



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:33 AM UTC

PDB ID : 2J3N / pdb_00002j3n
Title : X-ray structure of human thioredoxin reductase 1
Authors : Fritz-Wolf, K.; Urig, S.; Becker, K.
Deposited on : 2006-08-22
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

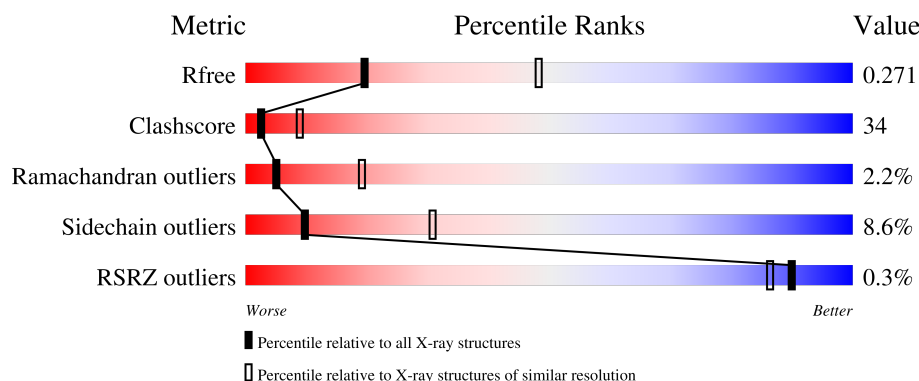
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	519	
1	B	519	
1	C	519	
1	D	519	
1	E	519	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	519	

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
3	NAP	A	601	X	-	-	-
3	NAP	B	601	X	-	-	-
3	NAP	C	601	X	-	-	-

2 Entry composition [i](#)

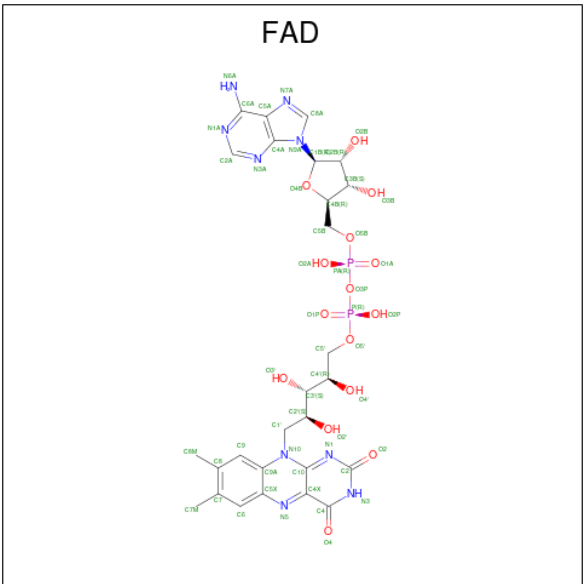
There are 5 unique types of molecules in this entry. The entry contains 23294 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 THIOREDOXIN REDUCTASE 1.

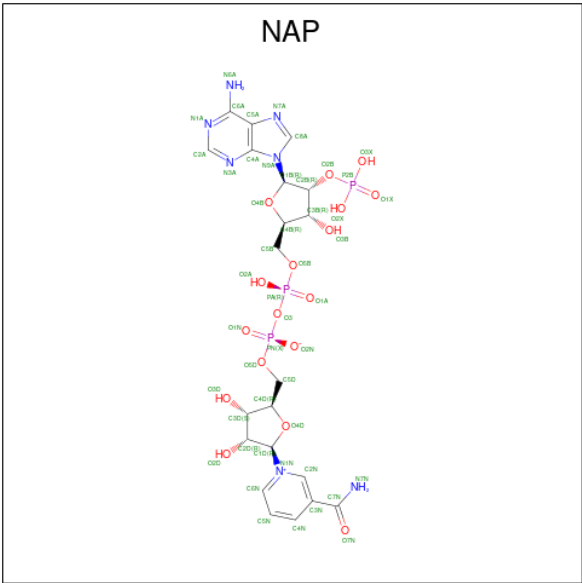
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	1
			3756	2387	642	708	19			
1	B	487	Total	C	N	O	S	0	0	1
			3760	2390	643	708	19			
1	C	490	Total	C	N	O	S	0	0	0
			3776	2397	645	713	21			
1	D	491	Total	C	N	O	S	0	0	0
			3785	2403	647	714	21			
1	E	490	Total	C	N	O	S	0	0	0
			3776	2397	645	713	21			
1	F	486	Total	C	N	O	S	0	0	1
			3751	2385	641	706	19			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



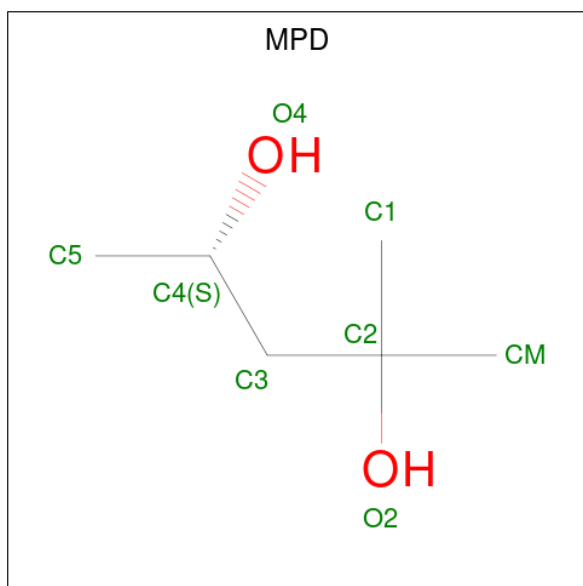
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	9	Total	O	0	0
			9	9		
5	C	7	Total	O	0	0
			7	7		

Continued on next page...

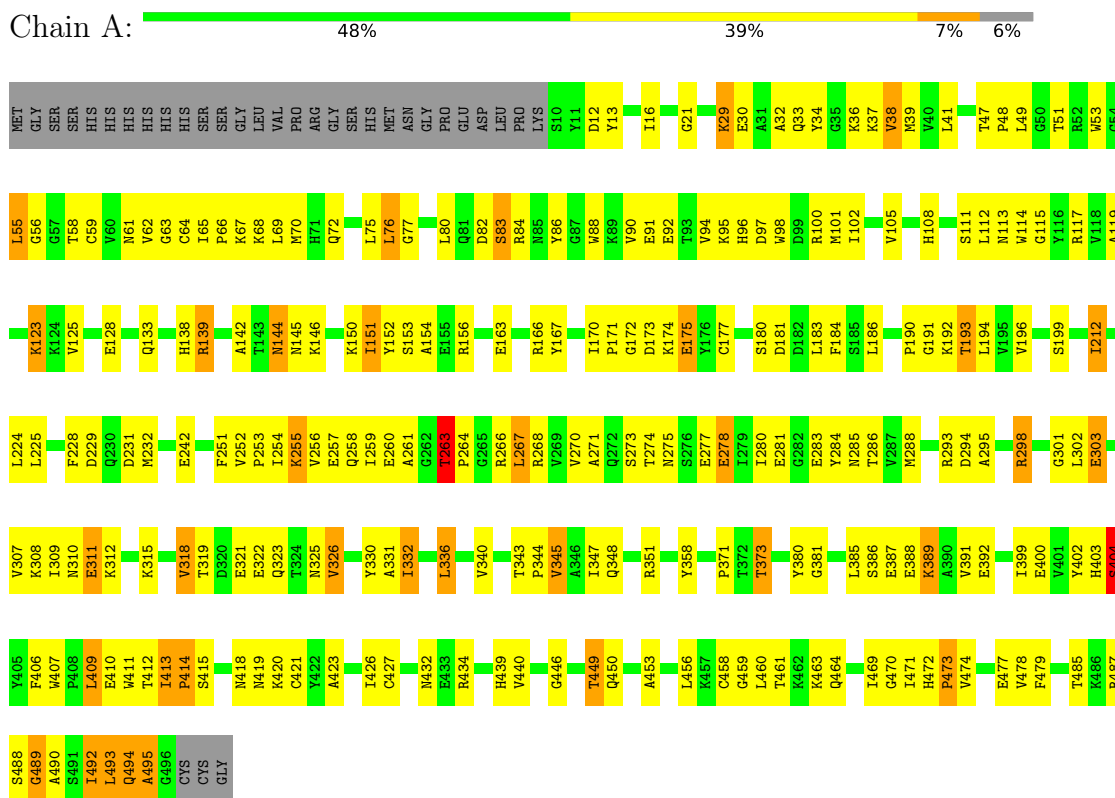
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	8	Total 8	O 8	0	0
5	E	4	Total 4	O 4	0	0
5	F	7	Total 7	O 7	0	0

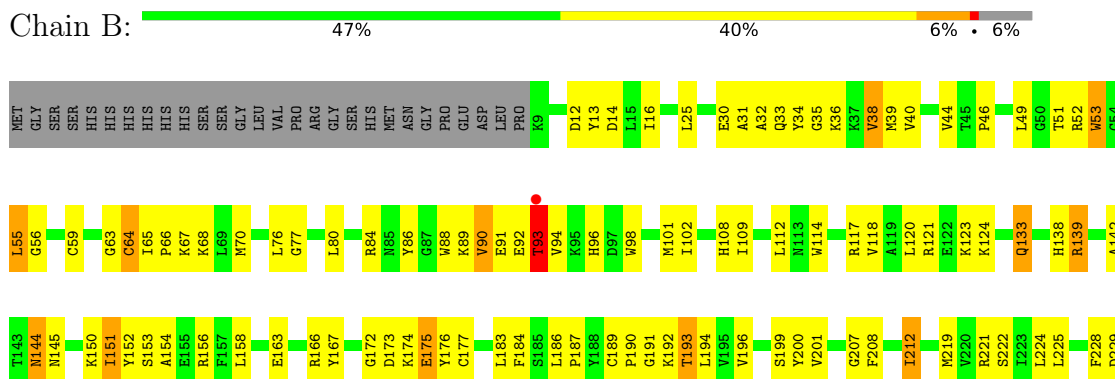
3 Residue-property plots

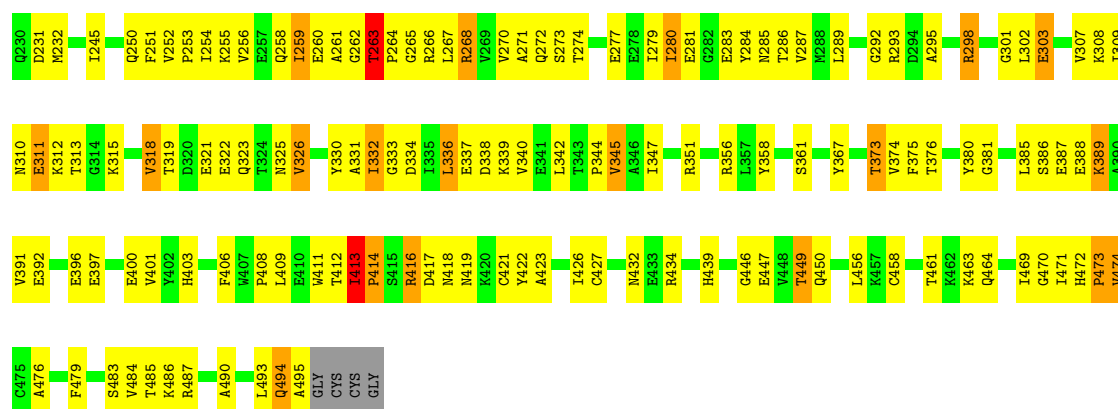
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: THIOREDOXIN REDUCTASE 1

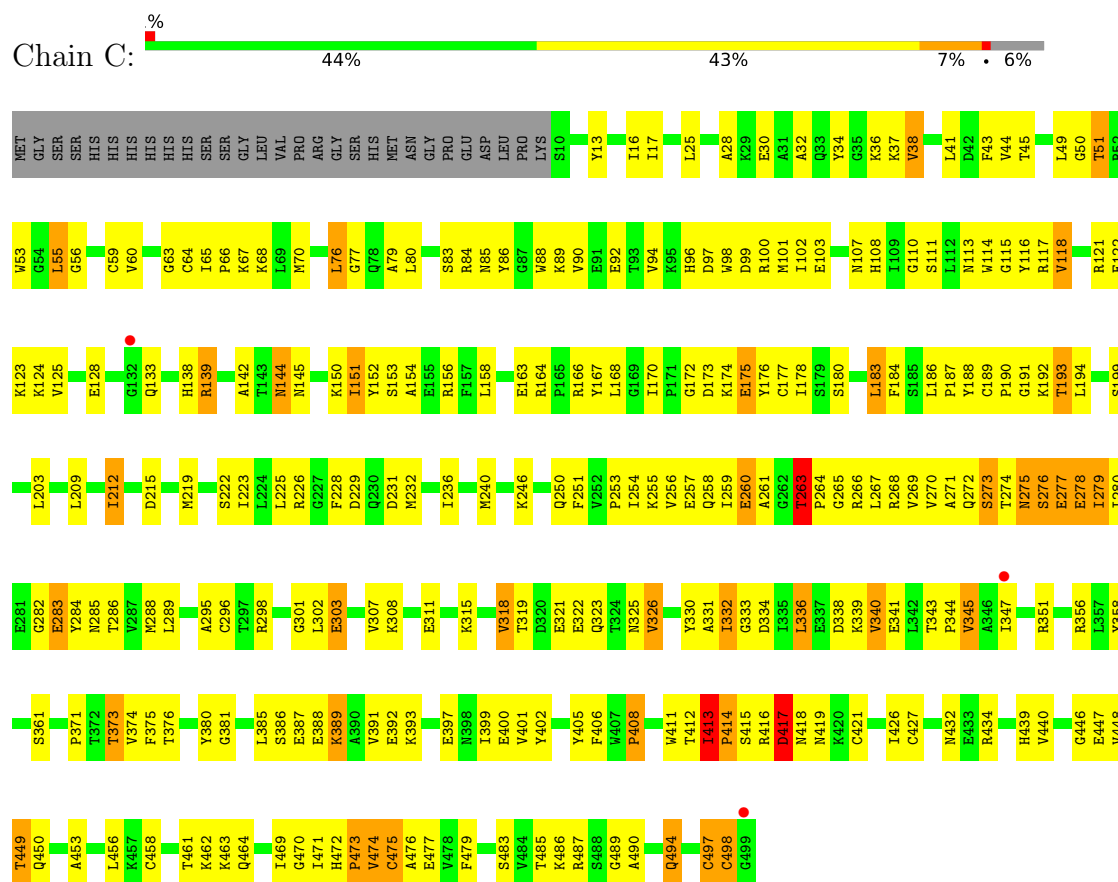


• Molecule 1: THIOREDOXIN REDUCTASE 1

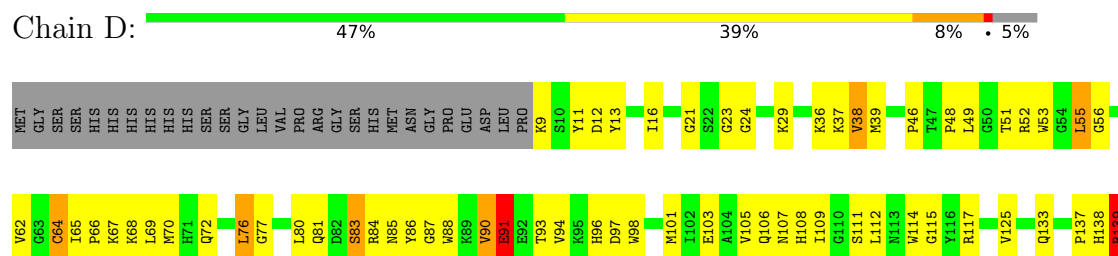


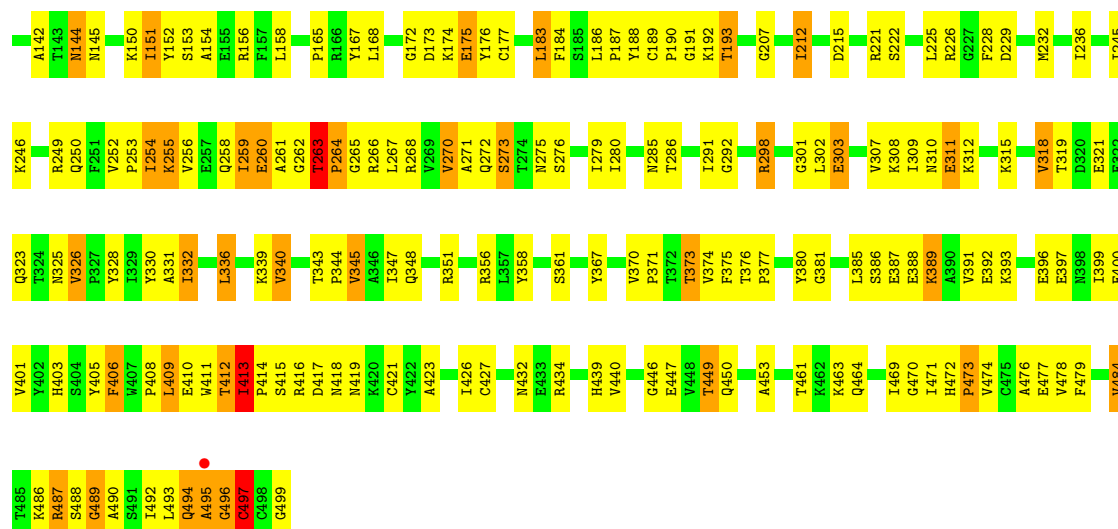


• Molecule 1: THIOREDOXIN REDUCTASE 1

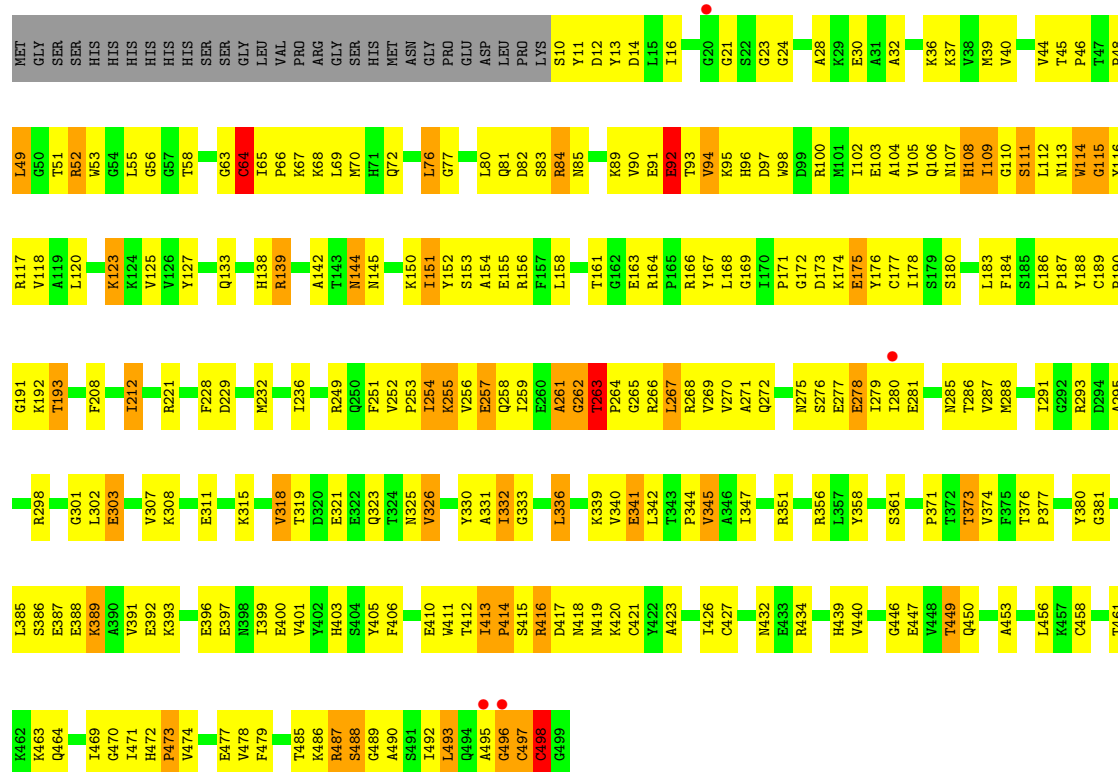
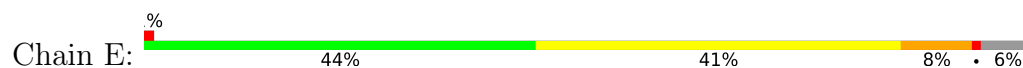


