
1:E:591:GLU:OE2	1:E:604:PRO:CB	2.67	0.42
1:E:745:GLU:HG3	8:E:2430:HOH:O	2.19	0.42
3:G:17:ASN:HB2	8:G:2010:HOH:O	2.19	0.42
3:G:58:LEU:HD12	3:G:58:LEU:O	2.20	0.42
3:G:70:ARG:HG3	3:G:71:PHE:CD2	2.54	0.42
1:A:81:ARG:HD2	1:A:630:THR:OG1	2.19	0.42
3:C:79:LEU:CD2	7:C:1252:UQ1:C8	2.98	0.42
3:C:169:SER:HA	3:C:170:PRO:HD3	1.82	0.42
1:E:151:TRP:O	1:E:156:LEU:HB3	2.19	0.42
1:E:673:ASP:OD2	1:E:721:THR:HG22	2.15	0.42
2:F:164:VAL:HG12	2:F:167:PRO:HB3	2.00	0.42
1:A:47:CYS:HB3	1:A:81:ARG:HH12	1.84	0.42
1:A:52:GLY:H	1:A:71:ASN:ND2	2.18	0.42
1:A:310:GLN:CG	8:A:2160:HOH:O	2.67	0.42
3:C:154:LEU:O	3:C:158:VAL:HG23	2.20	0.42
1:E:256:THR:HG23	1:E:256:THR:O	2.19	0.42
1:E:632:ALA:HB2	1:E:698:GLY:HA2	2.02	0.42
3:G:106:TYR:C	3:G:108:GLY:H	2.26	0.42
3:G:117:TRP:CB	8:G:2033:HOH:O	2.68	0.42
3:G:216:GLY:C	3:G:218:GLY:N	2.76	0.42
1:A:101:ARG:NH1	1:A:477:ASP:OD1	2.53	0.42
1:A:641:MET:CE	1:A:645:PRO:HA	2.50	0.42
1:A:644:ASP:HA	1:A:645:PRO:HD3	1.67	0.42
3:C:125:LEU:HD23	3:C:125:LEU:HA	1.87	0.42
1:E:46:GLY:O	1:E:630:THR:HG21	2.19	0.42
1:E:160:TRP:O	1:E:160:TRP:CD1	2.73	0.42
1:E:177:ARG:NH1	1:E:332:ARG:HA	2.35	0.42
1:E:548:LEU:HD23	1:E:548:LEU:HA	1.76	0.42
1:E:602:HIS:CE1	1:E:606:PRO:CD	3.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:154:THR:HG21	3:G:238:ARG:CG	2.45	0.42
3:G:184:LEU:O	3:G:188:LEU:HG	2.20	0.42
1:A:205:LEU:HB3	1:A:208:HIS:HB3	2.01	0.42
1:A:425:ILE:HD11	1:A:451:ARG:HG2	2.02	0.42
1:A:488:ARG:HD3	1:A:490:ASP:CG	2.45	0.42
2:B:12:LEU:HB2	2:B:139:CYS:HB3	2.01	0.42
2:B:22:ALA:CB	2:B:134:THR:HG21	2.47	0.42
1:E:412:ALA:CB	1:E:413:ARG:NH1	2.82	0.42
1:E:488:ARG:HG2	1:E:489:TYR:N	2.34	0.42
1:E:626:SER:O	1:E:628:VAL:N	2.52	0.42
1:E:629:HIS:HA	1:E:634:THR:HG21	2.00	0.42
2:F:135:CYS:HA	2:F:136:PRO:HD3	1.71	0.42
8:F:2052:HOH:O	3:G:88:ILE:HG13	2.19	0.42
3:G:142:LEU:HD23	3:G:197:ALA:HB1	2.02	0.42
3:G:165:LEU:HD22	3:G:224:ARG:HH11	1.83	0.42
1:A:82:GLY:HA3	4:A:1764:SF4:S3	2.60	0.42
1:A:333:HIS:O	1:A:336:TRP:NE1	2.51	0.42
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.87	0.42
1:A:591:GLU:HB3	1:A:603:GLN:HE21	1.76	0.42
1:A:678:GLY:N	8:A:2329:HOH:O	2.52	0.42
2:B:110:ALA:HB3	2:B:112:TYR:CE2	2.54	0.42
3:C:48:ARG:HH11	3:C:48:ARG:HD3	1.70	0.42
3:C:241:LEU:CD1	3:C:241:LEU:O	2.68	0.42
1:E:269:ILE:HG21	1:E:290:LYS:HG3	2.02	0.42
1:E:339:ASP:O	1:E:342:TYR:HB2	2.20	0.42
1:E:371:LEU:HD13	1:E:547:ARG:NH2	2.35	0.42
1:E:407:LYS:O	1:E:407:LYS:HG3	2.18	0.42
1:E:413:ARG:HH11	1:E:413:ARG:HD2	1.71	0.42
1:E:607:VAL:CG2	8:E:2145:HOH:O	2.61	0.42
8:F:2030:HOH:O	3:G:1:ALA:CB	2.66	0.42
1:A:71:ASN:ND2	1:A:74:SER:H	2.08	0.41
1:A:95:LEU:HG	1:A:467:VAL:O	2.20	0.41
1:A:346:ALA:CB	1:A:605:LEU:HD13	2.49	0.41
1:A:678:GLY:CA	8:A:2329:HOH:O	2.68	0.41
3:C:108:LEU:HB3	3:C:110:LYS:HD2	2.02	0.41
3:C:251:LEU:HD23	8:C:2087:HOH:O	2.20	0.41
1:E:87:GLN:OE1	1:E:637:ASN:HA	2.20	0.41
1:E:391:PRO:CD	1:E:595:GLN:OE1	2.68	0.41
1:E:604:PRO:CB	1:E:605:LEU:HD23	2.50	0.41
1:E:636:ASN:HB2	1:E:706:MET:CE	2.50	0.41
1:A:279:VAL:O	1:A:283:THR:HB	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:THR:CG2	8:A:2049:HOH:O	2.63	0.41
1:E:69:GLU:H	1:E:69:GLU:HG2	1.59	0.41
1:E:254:PRO:HG3	1:E:692:CYS:SG	2.60	0.41
3:G:124:LEU:HD23	3:G:124:LEU:HA	1.92	0.41
3:G:222:GLN:HB2	8:G:2068:HOH:O	2.20	0.41
1:A:283:THR:HA	1:A:588:GLY:O	2.20	0.41
1:A:335:VAL:HG13	1:A:733:GLY:N	2.35	0.41
1:A:498:LYS:HE3	8:A:2107:HOH:O	2.18	0.41
1:A:539:THR:HG22	1:A:542:GLU:H	1.85	0.41
1:A:723:TYR:CD1	1:A:732:ALA:HB1	2.56	0.41
3:C:109:GLY:C	3:C:110:LYS:HG2	2.44	0.41
1:E:310:GLN:O	1:E:314:GLU:HB2	2.20	0.41
3:G:78:LEU:HG	3:G:92:ALA:CB	2.50	0.41
3:G:146:LEU:HD23	3:G:146:LEU:HA	1.90	0.41
1:A:278:TYR:HD1	1:A:359:ARG:NH2	2.19	0.41
1:A:389:SER:HA	1:A:595:GLN:HE22	1.85	0.41
2:B:47:PRO:C	2:B:48:ASN:OD1	2.62	0.41
1:E:137:PRO:C	1:E:139:ALA:H	2.28	0.41
1:E:281:LYS:HE2	1:E:281:LYS:HB3	1.89	0.41
1:E:545:GLU:CD	1:E:555:LEU:HB2	2.45	0.41
1:E:651:ILE:O	1:E:684:PRO:O	2.39	0.41
2:F:24:LYS:NZ	2:F:30:PRO:O	2.53	0.41
2:F:67:VAL:CB	2:F:68:PRO:CD	2.97	0.41
2:F:117:THR:HG23	2:F:120:ALA:N	2.22	0.41
3:G:38:HIS:HE1	3:G:105:LEU:HD22	1.80	0.41
3:G:223:GLU:HB3	8:G:2069:HOH:O	2.19	0.41
1:A:342:TYR:CG	1:A:605:LEU:HA	2.56	0.41
1:A:722:ARG:HA	8:A:2352:HOH:O	2.20	0.41
2:B:128:VAL:HG11	8:B:2070:HOH:O	2.19	0.41
3:C:17:THR:HG22	3:C:67:GLU:HG3	1.91	0.41
3:C:18:ASN:O	3:C:21:HIS:HB3	2.21	0.41
3:C:163:LEU:O	3:C:167:LEU:HG	2.20	0.41
3:C:180:ALA:O	3:C:184:LEU:HG	2.21	0.41
1:E:77:ARG:NH2	2:F:138:TYR:CE2	2.88	0.41
1:E:160:TRP:CE3	1:E:529:LEU:HD13	2.55	0.41
1:E:595:GLN:HE21	1:E:595:GLN:HB2	1.48	0.41
3:G:52:ALA:O	3:G:56:ILE:CG1	2.68	0.41
1:A:371:LEU:HD23	1:A:371:LEU:HA	1.85	0.41
1:E:197:TRP:CD1	1:E:221:ASP:HB3	2.55	0.41
1:E:220:GLN:O	1:E:224:LEU:HB2	2.20	0.41
1:E:292:HIS:CD2	8:E:2084:HOH:O	2.71	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:430:TYR:HB2	1:E:431:PRO:CD	2.51	0.41
1:E:537:TRP:O	1:E:537:TRP:CE3	2.73	0.41
1:E:650:TRP:O	1:E:693:VAL:HA	2.20	0.41
1:E:651:ILE:CD1	1:E:656:ALA:HB2	2.49	0.41
3:G:97:LEU:HD23	3:G:97:LEU:HA	1.84	0.41
1:A:124:ILE:HG12	1:A:463:VAL:HG21	2.01	0.41
1:A:213:ASP:OD1	1:A:213:ASP:C	2.63	0.41
1:A:452:THR:O	1:A:456:LEU:HG	2.21	0.41
1:A:497:HIS:O	1:A:498:LYS:C	2.62	0.41
1:A:679:PRO:HG2	1:A:747:PRO:HB3	2.02	0.41
3:C:171:TRP:CE3	3:C:172:ALA:HB2	2.56	0.41
1:E:510:GLU:CG	8:E:2299:HOH:O	2.49	0.41
1:E:657:LYS:HE2	1:E:657:LYS:HB2	1.77	0.41
2:F:71:PRO:O	3:G:83:HIS:CD2	2.74	0.41
3:G:112:GLN:O	3:G:114:ALA:N	2.54	0.41
1:A:103:GLU:OE1	1:A:103:GLU:CA	2.69	0.41
1:A:123:HIS:CE1	8:A:2069:HOH:O	2.74	0.41
1:A:239:PHE:HB3	1:A:687:ARG:CB	2.49	0.41
1:A:519:TRP:CD2	1:A:540:ILE:CG2	3.03	0.41
1:A:539:THR:HG23	1:A:541:GLU:H	1.85	0.41
1:A:541:GLU:O	1:A:545:GLU:CG	2.69	0.41
3:C:64:LEU:HD23	7:C:1252:UQ1:HM22	2.03	0.41
1:E:183:TRP:HA	1:E:593:TYR:CE1	2.55	0.41
2:F:109:PRO:HG3	8:F:2014:HOH:O	2.19	0.41
1:A:37:VAL:HG12	1:A:38:LYS:H	1.83	0.41
1:A:81:ARG:HB2	4:A:1764:SF4:S1	2.61	0.41
1:A:213:ASP:OD2	1:A:218:GLN:NE2	2.53	0.41
1:A:427:GLY:C	1:A:430:TYR:O	2.63	0.41
1:A:498:LYS:HD2	8:A:2241:HOH:O	2.19	0.41
1:A:502:ILE:HD12	1:A:564:LEU:HD22	2.03	0.41
1:A:520:TRP:O	1:A:524:GLU:HG2	2.20	0.41
2:B:7:ALA:O	2:B:140:ARG:HA	2.21	0.41
2:B:10:LEU:HD22	2:B:53:PHE:O	2.21	0.41
2:B:48:ASN:ND2	2:F:157:LYS:HE2	2.36	0.41
2:B:72:THR:HG22	2:B:74:ALA:N	2.07	0.41
2:B:118:PHE:HD1	2:B:118:PHE:HA	1.63	0.41
3:C:66:ALA:O	3:C:71:ARG:NH1	2.54	0.41
1:E:100:ILE:HG12	1:E:478:VAL:CG1	2.51	0.41
1:E:403:PRO:O	1:E:404:ARG:C	2.62	0.41
2:F:81:GLY:O	2:F:174:LYS:NZ	2.47	0.41
2:F:86:ASP:OD1	2:F:88:LYS:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:118:PHE:HD1	2:F:118:PHE:HA	1.55	0.41
3:G:117:TRP:HB3	8:G:2033:HOH:O	2.21	0.41
3:G:165:LEU:HG	3:G:227:PRO:HB2	2.03	0.41
1:A:77:ARG:HD2	2:B:138:TYR:CE2	2.56	0.41
1:A:77:ARG:HH12	2:B:138:TYR:HE2	1.54	0.41
1:A:155:PHE:O	1:A:156:LEU:C	2.64	0.41
1:A:261:LEU:HD22	1:A:347:LEU:HA	2.03	0.41
1:A:269:ILE:HG21	1:A:290:LYS:HG3	2.02	0.41
1:A:546:THR:O	1:A:549:GLN:HB2	2.21	0.41
1:A:591:GLU:OE2	1:A:604:PRO:HG2	2.11	0.41
1:A:677:GLU:O	1:A:678:GLY:C	2.62	0.41
1:E:64:LYS:NZ	1:E:66:GLU:OE1	2.54	0.41
1:E:97:ARG:NH2	1:E:763:ARG:HH11	2.18	0.41
1:E:417:ILE:HG23	1:E:418:GLN:N	2.36	0.41
3:G:24:VAL:CG2	3:G:95:LEU:HD11	2.51	0.41
3:G:38:HIS:O	3:G:40:LYS:N	2.54	0.41
1:A:62:VAL:HG21	1:A:486:LEU:HD22	2.03	0.40
1:A:477:ASP:HB3	8:A:2069:HOH:O	2.20	0.40
1:A:510:GLU:HG3	1:A:510:GLU:H	1.62	0.40
2:B:78:THR:HB	2:B:82:LEU:O	2.21	0.40
2:B:101:PRO:HA	3:C:249:GLN:HE22	1.84	0.40
1:E:47:CYS:HB3	1:E:81:ARG:NH1	2.36	0.40
1:E:122:ASP:OD1	1:E:528:ARG:HD3	2.21	0.40
1:E:322:HIS:O	1:E:323:LYS:O	2.38	0.40
1:E:342:TYR:HD1	1:E:607:VAL:CG1	2.34	0.40
1:E:421:ILE:O	1:E:421:ILE:HG22	2.18	0.40
2:F:34:PHE:H	3:G:8:ASN:HD21	1.69	0.40
1:A:39:SER:HA	1:A:55:ALA:O	2.21	0.40
1:A:177:ARG:HA	1:A:344:VAL:HG11	2.03	0.40
1:A:293:VAL:HA	1:A:296:PHE:CD1	2.57	0.40
1:A:412:ALA:CB	1:A:728:ILE:O	2.69	0.40
1:A:552:GLY:O	8:A:2261:HOH:O	2.22	0.40
1:A:685:THR:CG2	8:B:2028:HOH:O	2.68	0.40
2:B:30:PRO:HG3	2:B:109:PRO:HD2	2.03	0.40
3:C:111:GLY:O	3:C:112:SER:HB3	2.21	0.40
1:E:95:LEU:HG	1:E:468:LEU:O	2.21	0.40
1:E:97:ARG:HA	1:E:514:ASP:HB3	2.03	0.40
1:E:116:THR:HG23	1:E:118:GLU:N	2.36	0.40
1:E:216:ASN:O	1:E:220:GLN:HG3	2.22	0.40
1:E:574:ASP:O	1:E:578:GLU:HG3	2.21	0.40
1:E:632:ALA:HA	1:E:635:GLN:NE2	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2:PRO:HB3	2:F:144:ASP:HB2	2.04	0.40
2:F:7:ALA:HB1	2:F:178:LEU:HD11	2.03	0.40
2:F:17:ALA:HB1	2:F:20:ALA:HB3	2.02	0.40
2:F:72:THR:CG2	2:F:89:LYS:O	2.65	0.40
3:G:20:HIS:CE1	3:G:59:ASP:CG	2.99	0.40
3:G:83:HIS:HA	3:G:84:PRO:HD2	1.87	0.40
1:A:286:PHE:O	1:A:286:PHE:CG	2.71	0.40
1:E:194:PRO:O	1:E:363:PHE:HA	2.21	0.40
1:E:443:PHE:CE1	1:E:472:HIS:HA	2.56	0.40
1:E:669:LEU:HD22	1:E:739:VAL:HG13	2.03	0.40
1:E:678:GLY:O	1:E:679:PRO:C	2.63	0.40
3:G:111:SER:C	3:G:115:LEU:HD12	2.44	0.40
1:A:417:ILE:HG23	1:A:418:GLN:N	2.36	0.40
1:A:589:LYS:O	1:A:592:LEU:CB	2.69	0.40
1:A:589:LYS:H	1:A:589:LYS:HG2	1.53	0.40
1:A:629:HIS:CB	1:A:634:THR:HG21	2.50	0.40
2:B:3:ARG:O	2:B:145:LEU:HB2	2.22	0.40
3:C:9:ASN:ND2	8:C:2009:HOH:O	2.39	0.40
3:C:64:LEU:CD2	7:C:1252:UQ1:C1	2.93	0.40
1:E:36:GLU:O	1:E:58:VAL:CB	2.66	0.40
1:E:42:GLN:CB	1:E:53:ILE:HG13	2.52	0.40
1:E:145:HIS:HD1	5:E:1765:MGD:PA	2.44	0.40
1:E:457:LYS:HE2	8:E:2061:HOH:O	2.21	0.40
1:E:487:GLU:C	1:E:507:PRO:HB3	2.46	0.40
1:E:667:VAL:HG11	1:E:741:LEU:HD13	2.04	0.40
2:F:46:TYR:C	2:F:48:ASN:H	2.28	0.40
1:A:42:GLN:OE1	1:A:505:ARG:HB2	2.21	0.40
1:A:116:THR:CG2	1:A:118:GLU:HB2	2.51	0.40
1:A:125:ALA:O	1:A:129:LEU:HG	2.22	0.40
1:A:177:ARG:NH2	1:A:193:GLU:OE1	2.52	0.40
1:A:209:HIS:CD2	5:A:1766:MGD:O2A	2.72	0.40
1:A:292:HIS:CD2	1:A:604:PRO:HB2	2.57	0.40
1:A:647:ASN:ND2	1:A:713:GLY:CA	2.85	0.40
1:A:670:VAL:HA	1:A:675:VAL:O	2.22	0.40
2:B:35:ASN:HD22	2:B:106:TYR:HE2	1.68	0.40
1:E:88:THR:CG2	1:E:467:VAL:CG1	3.00	0.40
1:E:156:LEU:HB3	1:E:157:PRO:HD3	2.03	0.40
1:E:187:ARG:HB3	1:E:188:PRO:HD2	2.03	0.40
1:E:621:LEU:HD22	1:E:622:LEU:H	1.85	0.40
3:G:150:LEU:HA	3:G:150:LEU:HD23	1.77	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLU:OE2	1:E:133:GLU:C[2_674]	1.77	0.43
1:A:399:GLU:OE2	1:E:134:LYS:N[2_674]	1.83	0.37
1:A:399:GLU:OE2	1:E:133:GLU:O[2_674]	2.04	0.16