• Molecule 1: THIOREDOXIN REDUCTASE 1





• Molecule 1: THIOREDOXIN REDUCTASE 1



• Molecule 1: THIOREDOXIN REDUCTASE 1



A453	L456	R457	C458	G459	I460	T461	R462	K463	Q464	I469	G470	I471	H472	P473	V474	C475	A476	E477	V478	F479	L482	S483	V484	T485	R486	R487	S488	G489	A490	S491	I492	L493	R494	ALA	GLY	CYS	CYS	GLY															
V374	F375	T376	P377	Y380	G381	L385	S386	E387	E388	K389	K390	V391	E392	K393	E397	R398	I399	E400	V401	Y402	H403	S404	Y405	F406	W407	P408	L409	E410	W411	T412	I413	P414	S415	R416	D417	N418	N419	K420	C421	I426	C427	N432	E433	R434	F438	H439	G446	E447	V448	T449	Q450		
Y284	M288	I291	G292	R293	D294	A295	R298	G301	L302	E303	V307	K308	E311	V318	T319	D320	E321	E322	Q323	T324	N325	V326	Y330	A331	T332	G333	D334	I335	L336	E337	D338	K339	V340	E341	L342	T343	P344	V345	A346	I347	Q348	R351	L352	L353	Y367	P371	T372	T373					
L203	E204	C205	A206	G207	F208	L209	I212	D215	I223	R226	G227	F228	D229	Q230	D231	M232	K235	M240	I245	K246	F251	V252	P253	I254	K255	V256	E257	Q258	I259	E260	A261	G262	T263	P264	G265	R266	L267	R268	V269	V270	A271	Q272	S273	T274	N275	S276	E277	I280	E281				
T47	P48	L49	R52	G57	T58	C59	V60	N61	V62	G63	C64	I65	K67	K68	L69	M70	H71	Q72	L75	L76	G77	Q78	A79	L80	Q81	D82	S83	R84	N85	Y86	G87	W88	K89	V90	E91	E92	T93	V94	K95	H96	D97	W98	M101	I102	E103	A104	N107	H108	I109	G110	S111	L112	N113
Y116	R117	V118	A119	L120	V125	Q133	H138	R139	I140	K141	A142	T143	N144	N145	K150	I151	Y152	S153	A154	E155	R156	F157	L158	T161	G162	E163	R164	Y167	L168	G172	D173	K174	E175	Y176	C177	I178	D181	D182	L183	F184	S185	L186	P190	G191	K192	T193	Y200						

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	144.63Å 90.64Å 166.60Å 90.00° 112.46° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.8 (15.00-2.80) 98.8 (15.00-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.287 (Not available) , 0.271	Depositor DCC
R_{free} test set	4885 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23294	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: FAD, MPD, NAP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	1/3830 (0.0%)	1.01	11/5187 (0.2%)
1	B	0.55	1/3834 (0.0%)	0.99	11/5191 (0.2%)
1	C	0.53	1/3850 (0.0%)	1.00	12/5211 (0.2%)
1	D	0.55	1/3859 (0.0%)	1.08	19/5222 (0.4%)
1	E	0.47	0/3850	0.99	18/5211 (0.3%)
1	F	0.48	1/3825 (0.0%)	0.99	13/5179 (0.3%)
All	All	0.52	5/23048 (0.0%)	1.01	84/31201 (0.3%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	413	ILE	CA-CB	7.69	1.59	1.53
1	F	493	LEU	C-N	-5.57	1.25	1.33
1	B	494	GLN	C-N	-5.56	1.25	1.33
1	A	495	ALA	C-N	-5.45	1.25	1.33
1	C	497	CYS	CA-C	5.10	1.59	1.52

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	263	THR	CA-C-N	-15.27	101.44	120.23
1	D	263	THR	C-N-CA	-15.27	101.44	120.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	ARG	NE-CZ-NH2	13.00	130.90	119.20
1	D	139	ARG	NE-CZ-NH1	-11.64	109.86	121.50
1	A	263	THR	CA-C-N	-11.59	105.72	120.79
1	A	263	THR	C-N-CA	-11.59	105.72	120.79
1	F	263	THR	CA-C-N	-11.22	106.43	120.23
1	F	263	THR	C-N-CA	-11.22	106.43	120.23
1	C	263	THR	CA-C-N	-10.86	106.27	119.84
1	C	263	THR	C-N-CA	-10.86	106.27	119.84
1	D	139	ARG	CD-NE-CZ	10.01	138.41	124.40
1	E	263	THR	CA-C-N	-9.78	107.62	119.84
1	E	263	THR	C-N-CA	-9.78	107.62	119.84
1	A	274	THR	N-CA-C	-8.61	102.91	113.50
1	B	263	THR	CA-C-N	-8.60	109.08	119.84
1	B	263	THR	C-N-CA	-8.60	109.08	119.84
1	B	413	ILE	CA-C-N	-7.70	111.86	119.64
1	B	413	ILE	C-N-CA	-7.70	111.86	119.64
1	D	484	VAL	N-CA-C	7.52	118.71	107.51
1	B	414	PRO	N-CA-C	-7.23	104.13	114.18
1	F	274	THR	N-CA-C	-7.02	103.63	111.28
1	E	109	ILE	N-CA-C	-6.90	103.80	110.42
1	A	492	ILE	N-CA-C	-6.90	106.50	113.47
1	A	92	GLU	N-CA-C	-6.79	101.12	110.35
1	D	264	PRO	N-CA-C	-6.79	99.85	110.50
1	D	412	THR	CA-C-N	-6.75	115.99	120.24
1	D	412	THR	C-N-CA	-6.75	115.99	120.24
1	C	414	PRO	N-CA-C	-6.75	104.80	114.18
1	E	92	GLU	N-CA-C	6.58	118.54	111.36
1	F	414	PRO	N-CA-C	-6.55	104.80	113.65
1	A	414	PRO	N-CA-C	-6.32	106.25	114.03
1	C	386	SER	N-CA-C	-6.22	102.50	110.53
1	D	326	VAL	CA-C-N	6.11	127.47	119.84
1	D	326	VAL	C-N-CA	6.11	127.47	119.84
1	D	413	ILE	N-CA-CB	6.10	114.34	110.50
1	B	386	SER	N-CA-C	-6.06	102.71	110.53
1	E	487	ARG	N-CA-C	-6.03	103.88	111.11
1	D	259	ILE	N-CA-C	-6.02	107.26	113.10
1	A	386	SER	N-CA-C	-5.97	102.82	110.53
1	C	326	VAL	CA-C-N	5.84	127.14	119.84
1	C	326	VAL	C-N-CA	5.84	127.14	119.84
1	E	498	CYS	N-CA-C	5.77	117.95	109.24
1	C	413	ILE	CA-C-N	-5.76	113.82	119.64
1	C	413	ILE	C-N-CA	-5.76	113.82	119.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	449	THR	N-CA-C	5.75	117.62	111.36
1	A	449	THR	N-CA-C	5.72	117.59	111.36
1	D	280	ILE	N-CA-C	5.72	117.15	108.80
1	F	326	VAL	CA-C-N	5.72	126.98	119.84
1	F	326	VAL	C-N-CA	5.72	126.98	119.84
1	E	414	PRO	N-CA-C	-5.69	106.44	113.84
1	E	326	VAL	CA-C-N	5.66	126.91	119.84
1	E	326	VAL	C-N-CA	5.66	126.91	119.84
1	A	326	VAL	CA-C-N	5.65	126.90	119.84
1	A	326	VAL	C-N-CA	5.65	126.90	119.84
1	B	326	VAL	CA-C-N	5.63	126.88	119.84
1	B	326	VAL	C-N-CA	5.63	126.88	119.84
1	F	61	ASN	N-CA-C	5.59	120.22	112.90
1	E	496	GLY	N-CA-C	5.58	126.42	113.18
1	F	386	SER	N-CA-C	-5.57	103.34	110.53
1	E	111	SER	N-CA-C	-5.55	104.62	111.33
1	F	375	PHE	N-CA-C	5.54	118.38	110.68
1	F	488	SER	N-CA-C	-5.53	101.86	110.10
1	B	53	TRP	N-CA-C	5.53	116.37	108.74
1	B	449	THR	N-CA-C	5.52	117.38	111.36
1	E	495	ALA	N-CA-C	5.48	118.20	110.14
1	E	497	CYS	N-CA-C	5.47	122.44	110.80
1	C	375	PHE	N-CA-C	5.45	118.26	110.68
1	E	386	SER	N-CA-C	-5.31	103.68	110.53
1	E	449	THR	N-CA-C	5.30	117.14	111.36
1	E	417	ASP	N-CA-C	5.29	118.92	111.52
1	E	108	HIS	N-CA-C	-5.25	106.94	113.55
1	D	449	THR	N-CA-C	5.24	117.08	111.36
1	A	61	ASN	N-CA-C	5.16	119.47	112.04
1	F	14	ASP	N-CA-C	-5.16	106.94	113.18
1	E	53	TRP	N-CA-C	5.14	115.14	107.88
1	D	53	TRP	N-CA-C	5.13	114.91	108.45
1	D	386	SER	N-CA-C	-5.11	103.30	110.35
1	F	96	HIS	N-CA-C	5.09	116.71	108.41
1	F	334	ASP	N-CA-C	5.07	117.19	111.11
1	B	375	PHE	N-CA-C	5.06	117.71	110.68
1	C	405	TYR	N-CA-C	-5.05	102.99	110.46
1	C	183	LEU	N-CA-C	5.04	117.17	111.02
1	D	183	LEU	N-CA-C	5.02	117.14	111.02
1	D	375	PHE	N-CA-C	5.01	117.64	110.68

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	13	TYR	Sidechain

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	3756	0	3764	261	0
1	B	3760	0	3772	272	0
1	C	3776	0	3780	288	0
1	D	3785	0	3793	272	0
1	E	3776	0	3778	344	0
1	F	3751	0	3764	298	0
2	A	53	0	31	2	0
2	B	53	0	31	1	0
2	C	53	0	31	0	0
2	D	53	0	31	5	0
2	E	53	0	31	4	0
2	F	53	0	31	10	0
3	A	48	0	24	1	0
3	B	48	0	24	6	0
3	C	48	0	24	1	0
3	D	48	0	25	4	0
3	E	48	0	25	2	0
3	F	48	0	25	1	0
4	A	8	0	14	2	0
4	B	16	0	28	5	0
4	D	8	0	14	3	0
4	F	8	0	14	5	0
5	A	9	0	0	2	0
5	B	9	0	0	3	0
5	C	7	0	0	1	0
5	D	8	0	0	3	0
5	E	4	0	0	2	0
5	F	7	0	0	2	0
All	All	23294	0	23054	1590	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 34.