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	733/765 (96%)	653 (89%)	45 (6%)	35 (5%)	2	11
1	E	733/765 (96%)	639 (87%)	59 (8%)	35 (5%)	2	11
2	B	192/195 (98%)	178 (93%)	11 (6%)	3 (2%)	7	30
2	F	192/195 (98%)	179 (93%)	9 (5%)	4 (2%)	5	25
3	C	249/253 (98%)	233 (94%)	11 (4%)	5 (2%)	6	25
3	G	249/253 (98%)	220 (88%)	21 (8%)	8 (3%)	3	18
All	All	2348/2426 (97%)	2102 (90%)	156 (7%)	90 (4%)	2	15

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	TRP
1	A	340	ASP
1	A	428	GLU
1	A	429	PRO
1	A	431	PRO
1	A	535	PHE
1	A	562	GLY
1	A	570	PRO
1	A	586	ALA
1	A	587	SER
1	A	593	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	605	LEU
1	A	678	GLY
1	A	687	ARG
1	A	730	GLY
2	B	17	ALA
3	C	208	PHE
3	C	250	GLY
1	E	92	PRO
1	E	93	ASP
1	E	109	GLU
1	E	396	HIS
1	E	397	GLU
1	E	428	GLU
1	E	429	PRO
1	E	552	GLY
1	E	567	ARG
1	E	583	PHE
1	E	593	TYR
1	E	607	VAL
1	E	631	PHE
1	E	678	GLY
1	E	686	ALA
2	F	46	TYR
3	G	108	GLY
3	G	113	ARG
3	G	222	GLN
1	A	365	ILE
1	A	399	GLU
1	A	430	TYR
1	A	434	GLY
1	A	582	PRO
1	A	592	LEU
1	A	607	VAL
1	A	631	PHE
1	A	633	ARG
2	B	193	HIS
3	C	112	SER
3	C	172	ALA
1	E	337	TYR
1	E	391	PRO
1	E	606	PRO
1	E	685	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	179	ASN
3	G	39	LEU
3	G	51	TYR
3	G	249	GLY
1	A	216	ASN
1	A	389	SER
1	A	398	PRO
1	E	466	ASP
1	E	469	PRO
1	E	478	VAL
1	E	513	PHE
1	E	570	PRO
1	E	627	PRO
2	F	45	GLU
2	F	178	LEU
1	A	478	VAL
2	B	115	LYS
3	C	113	GLN
1	E	389	SER
1	E	471	GLU
1	E	763	ARG
1	A	387	GLY
1	E	70	ALA
1	E	710	HIS
3	G	38	HIS
1	A	584	GLY
1	A	598	LYS
1	A	610	PRO
1	A	609	THR
1	A	684	PRO
1	E	434	GLY
1	E	610	PRO
3	G	110	GLY
1	E	468	LEU
1	E	604	PRO
1	A	362	GLY
1	E	609	THR

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	610/632 (96%)	491 (80%)	119 (20%)	1	6
1	E	610/632 (96%)	494 (81%)	116 (19%)	1	7
2	B	162/163 (99%)	140 (86%)	22 (14%)	3	16
2	F	162/163 (99%)	143 (88%)	19 (12%)	5	22
3	C	185/187 (99%)	160 (86%)	25 (14%)	4	16
3	G	185/187 (99%)	162 (88%)	23 (12%)	4	19
All	All	1914/1964 (98%)	1590 (83%)	324 (17%)	2	10