All (1590) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:PRO:HG3	1:F:52:ARG:HE	1.15	1.10
1:E:80:LEU:HD23	1:F:80:LEU:HD23	1.34	1.10
1:B:199:SER:HB3	3:B:601:NAP:H52A	1.37	1.05
1:D:418:ASN:HD21	1:D:495:ALA:HB2	1.19	1.05
1:A:199:SER:HB3	3:A:601:NAP:H52A	1.39	1.04
1:E:84:ARG:HH11	1:E:84:ARG:HB2	1.20	1.01
1:E:336:LEU:HD23	1:E:339:LYS:HG3	1.41	1.00
1:E:84:ARG:HB2	1:E:84:ARG:NH1	1.77	1.00
1:B:86:TYR:CD1	1:B:413:ILE:HD11	1.97	0.99
1:E:106:GLN:HE22	1:E:109:ILE:HD12	1.28	0.99
1:A:259:ILE:HD11	1:A:268:ARG:HB2	1.44	0.99
1:F:163:GLU:HG2	1:F:295:ALA:HA	1.43	0.99
1:A:53:TRP:CZ3	1:A:62:VAL:HG11	1.98	0.98
1:E:106:GLN:NE2	1:E:109:ILE:HD12	1.78	0.97
1:C:199:SER:HB3	3:C:601:NAP:H52A	1.43	0.97
1:D:308:LYS:H	1:D:325:ASN:ND2	1.63	0.97
1:B:308:LYS:H	1:B:325:ASN:ND2	1.63	0.96
1:E:308:LYS:H	1:E:325:ASN:ND2	1.63	0.96
1:F:308:LYS:H	1:F:325:ASN:ND2	1.63	0.95
1:C:418:ASN:ND2	1:C:419:ASN:H	1.64	0.95
1:C:308:LYS:H	1:C:325:ASN:ND2	1.64	0.95
1:A:308:LYS:H	1:A:325:ASN:ND2	1.62	0.95
1:B:260:GLU:HB3	1:B:266:ARG:HG3	1.48	0.93
1:F:46:PRO:HG3	1:F:52:ARG:NE	1.82	0.93
1:D:308:LYS:H	1:D:325:ASN:HD21	0.94	0.93
1:E:418:ASN:HD22	1:E:419:ASN:H	1.16	0.93
1:A:308:LYS:N	1:A:325:ASN:HD21	1.67	0.92
1:C:271:ALA:HB3	1:C:280:ILE:HG13	1.52	0.92
1:D:418:ASN:ND2	1:D:495:ALA:HB2	1.83	0.92
1:C:308:LYS:N	1:C:325:ASN:HD21	1.68	0.92
1:E:308:LYS:N	1:E:325:ASN:HD21	1.67	0.92
1:B:308:LYS:N	1:B:325:ASN:HD21	1.68	0.92
1:C:471:ILE:HG21	1:D:373:THR:CG2	1.98	0.92
1:C:308:LYS:H	1:C:325:ASN:HD21	0.94	0.92
1:E:259:ILE:HD11	1:E:268:ARG:HB2	1.52	0.91
1:E:120:LEU:HD13	1:E:127:TYR:HB2	1.51	0.91
1:F:70:MET:HG2	1:F:101:MET:HE3	1.52	0.91
1:F:30:GLU:O	1:F:33:GLN:HB3	1.70	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:PRO:CG	1:F:52:ARG:HE	1.84	0.91
1:E:497:CYS:SG	1:E:498:CYS:N	2.44	0.91
1:F:308:LYS:N	1:F:325:ASN:HD21	1.67	0.91
1:D:308:LYS:N	1:D:325:ASN:HD21	1.67	0.90
1:F:308:LYS:H	1:F:325:ASN:HD21	0.94	0.90
1:F:340:VAL:HG13	1:F:345:VAL:HG21	1.53	0.90
1:E:308:LYS:HG2	1:E:325:ASN:HD22	1.37	0.90
1:D:255:LYS:HE2	1:D:270:VAL:HG21	1.53	0.89
1:D:418:ASN:HD22	1:D:419:ASN:H	1.20	0.89
1:B:308:LYS:H	1:B:325:ASN:HD21	0.93	0.89
1:A:308:LYS:H	1:A:325:ASN:HD21	0.92	0.88
1:C:418:ASN:HD22	1:C:419:ASN:H	1.17	0.88
1:E:308:LYS:H	1:E:325:ASN:HD21	0.91	0.88
1:F:308:LYS:HG2	1:F:325:ASN:HD22	1.36	0.88
1:C:110:GLY:HA2	1:C:113:ASN:HD22	1.38	0.88
1:A:471:ILE:HG21	1:B:373:THR:CG2	2.04	0.88
1:E:90:VAL:HG22	1:F:94:VAL:HG21	1.54	0.88
1:A:308:LYS:HG2	1:A:325:ASN:HD22	1.40	0.87
1:D:411:TRP:CD1	1:D:416:ARG:HH12	1.93	0.86
1:E:168:LEU:HD23	1:E:291:ILE:HD13	1.55	0.86
1:E:139:ARG:HG3	1:E:151:ILE:HD11	1.56	0.86
1:B:411:TRP:HZ3	1:B:421:CYS:SG	1.98	0.86
1:F:21:GLY:HA3	2:F:600:FAD:H51A	1.57	0.86
1:A:139:ARG:HG3	1:A:151:ILE:HD11	1.57	0.86
1:C:255:LYS:HE2	1:C:270:VAL:HG21	1.57	0.86
1:D:308:LYS:HG2	1:D:325:ASN:HD22	1.41	0.85
1:A:493:LEU:H	1:A:493:LEU:HD12	1.40	0.85
1:E:259:ILE:HD11	1:E:268:ARG:HH11	1.41	0.85
1:B:70:MET:HG2	1:B:101:MET:HE3	1.59	0.85
1:E:373:THR:CG2	1:F:471:ILE:HG21	2.05	0.85
1:F:176:TYR:HB3	1:F:267:LEU:HD21	1.58	0.85
1:B:308:LYS:HG2	1:B:325:ASN:HD22	1.41	0.84
1:C:497:CYS:SG	1:C:498:CYS:N	2.50	0.84
1:E:80:LEU:HD13	1:E:94:VAL:HG11	1.59	0.84
1:C:413:ILE:HG13	1:C:414:PRO:HD3	1.60	0.84
1:C:259:ILE:HD11	1:C:268:ARG:HB2	1.59	0.84
1:D:139:ARG:HG2	1:D:151:ILE:HD11	1.58	0.83
1:E:163:GLU:HG2	1:E:295:ALA:HA	1.60	0.83
1:E:413:ILE:HD12	1:F:104:ALA:HB1	1.61	0.83
1:F:139:ARG:HG3	1:F:151:ILE:HD11	1.59	0.83
1:B:139:ARG:HG3	1:B:151:ILE:HD11	1.59	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ASN:HB3	1:C:413:ILE:HD12	1.62	0.82
1:C:139:ARG:HG3	1:C:151:ILE:HD11	1.59	0.82
1:B:411:TRP:CZ3	1:B:421:CYS:SG	2.73	0.81
1:C:268:ARG:HA	1:C:282:GLY:O	1.81	0.81
1:F:253:PRO:HA	1:F:271:ALA:HB2	1.62	0.81
1:B:484:VAL:HG13	1:B:490:ALA:HB3	1.62	0.81
1:E:259:ILE:HB	1:E:266:ARG:O	1.80	0.81
1:D:139:ARG:CG	1:D:151:ILE:HD11	2.11	0.81
1:C:497:CYS:HB2	1:D:112:LEU:HD23	1.64	0.80
1:E:485:THR:HB	5:E:2004:HOH:O	1.80	0.80
1:D:91:GLU:HG3	1:D:93:THR:H	1.47	0.80
1:C:373:THR:CG2	1:D:471:ILE:HG21	2.12	0.80
1:C:89:LYS:NZ	1:D:97:ASP:HB2	1.97	0.80
1:C:254:ILE:HD13	1:C:272:GLN:HB2	1.64	0.79
1:D:418:ASN:HD21	1:D:495:ALA:CB	1.92	0.79
1:C:450:GLN:HE22	1:D:470:GLY:HA2	1.47	0.79
1:A:80:LEU:HD23	1:B:80:LEU:HD23	1.63	0.79
1:A:254:ILE:HG23	1:A:271:ALA:HA	1.63	0.79
1:C:308:LYS:HG2	1:C:325:ASN:HD22	1.45	0.79
1:B:91:GLU:HB2	1:B:93:THR:HG22	1.65	0.79
1:E:471:ILE:HG21	1:F:373:THR:CG2	2.13	0.79
1:D:413:ILE:HG13	1:D:414:PRO:HD3	1.62	0.79
1:D:493:LEU:O	1:D:494:GLN:HG3	1.82	0.79
1:C:471:ILE:HG21	1:D:373:THR:HG23	1.65	0.78
1:D:12:ASP:O	1:D:37:LYS:HE2	1.83	0.78
1:D:254:ILE:HG12	1:D:271:ALA:HA	1.65	0.78
1:B:84:ARG:HH21	1:B:92:GLU:HG3	1.48	0.78
1:B:262:GLY:O	1:B:263:THR:C	2.25	0.78
1:B:408:PRO:HD2	1:B:411:TRP:CE3	2.16	0.78
1:B:163:GLU:HG2	1:B:295:ALA:HA	1.66	0.78
1:B:336:LEU:HB3	1:B:339:LYS:HG3	1.65	0.78
1:B:397:GLU:HA	1:B:487:ARG:NH2	1.97	0.78
1:B:263:THR:OG1	1:B:264:PRO:HD2	1.82	0.78
1:E:84:ARG:HH11	1:E:84:ARG:CB	1.97	0.77
1:F:258:GLN:HE22	1:F:261:ALA:HB2	1.49	0.77
1:C:98:TRP:O	1:C:102:ILE:HG12	1.85	0.77
1:D:399:ILE:HD12	1:D:399:ILE:O	1.84	0.77
1:F:254:ILE:HG12	1:F:271:ALA:HA	1.65	0.77
1:E:263:THR:HB	1:E:264:PRO:HD3	1.66	0.76
1:A:488:SER:O	1:A:490:ALA:N	2.17	0.76
1:E:418:ASN:ND2	1:E:419:ASN:H	1.84	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:418:ASN:ND2	1:D:419:ASN:H	1.83	0.76
1:B:406:PHE:CZ	1:B:421:CYS:HB3	2.21	0.76
1:D:13:TYR:CE1	1:D:37:LYS:HE3	2.21	0.76
1:E:308:LYS:HG2	1:E:325:ASN:ND2	2.00	0.76
1:C:163:GLU:HG2	1:C:295:ALA:HA	1.66	0.76
1:E:418:ASN:HD22	1:E:419:ASN:N	1.83	0.76
1:F:252:VAL:O	1:F:271:ALA:HB1	1.84	0.76
1:E:253:PRO:HA	1:E:271:ALA:HB2	1.68	0.76
1:B:259:ILE:HG13	1:B:268:ARG:HB2	1.68	0.75
1:F:340:VAL:CG1	1:F:345:VAL:HG21	2.16	0.75
1:B:268:ARG:HH21	1:B:281:GLU:CD	1.94	0.75
1:F:75:LEU:HB3	4:F:700:MPD:H51	1.69	0.75
1:A:470:GLY:HA2	1:B:450:GLN:HE22	1.52	0.75
1:C:258:GLN:HE22	1:C:261:ALA:HB2	1.51	0.75
1:F:308:LYS:HG2	1:F:325:ASN:ND2	2.00	0.75
1:A:293:ARG:HD3	5:A:2005:HOH:O	1.86	0.74
1:B:25:LEU:HD22	1:B:120:LEU:HD11	1.69	0.74
1:A:96:HIS:CD2	1:A:212:ILE:HG13	2.22	0.74
1:F:38:VAL:HG23	1:F:125:VAL:HG13	1.68	0.74
1:F:258:GLN:NE2	1:F:261:ALA:HB2	2.02	0.74
1:A:171:PRO:HB2	1:A:255:LYS:HG3	1.68	0.74
1:B:84:ARG:NH2	1:B:92:GLU:HG3	2.01	0.74
1:E:259:ILE:HD11	1:E:268:ARG:NH1	2.02	0.74
1:C:110:GLY:HA2	1:C:113:ASN:ND2	2.03	0.74
1:E:470:GLY:HA2	1:F:450:GLN:HE22	1.51	0.74
1:A:308:LYS:HG2	1:A:325:ASN:ND2	2.03	0.74
1:C:278:GLU:HG2	1:C:279:ILE:H	1.51	0.74
1:D:255:LYS:CE	1:D:270:VAL:HG21	2.18	0.74
1:F:340:VAL:HG11	1:F:345:VAL:HG11	1.68	0.74
1:A:258:GLN:HG3	1:A:260:GLU:O	1.88	0.74
1:C:38:VAL:HG22	1:C:125:VAL:HG13	1.70	0.74
1:B:419:ASN:HD21	1:B:494:GLN:C	1.96	0.74
1:F:163:GLU:HG2	1:F:295:ALA:CA	2.18	0.74
1:D:418:ASN:HD22	1:D:419:ASN:N	1.86	0.73
1:E:150:LYS:HD3	1:E:152:TYR:OH	1.88	0.73
1:A:13:TYR:HD1	1:A:37:LYS:HG2	1.52	0.73
1:C:164:ARG:HG2	1:C:296:CYS:SG	2.28	0.73
1:E:98:TRP:CZ2	1:E:102:ILE:HD11	2.23	0.73
1:A:450:GLN:HE22	1:B:470:GLY:HA2	1.53	0.73
1:B:380:TYR:OH	1:B:439:HIS:HD2	1.72	0.73
1:E:102:ILE:O	1:E:105:VAL:HG12	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:TRP:CZ2	1:B:77:GLY:HA3	2.24	0.72
1:B:86:TYR:CD1	1:B:413:ILE:CD1	2.71	0.72
1:E:84:ARG:NH2	1:E:92:GLU:HA	2.03	0.72
1:E:440:VAL:HB	1:E:479:PHE:HZ	1.53	0.72
1:D:255:LYS:HB3	1:D:270:VAL:CG2	2.18	0.72
1:A:373:THR:CG2	1:B:471:ILE:HG21	2.20	0.72
1:C:418:ASN:HD22	1:C:419:ASN:N	1.86	0.72
1:A:47:THR:HG23	1:A:51:THR:O	1.89	0.72
1:B:418:ASN:HB2	4:B:701:MPD:HM2	1.70	0.72
1:E:493:LEU:N	1:E:493:LEU:HD12	2.04	0.72
1:F:255:LYS:HE2	1:F:257:GLU:HB3	1.70	0.72
1:B:86:TYR:CG	1:B:413:ILE:HD11	2.24	0.72
1:D:308:LYS:HG2	1:D:325:ASN:ND2	2.04	0.72
1:C:402:TYR:CD2	1:C:462:LYS:HE3	2.25	0.71
1:F:273:SER:OG	1:F:275:ASN:HB2	1.91	0.71
1:C:80:LEU:HD23	1:D:80:LEU:HD23	1.70	0.71
1:A:86:TYR:HE2	1:A:414:PRO:HG3	1.55	0.71
1:B:416:ARG:HG2	1:B:416:ARG:HH11	1.55	0.71
1:B:259:ILE:HD11	1:B:268:ARG:HG3	1.72	0.71
1:B:313:THR:OG1	1:B:315:LYS:HG2	1.90	0.71
1:E:106:GLN:HA	1:E:106:GLN:HE21	1.56	0.70
1:E:49:LEU:N	1:E:49:LEU:HD22	2.06	0.70
1:E:399:ILE:HD12	1:E:399:ILE:O	1.90	0.70
1:F:344:PRO:O	1:F:347:ILE:HG12	1.90	0.70
1:E:344:PRO:O	1:E:347:ILE:HG12	1.91	0.70
1:B:308:LYS:HG2	1:B:325:ASN:ND2	2.06	0.70
1:B:344:PRO:O	1:B:347:ILE:HG12	1.92	0.70
1:D:46:PRO:HG3	1:D:52:ARG:CZ	2.22	0.70
1:C:418:ASN:ND2	1:C:419:ASN:N	2.39	0.70
1:A:29:LYS:HB2	1:A:29:LYS:NZ	2.07	0.70
1:A:478:VAL:HG23	4:A:701:MPD:H51	1.72	0.70
1:B:260:GLU:HB3	1:B:266:ARG:CG	2.22	0.70
1:C:469:ILE:HG21	1:D:345:VAL:HG12	1.73	0.70
1:E:485:THR:O	1:E:488:SER:HB3	1.91	0.70
1:D:315:LYS:HD2	1:D:336:LEU:O	1.92	0.69
1:E:193:THR:HB	1:E:286:THR:HB	1.73	0.69
1:E:254:ILE:HD11	1:E:270:VAL:HG12	1.75	0.69
1:E:164:ARG:O	1:E:293:ARG:HB3	1.92	0.69
1:A:487:ARG:C	1:A:489:GLY:H	2.01	0.69
1:F:49:LEU:HD22	1:F:49:LEU:N	2.07	0.69
1:B:133:GLN:NE2	5:B:2003:HOH:O	2.24	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:LYS:HE3	1:E:358:TYR:CD1	2.28	0.69
1:A:399:ILE:HD12	1:A:399:ILE:O	1.93	0.69
1:C:373:THR:HG23	1:D:471:ILE:HG21	1.75	0.69
1:C:470:GLY:HA2	1:D:450:GLN:HE22	1.56	0.69
1:D:260:GLU:OE2	1:D:266:ARG:HD3	1.92	0.69
1:A:150:LYS:HD3	1:A:152:TYR:OH	1.93	0.69
1:C:308:LYS:HG2	1:C:325:ASN:ND2	2.07	0.69
1:A:267:LEU:N	1:A:267:LEU:HD12	2.07	0.68
1:D:292:GLY:HA2	3:D:601:NAP:O1A	1.92	0.68
1:E:450:GLN:HE22	1:F:470:GLY:HA2	1.58	0.68
1:A:258:GLN:NE2	1:A:261:ALA:HB2	2.07	0.68
1:D:16:ILE:HG12	1:D:39:MET:HE2	1.75	0.68
1:A:432:ASN:HD22	1:A:463:LYS:NZ	1.92	0.68
1:C:413:ILE:HG13	1:C:414:PRO:CD	2.23	0.68
1:D:36:LYS:HE3	1:D:358:TYR:CD1	2.28	0.68
1:D:418:ASN:ND2	1:D:419:ASN:N	2.42	0.68
1:F:252:VAL:C	1:F:271:ALA:HB1	2.19	0.68