All (324) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	43	ILE
1	A	65	VAL
1	A	77	ARG
1	A	87	GLN
1	A	97	ARG
1	A	103	GLU
1	A	106	GLN
1	A	111	LYS
1	A	116	THR
1	A	119	GLU
1	A	126	LYS
1	A	134	LYS
1	A	156	LEU
1	A	167	LYS
1	A	170	VAL
1	A	174	THR
1	A	187	ARG
1	A	189	ILE
1	A	193	GLU
1	A	213	ASP
1	A	214	THR
1	A	217	THR
1	A	231	LYS
1	A	250	LEU
1	A	252	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	256	THR
1	A	260	LEU
1	A	281	LYS
1	A	283	THR
1	A	286	PHE
1	A	289	LEU
1	A	293	VAL
1	A	297	THR
1	A	299	GLU
1	A	302	GLU
1	A	305	THR
1	A	323	LYS
1	A	327	VAL
1	A	335	VAL
1	A	371	LEU
1	A	372	GLU
1	A	378	PRO
1	A	379	LEU
1	A	382	GLU
1	A	395	ASP
1	A	413	ARG
1	A	414	SER
1	A	415	THR
1	A	418	GLN
1	A	421	ILE
1	A	428	GLU
1	A	433	LYS
1	A	440	ILE
1	A	441	ASN
1	A	454	GLU
1	A	457	LYS
1	A	470	GLN
1	A	477	ASP
1	A	478	VAL
1	A	484	THR
1	A	504	LEU
1	A	510	GLU
1	A	512	LEU
1	A	515	THR
1	A	528	ARG
1	A	529	LEU
1	A	532	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	533	GLN
1	A	538	LYS
1	A	539	THR
1	A	540	ILE
1	A	541	GLU
1	A	542	GLU
1	A	549	GLN
1	A	550	SER
1	A	553	LEU
1	A	555	LEU
1	A	558	MET
1	A	561	MET
1	A	578	GLU
1	A	580	ARG
1	A	587	SER
1	A	589	LYS
1	A	591	GLU
1	A	592	LEU
1	A	594	CYS
1	A	595	GLN
1	A	596	ARG
1	A	603	GLN
1	A	605	LEU
1	A	608	PHE
1	A	616	GLU
1	A	621	LEU
1	A	633	ARG
1	A	647	ASN
1	A	648	GLU
1	A	649	VAL
1	A	651	ILE
1	A	662	LYS
1	A	663	GLU
1	A	667	VAL
1	A	671	ASN
1	A	672	GLN
1	A	680	VAL
1	A	683	LYS
1	A	685	THR
1	A	687	ARG
1	A	693	VAL
1	A	702	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	708	LEU
1	A	721	THR
1	A	725	LEU
1	A	736	VAL
1	A	739	VAL
1	A	741	LEU
1	A	743	LYS
1	A	746	ARG
1	A	762	GLU
2	B	1	MET
2	B	25	MET
2	B	39	ARG
2	B	41	ARG
2	B	45	GLU
2	B	54	ARG
2	B	69	VAL
2	B	72	THR
2	B	78	THR
2	B	105	ARG
2	B	114	SER
2	B	117	THR
2	B	118	PHE
2	B	125	LYS
2	B	131	CYS
2	B	141	THR
2	B	145	LEU
2	B	152	VAL
2	B	164	VAL
2	B	166	ARG
2	B	175	LEU
2	B	187	THR
3	C	11	GLN
3	C	17	THR
3	C	18	ASN
3	C	20	LEU
3	C	24	LEU
3	C	40	LEU
3	C	57	ILE
3	C	63	ILE
3	C	67	GLU
3	C	71	ARG
3	C	75	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	79	LEU
3	C	105	LEU
3	C	130	TYR
3	C	140	ASN
3	C	145	ASN
3	C	155	THR
3	C	163	LEU
3	C	193	THR
3	C	197	GLU
3	C	216	LEU
3	C	225	ARG
3	C	232	LEU
3	C	241	LEU
3	C	249	GLN
1	E	65	VAL
1	E	69	GLU
1	E	101	ARG
1	E	102	VAL
1	E	111	LYS
1	E	113	ARG
1	E	114	VAL
1	E	119	GLU
1	E	126	LYS
1	E	145	HIS
1	E	172	LEU
1	E	174	THR
1	E	189	ILE
1	E	193	GLU
1	E	208	HIS
1	E	213	ASP
1	E	214	THR
1	E	217	THR
1	E	224	LEU
1	E	250	LEU
1	E	256	THR
1	E	260	LEU
1	E	272	ASP
1	E	284	VAL
1	E	286	PHE
1	E	289	LEU
1	E	293	VAL
1	E	297	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	298	PRO
1	E	299	GLU
1	E	305	THR
1	E	310	GLN
1	E	314	GLU
1	E	323	LYS
1	E	327	VAL
1	E	335	VAL
1	E	360	PRO
1	E	371	LEU
1	E	389	SER
1	E	395	ASP
1	E	402	LYS
1	E	413	ARG
1	E	415	THR
1	E	418	GLN
1	E	421	ILE
1	E	428	GLU
1	E	440	ILE
1	E	441	ASN
1	E	457	LYS
1	E	466	ASP
1	E	467	VAL
1	E	470	GLN
1	E	484	THR
1	E	488	ARG
1	E	498	LYS
1	E	499	THR
1	E	504	LEU
1	E	510	GLU
1	E	512	LEU
1	E	515	THR
1	E	528	ARG
1	E	533	GLN
1	E	538	LYS
1	E	539	THR
1	E	540	ILE
1	E	541	GLU
1	E	554	ASP
1	E	555	LEU
1	E	558	MET
1	E	564	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	569	LYS
1	E	577	LYS
1	E	581	LEU
1	E	585	THR
1	E	589	LYS
1	E	590	ILE
1	E	591	GLU
1	E	595	GLN
1	E	596	ARG
1	E	602	HIS
1	E	605	LEU
1	E	607	VAL
1	E	608	PHE
1	E	609	THR
1	E	612	GLU
1	E	620	ARG
1	E	621	LEU
1	E	626	SER
1	E	628	VAL
1	E	633	ARG
1	E	647	ASN
1	E	649	VAL
1	E	651	ILE
1	E	657	LYS
1	E	663	GLU
1	E	667	VAL
1	E	671	ASN
1	E	672	GLN
1	E	676	LYS
1	E	680	VAL
1	E	685	THR
1	E	691	ASP
1	E	693	VAL
1	E	696	VAL
1	E	702	LYS
1	E	708	LEU
1	E	721	THR
1	E	725	LEU
1	E	736	VAL
1	E	739	VAL
1	E	740	ARG
1	E	741	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	746	ARG
1	E	748	ARG
1	E	751	SER
1	E	752	LEU
2	F	49	LEU
2	F	68	PRO
2	F	69	VAL
2	F	72	THR
2	F	78	THR
2	F	88	LYS
2	F	114	SER
2	F	117	THR
2	F	118	PHE
2	F	133	GLU
2	F	145	LEU
2	F	150	SER
2	F	152	VAL
2	F	164	VAL
2	F	166	ARG
2	F	171	THR
2	F	175	LEU
2	F	187	THR
2	F	191	GLU
3	G	10	GLN
3	G	17	ASN
3	G	39	LEU
3	G	40	LYS
3	G	64	TRP
3	G	66	GLU
3	G	74	THR
3	G	88	ILE
3	G	107	LEU
3	G	109	LYS
3	G	113	ARG
3	G	129	TYR
3	G	136	VAL
3	G	139	ASN
3	G	144	ASN
3	G	154	THR
3	G	162	LEU
3	G	167	LYS
3	G	192	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	196	GLU
3	G	204	GLU
3	G	215	LEU
3	G	240	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	71	ASN
1	A	83	GLN
1	A	123	HIS
1	A	192	HIS
1	A	209	HIS
1	A	220	GLN
1	A	247	HIS
1	A	322	HIS
1	A	367	GLN
1	A	396	HIS
1	A	441	ASN
1	A	470	GLN
1	A	472	HIS
1	A	509	HIS
1	A	533	GLN
1	A	595	GLN
1	A	602	HIS
1	A	603	GLN
1	A	647	ASN
1	A	671	ASN
1	A	672	GLN
1	A	717	ASN
2	B	27	ASN
2	B	35	ASN
2	B	48	ASN
2	B	57	GLN
2	B	77	GLN
2	B	179	ASN
3	C	9	ASN
3	C	11	GLN
3	C	39	HIS
3	C	84	HIS
3	C	140	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	145	ASN
3	C	249	GLN
1	E	60	ASN
1	E	71	ASN
1	E	83	GLN
1	E	123	HIS
1	E	192	HIS
1	E	208	HIS
1	E	209	HIS
1	E	218	GLN
1	E	220	GLN
1	E	247	HIS
1	E	292	HIS
1	E	322	HIS
1	E	396	HIS
1	E	418	GLN
1	E	441	ASN
1	E	444	HIS
1	E	470	GLN
1	E	509	HIS
1	E	533	GLN
1	E	595	GLN
1	E	602	HIS
1	E	603	GLN
1	E	635	GLN
1	E	647	ASN
1	E	671	ASN
1	E	672	GLN
1	E	717	ASN
2	F	27	ASN
2	F	35	ASN
2	F	48	ASN
2	F	57	GLN
2	F	77	GLN
2	F	169	GLN
2	F	179	ASN
3	G	8	ASN
3	G	10	GLN
3	G	38	HIS
3	G	83	HIS
3	G	137	ASN
3	G	139	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	200	HIS
3	G	248	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	MGD	A	1765	6	47,52,52	2.76	21 (44%)	58,81,81	3.05	19 (32%)
4	SF4	B	1196	2	0,12,12	-	-	-		
4	SF4	B	1195	2	0,12,12	-	-	-		
4	SF4	B	1197	2	0,12,12	-	-	-		
5	MGD	A	1766	6	47,52,52	2.91	23 (48%)	58,81,81	3.02	20 (34%)
4	SF4	B	1194	2	0,12,12	-	-	-		
4	SF4	E	1764	1	0,12,12	-	-	-		
4	SF4	F	1194	2	0,12,12	-	-	-		
4	SF4	A	1764	1	0,12,12	-	-	-		
7	UQ1	C	1252	3	18,18,18	1.08	2 (11%)	24,25,25	1.61	7 (29%)
5	MGD	E	1765	6	47,52,52	2.79	28 (59%)	58,81,81	3.13	22 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SF4	F	1196	2	0,12,12	-	-	-		
5	MGD	E	1766	6	47,52,52	3.01	21 (44%)	58,81,81	2.68	19 (32%)
4	SF4	F	1195	2	0,12,12	-	-	-		
4	SF4	F	1197	2	0,12,12	-	-	-		
7	UQ1	G	1251	-	18,18,18	1.07	2 (11%)	24,25,25	1.61	6 (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	MGD	A	1765	6	-	5/22/66/66	0/6/6/6
4	SF4	B	1196	2	-	-	0/6/5/5
4	SF4	B	1195	2	-	-	0/6/5/5
5	MGD	A	1766	6	-	1/22/66/66	0/6/6/6
4	SF4	B	1197	2	-	-	0/6/5/5
4	SF4	B	1194	2	-	-	0/6/5/5
4	SF4	E	1764	1	-	-	0/6/5/5
4	SF4	F	1194	2	-	-	0/6/5/5
4	SF4	A	1764	1	-	-	0/6/5/5
7	UQ1	C	1252	3	-	3/9/33/33	0/1/1/1
5	MGD	E	1765	6	-	2/22/66/66	0/6/6/6
4	SF4	F	1196	2	-	-	0/6/5/5
5	MGD	E	1766	6	-	1/22/66/66	0/6/6/6
4	SF4	F	1195	2	-	-	0/6/5/5
4	SF4	F	1197	2	-	-	0/6/5/5
7	UQ1	G	1251	-	-	3/9/33/33	0/1/1/1

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1766	MGD	C21-N22	-10.00	1.25	1.35
5	A	1765	MGD	C23-C14	-9.87	1.45	1.53
5	A	1766	MGD	C14-N15	-8.01	1.37	1.46
5	A	1766	MGD	C23-C14	-7.36	1.47	1.53
5	E	1765	MGD	C23-C14	-7.11	1.48	1.53
5	A	1766	MGD	C21-N22	-6.88	1.28	1.35
5	E	1766	MGD	C14-N15	-6.72	1.38	1.46
5	E	1766	MGD	C23-C14	-6.64	1.48	1.53
5	E	1765	MGD	C10-C11	-6.11	1.43	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1765	MGD	C5-N7	-5.31	1.28	1.39
5	A	1765	MGD	C21-N22	-5.09	1.30	1.35
5	A	1765	MGD	C10-C11	-4.98	1.44	1.51
5	A	1766	MGD	C6-N1	-4.92	1.29	1.38
5	A	1765	MGD	C17-N18	-4.84	1.29	1.38
5	A	1766	MGD	C10-C11	-4.66	1.45	1.51
5	E	1765	MGD	C8-N9	-4.59	1.27	1.37
5	E	1766	MGD	C5-N7	-4.58	1.29	1.39
5	A	1765	MGD	C21-N20	-4.45	1.29	1.36
5	E	1766	MGD	C6-N1	-4.16	1.31	1.38
5	E	1766	MGD	C19-N19	-4.14	1.24	1.34
5	A	1765	MGD	C23-N22	-4.14	1.38	1.45
5	E	1766	MGD	PB-O3B	-4.11	1.55	1.59
5	E	1766	MGD	C19-N18	-4.10	1.27	1.37
5	E	1766	MGD	C16-N15	-4.10	1.28	1.37
5	E	1765	MGD	C16-C21	4.07	1.45	1.38
5	A	1766	MGD	C23-N22	-4.00	1.38	1.45
5	E	1765	MGD	C17-N18	-3.97	1.31	1.38
5	E	1765	MGD	C14-N15	-3.94	1.42	1.46
5	E	1765	MGD	C21-N22	-3.91	1.31	1.35
5	A	1766	MGD	PA-O3B	-3.85	1.55	1.59
5	E	1766	MGD	O4'-C4'	-3.75	1.36	1.45
5	E	1765	MGD	C2-N1	-3.60	1.28	1.37
5	A	1765	MGD	C5-N7	-3.60	1.31	1.39
5	A	1766	MGD	PB-O3B	-3.58	1.55	1.59
5	E	1766	MGD	C23-N22	-3.57	1.39	1.45
5	E	1765	MGD	C3'-C4'	-3.54	1.44	1.53
5	A	1766	MGD	C5-N7	-3.49	1.32	1.39
5	E	1765	MGD	C19-N18	-3.44	1.29	1.37
5	A	1765	MGD	C8-N9	-3.36	1.30	1.37
5	E	1766	MGD	O11-C11	-3.32	1.37	1.43
5	E	1765	MGD	C23-N22	-3.28	1.39	1.45
5	A	1766	MGD	PB-O2B	-3.27	1.40	1.55
5	E	1765	MGD	C6-N1	-3.26	1.32	1.38
5	A	1766	MGD	O4'-C4'	-3.24	1.37	1.45
5	A	1765	MGD	C4-N9	-3.18	1.30	1.38
5	E	1765	MGD	C4-N9	-3.13	1.30	1.38
5	A	1765	MGD	O11-C23	-3.03	1.39	1.43
5	A	1765	MGD	C16-C21	2.99	1.43	1.38
5	E	1766	MGD	C17-N18	-2.97	1.33	1.38
5	A	1766	MGD	C4-N9	-2.97	1.30	1.38
5	E	1766	MGD	C16-C21	2.97	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1766	MGD	PA-O2A	-2.94	1.41	1.55
5	A	1765	MGD	O4'-C4'	-2.91	1.38	1.45
5	E	1765	MGD	O3'-C3'	-2.82	1.36	1.43
5	E	1766	MGD	C5-C4	2.82	1.46	1.38
5	A	1765	MGD	O2'-C2'	-2.71	1.36	1.43
5	A	1765	MGD	C3'-C4'	-2.64	1.46	1.53
5	A	1765	MGD	PB-O3B	-2.63	1.56	1.59
5	A	1765	MGD	C19-N18	-2.62	1.31	1.37
5	A	1765	MGD	C6-N1	-2.62	1.34	1.38
5	A	1766	MGD	PA-O1A	-2.61	1.41	1.50
5	A	1766	MGD	C17-N18	-2.60	1.34	1.38
5	E	1766	MGD	O17-C17	-2.54	1.18	1.23
5	E	1765	MGD	O11-C23	-2.54	1.39	1.43
5	A	1766	MGD	C19-N19	-2.52	1.28	1.34
5	E	1766	MGD	C10-C11	-2.51	1.48	1.51
5	A	1766	MGD	C16-C21	2.51	1.43	1.38
5	E	1765	MGD	O11-C11	-2.50	1.38	1.43
5	A	1765	MGD	O11-C11	-2.45	1.38	1.43
5	E	1766	MGD	PA-O1A	-2.45	1.42	1.50
5	E	1765	MGD	C2'-C1'	-2.44	1.45	1.53
5	E	1765	MGD	O4'-C4'	-2.41	1.39	1.45
5	E	1765	MGD	PB-O1B	-2.33	1.42	1.50
7	G	1251	UQ1	C6-C5	2.33	1.39	1.35
7	C	1252	UQ1	C6-C5	2.32	1.39	1.35
5	E	1765	MGD	C21-N20	-2.32	1.32	1.36
5	E	1765	MGD	O2'-C2'	-2.27	1.37	1.43
5	E	1766	MGD	C4-N9	-2.26	1.32	1.38
5	E	1765	MGD	O3A-C10	-2.26	1.36	1.44
5	A	1765	MGD	PA-O2A	-2.26	1.44	1.55
5	A	1766	MGD	C2'-C1'	-2.24	1.46	1.53
5	E	1765	MGD	PA-O2A	-2.23	1.45	1.55
5	E	1765	MGD	O6-C6	-2.23	1.19	1.23
5	A	1766	MGD	C19-N18	-2.21	1.32	1.37
5	A	1766	MGD	C2-N1	-2.19	1.32	1.37
5	A	1765	MGD	C5-C4	2.16	1.44	1.38
5	E	1765	MGD	C1'-N9	-2.12	1.41	1.47
5	A	1765	MGD	PB-O2B	-2.10	1.45	1.55
5	E	1765	MGD	C2'-C3'	-2.10	1.47	1.53
5	A	1766	MGD	O11-C11	-2.09	1.39	1.43
5	E	1766	MGD	O3'-C3'	2.09	1.48	1.43
5	A	1766	MGD	C5-C4	2.07	1.44	1.38
7	C	1252	UQ1	O1-C1	-2.06	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1765	MGD	C5-C4	2.03	1.44	1.38
5	A	1766	MGD	PB-O1B	-2.02	1.43	1.50
7	G	1251	UQ1	O1-C1	-2.02	1.18	1.23
5	E	1766	MGD	C8-N9	-2.01	1.33	1.37