1:F:39:MET:HE3	1:F:41:LEU:HD21	1.75	0.68
1:D:193:THR:HB	1:D:286:THR:HB	1.76	0.68
1:A:344:PRO:HG3	1:B:472:HIS:HB2	1.74	0.68
1:F:336:LEU:HD23	1:F:339:LYS:HG3	1.75	0.68
1:A:344:PRO:O	1:A:347:ILE:HG12	1.94	0.67
1:A:492:ILE:H	1:A:493:LEU:HD12	1.59	0.67
1:B:315:LYS:HE3	1:B:336:LEU:O	1.94	0.67
1:E:380:TYR:OH	1:E:439:HIS:HD2	1.76	0.67
1:E:106:GLN:NE2	1:E:106:GLN:HA	2.07	0.67
1:E:262:GLY:O	1:E:263:THR:C	2.38	0.67
1:F:339:LYS:HD2	1:F:367:TYR:CD2	2.30	0.67
1:A:471:ILE:HG21	1:B:373:THR:HG23	1.75	0.67
1:C:223:ILE:HG12	1:C:226:ARG:NH2	2.10	0.67
1:F:380:TYR:OH	1:F:439:HIS:HD2	1.77	0.67
1:C:89:LYS:HZ2	1:D:97:ASP:HB2	1.60	0.67
1:E:80:LEU:HD23	1:F:80:LEU:CD2	2.21	0.67
1:C:258:GLN:NE2	1:C:261:ALA:HB2	2.08	0.67
1:E:259:ILE:CD1	1:E:268:ARG:HB2	2.25	0.67
1:B:293:ARG:HD3	5:B:2007:HOH:O	1.95	0.66
1:E:55:LEU:HD13	1:E:56:GLY:N	2.10	0.66
1:F:150:LYS:HD3	1:F:152:TYR:OH	1.95	0.66
1:F:96:HIS:CD2	1:F:212:ILE:HG13	2.30	0.66
1:E:450:GLN:HE22	1:F:471:ILE:H	1.43	0.66
1:F:251:PHE:CE2	1:F:273:SER:HB2	2.30	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:GLU:HA	1:B:487:ARG:HH21	1.61	0.66
1:B:416:ARG:HD2	1:B:417:ASP:OD2	1.95	0.66
1:C:406:PHE:CZ	1:C:421:CYS:HB3	2.30	0.66
1:E:96:HIS:CD2	1:E:212:ILE:HG13	2.30	0.66
1:C:170:ILE:HB	1:C:254:ILE:O	1.95	0.66
1:D:150:LYS:HD3	1:D:152:TYR:OH	1.95	0.66
1:A:232:MET:HE2	1:A:439:HIS:HB3	1.77	0.66
1:A:315:LYS:HE3	1:A:336:LEU:O	1.95	0.66
1:C:447:GLU:CD	1:D:474:VAL:HG13	2.21	0.66
1:D:400:GLU:OE2	1:D:400:GLU:HA	1.94	0.66
1:E:103:GLU:HG2	1:E:107:ASN:HD21	1.61	0.66
1:E:315:LYS:HD2	1:E:336:LEU:O	1.96	0.66
1:A:194:LEU:HD22	1:A:284:TYR:CE1	2.30	0.66
1:B:92:GLU:C	1:B:94:VAL:H	2.04	0.66
1:B:339:LYS:HA	1:B:339:LYS:HE2	1.78	0.66
1:A:252:VAL:O	1:A:271:ALA:HB1	1.96	0.66
1:E:418:ASN:ND2	1:E:419:ASN:N	2.44	0.65
1:C:399:ILE:O	1:C:399:ILE:HD12	1.96	0.65
1:A:29:LYS:HE3	1:A:119:ALA:HB1	1.78	0.65
1:C:344:PRO:O	1:C:347:ILE:HG12	1.96	0.65
1:E:272:GLN:CB	1:E:279:ILE:HG12	2.27	0.65
1:E:405:TYR:HE1	1:E:493:LEU:HG	1.61	0.65
1:D:117:ARG:HA	1:D:117:ARG:HH11	1.61	0.65
1:C:432:ASN:HD22	1:C:463:LYS:NZ	1.93	0.65
1:E:373:THR:HB	1:E:381:GLY:HA2	1.79	0.65
1:E:401:VAL:HG11	1:E:486:LYS:HE3	1.78	0.65
1:F:417:ASP:OD1	1:F:420:LYS:HE3	1.96	0.65
1:A:13:TYR:CD1	1:A:37:LYS:HG2	2.32	0.65
1:A:139:ARG:CG	1:A:151:ILE:HD11	2.27	0.65
1:D:96:HIS:CD2	1:D:212:ILE:HG13	2.31	0.65
1:D:411:TRP:C	1:D:414:PRO:HD2	2.22	0.65
1:A:469:ILE:HG21	1:B:345:VAL:HG12	1.79	0.65
1:C:334:ASP:HA	1:C:341:GLU:HG3	1.78	0.65
1:D:344:PRO:O	1:D:347:ILE:HG12	1.96	0.65
1:C:259:ILE:HD11	1:C:268:ARG:CB	2.27	0.64
1:C:85:ASN:CB	1:C:413:ILE:HD12	2.27	0.64
1:C:150:LYS:HD3	1:C:152:TYR:OH	1.97	0.64
1:C:380:TYR:OH	1:C:439:HIS:HD2	1.81	0.64
1:D:172:GLY:HA2	1:D:175:GLU:CG	2.27	0.64
3:E:601:NAP:H6N	3:E:601:NAP:O2N	1.96	0.64
1:E:139:ARG:CG	1:E:151:ILE:HD11	2.26	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:ARG:HG2	1:F:90:VAL:HG12	1.78	0.64
1:C:474:VAL:HG21	1:D:446:GLY:HA3	1.78	0.64
1:D:432:ASN:HD22	1:D:463:LYS:NZ	1.96	0.64
1:B:260:GLU:CB	1:B:266:ARG:HG3	2.26	0.64
1:C:373:THR:HB	1:C:381:GLY:HA2	1.80	0.64
1:E:411:TRP:C	1:E:414:PRO:HD2	2.23	0.64
1:E:120:LEU:CD1	1:E:127:TYR:HB2	2.27	0.64
1:B:432:ASN:HD22	1:B:463:LYS:NZ	1.95	0.64
1:D:254:ILE:O	1:D:255:LYS:HB2	1.96	0.64
1:E:108:HIS:CD2	1:F:412:THR:HB	2.33	0.64
1:E:163:GLU:O	1:E:164:ARG:HG2	1.98	0.64
1:E:474:VAL:HG13	1:F:447:GLU:CD	2.23	0.64
1:F:31:ALA:O	1:F:33:GLN:N	2.31	0.64
1:A:95:LYS:HB2	1:B:89:LYS:HD2	1.80	0.64
1:E:104:ALA:HB1	1:F:413:ILE:HD12	1.78	0.64
1:A:472:HIS:HB2	1:B:344:PRO:HG3	1.79	0.64
1:B:373:THR:HB	1:B:381:GLY:HA2	1.80	0.64
1:C:123:LYS:O	1:C:124:LYS:HB2	1.96	0.64
1:A:76:LEU:HD23	1:B:86:TYR:CD2	2.32	0.64
1:A:173:ASP:OD1	1:A:174:LYS:N	2.31	0.64
1:F:302:LEU:HD22	1:F:307:VAL:HB	1.80	0.63
1:A:493:LEU:HD12	1:A:493:LEU:N	2.12	0.63
1:C:172:GLY:HA2	1:C:175:GLU:CG	2.29	0.63
1:C:263:THR:OG1	1:C:264:PRO:CD	2.47	0.63
1:E:336:LEU:HD23	1:E:339:LYS:CG	2.22	0.63
1:E:13:TYR:HD1	1:E:37:LYS:HG2	1.64	0.63
1:D:172:GLY:HA2	1:D:175:GLU:HG2	1.80	0.63
1:F:172:GLY:HA2	1:F:175:GLU:CG	2.29	0.63
1:F:484:VAL:HG13	1:F:490:ALA:HB3	1.80	0.63
1:E:52:ARG:HH11	1:E:52:ARG:HB2	1.64	0.63
1:E:336:LEU:HB3	1:E:339:LYS:HG2	1.79	0.63
1:F:173:ASP:OD1	1:F:174:LYS:N	2.32	0.63
1:B:86:TYR:CE1	1:B:413:ILE:CD1	2.82	0.63
1:B:172:GLY:HA2	1:B:175:GLU:CG	2.28	0.63
1:E:172:GLY:HA2	1:E:175:GLU:CG	2.29	0.63
1:F:269:VAL:O	1:F:281:GLU:HA	1.99	0.63
1:A:191:GLY:O	1:A:193:THR:HG22	1.98	0.63
1:E:172:GLY:HA2	1:E:175:GLU:HG2	1.81	0.63
1:A:461:THR:OG1	1:A:464:GLN:HG3	1.98	0.62
1:B:96:HIS:CD2	1:B:212:ILE:HG13	2.35	0.62
1:B:150:LYS:HD3	1:B:152:TYR:OH	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:397:GLU:HA	1:E:487:ARG:HH22	1.64	0.62
1:C:163:GLU:O	1:C:164:ARG:HD2	1.99	0.62
1:F:25:LEU:HD22	1:F:120:LEU:HD11	1.81	0.62
1:F:406:PHE:O	1:F:421:CYS:HB2	1.98	0.62
1:D:38:VAL:HG22	1:D:125:VAL:HG13	1.80	0.62
1:E:261:ALA:O	1:E:262:GLY:O	2.17	0.62
1:F:403:HIS:CE1	1:F:492:ILE:HD13	2.35	0.62
1:F:427:CYS:HA	1:F:434:ARG:O	1.99	0.62
1:A:193:THR:HB	1:A:286:THR:HB	1.82	0.62
1:A:493:LEU:H	1:A:493:LEU:CD1	2.11	0.62
1:D:496:GLY:O	1:D:499:GLY:N	2.30	0.62
1:E:391:VAL:HG12	1:E:399:ILE:HD11	1.79	0.62
1:B:411:TRP:C	1:B:414:PRO:HD2	2.24	0.62
1:C:450:GLN:HE22	1:D:470:GLY:CA	2.12	0.62
1:C:70:MET:HG2	1:C:101:MET:HE3	1.80	0.62
1:D:262:GLY:O	1:D:263:THR:C	2.42	0.62
1:D:380:TYR:OH	1:D:439:HIS:HD2	1.81	0.62
1:D:418:ASN:CG	1:D:495:ALA:HB2	2.24	0.62
1:F:172:GLY:HA2	1:F:175:GLU:HG2	1.82	0.62
1:D:373:THR:HB	1:D:381:GLY:HA2	1.82	0.62
1:B:272:GLN:HB2	1:B:279:ILE:HG12	1.81	0.62
1:E:373:THR:HG22	1:F:471:ILE:HG21	1.80	0.62
1:C:263:THR:OG1	1:C:264:PRO:HD3	2.00	0.62
1:D:13:TYR:CD1	1:D:37:LYS:HE3	2.35	0.62
1:D:336:LEU:HD23	1:D:339:LYS:HG3	1.81	0.62
1:E:401:VAL:HG22	1:E:426:ILE:HG12	1.81	0.62
1:A:172:GLY:HA2	1:A:175:GLU:HG2	1.82	0.61
1:B:196:VAL:HB	1:B:289:LEU:HD23	1.81	0.61
1:E:168:LEU:CD2	1:E:291:ILE:HD13	2.30	0.61
1:C:167:TYR:CD2	1:C:289:LEU:HD12	2.34	0.61
1:E:267:LEU:N	1:E:267:LEU:HD12	2.15	0.61
1:A:450:GLN:HE22	1:B:471:ILE:H	1.47	0.61
1:E:470:GLY:CA	1:F:450:GLN:HE22	2.12	0.61
1:C:477:GLU:HA	1:D:450:GLN:HE21	1.65	0.61
1:D:302:LEU:HD22	1:D:307:VAL:HB	1.82	0.61
1:E:474:VAL:HG12	1:F:447:GLU:OE1	2.00	0.61
1:F:48:PRO:C	1:F:49:LEU:HD13	2.26	0.61
1:A:419:ASN:OD1	1:A:495:ALA:HB3	2.00	0.61
1:D:13:TYR:O	1:D:154:ALA:HA	1.99	0.61
1:E:474:VAL:CG1	1:F:447:GLU:CD	2.74	0.61
1:B:461:THR:OG1	1:B:464:GLN:HG3	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:GLN:HG2	1:D:275:ASN:ND2	2.15	0.61
1:E:471:ILE:H	1:F:450:GLN:HE22	1.48	0.61
1:F:256:VAL:O	1:F:256:VAL:HG13	2.01	0.61
1:A:380:TYR:OH	1:A:439:HIS:HD2	1.82	0.61
1:B:172:GLY:HA2	1:B:175:GLU:HG2	1.81	0.61
1:E:432:ASN:HD22	1:E:463:LYS:NZ	1.98	0.61
1:F:263:THR:OG1	1:F:264:PRO:CD	2.48	0.61
1:F:432:ASN:HD22	1:F:463:LYS:NZ	1.98	0.61
1:C:277:GLU:O	1:C:277:GLU:OE1	2.19	0.60
1:F:139:ARG:CG	1:F:151:ILE:HD11	2.30	0.60
1:F:373:THR:HB	1:F:381:GLY:HA2	1.82	0.60
1:F:471:ILE:HA	5:F:2006:HOH:O	2.01	0.60
1:C:173:ASP:OD1	1:C:174:LYS:N	2.33	0.60
1:C:251:PHE:CD2	1:C:273:SER:HA	2.36	0.60
1:D:173:ASP:OD1	1:D:174:LYS:N	2.35	0.60
1:E:13:TYR:HB3	1:E:37:LYS:O	2.01	0.60
1:A:123:LYS:HB2	1:A:123:LYS:HZ2	1.66	0.60
1:B:139:ARG:CG	1:B:151:ILE:HD11	2.27	0.60
1:C:172:GLY:HA2	1:C:175:GLU:HG2	1.82	0.60
1:D:259:ILE:HD11	1:D:268:ARG:HB2	1.82	0.60
1:F:226:ARG:HG3	1:F:226:ARG:HH11	1.66	0.60
1:C:139:ARG:CG	1:C:151:ILE:HD11	2.29	0.60
1:E:89:LYS:O	1:F:94:VAL:HG13	2.01	0.60
1:C:278:GLU:CG	1:C:279:ILE:H	2.14	0.60
1:E:344:PRO:HG3	1:F:472:HIS:HB2	1.82	0.60
1:F:82:ASP:CG	1:F:416:ARG:HH12	2.09	0.60
1:A:88:TRP:CZ2	1:B:77:GLY:CA	2.84	0.60
1:B:302:LEU:HD22	1:B:307:VAL:HB	1.83	0.60
1:C:250:GLN:HB3	1:C:274:THR:HB	1.84	0.60
1:A:21:GLY:HA3	2:A:600:FAD:H52A	1.83	0.60
1:A:166:ARG:HB2	1:A:294:ASP:OD2	2.01	0.60
1:B:427:CYS:HA	1:B:434:ARG:O	2.02	0.60
1:C:498:CYS:SG	1:D:29:LYS:NZ	2.75	0.60
1:F:266:ARG:C	1:F:267:LEU:HD12	2.26	0.60
1:C:86:TYR:CE1	1:C:413:ILE:HG12	2.36	0.60
1:F:340:VAL:CG1	1:F:345:VAL:HG11	2.32	0.60
1:A:242:GLU:OE2	1:A:420:LYS:NZ	2.35	0.60
1:C:13:TYR:O	1:C:154:ALA:HA	2.02	0.60
1:E:397:GLU:HA	1:E:487:ARG:NH2	2.17	0.60
1:A:76:LEU:HD13	4:B:700:MPD:H51	1.82	0.60
1:A:114:TRP:O	1:A:117:ARG:HB2	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:GLU:CD	1:D:474:VAL:CG1	2.75	0.60
1:E:472:HIS:ND1	1:E:473:PRO:HA	2.17	0.60
1:A:186:LEU:HD12	1:A:190:PRO:HG3	1.84	0.59
1:A:470:GLY:CA	1:B:450:GLN:HE22	2.14	0.59
1:B:91:GLU:HB2	1:B:93:THR:CG2	2.32	0.59
1:B:173:ASP:OD1	1:B:174:LYS:N	2.35	0.59
1:C:50:GLY:O	1:C:51:THR:C	2.45	0.59
1:D:259:ILE:O	1:D:260:GLU:HB2	2.01	0.59
1:D:401:VAL:HG11	1:D:486:LYS:HD2	1.84	0.59
1:E:16:ILE:HG13	1:E:154:ALA:HB2	1.83	0.59
1:E:80:LEU:CD2	1:F:80:LEU:HD23	2.21	0.59
1:E:173:ASP:OD1	1:E:174:LYS:N	2.35	0.59
1:E:259:ILE:HD11	1:E:268:ARG:CB	2.31	0.59
1:A:172:GLY:HA2	1:A:175:GLU:CG	2.32	0.59
1:C:70:MET:HE1	1:C:184:PHE:HA	1.83	0.59
1:C:401:VAL:HG11	1:C:486:LYS:HD2	1.84	0.59
1:F:403:HIS:NE2	1:F:492:ILE:HD13	2.17	0.59
1:A:112:LEU:O	1:A:113:ASN:C	2.45	0.59
1:B:70:MET:CG	1:B:101:MET:HE3	2.31	0.59
1:C:302:LEU:HD22	1:C:307:VAL:HB	1.85	0.59
1:D:16:ILE:HG13	1:D:154:ALA:HB2	1.84	0.59
1:F:58:THR:HG22	1:F:59:CYS:N	2.17	0.59
1:B:49:LEU:N	1:B:49:LEU:HD22	2.16	0.59
1:E:191:GLY:O	1:E:193:THR:HG22	2.02	0.59
1:A:263:THR:OG1	1:A:264:PRO:HD3	2.03	0.59
1:A:267:LEU:N	1:A:267:LEU:CD1	2.65	0.59
1:B:292:GLY:HA3	3:B:601:NAP:O2N	2.02	0.59
1:C:472:HIS:ND1	1:C:473:PRO:HA	2.18	0.59
1:A:77:GLY:HA3	1:B:88:TRP:CZ2	2.37	0.59
3:B:601:NAP:O1A	3:B:601:NAP:H52N	2.02	0.59
1:E:70:MET:HE1	1:E:184:PHE:HA	1.85	0.59
1:F:16:ILE:HG13	1:F:154:ALA:HB2	1.84	0.59
1:A:192:LYS:HE2	1:A:284:TYR:CD2	2.38	0.59
1:D:344:PRO:HD3	2:D:600:FAD:O2	2.03	0.59
1:F:402:TYR:HB3	1:F:482:LEU:HB3	1.83	0.59