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1766	MGD	O11-C23-C14	14.24	118.46	108.96
5	A	1765	MGD	O11-C23-C14	12.67	117.42	108.96
5	E	1765	MGD	O11-C23-N22	-11.11	98.53	108.61
5	E	1766	MGD	O11-C23-C14	10.85	116.20	108.96
5	E	1765	MGD	C23-C14-N15	9.17	116.88	107.87
5	A	1765	MGD	C23-C14-N15	8.30	116.02	107.87
5	A	1765	MGD	C2-N3-C4	7.30	124.88	112.30
5	E	1766	MGD	C5-C4-N3	-7.16	117.00	128.39
5	A	1765	MGD	C5-C4-N3	-7.10	117.09	128.39
5	E	1765	MGD	C5-C4-N3	-6.83	117.53	128.39
5	E	1765	MGD	O11-C23-C14	-6.77	104.45	108.96
5	E	1765	MGD	C2-N3-C4	6.59	123.66	112.30
5	A	1766	MGD	C5-C4-N3	-6.26	118.42	128.39
5	E	1765	MGD	C19-N20-C21	5.88	123.74	113.36
5	E	1766	MGD	O17-C17-C16	-5.54	113.91	127.26
5	A	1765	MGD	C19-N20-C21	5.47	123.01	113.36
5	E	1766	MGD	C23-C14-N15	5.36	113.13	107.87
5	E	1765	MGD	C6-C5-N7	5.27	139.88	130.29
5	A	1766	MGD	C2-N3-C4	5.18	121.22	112.30
5	A	1766	MGD	N9-C4-N3	5.10	136.14	125.95
5	A	1766	MGD	O4'-C1'-N9	4.93	119.52	108.36
5	E	1766	MGD	C2-N3-C4	4.74	120.47	112.30
5	A	1766	MGD	C23-C14-N15	4.67	112.46	107.87
5	A	1766	MGD	O3B-PB-O1B	-4.56	96.97	110.70
5	E	1766	MGD	N9-C4-N3	4.55	135.06	125.95
5	A	1765	MGD	N9-C4-N3	4.52	134.99	125.95
5	E	1765	MGD	C4-C5-N7	-4.22	103.98	110.67
5	A	1766	MGD	O11-C23-N22	4.19	112.41	108.61
5	E	1765	MGD	N9-C4-N3	4.06	134.07	125.95
5	A	1765	MGD	C6-C5-N7	4.05	137.66	130.29
5	E	1766	MGD	C19-N20-C21	3.97	120.36	113.36
5	A	1765	MGD	C17-C16-N15	3.89	126.88	116.27
5	A	1765	MGD	C4-C5-N7	-3.64	104.91	110.67
5	A	1766	MGD	C19-N18-C17	-3.62	118.55	125.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1766	MGD	C16-C17-N18	3.51	121.77	112.13
5	A	1766	MGD	O6-C6-C5	-3.51	117.28	126.53
5	E	1765	MGD	C17-C16-N15	3.46	125.70	116.27
5	A	1765	MGD	O2B-PB-O3B	3.43	116.53	107.27
5	E	1766	MGD	O4'-C1'-N9	3.36	115.97	108.36
7	G	1251	UQ1	C10-C9-C8	-3.33	112.66	122.66
7	C	1252	UQ1	C10-C9-C8	-3.32	112.69	122.66
5	A	1766	MGD	O17-C17-C16	-3.31	119.27	127.26
5	A	1766	MGD	O2B-PB-O3B	3.31	116.22	107.27
5	A	1766	MGD	C17-C16-N15	3.22	125.06	116.27
5	E	1766	MGD	O11-C23-N22	-3.11	105.78	108.61
5	A	1765	MGD	N2-C2-N1	3.11	123.33	116.76
5	E	1765	MGD	C16-C17-N18	3.04	120.48	112.13
5	E	1766	MGD	O2A-PA-O1A	3.02	126.49	112.44
7	G	1251	UQ1	C5-C6-C1	-2.78	116.92	119.62
7	C	1252	UQ1	C5-C6-C1	-2.76	116.93	119.62
5	E	1766	MGD	C2-N1-C6	-2.76	120.10	125.11
5	E	1765	MGD	O3'-C3'-C4'	-2.74	103.21	111.08
5	E	1765	MGD	O2A-PA-O3B	-2.74	99.87	107.27
5	A	1766	MGD	O5'-C5'-C4'	-2.74	99.67	108.99
5	A	1765	MGD	O3B-PA-O1A	-2.72	102.53	110.70
5	A	1766	MGD	C16-C17-N18	2.71	119.58	112.13
5	E	1766	MGD	O3'-C3'-C4'	2.69	118.81	111.08
5	A	1765	MGD	O17-C17-C16	-2.68	120.79	127.26
5	E	1766	MGD	C19-N18-C17	-2.67	120.27	125.11
5	A	1766	MGD	C6-C5-N7	2.63	135.08	130.29
5	E	1766	MGD	O6-C6-C5	-2.61	119.64	126.53
5	A	1765	MGD	O4'-C1'-C2'	-2.60	101.05	106.62
5	E	1765	MGD	C8-N7-C5	2.60	108.89	104.26
5	A	1765	MGD	O4'-C4'-C5'	-2.59	101.04	109.33
5	E	1766	MGD	C4-C5-N7	-2.56	106.61	110.67
7	C	1252	UQ1	O1-C1-C6	-2.51	116.94	121.79
7	G	1251	UQ1	O1-C1-C6	-2.51	116.94	121.79
5	A	1765	MGD	O3B-PB-O1B	-2.48	103.23	110.70
5	E	1765	MGD	O2B-PB-O1B	2.48	123.98	112.44
5	A	1765	MGD	N19-C19-N18	2.48	121.99	116.76
5	E	1765	MGD	O6-C6-C5	-2.47	120.01	126.53
5	E	1765	MGD	O3B-PB-O1B	-2.47	103.28	110.70
7	C	1252	UQ1	C11-C9-C8	2.43	129.96	122.66
7	G	1251	UQ1	C11-C9-C8	2.43	129.96	122.66
7	C	1252	UQ1	C6-C5-C4	2.38	121.05	119.17
5	E	1765	MGD	O17-C17-C16	-2.38	121.52	127.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1766	MGD	C19-N20-C21	2.36	117.52	113.36
7	G	1251	UQ1	C6-C5-C4	2.35	121.02	119.17
5	A	1766	MGD	O4'-C4'-C5'	-2.34	101.84	109.33
5	E	1766	MGD	C6-C5-N7	2.34	134.54	130.29
5	A	1766	MGD	C5-C6-N1	2.33	119.18	113.25
5	E	1765	MGD	O2B-PB-O3B	-2.29	101.08	107.27
5	E	1765	MGD	C19-N18-C17	-2.27	121.00	125.11
7	G	1251	UQ1	CM3-O3-C3	-2.21	108.69	116.47
5	E	1766	MGD	O17-C17-N18	2.21	124.27	120.11
5	E	1765	MGD	O2A-PA-O1A	2.21	122.72	112.44
7	C	1252	UQ1	CM3-O3-C3	-2.20	108.73	116.47
5	A	1766	MGD	C2'-C1'-N9	2.12	119.15	113.25
5	A	1765	MGD	C2'-C1'-N9	2.11	119.12	113.25
5	E	1765	MGD	N2-C2-N1	2.10	121.19	116.76
5	E	1766	MGD	C4'-O4'-C1'	-2.10	104.84	109.47
5	A	1765	MGD	C16-C17-N18	2.10	117.88	112.13
7	C	1252	UQ1	O4-C4-C3	-2.00	116.79	121.03

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1765	MGD	C5'-O5'-PB-O2B
5	A	1765	MGD	C5'-O5'-PB-O3B
7	C	1252	UQ1	C1-C6-C7-C8
7	C	1252	UQ1	C5-C6-C7-C8
7	G	1251	UQ1	C1-C6-C7-C8
7	G	1251	UQ1	C5-C6-C7-C8
5	E	1765	MGD	O4'-C4'-C5'-O5'
5	A	1765	MGD	PA-O3B-PB-O5'
5	E	1765	MGD	PA-O3B-PB-O5'
5	A	1766	MGD	C11-C10-O3A-PA
5	A	1765	MGD	C5'-O5'-PB-O1B
5	E	1766	MGD	C11-C10-O3A-PA
5	A	1765	MGD	PA-O3B-PB-O1B
7	C	1252	UQ1	C4-C3-O3-CM3
7	G	1251	UQ1	C4-C3-O3-CM3

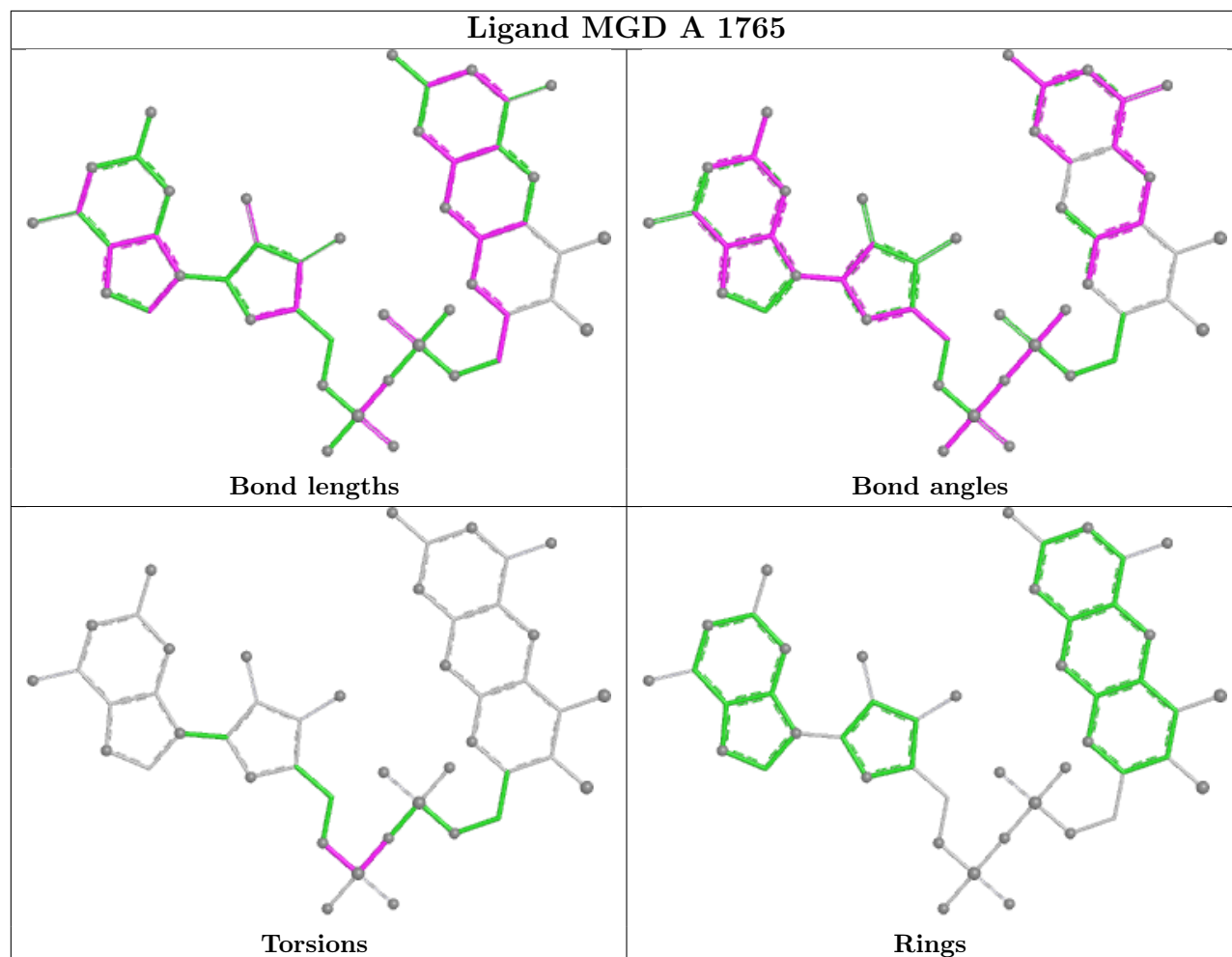
There are no ring outliers.

14 monomers are involved in 100 short contacts:

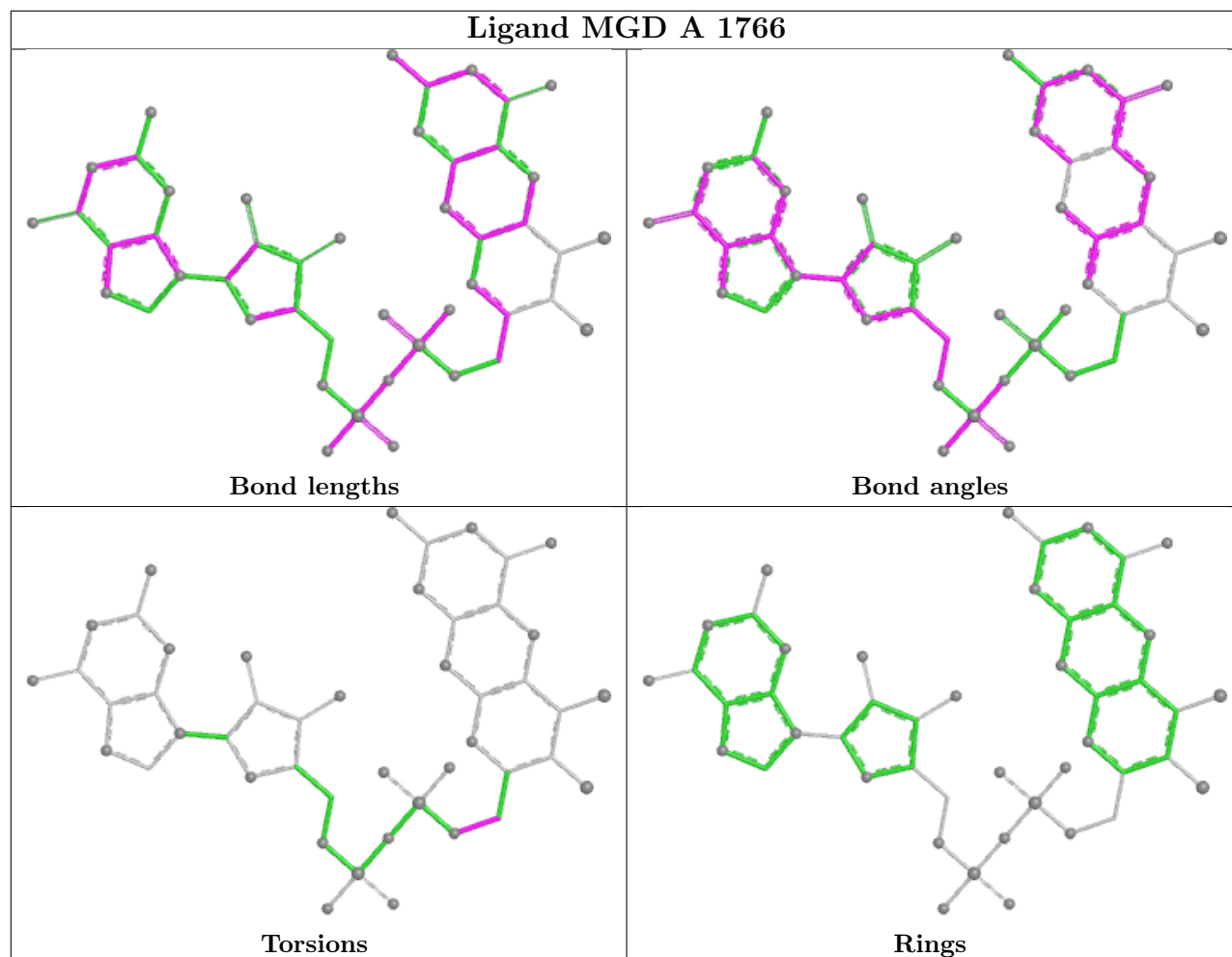
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1765	MGD	7	0
4	B	1196	SF4	2	0
4	B	1195	SF4	3	0
5	A	1766	MGD	5	0
4	B	1194	SF4	3	0
4	E	1764	SF4	1	0
4	F	1194	SF4	3	0
4	A	1764	SF4	2	0
7	C	1252	UQ1	26	0
5	E	1765	MGD	10	0
4	F	1196	SF4	1	0
5	E	1766	MGD	13	0
4	F	1195	SF4	2	0
7	G	1251	UQ1	22	0

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.