1:E:280:ILE:HD12	1:E:281:GLU:H	1.65	0.59
1:C:256:VAL:HG13	1:C:269:VAL:HG22	1.83	0.58
1:A:450:GLN:NE2	1:B:471:ILE:H	2.01	0.58
1:E:180:SER:HA	1:E:288:MET:CE	2.33	0.58
1:F:48:PRO:HG2	1:F:167:TYR:CE1	2.38	0.58
1:C:345:VAL:HG12	1:D:469:ILE:HG21	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:GLN:HB2	1:E:279:ILE:HG12	1.85	0.58
1:E:302:LEU:HD22	1:E:307:VAL:HB	1.84	0.58
1:F:397:GLU:HA	1:F:487:ARG:HH22	1.67	0.58
1:B:319:THR:HG23	1:B:323:GLN:O	2.04	0.58
1:E:76:LEU:HD23	1:F:86:TYR:CD2	2.38	0.58
1:F:407:TRP:CZ2	1:F:412:THR:HA	2.38	0.58
1:A:270:VAL:HG22	1:A:281:GLU:HB3	1.84	0.58
1:A:373:THR:HB	1:A:381:GLY:HA2	1.84	0.58
1:C:191:GLY:O	1:C:193:THR:HG22	2.04	0.58
1:E:123:LYS:HB2	1:E:123:LYS:NZ	2.17	0.58
1:E:450:GLN:NE2	1:F:471:ILE:H	2.00	0.58
1:E:471:ILE:H	1:F:450:GLN:NE2	2.01	0.58
1:F:484:VAL:HG13	1:F:490:ALA:CB	2.34	0.58
1:B:70:MET:HE1	1:B:184:PHE:HA	1.86	0.58
1:C:259:ILE:CD1	1:C:268:ARG:HB2	2.30	0.58
1:D:12:ASP:HB2	1:D:153:SER:H	1.68	0.58
1:B:338:ASP:O	1:B:339:LYS:HE3	2.04	0.58
1:D:255:LYS:HB3	1:D:270:VAL:HG23	1.84	0.58
1:E:85:ASN:C	1:E:413:ILE:HD11	2.29	0.58
1:E:186:LEU:HD12	1:E:190:PRO:HG3	1.86	0.58
1:D:385:LEU:HD22	1:D:389:LYS:HG3	1.86	0.58
1:E:102:ILE:O	1:E:106:GLN:HG2	2.03	0.58
1:F:319:THR:HG23	1:F:323:GLN:O	2.03	0.58
1:A:302:LEU:HD22	1:A:307:VAL:HB	1.86	0.58
1:A:450:GLN:HE22	1:B:470:GLY:CA	2.15	0.58
1:B:91:GLU:CB	1:B:93:THR:HG22	2.32	0.58
1:B:254:ILE:HD11	1:B:270:VAL:HG12	1.85	0.58
1:D:427:CYS:HA	1:D:434:ARG:O	2.04	0.58
1:E:263:THR:CB	1:E:264:PRO:HD3	2.32	0.58
1:E:275:ASN:OD1	1:E:276:SER:N	2.37	0.58
1:E:440:VAL:HB	1:E:479:PHE:CZ	2.37	0.58
1:F:151:ILE:HD13	1:F:151:ILE:C	2.29	0.58
1:B:266:ARG:NH2	1:B:283:GLU:OE2	2.37	0.57
1:E:450:GLN:HE22	1:F:470:GLY:CA	2.16	0.57
1:C:194:LEU:HD22	1:C:284:TYR:CE1	2.38	0.57
1:A:171:PRO:HB2	1:A:255:LYS:CG	2.34	0.57
1:A:446:GLY:HA3	1:B:474:VAL:HG21	1.86	0.57
1:C:44:VAL:HG11	1:C:53:TRP:CE2	2.39	0.57
1:C:259:ILE:HG22	1:C:259:ILE:O	2.02	0.57
1:C:417:ASP:OD2	1:C:417:ASP:N	2.35	0.57
1:D:117:ARG:HH11	1:D:117:ARG:CA	2.17	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:LYS:HD2	1:D:367:TYR:CE2	2.39	0.57
1:F:186:LEU:HD12	1:F:190:PRO:HG3	1.86	0.57
1:A:194:LEU:HD22	1:A:284:TYR:HE1	1.68	0.57
1:B:401:VAL:HB	1:B:486:LYS:HG3	1.87	0.57
1:D:81:GLN:OE1	1:D:84:ARG:NH2	2.32	0.57
1:D:411:TRP:CG	1:D:416:ARG:HH12	2.23	0.57
1:F:413:ILE:HG23	1:F:414:PRO:HD3	1.84	0.57
1:B:396:GLU:OE2	1:B:487:ARG:NH2	2.37	0.57
1:C:432:ASN:HD22	1:C:463:LYS:HZ1	1.52	0.57
1:C:461:THR:OG1	1:C:464:GLN:HG3	2.05	0.57
1:D:319:THR:HG23	1:D:323:GLN:O	2.05	0.57
1:B:35:GLY:O	1:B:36:LYS:C	2.47	0.57
1:B:46:PRO:HA	1:B:51:THR:O	2.04	0.57
1:D:496:GLY:O	1:D:497:CYS:C	2.46	0.57
1:A:53:TRP:HH2	1:A:181:ASP:CG	2.13	0.57
1:E:97:ASP:OD2	1:E:100:ARG:HB2	2.04	0.57
1:E:345:VAL:HG12	1:F:469:ILE:HG21	1.87	0.57
1:E:413:ILE:HD12	1:F:104:ALA:CB	2.33	0.57
1:B:166:ARG:HG3	5:B:2006:HOH:O	2.05	0.57
1:B:418:ASN:CB	4:B:701:MPD:HM2	2.34	0.57
1:C:258:GLN:HE21	1:C:260:GLU:C	2.12	0.57
1:C:427:CYS:HA	1:C:434:ARG:O	2.04	0.57
1:E:49:LEU:N	1:E:49:LEU:CD2	2.68	0.57
1:E:49:LEU:CD2	1:E:49:LEU:H	2.18	0.57
1:E:178:ILE:O	1:E:288:MET:HA	2.05	0.57
1:F:38:VAL:CG2	1:F:125:VAL:HG13	2.33	0.57
1:F:70:MET:HE1	1:F:184:PHE:HA	1.86	0.57
1:B:191:GLY:O	1:B:193:THR:HG22	2.05	0.56
1:C:151:ILE:C	1:C:151:ILE:HD13	2.30	0.56
1:E:413:ILE:HG23	1:E:414:PRO:HD3	1.87	0.56
1:E:478:VAL:HG13	1:E:479:PHE:N	2.20	0.56
1:A:432:ASN:HD22	1:A:463:LYS:HZ1	1.52	0.56
1:C:186:LEU:HD12	1:C:190:PRO:HG3	1.87	0.56
1:C:278:GLU:O	1:C:279:ILE:HG13	2.05	0.56
1:D:339:LYS:HD2	1:D:367:TYR:CD2	2.40	0.56
1:E:163:GLU:HG2	1:E:295:ALA:CA	2.34	0.56
1:C:101:MET:HE2	1:C:102:ILE:HD13	1.86	0.56
1:D:408:PRO:O	1:D:409:LEU:C	2.49	0.56
1:F:448:VAL:HG22	1:F:476:ALA:HB2	1.88	0.56
1:C:76:LEU:HD23	1:D:86:TYR:CD2	2.41	0.56
1:F:70:MET:CG	1:F:101:MET:HE3	2.30	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:403:HIS:CD2	1:F:492:ILE:HG21	2.40	0.56
1:D:432:ASN:HD22	1:D:463:LYS:HZ1	1.54	0.56
1:B:272:GLN:HG2	1:B:273:SER:O	2.05	0.56
1:A:450:GLN:NE2	1:B:470:GLY:HA2	2.20	0.56
1:B:267:LEU:HD23	1:B:287:VAL:HG23	1.87	0.56
1:D:259:ILE:CD1	1:D:268:ARG:HB2	2.36	0.56
1:E:259:ILE:HG22	1:E:259:ILE:O	2.05	0.56
1:E:416:ARG:HH11	1:E:416:ARG:HG2	1.71	0.56
1:A:192:LYS:HE2	1:A:284:TYR:HD2	1.71	0.56
1:E:123:LYS:HB2	1:E:123:LYS:HZ3	1.71	0.56
1:A:151:ILE:HD13	1:A:151:ILE:C	2.31	0.55
1:B:416:ARG:CD	1:B:417:ASP:OD2	2.54	0.55
1:C:255:LYS:HB3	1:C:270:VAL:CG2	2.36	0.55
1:E:171:PRO:HB2	1:E:255:LYS:HG3	1.89	0.55
1:E:254:ILE:O	1:E:255:LYS:HB2	2.06	0.55
1:E:470:GLY:HA2	1:F:450:GLN:NE2	2.21	0.55
1:C:16:ILE:HG13	1:C:154:ALA:HB2	1.89	0.55
1:C:475:CYS:HB2	1:D:447:GLU:OE2	2.07	0.55
1:D:250:GLN:HG2	1:D:275:ASN:HD21	1.71	0.55
1:E:252:VAL:O	1:E:271:ALA:HB1	2.06	0.55
1:E:262:GLY:O	1:E:263:THR:O	2.24	0.55
1:A:70:MET:HE1	1:A:184:PHE:HA	1.88	0.55
1:B:93:THR:O	1:B:93:THR:OG1	2.25	0.55
1:B:259:ILE:CG1	1:B:268:ARG:HB2	2.36	0.55
1:B:406:PHE:CE1	1:B:421:CYS:HB3	2.41	0.55
1:B:416:ARG:HG2	1:B:416:ARG:NH1	2.20	0.55
1:C:192:LYS:H	1:C:285:ASN:HD22	1.54	0.55
1:C:319:THR:HG23	1:C:323:GLN:O	2.06	0.55
1:C:450:GLN:NE2	1:D:470:GLY:HA2	2.19	0.55
1:E:410:GLU:OE2	1:F:68:LYS:HE2	2.06	0.55
1:B:416:ARG:HD2	1:B:417:ASP:CG	2.31	0.55
1:E:319:THR:HG23	1:E:323:GLN:O	2.06	0.55
1:E:427:CYS:HA	1:E:434:ARG:O	2.07	0.55
1:C:273:SER:HB2	1:C:278:GLU:HB3	1.89	0.55
1:C:278:GLU:HG2	1:C:279:ILE:N	2.20	0.55
1:E:55:LEU:O	1:E:113:ASN:ND2	2.40	0.55
1:F:263:THR:OG1	1:F:264:PRO:HD3	2.07	0.55
1:A:427:CYS:HA	1:A:434:ARG:O	2.06	0.55
1:E:151:ILE:C	1:E:151:ILE:HD13	2.32	0.55
1:F:235:LYS:NZ	1:F:405:TYR:OH	2.40	0.55
1:F:411:TRP:CZ3	1:F:421:CYS:SG	2.99	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LYS:HB2	1:A:123:LYS:NZ	2.21	0.55
1:E:49:LEU:HD22	1:E:49:LEU:H	1.72	0.55
1:E:232:MET:HE2	1:E:439:HIS:HB3	1.88	0.55
1:E:272:GLN:HB3	1:E:279:ILE:HG12	1.89	0.55
1:F:461:THR:OG1	1:F:464:GLN:HG3	2.06	0.55
1:A:477:GLU:HA	1:B:450:GLN:HE21	1.71	0.55
1:C:388:GLU:O	1:C:391:VAL:HG22	2.07	0.55
1:D:343:THR:OG1	2:D:600:FAD:H2'	2.07	0.55
1:E:279:ILE:HG22	1:E:280:ILE:N	2.21	0.55
1:E:472:HIS:HB2	1:F:344:PRO:HG3	1.87	0.55
1:F:57:GLY:HA2	2:F:600:FAD:H3B	1.89	0.55
1:F:151:ILE:HD13	1:F:152:TYR:N	2.22	0.55
1:A:128:GLU:CD	1:C:100:ARG:HH12	2.15	0.55
1:B:186:LEU:HD12	1:B:190:PRO:HG3	1.87	0.55
1:F:191:GLY:O	1:F:193:THR:HG22	2.07	0.55
1:B:30:GLU:O	1:B:33:GLN:HB3	2.07	0.54
1:C:408:PRO:HG3	1:C:475:CYS:SG	2.48	0.54
1:C:497:CYS:HB3	1:D:115:GLY:HA3	1.88	0.54
1:D:48:PRO:HG2	1:D:167:TYR:CE1	2.42	0.54
1:D:70:MET:HE1	1:D:184:PHE:HA	1.89	0.54
1:F:226:ARG:HG3	1:F:226:ARG:NH1	2.21	0.54
1:F:266:ARG:O	1:F:267:LEU:HD12	2.07	0.54
1:A:16:ILE:HG13	1:A:154:ALA:HB2	1.89	0.54
1:A:266:ARG:C	1:A:267:LEU:HD12	2.32	0.54
1:B:12:ASP:HB2	1:B:153:SER:O	2.07	0.54
1:B:263:THR:OG1	1:B:264:PRO:CD	2.55	0.54
1:C:470:GLY:CA	1:D:450:GLN:HE22	2.20	0.54
1:C:450:GLN:HE22	1:D:471:ILE:H	1.56	0.54
1:F:167:TYR:CE2	1:F:174:LYS:HA	2.43	0.54
1:A:319:THR:HG23	1:A:323:GLN:O	2.08	0.54
1:B:487:ARG:O	1:B:487:ARG:HG2	2.08	0.54
1:C:448:VAL:HG22	1:C:476:ALA:HB2	1.89	0.54
1:C:472:HIS:HB2	1:D:344:PRO:HG3	1.88	0.54
1:E:192:LYS:H	1:E:285:ASN:HD22	1.53	0.54
1:E:461:THR:OG1	1:E:464:GLN:HG3	2.07	0.54
1:A:450:GLN:HE22	1:B:471:ILE:N	2.05	0.54
1:D:232:MET:HE2	1:D:439:HIS:HB3	1.88	0.54
1:D:191:GLY:O	1:D:193:THR:HG22	2.08	0.54
1:D:400:GLU:OE1	1:D:487:ARG:HD2	2.08	0.54
1:E:151:ILE:HD13	1:E:152:TYR:N	2.23	0.54
1:F:25:LEU:HD13	1:F:116:TYR:CD1	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ILE:HG12	1:A:270:VAL:O	2.07	0.54
1:C:86:TYR:CD2	1:C:413:ILE:HD11	2.43	0.54
1:C:259:ILE:HD12	1:C:283:GLU:OE1	2.08	0.54
1:B:232:MET:HE2	1:B:439:HIS:HB3	1.89	0.54
1:F:262:GLY:O	1:F:263:THR:O	2.26	0.54
1:A:170:ILE:HD12	1:A:255:LYS:HA	1.89	0.54
1:D:156:ARG:HG3	1:D:156:ARG:HH11	1.72	0.54
1:D:273:SER:OG	1:D:276:SER:HB3	2.08	0.54
1:E:32:ALA:HB2	1:E:125:VAL:HG22	1.90	0.54
1:A:32:ALA:C	1:A:34:TYR:H	2.16	0.54
1:A:36:LYS:HE3	1:A:358:TYR:CD1	2.43	0.54
1:D:472:HIS:ND1	1:D:473:PRO:HA	2.23	0.54
1:E:403:HIS:CD2	1:E:492:ILE:HG21	2.43	0.54
1:C:450:GLN:NE2	1:D:471:ILE:H	2.07	0.53
1:E:82:ASP:O	1:E:83:SER:C	2.51	0.53
1:A:39:MET:HE3	1:A:41:LEU:HD21	1.90	0.53
1:A:260:GLU:HB2	1:A:266:ARG:HB2	1.91	0.53
1:A:263:THR:OG1	1:A:264:PRO:CD	2.57	0.53
1:A:388:GLU:O	1:A:391:VAL:HG22	2.08	0.53
1:E:387:GLU:OE2	1:E:486:LYS:NZ	2.41	0.53
1:F:42:ASP:OD1	2:F:600:FAD:H1B	2.08	0.53
1:B:156:ARG:HG3	1:B:156:ARG:HH11	1.73	0.53
1:B:336:LEU:HD23	1:B:339:LYS:HG3	1.91	0.53
1:C:259:ILE:O	1:C:260:GLU:HB2	2.07	0.53
1:C:263:THR:O	1:C:265:GLY:N	2.41	0.53
1:C:387:GLU:OE2	1:C:486:LYS:NZ	2.41	0.53
1:E:11:TYR:CZ	1:E:155:GLU:HA	2.43	0.53
1:E:493:LEU:N	1:E:493:LEU:CD1	2.70	0.53
1:F:253:PRO:HA	1:F:271:ALA:CB	2.36	0.53
1:E:105:VAL:HG13	1:E:106:GLN:N	2.23	0.53
1:F:49:LEU:HD22	1:F:49:LEU:H	1.74	0.53
1:F:84:ARG:CG	1:F:90:VAL:HG12	2.37	0.53
1:B:86:TYR:CE1	1:B:413:ILE:HD13	2.44	0.53
1:C:139:ARG:NH1	5:C:2003:HOH:O	2.41	0.53
1:E:12:ASP:HB2	1:E:153:SER:O	2.08	0.53
1:E:55:LEU:HD13	1:E:56:GLY:H	1.73	0.53
1:F:49:LEU:HD11	1:F:174:LYS:O	2.08	0.53
1:A:400:GLU:OE1	1:A:487:ARG:NH1	2.42	0.53
1:C:86:TYR:CD2	1:D:76:LEU:HD23	2.42	0.53
1:C:412:THR:HG21	1:D:108:HIS:CE1	2.43	0.53
1:A:254:ILE:HG12	1:A:270:VAL:HG12	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:488:SER:O	1:D:490:ALA:N	2.41	0.53
1:D:413:ILE:HG13	1:D:414:PRO:CD	2.35	0.53
1:E:450:GLN:HE22	1:F:471:ILE:N	2.07	0.53
1:A:347:ILE:O	1:A:351:ARG:HG3	2.09	0.53
1:D:259:ILE:O	1:D:259:ILE:HG22	2.08	0.53
1:E:114:TRP:O	1:E:115:GLY:C	2.51	0.53
1:F:58:THR:O	1:F:59:CYS:C	2.52	0.53
1:A:32:ALA:C	1:A:34:TYR:N	2.67	0.52
1:A:318:VAL:HG13	1:A:319:THR:O	2.09	0.52
1:A:400:GLU:OE2	1:A:400:GLU:HA	2.08	0.52
1:B:325:ASN:OD1	1:B:326:VAL:HG23	2.09	0.52
1:D:186:LEU:HD12	1:D:190:PRO:HG3	1.90	0.52
1:E:450:GLN:HE21	1:F:477:GLU:HA	1.74	0.52
1:F:162:GLY:HA3	2:F:600:FAD:O1A	2.08	0.52
1:B:151:ILE:HD13	1:B:151:ILE:C	2.34	0.52
1:B:388:GLU:O	1:B:391:VAL:HG22	2.09	0.52
1:D:423:ALA:HB1	1:D:479:PHE:CZ	2.44	0.52
1:A:76:LEU:CD2	1:B:86:TYR:CD2	2.92	0.52
1:A:263:THR:CB	1:A:264:PRO:HD3	2.39	0.52
1:B:373:THR:HG21	1:B:446:GLY:HA2	1.89	0.52
1:C:86:TYR:CZ	1:C:413:ILE:HG12	2.45	0.52
1:C:347:ILE:O	1:C:351:ARG:HG3	2.10	0.52
1:D:388:GLU:O	1:D:391:VAL:HG22	2.08	0.52
1:E:280:ILE:HG13	1:E:281:GLU:N	2.25	0.52
1:F:232:MET:HE2	1:F:439:HIS:HB3	1.90	0.52
1:D:91:GLU:HG3	1:D:93:THR:N	2.21	0.52
1:D:139:ARG:HG3	1:D:151:ILE:HD11	1.88	0.52
1:E:373:THR:HG23	1:F:471:ILE:HG21	1.86	0.52
1:F:110:GLY:HA2	1:F:113:ASN:HD22	1.75	0.52
1:F:272:GLN:HE21	1:F:277:GLU:HA	1.75	0.52
1:F:411:TRP:C	1:F:414:PRO:HD2	2.35	0.52
1:A:404:SER:HA	1:A:492:ILE:HD12	1.92	0.52
1:C:232:MET:HE2	1:C:439:HIS:HB3	1.91	0.52
1:C:373:THR:HG21	1:C:446:GLY:HA2	1.91	0.52
1:C:471:ILE:CG2	1:D:373:THR:HG23	2.36	0.52
1:D:106:GLN:HA	1:D:109:ILE:HD12	1.92	0.52
1:A:407:TRP:CG	1:A:418:ASN:HD22	2.28	0.52
1:B:251:PHE:CE2	1:B:280:ILE:HD12	2.44	0.52
1:B:262:GLY:O	1:B:263:THR:O	2.27	0.52
1:C:258:GLN:C	1:C:260:GLU:H	2.18	0.52
1:D:292:GLY:HA3	3:D:601:NAP:O2A	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:ARG:HG2	1:E:361:SER:O	2.08	0.52
1:A:385:LEU:HD22	1:A:389:LYS:HG3	1.91	0.52
1:B:258:GLN:O	1:B:259:ILE:C	2.52	0.52
1:D:461:THR:OG1	1:D:464:GLN:HG3	2.09	0.52
1:F:325:ASN:OD1	1:F:326:VAL:HG23	2.10	0.52
1:C:192:LYS:N	1:C:285:ASN:HD22	2.08	0.52
1:D:340:VAL:HG11	1:D:370:VAL:HG21	1.92	0.52
1:D:348:GLN:NE2	1:D:351:ARG:HH12	2.08	0.52
1:A:32:ALA:O	1:A:34:TYR:N	2.43	0.52
1:A:472:HIS:ND1	1:A:473:PRO:HA	2.25	0.52
1:B:493:LEU:N	1:B:493:LEU:HD12	2.25	0.52
1:C:194:LEU:HB2	1:C:284:TYR:CE1	2.45	0.52
1:D:151:ILE:HD13	1:D:151:ILE:C	2.34	0.52
1:D:221:ARG:HH21	3:D:601:NAP:P2B	2.33	0.52
1:E:388:GLU:O	1:E:391:VAL:HG22	2.10	0.52
1:F:21:GLY:CA	2:F:600:FAD:H51A	2.36	0.52
1:E:263:THR:CB	1:E:264:PRO:CD	2.87	0.51
1:C:255:LYS:HE3	1:C:257:GLU:HG3	1.91	0.51
1:E:98:TRP:CE2	1:E:102:ILE:HD11	2.45	0.51
1:E:256:VAL:C	1:E:257:GLU:HG2	2.34	0.51
1:A:348:GLN:HG3	1:B:469:ILE:HD12	1.92	0.51
1:C:255:LYS:HB3	1:C:270:VAL:HG21	1.92	0.51
1:E:30:GLU:HG3	1:E:351:ARG:HA	1.92	0.51
1:E:85:ASN:O	1:E:413:ILE:HD11	2.09	0.51
1:E:114:TRP:O	1:E:117:ARG:N	2.43	0.51
1:F:25:LEU:CD2	1:F:120:LEU:HD11	2.41	0.51
1:F:31:ALA:O	1:F:32:ALA:C	2.54	0.51
1:B:114:TRP:CE2	1:B:117:ARG:NH2	2.74	0.51
1:C:254:ILE:CD1	1:C:272:GLN:HB2	2.35	0.51
1:C:485:THR:C	1:C:487:ARG:H	2.17	0.51
1:E:115:GLY:O	1:E:118:VAL:HB	2.10	0.51
1:E:291:ILE:O	1:E:291:ILE:HG13	2.10	0.51
1:E:340:VAL:HG13	1:E:345:VAL:HG21	1.92	0.51
1:F:343:THR:OG1	2:F:600:FAD:H2'	2.10	0.51
1:F:399:ILE:C	1:F:399:ILE:HD12	2.35	0.51
1:A:411:TRP:CZ3	1:A:421:CYS:SG	3.03	0.51
1:A:470:GLY:HA2	1:B:450:GLN:NE2	2.23	0.51
1:A:474:VAL:HG12	1:B:447:GLU:CD	2.36	0.51
1:C:344:PRO:HG3	1:D:472:HIS:HB2	1.92	0.51
1:E:104:ALA:CB	1:F:413:ILE:HD12	2.41	0.51
1:E:169:GLY:N	1:E:173:ASP:OD2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:VAL:HG13	1:C:319:THR:O	2.11	0.51
1:E:256:VAL:HG23	1:E:269:VAL:HG22	1.91	0.51
1:A:273:SER:OG	1:A:275:ASN:N	2.44	0.51
1:F:271:ALA:O	1:F:280:ILE:HG12	2.11	0.51
1:F:474:VAL:HG12	1:F:475:CYS:N	2.26	0.51
1:A:146:LYS:HE2	1:C:187:PRO:O	2.11	0.51
1:C:151:ILE:HD13	1:C:152:TYR:N	2.25	0.51
1:C:173:ASP:O	1:C:177:CYS:HB2	2.10	0.51
1:D:85:ASN:HB2	1:D:413:ILE:CD1	2.41	0.51
1:E:84:ARG:HH21	1:E:92:GLU:HA	1.74	0.51
1:C:222:SER:OG	1:C:226:ARG:NH2	2.43	0.51
1:C:258:GLN:HE21	1:C:261:ALA:N	2.09	0.51
1:A:156:ARG:HD3	1:A:330:TYR:HE2	1.76	0.50
1:C:98:TRP:NE1	1:C:102:ILE:HG13	2.25	0.50
1:D:318:VAL:HG13	1:D:319:THR:O	2.11	0.50
1:A:487:ARG:C	1:A:489:GLY:N	2.65	0.50
1:C:325:ASN:OD1	1:C:326:VAL:HG23	2.12	0.50
1:D:325:ASN:OD1	1:D:326:VAL:HG23	2.10	0.50
1:E:474:VAL:CG1	1:F:447:GLU:OE1	2.59	0.50
1:A:471:ILE:H	1:B:450:GLN:HE22	1.58	0.50
1:B:92:GLU:C	1:B:94:VAL:N	2.68	0.50
1:E:46:PRO:HG3	1:E:52:ARG:CZ	2.41	0.50
1:E:385:LEU:HD22	1:E:389:LYS:HG3	1.93	0.50
1:D:348:GLN:NE2	1:D:351:ARG:NH1	2.58	0.50
4:D:700:MPD:O4	4:D:700:MPD:H11	2.12	0.50
1:E:48:PRO:HB2	1:E:49:LEU:HD22	1.93	0.50
1:E:72:GLN:CD	1:F:410:GLU:HG3	2.37	0.50
1:E:164:ARG:NH1	1:E:164:ARG:HG3	2.27	0.50
1:F:156:ARG:HG3	1:F:156:ARG:HH11	1.77	0.50
1:B:408:PRO:O	1:B:409:LEU:C	2.53	0.50
1:C:447:GLU:OE1	1:D:474:VAL:HG12	2.12	0.50
1:D:13:TYR:HA	1:D:37:LYS:HD3	1.92	0.50
1:E:28:ALA:HB2	1:E:40:VAL:CG2	2.42	0.50
1:E:106:GLN:C	1:E:108:HIS:H	2.19	0.50
1:E:168:LEU:HD21	1:E:291:ILE:HG21	1.93	0.50
1:E:318:VAL:HG13	1:E:319:THR:O	2.12	0.50
1:F:39:MET:HE3	1:F:41:LEU:CD2	2.41	0.50
1:A:29:LYS:HB2	1:A:29:LYS:HZ3	1.73	0.50
1:A:277:GLU:O	1:A:278:GLU:C	2.54	0.50
1:B:418:ASN:ND2	1:B:419:ASN:H	2.09	0.50
1:B:432:ASN:HD22	1:B:463:LYS:HZ1	1.58	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:LEU:HD13	1:D:253:PRO:HB2	1.93	0.50
1:D:418:ASN:OD1	1:D:495:ALA:HB2	2.12	0.50
1:E:471:ILE:N	1:F:450:GLN:HE22	2.09	0.50
1:A:94:VAL:HG11	1:B:90:VAL:HG22	1.94	0.50
1:A:325:ASN:OD1	1:A:326:VAL:HG23	2.11	0.50
1:B:340:VAL:HG13	1:B:345:VAL:HG21	1.94	0.50
1:B:55:LEU:HD23	1:B:56:GLY:H	1.76	0.50
1:B:222:SER:OG	3:B:601:NAP:O3X	2.26	0.50
1:C:259:ILE:HD11	1:C:268:ARG:HD2	1.93	0.50
1:C:259:ILE:O	1:C:260:GLU:CB	2.59	0.50
1:D:151:ILE:HD13	1:D:152:TYR:N	2.26	0.50
1:D:387:GLU:HA	1:D:426:ILE:HD13	1.93	0.50
1:E:266:ARG:HH11	1:E:266:ARG:HB2	1.76	0.50
1:F:488:SER:C	1:F:490:ALA:H	2.20	0.50
1:A:53:TRP:CH2	1:A:62:VAL:HG11	2.45	0.49
4:A:701:MPD:O4	4:A:701:MPD:HM1	2.12	0.49
1:B:176:TYR:CE1	1:B:258:GLN:HB2	2.47	0.49
1:B:387:GLU:HA	1:B:426:ILE:HD13	1.93	0.49
1:C:32:ALA:C	1:C:34:TYR:H	2.20	0.49
1:E:114:TRP:O	1:E:116:TYR:N	2.44	0.49
1:D:374:VAL:HG12	1:D:376:THR:HG23	1.94	0.49
1:D:373:THR:HG21	1:D:446:GLY:HA2	1.93	0.49
1:E:252:VAL:C	1:E:271:ALA:HB1	2.37	0.49
1:E:387:GLU:HA	1:E:426:ILE:HD13	1.93	0.49
1:F:251:PHE:CZ	1:F:273:SER:HB2	2.46	0.49
1:B:46:PRO:HG3	1:B:52:ARG:HB3	1.95	0.49
1:B:151:ILE:HD13	1:B:152:TYR:N	2.27	0.49
1:C:331:ALA:O	1:C:332:ILE:HD12	2.13	0.49
1:C:400:GLU:OE1	1:C:487:ARG:NH1	2.45	0.49
1:D:356:ARG:HG2	1:D:361:SER:O	2.13	0.49
1:D:406:PHE:CZ	1:D:421:CYS:HB3	2.47	0.49
1:E:167:TYR:CE2	1:E:174:LYS:HA	2.47	0.49
1:E:400:GLU:OE1	1:E:487:ARG:HD2	2.13	0.49
1:E:487:ARG:O	1:E:489:GLY:N	2.46	0.49
1:F:31:ALA:C	1:F:33:GLN:N	2.71	0.49
1:F:303:GLU:CD	1:F:303:GLU:H	2.20	0.49
1:F:318:VAL:HG13	1:F:319:THR:O	2.13	0.49
1:F:331:ALA:O	1:F:332:ILE:HD12	2.13	0.49
1:B:167:TYR:CE2	1:B:174:LYS:HG2	2.48	0.49
1:B:194:LEU:HB2	1:B:284:TYR:CE2	2.47	0.49
1:B:200:TYR:CD2	1:B:201:VAL:N	2.80	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ILE:HG22	1:C:266:ARG:HH21	1.77	0.49
1:C:402:TYR:CE2	1:C:462:LYS:HE3	2.47	0.49
1:E:96:HIS:HB2	1:F:88:TRP:CZ3	2.48	0.49
1:E:254:ILE:HG12	1:E:271:ALA:HA	1.95	0.49
1:E:278:GLU:HG2	1:E:279:ILE:N	2.24	0.49
1:F:263:THR:CB	1:F:264:PRO:HD3	2.43	0.49
1:B:16:ILE:HG13	1:B:154:ALA:HB2	1.94	0.49
1:B:258:GLN:O	1:B:258:GLN:CG	2.60	0.49
1:E:389:LYS:O	1:E:389:LYS:HD3	2.12	0.49
1:B:193:THR:HB	1:B:286:THR:HB	1.95	0.49
1:D:173:ASP:O	1:D:177:CYS:HB2	2.12	0.49
1:D:413:ILE:C	1:D:413:ILE:HD12	2.38	0.49
1:E:301:GLY:HA2	1:E:303:GLU:OE2	2.13	0.49
1:E:373:THR:HG21	1:E:446:GLY:HA2	1.95	0.49
1:A:253:PRO:HA	1:A:271:ALA:HB2	1.95	0.49
1:D:85:ASN:HB2	1:D:413:ILE:HD12	1.94	0.49
1:E:123:LYS:O	1:E:123:LYS:HG3	2.13	0.49
1:E:396:GLU:OE2	1:E:487:ARG:NH2	2.46	0.49
1:F:90:VAL:O	1:F:91:GLU:C	2.55	0.49
1:F:388:GLU:O	1:F:391:VAL:HG22	2.12	0.49
1:B:55:LEU:CD2	1:B:56:GLY:N	2.76	0.49
1:B:408:PRO:O	1:B:411:TRP:N	2.37	0.49
1:C:43:PHE:C	1:C:43:PHE:CD2	2.91	0.49
1:C:84:ARG:HE	1:C:90:VAL:HG23	1.78	0.49
1:D:255:LYS:HB3	1:D:270:VAL:HG21	1.95	0.49
1:F:110:GLY:HA2	1:F:113:ASN:ND2	2.27	0.49
1:F:178:ILE:O	1:F:288:MET:HA	2.12	0.49
1:B:144:ASN:CG	1:B:145:ASN:N	2.71	0.48
1:C:76:LEU:CD2	1:D:86:TYR:CD2	2.95	0.48
1:D:228:PHE:O	1:D:229:ASP:C	2.55	0.48
1:D:476:ALA:C	1:D:478:VAL:N	2.71	0.48
1:F:98:TRP:CZ2	1:F:102:ILE:HD11	2.48	0.48
4:F:700:MPD:O4	4:F:700:MPD:H11	2.13	0.48
1:B:30:GLU:HG2	1:B:351:ARG:HG2	1.94	0.48
1:B:63:GLY:O	1:B:66:PRO:HG2	2.13	0.48
1:B:114:TRP:O	1:B:118:VAL:HG23	2.13	0.48
1:C:188:TYR:CB	1:C:263:THR:HB	2.43	0.48
1:C:194:LEU:HB2	1:C:284:TYR:CD1	2.49	0.48
1:E:280:ILE:CD1	1:E:281:GLU:H	2.26	0.48
1:E:447:GLU:OE1	1:F:474:VAL:HG12	2.13	0.48
1:E:469:ILE:HG21	1:F:345:VAL:HG12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:491:SER:OG	1:F:492:ILE:N	2.46	0.48
1:A:163:GLU:HG2	1:A:295:ALA:HA	1.95	0.48
1:A:171:PRO:HB2	1:A:255:LYS:HD2	1.95	0.48
1:B:253:PRO:HA	1:B:271:ALA:HB2	1.94	0.48
1:C:88:TRP:CZ3	1:D:96:HIS:HB2	2.49	0.48
1:D:188:TYR:HB2	1:D:264:PRO:HD3	1.95	0.48
1:E:277:GLU:O	1:E:278:GLU:C	2.56	0.48
1:F:173:ASP:O	1:F:177:CYS:HB2	2.13	0.48
1:A:471:ILE:HB	1:A:474:VAL:HG21	1.94	0.48
1:B:391:VAL:CG2	1:B:392:GLU:N	2.76	0.48
1:C:108:HIS:CE1	1:D:412:THR:HG21	2.48	0.48
1:C:259:ILE:CG1	1:C:268:ARG:HB2	2.44	0.48
1:D:86:TYR:CE1	1:D:413:ILE:HG12	2.49	0.48
1:E:266:ARG:NH1	1:E:266:ARG:CB	2.76	0.48
1:E:471:ILE:HG21	1:F:373:THR:HG23	1.90	0.48
1:F:339:LYS:HD2	1:F:367:TYR:CE2	2.48	0.48
1:A:65:ILE:HB	1:A:66:PRO:CD	2.44	0.48
1:A:251:PHE:CD2	1:A:280:ILE:HD11	2.49	0.48
1:B:44:VAL:HG21	1:B:53:TRP:CD1	2.48	0.48
1:C:32:ALA:C	1:C:34:TYR:N	2.72	0.48
1:D:212:ILE:HD12	1:D:212:ILE:HA	1.70	0.48
1:D:403:HIS:CE1	1:D:492:ILE:HD13	2.48	0.48
1:D:476:ALA:O	1:D:478:VAL:N	2.47	0.48
1:A:144:ASN:CG	1:A:145:ASN:N	2.72	0.48
1:B:101:MET:O	1:B:102:ILE:C	2.56	0.48
1:B:403:HIS:CD2	1:B:403:HIS:H	2.32	0.48
1:C:275:ASN:CG	1:C:276:SER:H	2.21	0.48
1:D:64:CYS:SG	2:D:600:FAD:C10	3.02	0.48
1:D:65:ILE:HB	1:D:66:PRO:CD	2.43	0.48
1:B:200:TYR:CE2	1:B:201:VAL:HG23	2.48	0.48