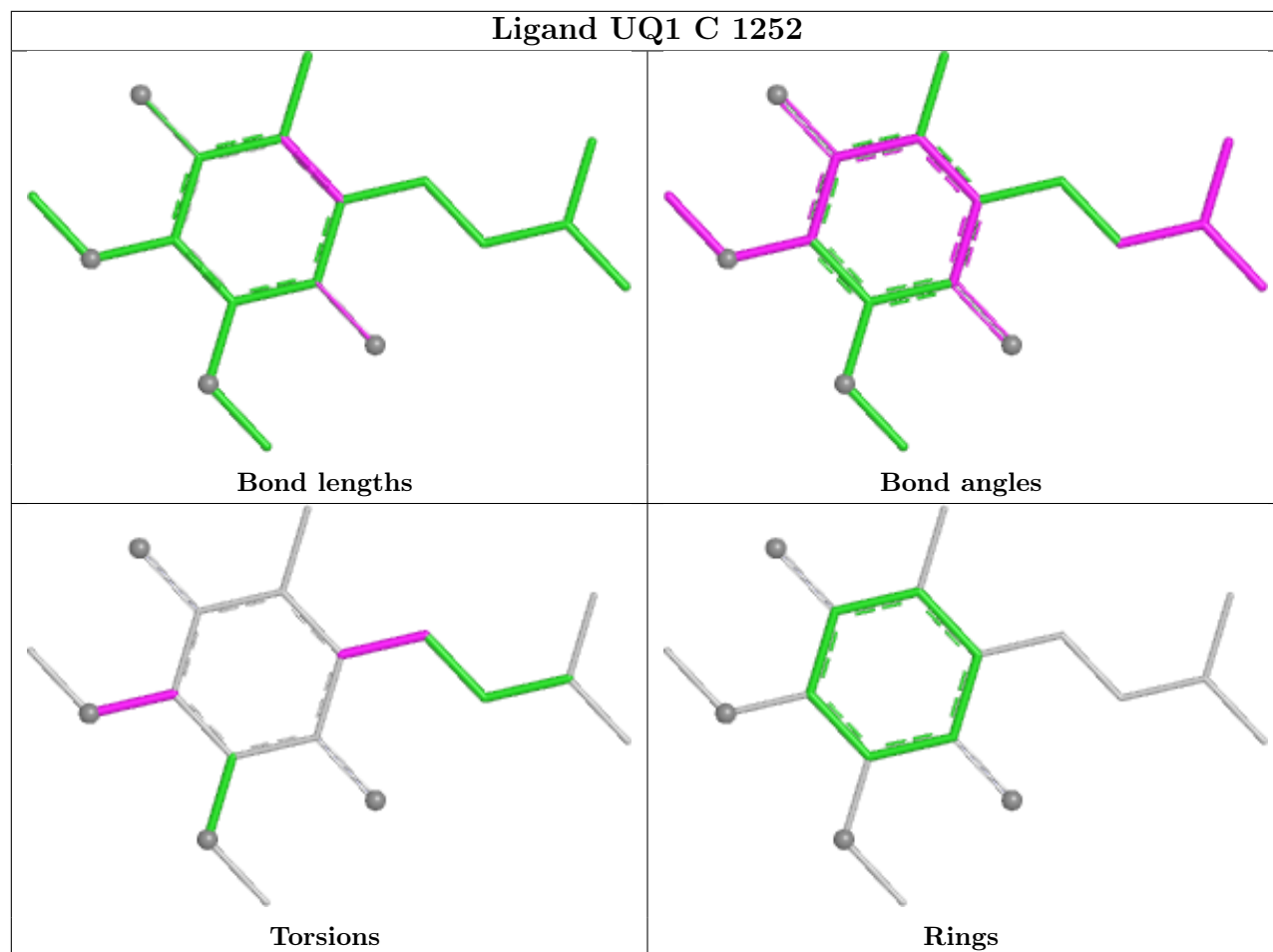
Ligand MGD A 1765

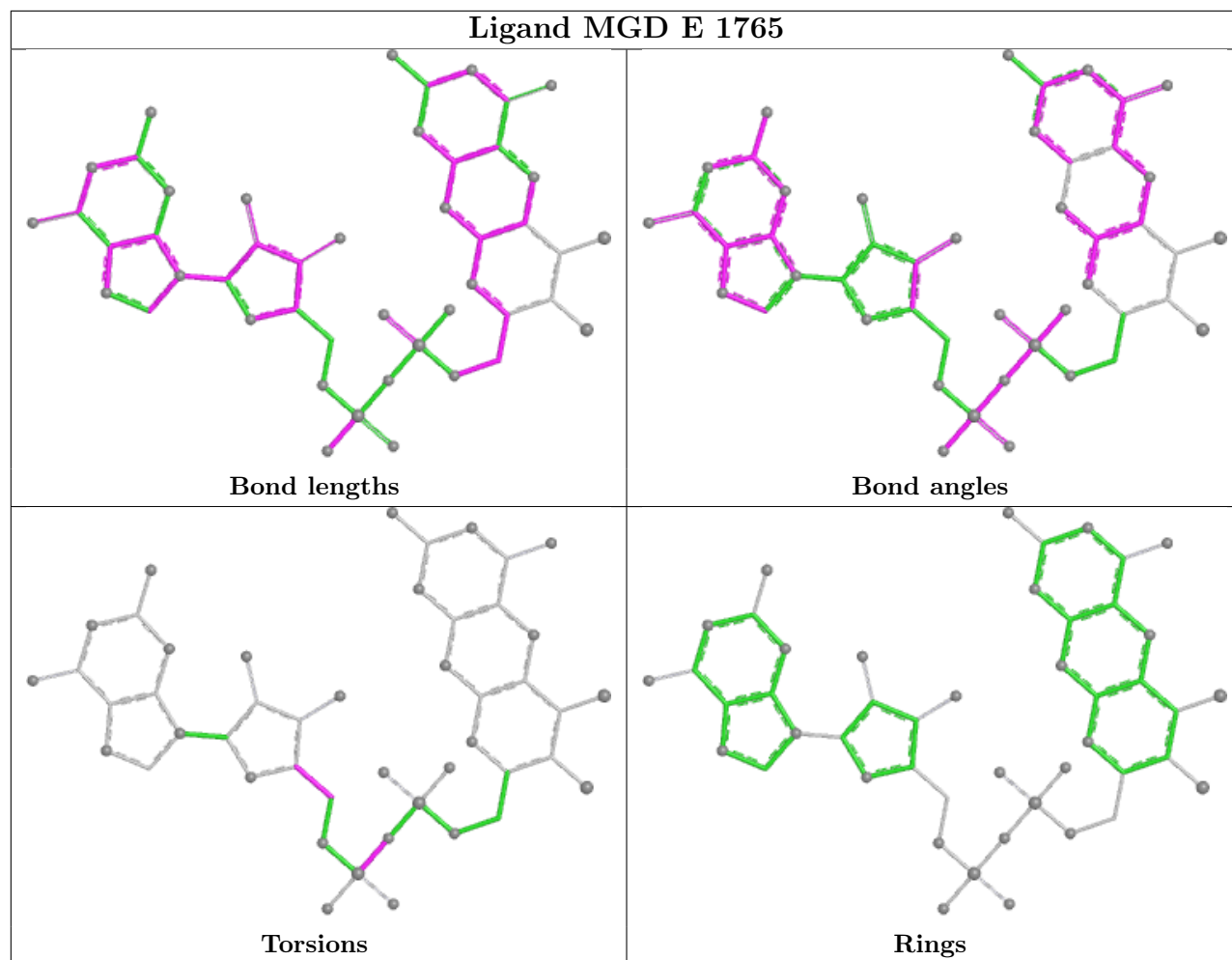


Ligand MGD A 1766

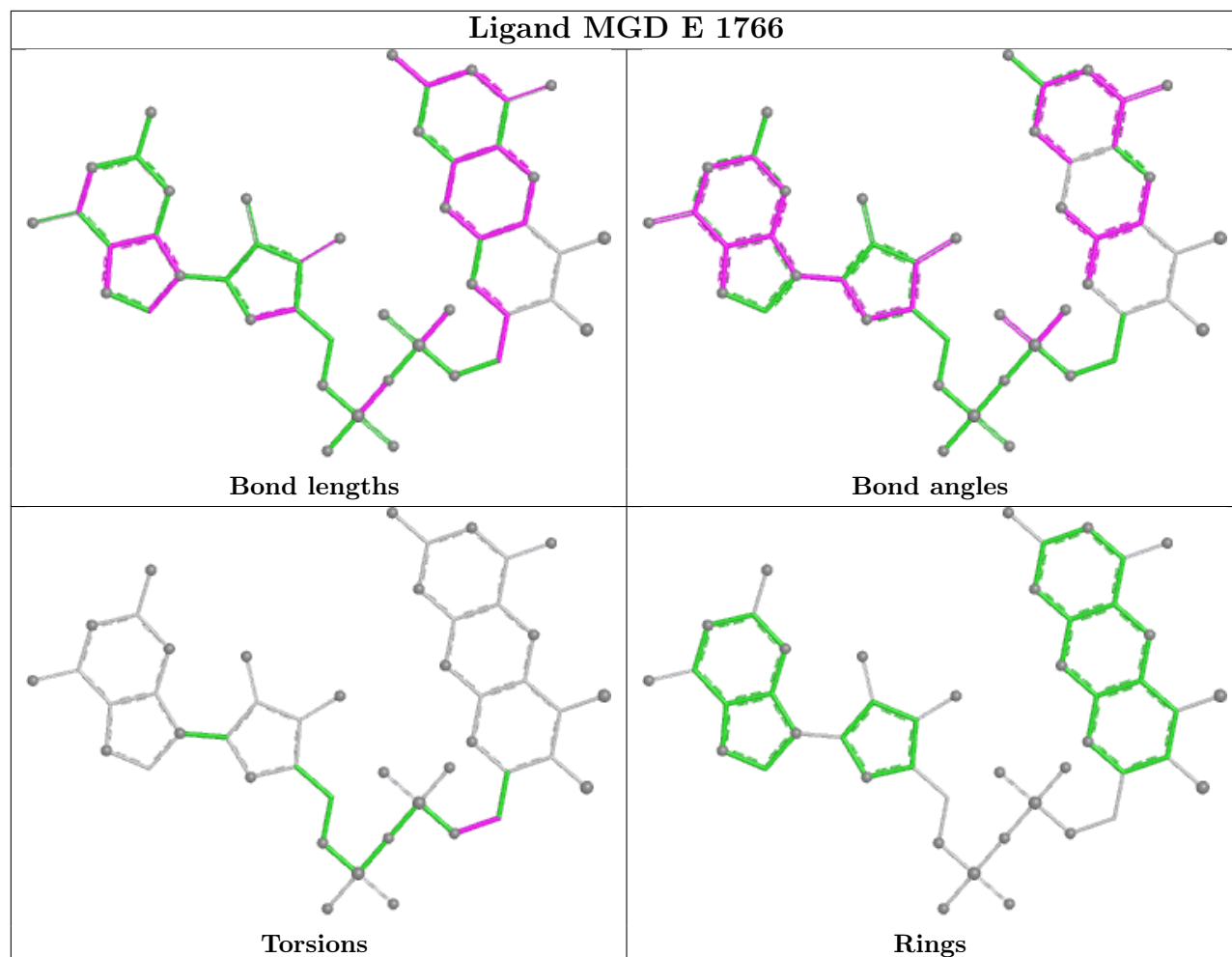


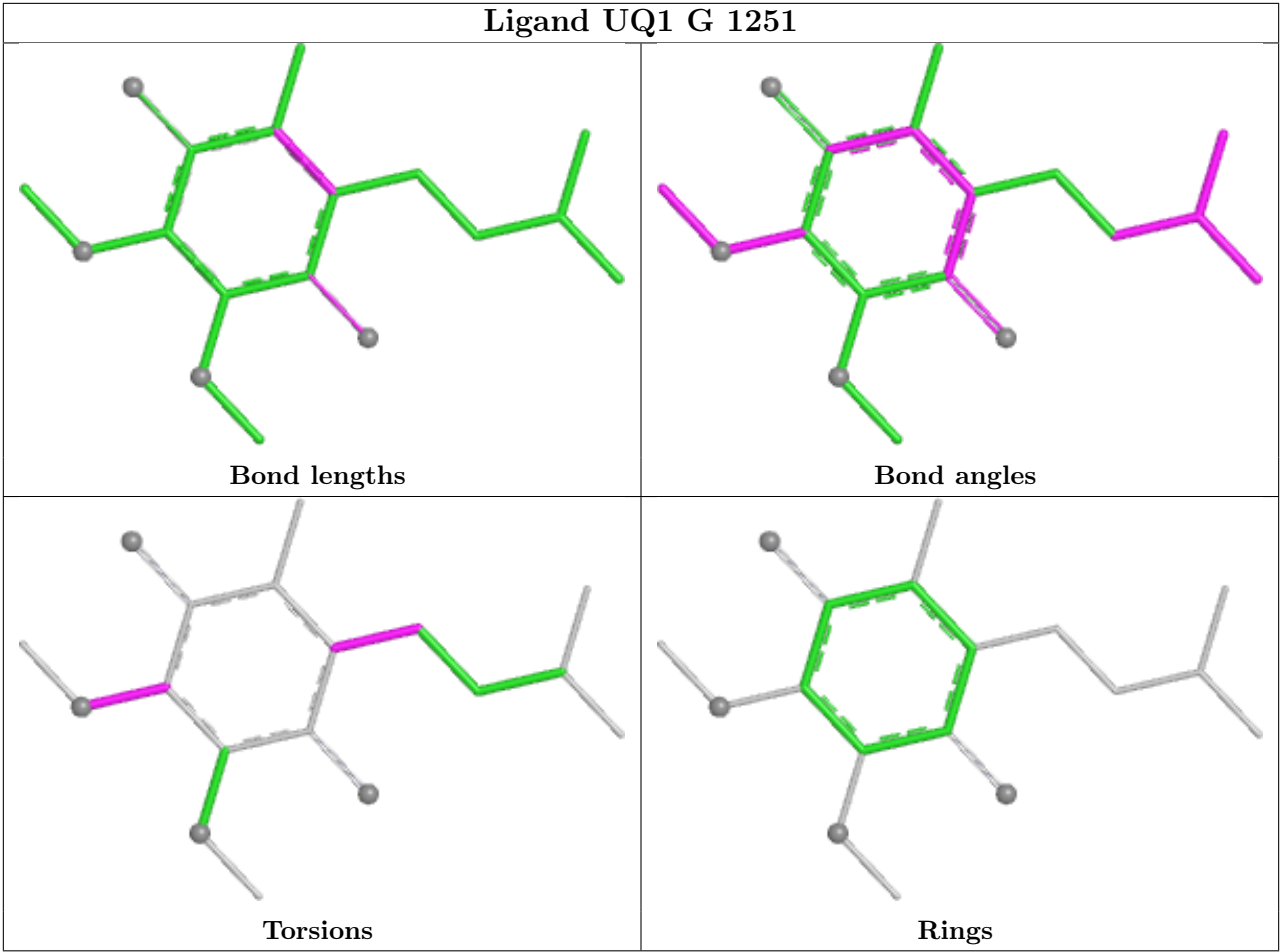
Ligand UQ1 C 1252





Ligand MGD E 1766





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	387:GLY	C	388:CYS	N	1.17

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	735/765 (96%)	1.44	175 (23%) 2 1	42, 73, 106, 157	0
1	E	735/765 (96%)	1.70	231 (31%) 1 1	44, 75, 104, 157	0
2	B	194/195 (99%)	0.74	11 (5%) 29 16	43, 61, 83, 106	0
2	F	194/195 (99%)	1.94	81 (41%) 0 0	50, 73, 91, 109	0
3	C	251/253 (99%)	1.34	50 (19%) 3 1	45, 75, 103, 119	0
3	G	251/253 (99%)	1.87	105 (41%) 0 0	55, 86, 115, 132	0
All	All	2360/2426 (97%)	1.54	653 (27%) 1 1	42, 74, 106, 157	0