1:C:391:VAL:CG2	1:C:392:GLU:N	2.77	0.48
1:E:156:ARG:HH11	1:E:156:ARG:HG3	1.78	0.48
1:E:192:LYS:N	1:E:285:ASN:HD22	2.11	0.48
1:F:78:GLN:NE2	1:F:82:ASP:OD1	2.42	0.48
1:F:116:TYR:C	1:F:118:VAL:N	2.70	0.48
1:F:389:LYS:O	1:F:389:LYS:HD3	2.14	0.48
1:F:477:GLU:O	1:F:477:GLU:HG3	2.14	0.48
1:A:150:LYS:HD3	1:A:152:TYR:CZ	2.48	0.48
1:B:385:LEU:HD22	1:B:389:LYS:HG3	1.95	0.48
1:C:49:LEU:N	1:C:49:LEU:HD22	2.28	0.48
1:D:156:ARG:HG3	1:D:156:ARG:NH1	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:THR:O	1:D:264:PRO:C	2.50	0.48
1:D:263:THR:OG1	1:D:264:PRO:CD	2.62	0.48
1:E:150:LYS:HD3	1:E:152:TYR:CZ	2.48	0.48
1:F:176:TYR:HB3	1:F:267:LEU:CD2	2.35	0.48
1:F:203:LEU:HD22	1:F:240:MET:SD	2.54	0.48
1:A:471:ILE:H	1:B:450:GLN:NE2	2.11	0.48
1:B:400:GLU:OE1	1:B:487:ARG:HD2	2.14	0.48
1:B:423:ALA:HB1	1:B:479:PHE:CZ	2.49	0.48
1:E:52:ARG:HB2	1:E:52:ARG:NH1	2.29	0.48
1:F:257:GLU:OE2	1:F:268:ARG:NH1	2.47	0.48
1:A:98:TRP:CZ2	1:A:102:ILE:HD11	2.49	0.48
1:C:411:TRP:C	1:C:414:PRO:HD2	2.39	0.48
1:D:340:VAL:O	1:D:340:VAL:HG22	2.13	0.48
1:D:385:LEU:HD22	1:D:389:LYS:CG	2.44	0.48
1:E:14:ASP:CG	1:E:36:LYS:HD2	2.39	0.48
1:E:98:TRP:O	1:E:102:ILE:HG12	2.14	0.48
1:F:385:LEU:HD22	1:F:389:LYS:HG3	1.95	0.48
1:A:108:HIS:CD2	1:B:412:THR:HB	2.49	0.47
1:C:101:MET:HG3	1:D:86:TYR:O	2.14	0.47
1:C:272:GLN:HA	1:C:279:ILE:HG12	1.95	0.47
1:C:412:THR:O	1:C:415:SER:N	2.47	0.47
1:C:471:ILE:HD13	1:D:373:THR:HG22	1.96	0.47
1:D:262:GLY:O	1:D:264:PRO:C	2.57	0.47
1:E:69:LEU:CD1	1:E:105:VAL:HG23	2.44	0.47
1:E:106:GLN:HE21	1:E:106:GLN:CA	2.19	0.47
1:E:138:HIS:O	1:E:153:SER:HA	2.14	0.47
1:E:341:GLU:CD	1:E:341:GLU:H	2.22	0.47
1:E:478:VAL:CG1	1:E:479:PHE:N	2.77	0.47
1:F:58:THR:O	1:F:60:VAL:N	2.47	0.47
1:F:156:ARG:HD3	1:F:330:TYR:HE2	1.79	0.47
1:B:192:LYS:H	1:B:285:ASN:HD22	1.61	0.47
1:B:401:VAL:O	1:B:485:THR:HA	2.13	0.47
1:C:263:THR:CB	1:C:264:PRO:HD3	2.44	0.47
1:D:222:SER:OG	1:D:226:ARG:NH2	2.47	0.47
1:E:469:ILE:HD12	1:F:348:GLN:HG3	1.95	0.47
1:F:403:HIS:CD2	1:F:492:ILE:HD13	2.49	0.47
1:A:55:LEU:CD2	1:A:56:GLY:H	2.26	0.47
1:B:389:LYS:O	1:B:389:LYS:HD3	2.15	0.47
1:E:98:TRP:CD1	1:E:98:TRP:C	2.91	0.47
1:F:144:ASN:CG	1:F:145:ASN:N	2.72	0.47
1:F:270:VAL:HG13	1:F:280:ILE:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:484:VAL:HG11	1:F:491:SER:O	2.13	0.47
1:A:151:ILE:HD13	1:A:152:TYR:N	2.29	0.47
1:C:416:ARG:O	1:C:417:ASP:C	2.58	0.47
1:E:106:GLN:C	1:E:108:HIS:N	2.70	0.47
1:E:325:ASN:OD1	1:E:326:VAL:HG23	2.14	0.47
1:F:351:ARG:HD3	5:F:2005:HOH:O	2.13	0.47
1:A:228:PHE:O	1:A:229:ASP:C	2.57	0.47
1:A:391:VAL:CG2	1:A:392:GLU:N	2.78	0.47
1:B:86:TYR:CE1	1:B:413:ILE:HD11	2.41	0.47
1:E:166:ARG:HG2	1:E:291:ILE:HD11	1.97	0.47
1:E:265:GLY:O	1:E:285:ASN:HA	2.14	0.47
1:E:488:SER:C	1:E:490:ALA:H	2.23	0.47
1:A:82:ASP:O	1:A:83:SER:C	2.57	0.47
1:A:259:ILE:HB	1:A:266:ARG:O	2.14	0.47
1:B:318:VAL:HG13	1:B:319:THR:O	2.13	0.47
1:B:403:HIS:HB2	1:B:422:TYR:CE1	2.49	0.47
1:C:450:GLN:HE21	1:D:477:GLU:HA	1.79	0.47
1:E:58:THR:O	1:E:63:GLY:N	2.48	0.47
1:E:303:GLU:CD	1:E:303:GLU:H	2.22	0.47
1:F:79:ALA:HB2	4:F:700:MPD:HM2	1.97	0.47
1:F:474:VAL:HG12	1:F:475:CYS:H	1.79	0.47
1:B:262:GLY:O	1:B:265:GLY:N	2.47	0.47
1:C:96:HIS:HA	1:D:87:GLY:O	2.15	0.47
1:C:100:ARG:O	1:C:103:GLU:HB3	2.14	0.47
1:C:168:LEU:HD13	1:C:253:PRO:HB2	1.96	0.47
1:D:55:LEU:HD22	1:D:56:GLY:N	2.29	0.47
1:D:90:VAL:CG2	1:D:91:GLU:N	2.77	0.47
1:D:150:LYS:HD3	1:D:152:TYR:CZ	2.50	0.47
1:E:116:TYR:O	1:E:117:ARG:C	2.57	0.47
1:E:287:VAL:O	1:E:287:VAL:HG12	2.14	0.47
1:E:410:GLU:OE2	1:F:68:LYS:NZ	2.46	0.47
1:A:29:LYS:CE	1:A:119:ALA:HB1	2.44	0.47
1:A:170:ILE:HB	1:A:254:ILE:O	2.14	0.47
1:B:30:GLU:HG3	1:B:351:ARG:HA	1.96	0.47
1:D:21:GLY:HA3	2:D:600:FAD:H52A	1.96	0.47
1:E:90:VAL:HG21	1:F:80:LEU:CD2	2.45	0.47
1:E:396:GLU:O	1:E:487:ARG:NH2	2.48	0.47
1:B:123:LYS:O	1:B:124:LYS:HB2	2.13	0.47
1:B:301:GLY:HA2	1:B:303:GLU:OE2	2.15	0.47
1:C:79:ALA:HB2	4:D:700:MPD:HM2	1.96	0.47
1:C:97:ASP:OD1	1:C:99:ASP:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:MET:HE1	1:C:271:ALA:HB2	1.96	0.47
1:C:389:LYS:HB2	1:C:389:LYS:NZ	2.30	0.47
1:E:336:LEU:HB3	1:E:339:LYS:CG	2.44	0.47
1:B:55:LEU:CD2	1:B:56:GLY:H	2.28	0.47
1:C:225:LEU:HB3	1:C:228:PHE:CD2	2.50	0.47
1:E:432:ASN:HD22	1:E:463:LYS:HZ1	1.62	0.47
1:C:254:ILE:HD11	1:C:270:VAL:HG12	1.97	0.46
1:D:262:GLY:O	1:D:263:THR:O	2.32	0.46
1:E:254:ILE:H	1:E:271:ALA:HA	1.78	0.46
1:E:279:ILE:CG2	1:E:280:ILE:N	2.78	0.46
1:F:67:LYS:HD2	1:F:68:LYS:N	2.30	0.46
1:F:223:ILE:HG12	1:F:226:ARG:NH2	2.30	0.46
1:F:387:GLU:HA	1:F:426:ILE:HD13	1.97	0.46
1:F:412:THR:O	1:F:415:SER:N	2.48	0.46
1:A:173:ASP:O	1:A:177:CYS:HB2	2.15	0.46
1:A:389:LYS:O	1:A:389:LYS:HD3	2.15	0.46
1:B:292:GLY:CA	3:B:601:NAP:O2N	2.63	0.46
1:C:32:ALA:O	1:C:34:TYR:N	2.48	0.46
1:C:259:ILE:HD11	1:C:268:ARG:CG	2.44	0.46
1:D:212:ILE:HG23	1:D:212:ILE:O	2.15	0.46
1:E:400:GLU:HA	1:E:400:GLU:OE2	2.16	0.46
1:B:419:ASN:HD21	1:B:495:ALA:N	2.12	0.46
1:C:401:VAL:HB	1:C:486:LYS:HB2	1.98	0.46
1:C:440:VAL:HB	1:C:479:PHE:HZ	1.80	0.46
1:D:62:VAL:HG23	1:D:62:VAL:O	2.16	0.46
1:E:106:GLN:NE2	1:E:106:GLN:CA	2.73	0.46
1:F:57:GLY:HA3	2:F:600:FAD:H52A	1.96	0.46
1:F:82:ASP:OD2	1:F:416:ARG:NH1	2.47	0.46
1:F:168:LEU:HD23	1:F:291:ILE:HD13	1.97	0.46
1:A:30:GLU:OE1	1:A:34:TYR:HE2	1.99	0.46
1:A:101:MET:HB2	1:B:86:TYR:O	2.16	0.46
1:C:77:GLY:HA2	1:C:80:LEU:HD12	1.97	0.46
1:C:477:GLU:HA	1:D:450:GLN:NE2	2.30	0.46
1:E:72:GLN:CD	1:F:410:GLU:CG	2.88	0.46
1:E:105:VAL:CG1	1:E:106:GLN:N	2.79	0.46
1:B:25:LEU:CD2	1:B:120:LEU:HD11	2.43	0.46
1:B:55:LEU:HD22	1:B:56:GLY:N	2.31	0.46
1:B:156:ARG:HG3	1:B:156:ARG:NH1	2.30	0.46
1:C:92:GLU:OE2	1:E:150:LYS:CE	2.63	0.46
1:E:12:ASP:O	1:E:37:LYS:CE	2.64	0.46
1:E:46:PRO:HG3	1:E:52:ARG:NH2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:TRP:NE1	1:E:102:ILE:HG13	2.30	0.46
1:E:103:GLU:O	1:E:104:ALA:C	2.58	0.46
1:E:315:LYS:HZ2	3:E:601:NAP:H4D	1.80	0.46
1:F:66:PRO:HB3	1:F:109:ILE:HD11	1.96	0.46
1:A:138:HIS:O	1:A:153:SER:HA	2.15	0.46
1:A:212:ILE:HD12	1:A:212:ILE:HA	1.66	0.46
1:C:283:GLU:O	1:C:283:GLU:HG3	2.12	0.46
1:C:471:ILE:HG21	1:D:373:THR:HG22	1.90	0.46
1:D:83:SER:O	1:D:86:TYR:N	2.48	0.46
1:D:303:GLU:CD	1:D:303:GLU:H	2.23	0.46
1:D:440:VAL:HB	1:D:479:PHE:CZ	2.51	0.46
1:E:164:ARG:HG3	1:E:164:ARG:HH11	1.80	0.46
1:A:77:GLY:HA2	1:A:80:LEU:HD12	1.97	0.46
1:A:108:HIS:NE2	1:B:412:THR:HB	2.31	0.46
1:A:156:ARG:HG3	1:A:156:ARG:HH11	1.81	0.46
1:A:387:GLU:HA	1:A:426:ILE:HD13	1.96	0.46
1:A:423:ALA:HB1	1:A:479:PHE:CZ	2.51	0.46
1:C:260:GLU:HG2	1:C:261:ALA:O	2.16	0.46
1:D:331:ALA:O	1:D:332:ILE:HD12	2.16	0.46
1:D:406:PHE:CE1	1:D:421:CYS:HB3	2.51	0.46
1:E:256:VAL:HG22	1:E:257:GLU:N	2.30	0.46
1:E:477:GLU:HA	1:F:450:GLN:HE21	1.81	0.46
1:A:53:TRP:CZ3	1:A:62:VAL:CG1	2.86	0.46
1:A:69:LEU:HD12	1:A:105:VAL:HG13	1.97	0.46
1:E:77:GLY:HA2	1:E:80:LEU:HD12	1.97	0.46
1:E:176:TYR:CE1	1:E:258:GLN:HB2	2.50	0.46
1:F:62:VAL:O	1:F:62:VAL:HG23	2.16	0.46
1:F:118:VAL:O	1:F:119:ALA:C	2.59	0.46
1:A:471:ILE:CG2	1:B:373:THR:HG23	2.44	0.46
1:B:98:TRP:CE2	1:B:190:PRO:HD3	2.50	0.46
1:C:385:LEU:HD22	1:C:389:LYS:HG3	1.97	0.46
1:E:280:ILE:CG1	1:E:281:GLU:N	2.79	0.46
1:E:331:ALA:O	1:E:332:ILE:HD12	2.16	0.46
1:B:36:LYS:HD2	1:B:358:TYR:CD1	2.51	0.46
1:B:221:ARG:HD3	3:B:601:NAP:C2A	2.46	0.46
1:B:266:ARG:NE	1:B:283:GLU:OE2	2.49	0.46
1:D:416:ARG:HG2	1:D:416:ARG:HH11	1.81	0.46
1:F:26:ALA:O	1:F:30:GLU:HB2	2.16	0.46
1:F:138:HIS:O	1:F:153:SER:HA	2.16	0.46
1:C:180:SER:HA	1:C:288:MET:CE	2.46	0.45
1:C:387:GLU:HA	1:C:426:ILE:HD13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:TRP:CE2	1:D:190:PRO:HD3	2.52	0.45
1:D:449:THR:O	1:D:450:GLN:C	2.57	0.45
1:E:44:VAL:HG22	2:E:600:FAD:O2B	2.16	0.45
1:A:252:VAL:C	1:A:271:ALA:HB1	2.40	0.45
1:A:345:VAL:HG12	1:B:469:ILE:HG21	1.98	0.45
1:B:263:THR:CB	1:B:264:PRO:CD	2.94	0.45
1:B:303:GLU:H	1:B:303:GLU:CD	2.22	0.45
1:C:303:GLU:CD	1:C:303:GLU:H	2.23	0.45
1:C:487:ARG:C	1:C:489:GLY:N	2.73	0.45
1:E:186:LEU:HA	1:E:187:PRO:HD3	1.82	0.45
1:E:253:PRO:HA	1:E:271:ALA:CB	2.40	0.45
1:F:78:GLN:NE2	1:F:416:ARG:NH1	2.64	0.45
1:F:319:THR:C	1:F:321:GLU:H	2.25	0.45
1:F:340:VAL:HG13	1:F:345:VAL:CG2	2.37	0.45
1:A:82:ASP:O	1:A:84:ARG:N	2.50	0.45
1:A:98:TRP:CD1	1:A:98:TRP:C	2.93	0.45
1:A:344:PRO:HD3	2:A:600:FAD:O2	2.17	0.45
4:B:701:MPD:HM1	4:B:701:MPD:O4	2.17	0.45
1:D:138:HIS:O	1:D:153:SER:HA	2.16	0.45
1:D:411:TRP:CZ3	1:D:421:CYS:SG	3.10	0.45
1:E:65:ILE:HB	1:E:66:PRO:CD	2.46	0.45
1:E:84:ARG:HH22	1:E:91:GLU:C	2.24	0.45
1:A:29:LYS:HD2	1:A:123:LYS:NZ	2.31	0.45
1:B:166:ARG:HG2	1:B:167:TYR:N	2.31	0.45
1:C:65:ILE:HB	1:C:66:PRO:CD	2.47	0.45
1:C:176:TYR:CE1	1:C:258:GLN:OE1	2.70	0.45
1:C:450:GLN:HE22	1:D:471:ILE:N	2.15	0.45
1:D:484:VAL:O	1:D:484:VAL:HG12	2.16	0.45
1:E:70:MET:HE3	1:E:184:PHE:HD1	1.81	0.45
1:E:144:ASN:CG	1:E:145:ASN:N	2.73	0.45
1:E:267:LEU:HD12	1:E:267:LEU:H	1.81	0.45
1:A:283:GLU:O	1:A:284:TYR:CD2	2.69	0.45
1:E:21:GLY:HA3	2:E:600:FAD:O2A	2.16	0.45
1:E:120:LEU:HD22	1:E:125:VAL:CG1	2.46	0.45
1:A:38:VAL:HG13	1:A:125:VAL:HG22	1.97	0.45
1:A:446:GLY:C	1:B:474:VAL:HG21	2.41	0.45
1:B:65:ILE:HB	1:B:66:PRO:CD	2.46	0.45
1:B:67:LYS:HD2	1:B:67:LYS:C	2.41	0.45
1:B:138:HIS:O	1:B:153:SER:HA	2.17	0.45
1:C:142:ALA:HB3	1:C:152:TYR:HE1	1.81	0.45
1:C:277:GLU:O	1:C:278:GLU:O	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:476:ALA:O	1:D:477:GLU:C	2.59	0.45
1:E:90:VAL:HG21	1:F:80:LEU:HD21	1.97	0.45
1:E:161:THR:O	2:E:600:FAD:H8A	2.17	0.45
1:E:450:GLN:NE2	1:F:470:GLY:HA2	2.26	0.45
1:F:47:THR:C	1:F:49:LEU:N	2.74	0.45
1:F:158:LEU:HD11	1:F:332:ILE:HB	1.98	0.45
1:F:192:LYS:HE2	1:F:284:TYR:CD2	2.52	0.45
1:F:373:THR:HG21	1:F:446:GLY:HA2	1.97	0.45
1:B:389:LYS:HB2	1:B:389:LYS:NZ	2.32	0.45
1:C:86:TYR:O	1:D:101:MET:HG3	2.17	0.45
1:C:340:VAL:HG22	1:C:340:VAL:O	2.17	0.45