All (653) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	251	GLY	13.8
3	C	252	GLY	9.8
1	E	518	GLY	8.5
1	A	362	GLY	7.7
1	A	570	PRO	7.4
1	A	764	ARG	7.3
1	A	396	HIS	7.0
3	C	224	GLU	6.8
3	C	111	GLY	6.7
1	E	495	VAL	5.8
3	G	17	ASN	5.8
1	A	583	PHE	5.8
3	G	78	LEU	5.8
1	E	592	LEU	5.7
1	E	606	PRO	5.7
2	F	131	CYS	5.6
1	E	491	ASP	5.6
1	A	685	THR	5.6
2	F	72	THR	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	362	GLY	5.6
3	G	81	SER	5.5
1	A	285	GLY	5.4
2	F	75	SER	5.4
1	E	555	LEU	5.3
2	F	128	VAL	5.3
1	A	384	ALA	5.2
3	G	42	ASP	5.2
1	E	166	ALA	5.1
1	A	434	GLY	5.1
1	E	494	LEU	5.1
1	A	535	PHE	5.0
2	F	76	TYR	5.0
3	G	75	HIS	5.0
1	A	566	GLN	5.0
1	E	582	PRO	4.9
1	E	164	ASN	4.8
3	G	77	TRP	4.8
1	E	558	MET	4.7
2	F	4	TYR	4.7
1	E	512	LEU	4.7
1	E	84	GLY	4.7
1	A	591	GLU	4.7
3	C	110	LYS	4.7
1	A	586	ALA	4.6
1	A	539	THR	4.6
1	E	44	CYS	4.6
1	E	56	HIS	4.6
3	G	21	PHE	4.5
2	F	32	GLY	4.5
1	E	85	ALA	4.5
1	E	66	GLU	4.4
2	F	117	THR	4.4
1	E	581	LEU	4.4
2	F	126	GLY	4.4
1	E	384	ALA	4.3
1	E	465	ILE	4.3
1	E	221	ASP	4.3
3	C	60	ASP	4.3
1	A	522	ALA	4.3
1	E	374	TYR	4.3
1	E	607	VAL	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	398	PRO	4.2
2	F	20	ALA	4.2
1	E	591	GLU	4.2
3	G	250	LEU	4.2
1	A	30	ALA	4.2
1	A	607	VAL	4.1
1	A	207	GLY	4.1
1	A	534	TYR	4.1
1	E	470	GLN	4.1
1	E	437	ALA	4.1
2	F	26	GLU	4.1
1	A	581	LEU	4.1
3	G	71	PHE	4.1
3	C	172	ALA	4.1
2	F	61	CYS	4.1
1	E	386	GLY	4.1
1	E	583	PHE	4.0
2	F	82	LEU	4.0
1	E	117	TRP	4.0
1	E	482	GLU	4.0
2	F	19	CYS	4.0
1	E	517	PRO	4.0
3	G	13	TRP	4.0
3	G	62	ILE	4.0
1	E	496	ALA	4.0
3	C	235	ALA	4.0
3	G	244	ALA	3.9
3	G	45	ALA	3.9
1	E	539	THR	3.9
1	E	30	ALA	3.9
2	F	23	CYS	3.8
2	F	69	VAL	3.8
1	E	546	THR	3.8
1	A	183	TRP	3.8
2	F	74	ALA	3.8
1	E	469	PRO	3.8
1	A	69	GLU	3.8
3	G	66	GLU	3.8
3	C	19	ALA	3.8
1	E	39	SER	3.8
1	E	387	GLY	3.8
1	E	60	ASN	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	68	TYR	3.7
1	E	464	ALA	3.7
2	F	84	LEU	3.7
1	A	585	THR	3.7
1	A	592	LEU	3.7
1	A	729	SER	3.7
1	A	608	PHE	3.7
3	G	74	THR	3.7
1	A	571	TRP	3.7
2	F	87	PRO	3.7
1	E	47	CYS	3.7
3	G	98	GLY	3.7
1	E	485	TYR	3.6
2	F	147	ASP	3.6
1	A	617	GLY	3.6
1	E	509	HIS	3.6
2	F	173	PRO	3.6
1	A	546	THR	3.6
1	A	605	LEU	3.6
2	F	27	ASN	3.6
1	E	593	TYR	3.6
1	E	506	THR	3.6
2	F	25	MET	3.6
1	E	63	TYR	3.6
3	G	85	THR	3.6
1	E	503	GLN	3.5
1	E	37	VAL	3.5
3	G	37	LEU	3.5
1	A	590	ILE	3.5
2	F	122	ARG	3.5
2	F	34	PHE	3.5
1	E	40	VAL	3.5
1	A	564	LEU	3.5
1	E	152	PHE	3.5
1	A	529	LEU	3.5
1	E	525	LEU	3.5
2	F	129	PRO	3.5
1	E	515	THR	3.4
1	E	366	ALA	3.4
3	C	79	LEU	3.4
1	A	606	PRO	3.4
1	E	189	ILE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	434	GLY	3.4
1	E	630	THR	3.4
1	A	582	PRO	3.4
1	E	493	VAL	3.4
3	G	110	GLY	3.4
3	G	63	LEU	3.4
1	A	568	GLY	3.4
1	E	533	GLN	3.4
1	E	537	TRP	3.4
1	A	388	CYS	3.4
3	G	59	ASP	3.4
1	A	597	PHE	3.3
2	F	6	MET	3.3
1	A	551	LEU	3.3
1	A	576	GLU	3.3
1	A	366	ALA	3.3
1	E	124	ILE	3.3
2	F	115	LYS	3.3
1	A	361	GLY	3.3
1	A	391	PRO	3.3
1	E	507	PRO	3.3
2	F	113	VAL	3.3
1	E	46	GLY	3.3
3	C	109	GLY	3.3
2	F	112	TYR	3.3
1	A	284	VAL	3.3
1	E	58	VAL	3.3
2	F	83	VAL	3.3
1	E	393	GLY	3.3
3	C	219	GLY	3.3
1	E	202	TYR	3.2
2	B	1	MET	3.2
1	A	430	TYR	3.2
3	G	104	LEU	3.2
1	E	483	ALA	3.2
1	A	164	ASN	3.2
1	E	369	PRO	3.2
1	A	36	GLU	3.2
1	A	593	TYR	3.2
1	A	70	ALA	3.2
3	G	225	LEU	3.2
1	E	383	PRO	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	672	GLN	3.2
3	G	224	ARG	3.2
1	A	686	ALA	3.2
1	E	196	ASP	3.1
1	E	621	LEU	3.1
1	A	286	PHE	3.1
1	A	293	VAL	3.1
2	F	85	VAL	3.1
3	G	207	PHE	3.1
1	A	280	ALA	3.1
3	C	112	SER	3.1
3	G	169	PRO	3.1
1	A	376	LEU	3.1
3	G	39	LEU	3.1
3	G	172	LEU	3.1
1	E	149	ASP	3.1
3	G	170	TRP	3.1
1	E	599	GLU	3.1
1	E	51	CYS	3.1
1	E	113	ARG	3.1
1	A	447	PRO	3.1
1	E	706	MET	3.1
3	G	38	HIS	3.1
1	A	394	GLY	3.1
1	A	721	THR	3.1
1	E	568	GLY	3.1
3	G	12	PHE	3.1
1	A	589	LYS	3.1
1	E	391	PRO	3.1
3	G	14	HIS	3.1
3	G	83	HIS	3.1
3	C	29	GLY	3.1
3	G	129	TYR	3.1
1	A	156	LEU	3.0
1	E	637	ASN	3.0
2	B	73	GLY	3.0
1	E	569	LYS	3.0
1	A	383	PRO	3.0
1	E	511	PRO	3.0
1	E	590	ILE	3.0
1	A	504	LEU	3.0
1	A	333	HIS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	64	LYS	3.0
1	E	65	VAL	3.0
1	E	484	THR	3.0
1	A	395	ASP	3.0
1	E	551	LEU	3.0
1	E	88	THR	3.0
1	E	685	THR	3.0
1	E	398	PRO	3.0
1	A	587	SER	3.0
3	G	53	LEU	3.0
1	A	514	ASP	3.0
1	E	566	GLN	3.0
1	A	558	MET	3.0
1	E	31	PRO	3.0
1	A	618	PHE	3.0
1	E	597	PHE	3.0
2	F	116	CYS	3.0
1	E	521	ILE	3.0
1	E	508	ALA	2.9
2	F	190	SER	2.9
1	E	629	HIS	2.9
1	E	486	LEU	2.9
3	G	36	LEU	2.9
1	E	600	ALA	2.9
1	A	569	LYS	2.9
1	A	500	PRO	2.9
1	A	392	SER	2.9
3	G	113	ARG	2.9
1	E	323	LYS	2.9
1	A	517	PRO	2.9
1	A	385	ALA	2.9
3	G	114	ALA	2.9
1	E	151	TRP	2.9
1	E	142	PHE	2.9
3	G	99	PHE	2.9
1	E	502	ILE	2.9
2	F	59	LEU	2.9
1	E	396	HIS	2.8
1	A	418	GLN	2.8
1	A	168	PRO	2.8
1	E	375	PRO	2.8
1	E	32	TRP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	66	CYS	2.8
2	F	15	GLY	2.8
1	E	70	ALA	2.8
3	G	7	PRO	2.8
2	F	103	ASP	2.8
1	A	537	TRP	2.8
1	E	638	TRP	2.8
1	A	526	GLY	2.8
1	A	141	ALA	2.8
1	E	115	ALA	2.8
1	E	165	ALA	2.8
1	E	62	VAL	2.8
1	E	467	VAL	2.8
3	G	124	LEU	2.8
3	G	231	LEU	2.8
1	E	148	GLY	2.8
1	E	355	GLY	2.8
1	E	543	TYR	2.8
2	F	121	HIS	2.8
3	C	113	GLN	2.8
1	E	392	SER	2.8
3	G	111	SER	2.8
1	E	640	LEU	2.8
1	A	296	PHE	2.8
2	F	73	GLY	2.8
3	C	114	ARG	2.8
1	A	298	PRO	2.8
3	G	125	VAL	2.8
2	F	118	PHE	2.7
1	E	584	GLY	2.7
1	E	588	GLY	2.7
3	G	221	TRP	2.7
2	F	127	LYS	2.7
3	G	227	PRO	2.7
1	A	386	GLY	2.7
1	E	448	ASN	2.7
1	E	34	ALA	2.7
1	A	37	VAL	2.7
3	G	246	GLN	2.7
1	E	92	PRO	2.7
1	E	371	LEU	2.7
2	F	93	CYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	1	MET	2.7
1	A	567	ARG	2.7
2	F	102	TYR	2.7
1	E	602	HIS	2.7
1	A	572	LEU	2.7
3	G	243	LEU	2.7
1	E	436	PHE	2.7
1	A	596	ARG	2.7
3	G	5	GLY	2.7
1	E	634	THR	2.7
1	E	368	SER	2.7
1	A	339	ASP	2.7
1	A	565	VAL	2.7
2	F	67	VAL	2.7
1	A	369	PRO	2.7
1	A	375	PRO	2.7
1	E	35	GLN	2.7
3	G	87	PRO	2.7
1	A	561	MET	2.7
1	A	387	GLY	2.7
1	E	585	THR	2.7
2	F	130	ALA	2.7
3	G	116	ALA	2.7
1	A	553	LEU	2.7
3	C	108	LEU	2.7
3	C	126	VAL	2.7
1	E	80	PRO	2.6
3	G	79	PHE	2.6
1	E	478	VAL	2.6
3	C	227	ALA	2.6
1	E	342	TYR	2.6
1	E	421	ILE	2.6
1	A	191	GLY	2.6
1	E	674	GLY	2.6
1	E	571	TRP	2.6
1	A	153	VAL	2.6
3	G	18	ALA	2.6
3	G	160	LEU	2.6
1	A	540	ILE	2.6
1	E	559	LYS	2.6
1	E	481	PRO	2.6
1	E	36	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	570	PRO	2.6
2	F	65	PRO	2.6
2	F	81	GLY	2.6
3	G	8	ASN	2.6
1	A	288	GLU	2.6
1	E	544	LEU	2.6
3	G	120	LEU	2.6
3	G	240	LEU	2.6
3	G	109	LYS	2.6
1	E	194	PRO	2.6
1	A	148	GLY	2.6
1	A	588	GLY	2.6
1	E	108	GLY	2.6
3	C	7	LEU	2.6
3	C	216	LEU	2.6
1	E	54	VAL	2.6
1	E	563	THR	2.6
2	F	78	THR	2.6
1	E	513	PHE	2.5
1	E	33	TYR	2.5
1	E	462	TYR	2.5
1	A	136	GLY	2.5
1	E	52	GLY	2.5
3	G	23	LEU	2.5
1	E	466	ASP	2.5
2	F	192	VAL	2.5
3	G	72	ARG	2.5
2	F	92	ALA	2.5
1	A	575	TRP	2.5
1	E	140	ILE	2.5
1	A	364	TYR	2.5
2	B	46	TYR	2.5
2	F	64	PRO	2.5
3	G	26	LEU	2.5
3	G	67	SER	2.5
3	G	107	LEU	2.5
3	G	171	ALA	2.5
1	A	43	ILE	2.5
1	A	331	THR	2.5
3	C	75	THR	2.5
2	F	31	PRO	2.5
3	C	228	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	402	LYS	2.5
1	A	461	LEU	2.5
1	A	603	GLN	2.5
1	E	367	GLN	2.5
1	E	463	VAL	2.5
1	E	471	GLU	2.5
1	E	510	GLU	2.5
1	A	269	ILE	2.5
1	E	490	ASP	2.5
1	E	48	PHE	2.5
3	G	15	TRP	2.5
3	G	82	PHE	2.5
1	A	132	ARG	2.5
1	A	381	LEU	2.5
1	A	725	LEU	2.5
1	E	192	HIS	2.5
1	E	534	TYR	2.5
1	E	564	LEU	2.5
1	E	67	GLY	2.5
1	E	678	GLY	2.5
3	G	206	GLY	2.5
3	C	46	ALA	2.5
3	C	183	SER	2.5
3	G	168	SER	2.5
1	A	48	PHE	2.5
1	A	441	ASN	2.5
1	E	395	ASP	2.5
1	E	443	PHE	2.5
1	A	160	TRP	2.5
1	A	432	ILE	2.4
2	F	139	CYS	2.4
1	A	66	GLU	2.4
1	E	762	GLU	2.4
1	E	580	ARG	2.4
1	E	499	THR	2.4
2	B	72	THR	2.4
1	E	168	PRO	2.4
3	C	15	HIS	2.4
1	A	421	ILE	2.4
1	E	715	SER	2.4
1	A	559	LYS	2.4
3	G	122	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	G	64	TRP	2.4
1	E	153	VAL	2.4
1	E	560	GLY	2.4
1	E	756	ALA	2.4
3	G	43	ALA	2.4
3	G	56	ILE	2.4
1	E	128	MET	2.4
3	G	40	LYS	2.4
1	A	95	LEU	2.4
2	B	192	VAL	2.4
3	G	245	GLY	2.4
1	E	669	LEU	2.4
3	G	97	LEU	2.4
1	E	214	THR	2.4
2	F	21	VAL	2.4
3	G	49	THR	2.4
1	A	406	ASP	2.4
1	E	90	TYR	2.4
1	E	125	ALA	2.4
2	B	20	ALA	2.4
3	G	48	TYR	2.4
1	E	596	ARG	2.4
1	A	42	GLN	2.4
1	E	87	GLN	2.4
1	A	739	VAL	2.4
1	E	611	PRO	2.4
3	C	25	VAL	2.4
1	A	728	ILE	2.3
1	A	599	GLU	2.3
1	E	565	VAL	2.3
1	E	385	ALA	2.3
3	C	115	ALA	2.3
3	G	1	ALA	2.3
1	A	270	TYR	2.3
3	G	60	LEU	2.3
3	G	119	LEU	2.3
1	A	595	GLN	2.3
2	F	28	GLU	2.3
3	C	45	GLU	2.3
1	E	552	GLY	2.3
3	G	143	TRP	2.3
1	A	283	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	106	TYR	2.3
1	E	760	PHE	2.3
1	E	549	GLN	2.3
1	E	133	GLU	2.3
2	F	152	VAL	2.3
1	A	101	ARG	2.3
1	A	336	TRP	2.3
3	C	187	ALA	2.3
3	G	89	TRP	2.3
1	A	634	THR	2.3
1	E	364	TYR	2.3
1	A	397	GLU	2.3
1	E	109	GLU	2.3
3	G	223	GLU	2.3
1	A	131	ILE	2.3
1	A	157	PRO	2.3
1	A	450	PRO	2.3
1	A	518	GLY	2.3
1	A	562	GLY	2.3
1	A	711	GLY	2.3
3	C	65	TRP	2.3
1	E	217	THR	2.3
3	C	50	THR	2.3
3	G	237	LEU	2.3
1	A	401	PHE	2.3
3	G	173	PHE	2.3
2	F	24	LYS	2.3
3	C	67	GLU	2.2
1	A	425	ILE	2.2
1	E	540	ILE	2.2
2	F	97	ILE	2.2
3	G	88	ILE	2.2
1	E	394	GLY	2.2
2	B	87	PRO	2.2
2	B	170	GLY	2.2
2	F	94	GLY	2.2
2	F	142	PHE	2.2
2	F	194	HIS	2.2
1	A	342	TYR	2.2
1	A	349	TYR	2.2
1	A	389	SER	2.2
3	C	68	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	169	SER	2.2
1	E	603	GLN	2.2
2	F	124	GLU	2.2
1	A	371	LEU	2.2
1	E	461	LEU	2.2
1	E	480	LEU	2.2
3	G	191	LEU	2.2
1	A	174	THR	2.2
1	A	563	THR	2.2
2	F	60	HIS	2.2
1	A	521	ILE	2.2
1	A	429	PRO	2.2
1	E	121	LEU	2.2
3	C	42	GLY	2.2
3	G	6	LEU	2.2
3	G	126	ALA	2.2
3	C	74	PHE	2.2
1	E	633	ARG	2.2
2	B	172	ARG	2.2
3	G	93	TRP	2.2
2	F	33	VAL	2.2
1	A	100	ILE	2.2
1	E	99	LEU	2.2
1	E	330	PRO	2.2
2	F	104	ALA	2.2
3	C	230	ALA	2.2
1	E	373	LYS	2.2
3	C	94	TRP	2.2
1	A	292	HIS	2.2
1	A	40	VAL	2.2
3	G	30	VAL	2.2
1	E	389	SER	2.2
1	A	290	LYS	2.2
1	A	448	ASN	2.2
1	A	400	GLY	2.2
1	E	400	GLY	2.2
1	E	500	PRO	2.2
3	G	117	TRP	2.2
1	E	89	THR	2.1
1	E	680	VAL	2.1
2	F	29	VAL	2.1
3	G	16	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	651	ILE	2.1
1	A	672	GLN	2.1
3	C	212	LEU	2.1
3	G	175	LEU	2.1
3	G	241	LEU	2.1
1	A	433	LYS	2.1
2	F	95	ALA	2.1
1	E	144	GLY	2.1
1	A	170	VAL	2.1
1	A	478	VAL	2.1
1	E	623	TYR	2.1
2	F	138	TYR	2.1
1	A	134	LYS	2.1
3	C	56	LEU	2.1
3	G	80	LEU	2.1
1	A	496	ALA	2.1
1	E	488	ARG	2.1
1	E	522	ALA	2.1
3	G	92	ALA	2.1
1	E	138	GLU	2.1
1	E	579	GLY	2.1
1	E	492	PHE	2.1
3	G	212	PHE	2.1
1	A	151	TRP	2.1
1	E	114	VAL	2.1
1	E	160	TRP	2.1
2	B	135	CYS	2.1
2	F	70	CYS	2.1
3	C	130	TYR	2.1
3	G	106	TYR	2.1
1	E	106	GLN	2.1
1	A	138	GLU	2.1
1	A	443	PHE	2.1
1	A	335	VAL	2.1
1	A	123	HIS	2.1
1	A	598	LYS	2.1
1	E	172	LEU	2.1
2	F	16	CYS	2.1
3	C	176	LEU	2.1
3	C	218	LEU	2.1
1	E	561	MET	2.1
2	F	120	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	155	ALA	2.1
2	F	77	GLN	2.1
1	E	59	GLY	2.1
1	A	542	GLU	2.1
2	B	191	GLU	2.1
3	G	61	PHE	2.1
1	A	169	SER	2.1
1	A	480	LEU	2.1
1	E	625	ARG	2.1
3	G	76	ILE	2.1
1	E	701	HIS	2.1
3	C	39	HIS	2.1
1	E	365	ILE	2.0
1	E	529	LEU	2.0
2	F	123	LEU	2.0
2	F	188	ARG	2.0
3	C	47	ARG	2.0
3	G	105	LEU	2.0
1	A	128	MET	2.0
1	E	406	ASP	2.0
1	E	476	ALA	2.0
3	C	196	PRO	2.0
1	E	435	LEU	2.0
1	E	553	LEU	2.0
3	C	61	LEU	2.0
1	E	105	SER	2.0
1	A	458	ASN	2.0
3	C	78	TRP	2.0
1	A	506	THR	2.0
1	A	609	THR	2.0
1	E	554	ASP	2.0
1	A	52	GLY	2.0
2	F	135	CYS	2.0
1	A	470	GLN	2.0
2	F	109	PRO	2.0
3	C	175	PRO	2.0
1	E	103	GLU	2.0
1	E	545	GLU	2.0
2	F	191	GLU	2.0
1	A	177	ARG	2.0
1	E	50	ARG	2.0
1	E	81	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	G	121	VAL	2.0
3	C	96	LEU	2.0
3	G	33	LEU	2.0
1	A	417	ILE	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 [i](#)

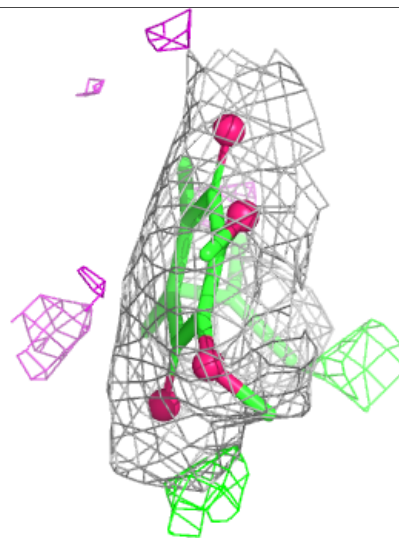
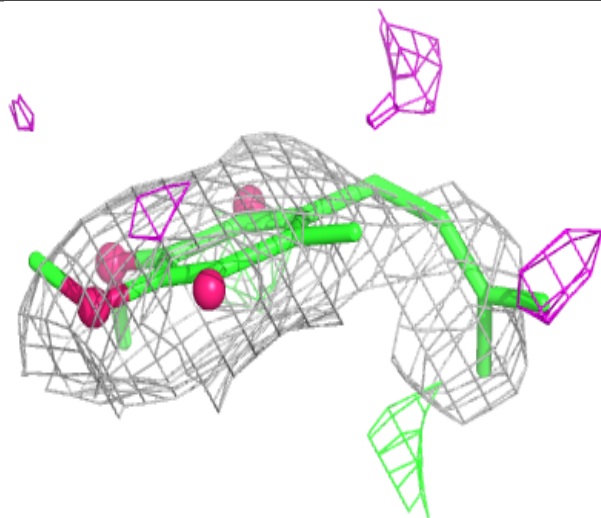
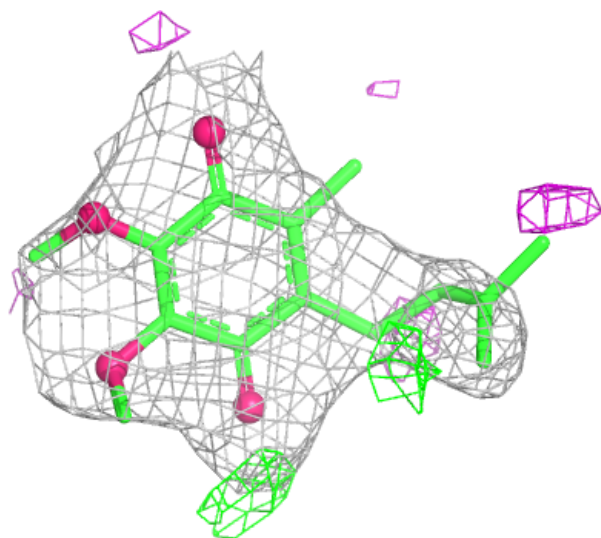
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	UQ1	G	1251	18/18	0.79	0.22	82,86,87,88	0
4	SF4	E	1764	8/8	0.88	0.15	60,69,74,77	0
4	SF4	F	1196	8/8	0.89	0.14	66,72,74,79	0
4	SF4	F	1197	8/8	0.89	0.13	77,82,85,86	0
5	MGD	E	1765	47/47	0.89	0.15	50,61,75,76	0
4	SF4	F	1195	8/8	0.89	0.15	56,63,69,69	0
5	MGD	E	1766	47/47	0.91	0.14	45,54,61,62	0
6	MO	A	1767	1/1	0.91	0.08	55,55,55,55	0
4	SF4	F	1194	8/8	0.91	0.13	67,71,72,73	0
5	MGD	A	1765	47/47	0.93	0.11	52,55,58,59	0
5	MGD	A	1766	47/47	0.93	0.13	46,50,63,64	0
4	SF4	B	1196	8/8	0.93	0.12	48,56,63,63	0
7	UQ1	C	1252	18/18	0.94	0.14	75,77,80,80	0
4	SF4	B	1194	8/8	0.96	0.08	62,65,67,68	0
6	MO	E	1767	1/1	0.96	0.07	60,60,60,60	0
4	SF4	A	1764	8/8	0.97	0.08	50,54,57,57	0
4	SF4	B	1195	8/8	0.97	0.07	60,61,63,65	0
4	SF4	B	1197	8/8	0.98	0.06	52,55,56,57	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.

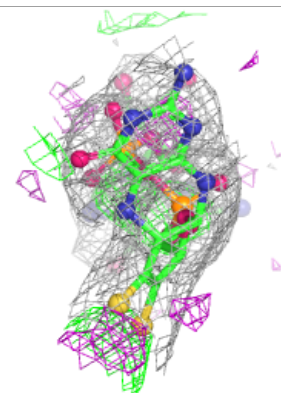
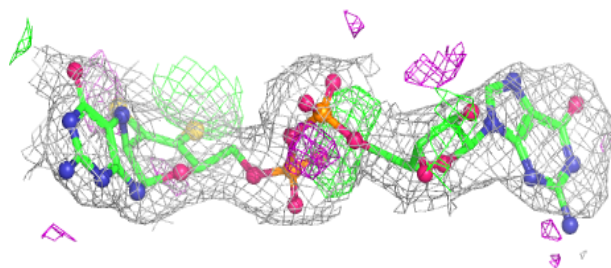
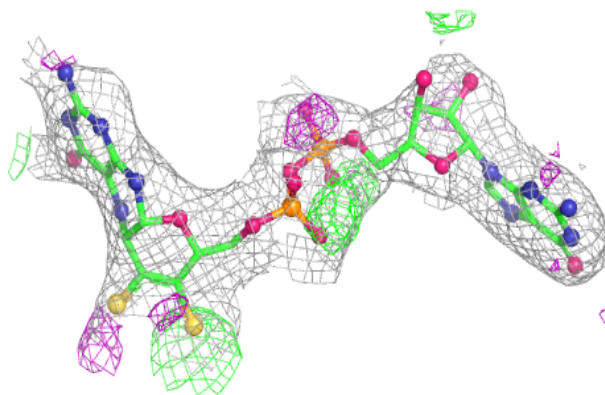
Electron density around UQ1 G 1251:

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

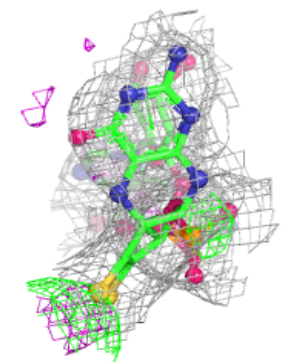
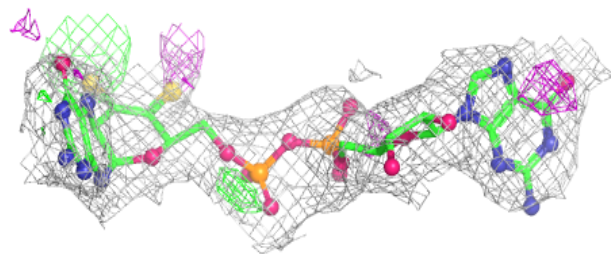
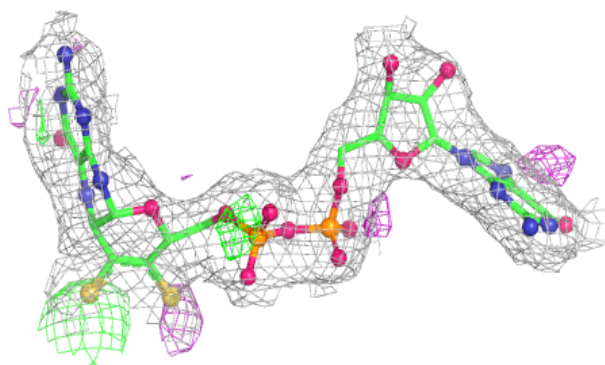


Electron density around MGD E 1765:

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

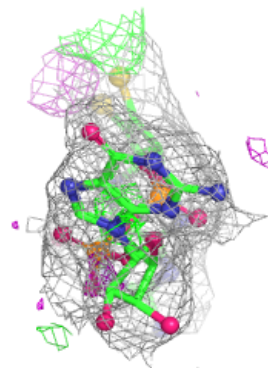
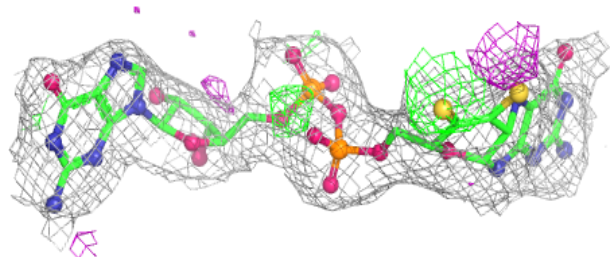
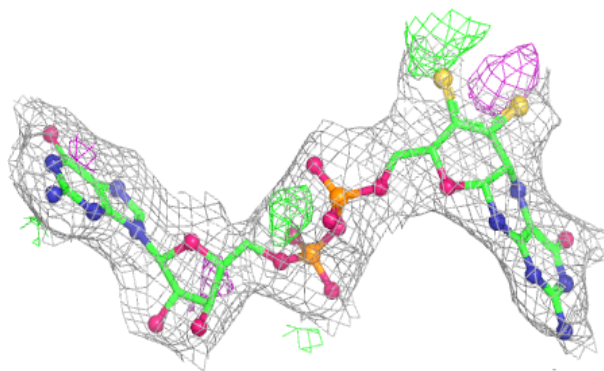
**Electron density around MGD E 1766:**

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

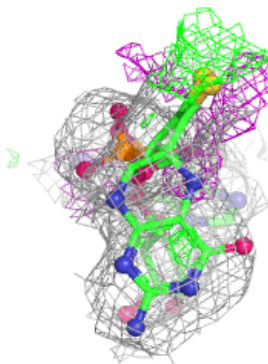
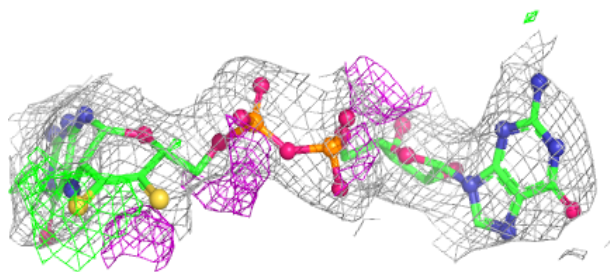
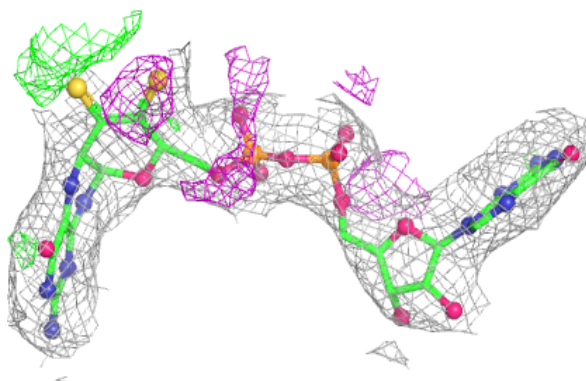


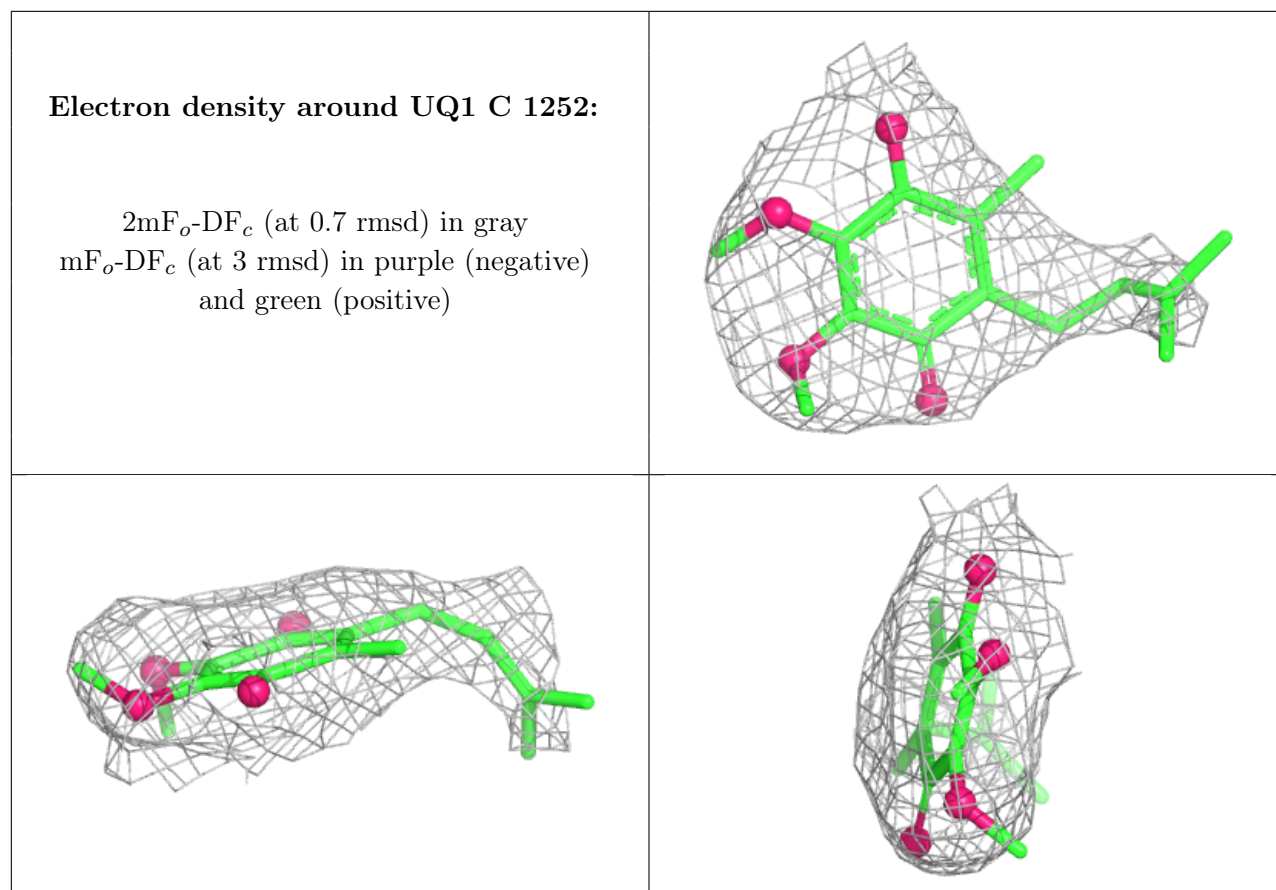
Electron density around MGD A 1765:

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

**Electron density around MGD A 1766:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.