1:C:389:LYS:HD3	1:C:389:LYS:O	2.16	0.45
1:D:301:GLY:HA2	1:D:303:GLU:OE2	2.17	0.45
1:D:403:HIS:ND1	1:D:486:LYS:HE3	2.32	0.45
1:E:81:GLN:O	1:E:84:ARG:HB3	2.16	0.45
1:E:340:VAL:HG13	1:E:345:VAL:HG11	1.98	0.45
1:E:412:THR:HG21	1:F:108:HIS:CE1	2.51	0.45
1:F:156:ARG:HG3	1:F:156:ARG:NH1	2.32	0.45
1:F:292:GLY:HA3	3:F:601:NAP:O1A	2.16	0.45
1:F:412:THR:OG1	1:F:413:ILE:N	2.50	0.45
1:A:373:THR:HG23	1:B:471:ILE:HG21	1.96	0.45
1:A:403:HIS:CE1	1:A:492:ILE:CD1	3.00	0.45
1:B:374:VAL:HG12	1:B:376:THR:HG23	1.97	0.45
1:C:43:PHE:C	1:C:43:PHE:HD2	2.25	0.45
1:C:94:VAL:HG12	1:D:88:TRP:HE3	1.80	0.45
1:C:121:ARG:HG2	1:C:122:GLU:N	2.30	0.45
1:C:166:ARG:HG2	1:C:167:TYR:N	2.32	0.45
1:A:301:GLY:HA2	1:A:303:GLU:OE2	2.16	0.45
1:C:114:TRP:O	1:C:117:ARG:N	2.49	0.45
1:D:192:LYS:H	1:D:285:ASN:HD22	1.64	0.45
1:E:156:ARG:HD3	1:E:330:TYR:HE2	1.81	0.45
1:E:173:ASP:O	1:E:177:CYS:HB2	2.17	0.45
1:E:447:GLU:CD	1:F:474:VAL:CG1	2.90	0.45
1:F:65:ILE:HB	1:F:66:PRO:CD	2.47	0.45
1:F:150:LYS:HD3	1:F:152:TYR:CZ	2.51	0.45
1:A:53:TRP:CE3	1:A:62:VAL:HG11	2.48	0.45
1:B:30:GLU:O	1:B:31:ALA:C	2.59	0.45
1:B:207:GLY:HA2	1:B:245:ILE:HD11	1.98	0.45
1:B:391:VAL:HG23	1:B:392:GLU:N	2.32	0.45
1:C:250:GLN:C	1:C:274:THR:OG1	2.60	0.45
1:D:46:PRO:CG	1:D:52:ARG:CZ	2.93	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:GLY:O	1:E:193:THR:CG2	2.65	0.45
1:E:371:PRO:HB3	1:E:453:ALA:HB2	1.99	0.45
1:E:486:LYS:O	1:E:487:ARG:C	2.56	0.45
1:F:33:GLN:O	1:F:33:GLN:NE2	2.50	0.45
1:F:212:ILE:HD12	1:F:212:ILE:HA	1.64	0.45
1:F:268:ARG:HE	1:F:281:GLU:CD	2.25	0.45
1:B:224:LEU:O	1:B:225:LEU:C	2.60	0.44
1:D:265:GLY:O	1:D:285:ASN:OD1	2.35	0.44
1:E:391:VAL:CG2	1:E:392:GLU:N	2.80	0.44
1:F:57:GLY:HA2	2:F:600:FAD:C3B	2.47	0.44
1:F:308:LYS:N	1:F:325:ASN:ND2	2.44	0.44
1:A:139:ARG:NH1	5:A:2002:HOH:O	2.50	0.44
1:E:266:ARG:HH11	1:E:266:ARG:CB	2.30	0.44
1:E:485:THR:OG1	1:E:488:SER:CB	2.65	0.44
1:B:67:LYS:HD2	1:B:68:LYS:N	2.32	0.44
1:B:310:ASN:O	1:B:312:LYS:N	2.50	0.44
1:B:356:ARG:HG2	1:B:361:SER:O	2.16	0.44
1:D:144:ASN:CG	1:D:145:ASN:N	2.74	0.44
1:D:408:PRO:O	1:D:410:GLU:N	2.51	0.44
1:E:392:GLU:O	1:E:392:GLU:HG2	2.17	0.44
1:F:67:LYS:HD2	1:F:67:LYS:C	2.42	0.44
1:F:91:GLU:O	1:F:92:GLU:C	2.61	0.44
1:A:343:THR:HB	1:A:344:PRO:HD3	2.00	0.44
1:B:59:CYS:HA	1:B:63:GLY:HA3	1.99	0.44
1:B:403:HIS:H	1:B:403:HIS:HD2	1.64	0.44
1:C:25:LEU:HD13	1:C:116:TYR:CD1	2.51	0.44
1:C:92:GLU:OE2	1:E:150:LYS:HE2	2.17	0.44
1:C:138:HIS:O	1:C:153:SER:HA	2.17	0.44
1:E:106:GLN:HE22	1:E:109:ILE:CD1	2.13	0.44
1:F:58:THR:HG23	1:F:62:VAL:HG23	1.99	0.44
1:A:86:TYR:CE2	1:A:414:PRO:HG3	2.44	0.44
1:C:163:GLU:OE1	1:C:334:ASP:HB3	2.18	0.44
1:C:178:ILE:O	1:C:288:MET:HA	2.17	0.44
1:C:258:GLN:HE21	1:C:261:ALA:CA	2.31	0.44
1:C:477:GLU:CA	1:D:450:GLN:HE21	2.30	0.44
1:D:319:THR:C	1:D:321:GLU:H	2.25	0.44
1:E:69:LEU:HD22	1:F:413:ILE:CG2	2.47	0.44
1:F:47:THR:HG21	1:F:181:ASP:HB3	1.99	0.44
1:A:191:GLY:O	1:A:193:THR:CG2	2.66	0.44
1:A:310:ASN:O	1:A:312:LYS:N	2.50	0.44
1:A:373:THR:HG21	1:A:446:GLY:HA2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:VAL:HG23	1:A:392:GLU:N	2.33	0.44
1:B:186:LEU:HA	1:B:187:PRO:HD3	1.83	0.44
1:C:114:TRP:O	1:C:118:VAL:HG23	2.18	0.44
1:D:252:VAL:O	1:D:271:ALA:HB1	2.18	0.44
1:D:391:VAL:CG2	1:D:392:GLU:N	2.80	0.44
1:E:221:ARG:HG3	1:E:252:VAL:CG2	2.48	0.44
1:E:447:GLU:CD	1:F:474:VAL:HG12	2.42	0.44
1:F:57:GLY:O	1:F:58:THR:O	2.35	0.44
1:F:432:ASN:HD22	1:F:463:LYS:HZ3	1.63	0.44
1:A:100:ARG:HG3	1:A:100:ARG:HH11	1.83	0.44
1:A:471:ILE:HG21	1:B:373:THR:HG22	1.94	0.44
1:C:373:THR:HG21	1:C:446:GLY:CA	2.47	0.44
1:D:105:VAL:HG12	1:D:106:GLN:N	2.32	0.44
1:F:47:THR:C	1:F:49:LEU:H	2.26	0.44
1:F:49:LEU:N	1:F:49:LEU:CD2	2.78	0.44
1:A:67:LYS:C	1:A:67:LYS:HD2	2.43	0.44
1:B:94:VAL:O	1:B:94:VAL:HG23	2.16	0.44
1:C:193:THR:HB	1:C:286:THR:HB	1.99	0.44
1:E:51:THR:HG22	1:E:52:ARG:N	2.32	0.44
1:C:259:ILE:HG22	1:C:266:ARG:NH2	2.33	0.44
1:D:249:ARG:NH1	5:D:2004:HOH:O	2.51	0.44
1:D:262:GLY:O	1:D:265:GLY:N	2.51	0.44
1:D:389:LYS:HB2	1:D:389:LYS:NZ	2.32	0.44
1:E:340:VAL:CG1	1:E:345:VAL:HG11	2.48	0.44
1:F:205:CYS:HA	1:F:208:PHE:CE2	2.53	0.44
1:F:391:VAL:CG2	1:F:392:GLU:N	2.80	0.44
1:A:49:LEU:HD22	1:A:49:LEU:N	2.33	0.43
1:A:196:VAL:HG21	1:A:253:PRO:HG2	2.00	0.43
1:A:303:GLU:CD	1:A:303:GLU:H	2.24	0.43
1:A:413:ILE:C	1:A:415:SER:H	2.25	0.43
1:B:156:ARG:HD3	1:B:330:TYR:HE2	1.82	0.43
1:C:36:LYS:HE3	1:C:358:TYR:CD1	2.53	0.43
1:C:144:ASN:CG	1:C:145:ASN:N	2.76	0.43
1:C:150:LYS:HD3	1:C:152:TYR:CZ	2.52	0.43
1:C:255:LYS:HE3	1:C:257:GLU:CG	2.48	0.43
1:D:117:ARG:NH1	1:D:117:ARG:HB3	2.33	0.43
1:F:58:THR:O	1:F:61:ASN:N	2.51	0.43
1:F:228:PHE:O	1:F:229:ASP:C	2.60	0.43
1:A:413:ILE:C	1:A:415:SER:N	2.71	0.43
1:B:36:LYS:HG3	1:B:358:TYR:CG	2.53	0.43
1:B:333:GLY:O	1:B:336:LEU:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:MET:HG2	1:C:101:MET:CE	2.45	0.43
1:C:278:GLU:CG	1:C:279:ILE:N	2.78	0.43
1:C:494:GLN:HE21	1:C:494:GLN:HB3	1.60	0.43
1:E:405:TYR:CE1	1:E:493:LEU:HG	2.48	0.43
1:E:413:ILE:C	1:E:415:SER:N	2.73	0.43
1:F:86:TYR:CE2	1:F:414:PRO:HG3	2.53	0.43
1:F:167:TYR:CD2	1:F:174:LYS:HG2	2.53	0.43
1:F:301:GLY:HA2	1:F:303:GLU:OE2	2.18	0.43
1:F:371:PRO:HB3	1:F:453:ALA:HB2	2.00	0.43
1:A:407:TRP:CD1	1:A:418:ASN:HA	2.53	0.43
1:B:339:LYS:HA	1:B:339:LYS:CE	2.46	0.43
1:B:408:PRO:HG2	1:B:411:TRP:CZ3	2.53	0.43
1:D:51:THR:HA	5:D:2001:HOH:O	2.17	0.43
1:D:225:LEU:HB3	1:D:228:PHE:CD2	2.53	0.43
1:B:91:GLU:HB3	1:B:92:GLU:H	1.62	0.43
1:C:192:LYS:HE2	1:C:284:TYR:CD2	2.53	0.43
1:C:447:GLU:OE1	1:D:474:VAL:CG1	2.66	0.43
1:D:258:GLN:NE2	1:D:261:ALA:HB2	2.32	0.43
1:D:310:ASN:O	1:D:312:LYS:N	2.51	0.43
1:E:485:THR:OG1	1:E:488:SER:HB2	2.19	0.43
1:F:176:TYR:CE1	1:F:258:GLN:OE1	2.72	0.43
1:A:38:VAL:CG2	1:A:39:MET:N	2.81	0.43
1:A:146:LYS:HE3	1:C:187:PRO:HB3	2.01	0.43
1:B:173:ASP:O	1:B:177:CYS:HB2	2.19	0.43
1:B:331:ALA:O	1:B:332:ILE:HD12	2.18	0.43
1:B:373:THR:HG21	1:B:446:GLY:CA	2.48	0.43
1:B:413:ILE:N	1:B:414:PRO:CD	2.82	0.43
1:C:88:TRP:HE3	1:D:94:VAL:HG12	1.83	0.43
1:C:156:ARG:HD3	1:C:330:TYR:HE2	1.82	0.43
1:D:488:SER:O	1:D:489:GLY:C	2.61	0.43
1:E:13:TYR:CD1	1:E:37:LYS:HG2	2.48	0.43
1:E:67:LYS:HD2	1:E:68:LYS:N	2.33	0.43
1:E:158:LEU:HD11	1:E:332:ILE:HB	2.01	0.43
1:E:212:ILE:O	1:E:212:ILE:HG23	2.18	0.43
1:A:371:PRO:HB3	1:A:453:ALA:HB2	1.99	0.43
1:B:77:GLY:HA2	1:B:80:LEU:HD12	2.00	0.43
1:B:319:THR:C	1:B:321:GLU:H	2.26	0.43
1:C:44:VAL:CG1	1:C:53:TRP:CE2	3.01	0.43
1:C:85:ASN:CB	1:C:413:ILE:CD1	2.96	0.43
1:C:97:ASP:OD1	1:C:97:ASP:C	2.61	0.43
1:C:315:LYS:HD2	1:C:336:LEU:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:CYS:SG	2:D:600:FAD:C4X	3.06	0.43
1:D:70:MET:HE3	1:D:184:PHE:HD1	1.82	0.43
1:E:256:VAL:HG22	1:E:257:GLU:H	1.82	0.43
1:A:487:ARG:O	1:A:489:GLY:N	2.43	0.43
1:B:336:LEU:CB	1:B:339:LYS:HG3	2.43	0.43
1:D:262:GLY:O	1:D:265:GLY:CA	2.67	0.43
1:E:156:ARG:HG3	1:E:156:ARG:NH1	2.33	0.43
1:E:389:LYS:HB2	1:E:389:LYS:NZ	2.33	0.43
1:E:399:ILE:HA	1:E:427:CYS:O	2.18	0.43
1:E:410:GLU:OE2	1:F:68:LYS:CE	2.65	0.43
1:E:420:LYS:HD3	1:E:420:LYS:HA	1.69	0.43
1:F:411:TRP:HZ3	1:F:421:CYS:SG	2.42	0.43
1:A:67:LYS:HD2	1:A:68:LYS:N	2.33	0.43
1:A:255:LYS:HE2	1:A:257:GLU:HG2	2.01	0.43
1:B:432:ASN:HD22	1:B:463:LYS:HZ3	1.65	0.43
1:C:67:LYS:HD2	1:C:68:LYS:N	2.34	0.43
1:C:269:VAL:N	1:C:282:GLY:O	2.47	0.43
1:D:165:PRO:HG3	5:D:2005:HOH:O	2.18	0.43
1:D:186:LEU:HA	1:D:187:PRO:HD3	1.84	0.43
1:D:371:PRO:HB3	1:D:453:ALA:HB2	2.01	0.43
1:D:413:ILE:N	1:D:414:PRO:CD	2.82	0.43
1:E:10:SER:OG	1:E:11:TYR:N	2.49	0.43
1:E:236:ILE:HD11	1:E:380:TYR:CB	2.49	0.43
1:F:77:GLY:HA2	1:F:80:LEU:HD12	2.00	0.43
1:F:449:THR:O	1:F:450:GLN:C	2.60	0.43
1:A:59:CYS:SG	1:B:472:HIS:CD2	3.12	0.43
1:A:298:ARG:H	1:A:298:ARG:HG2	1.51	0.43
1:B:344:PRO:HD3	2:B:600:FAD:O2	2.19	0.43
1:C:114:TRP:O	1:C:115:GLY:C	2.61	0.43
1:C:391:VAL:HG23	1:C:392:GLU:N	2.32	0.43
1:E:13:TYR:O	1:E:154:ALA:HA	2.19	0.43
1:E:228:PHE:O	1:E:229:ASP:C	2.60	0.43
1:E:319:THR:C	1:E:321:GLU:H	2.26	0.43
1:F:432:ASN:HD22	1:F:463:LYS:HZ1	1.64	0.43
1:A:53:TRP:CE3	1:A:62:VAL:CG1	3.02	0.43
1:C:392:GLU:O	1:C:392:GLU:HG2	2.18	0.43
1:C:485:THR:C	1:C:487:ARG:N	2.76	0.43
1:D:298:ARG:H	1:D:298:ARG:HG2	1.51	0.43
1:E:23:GLY:O	1:E:24:GLY:C	2.62	0.43
1:E:67:LYS:HD2	1:E:67:LYS:C	2.44	0.43
1:A:69:LEU:O	1:A:72:GLN:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASP:OD1	1:A:231:ASP:HB3	2.19	0.42
1:A:403:HIS:CE1	1:A:492:ILE:HD13	2.53	0.42
1:B:64:CYS:O	1:B:65:ILE:C	2.63	0.42
1:B:200:TYR:CD2	1:B:200:TYR:C	2.97	0.42
1:D:67:LYS:HD2	1:D:67:LYS:C	2.44	0.42
1:D:389:LYS:O	1:D:389:LYS:HD3	2.19	0.42
1:E:374:VAL:HG12	1:E:376:THR:HG23	2.01	0.42
1:E:471:ILE:HG21	1:F:373:THR:HG22	1.99	0.42
1:F:337:GLU:HG2	1:F:338:ASP:OD2	2.18	0.42
1:F:342:LEU:O	1:F:345:VAL:HG22	2.19	0.42
1:B:258:GLN:HE21	1:B:261:ALA:HA	1.84	0.42
1:C:59:CYS:HA	1:C:63:GLY:HA3	2.00	0.42
1:C:258:GLN:C	1:C:260:GLU:N	2.78	0.42
1:C:338:ASP:O	1:C:339:LYS:HD3	2.18	0.42
1:C:343:THR:HB	1:C:344:PRO:HD3	2.01	0.42
1:D:55:LEU:CD2	1:D:56:GLY:N	2.82	0.42
1:D:83:SER:O	1:D:84:ARG:C	2.62	0.42
1:D:93:THR:O	1:D:93:THR:HG22	2.20	0.42
1:E:249:ARG:NH1	5:E:2001:HOH:O	2.50	0.42
1:F:272:GLN:HG2	1:F:273:SER:H	1.85	0.42
1:A:55:LEU:HD22	1:A:56:GLY:N	2.35	0.42
1:B:208:PHE:CD1	1:B:208:PHE:C	2.97	0.42
1:B:273:SER:OG	1:B:274:THR:N	2.52	0.42
1:C:471:ILE:H	1:D:450:GLN:HE22	1.68	0.42
1:D:397:GLU:HA	1:D:487:ARG:NH2	2.34	0.42
1:E:112:LEU:O	1:E:113:ASN:C	2.62	0.42
1:E:267:LEU:N	1:E:267:LEU:CD1	2.82	0.42
1:F:215:ASP:CG	1:F:246:LYS:HZ1	2.26	0.42
1:F:389:LYS:HB2	1:F:389:LYS:NZ	2.34	0.42
1:A:406:PHE:O	1:A:421:CYS:HB2	2.19	0.42
1:A:412:THR:HB	1:B:108:HIS:CD2	2.53	0.42
1:B:339:LYS:HD3	1:B:367:TYR:CE2	2.54	0.42
1:C:156:ARG:HG3	1:C:156:ARG:HH11	1.83	0.42
1:C:176:TYR:HB3	1:C:267:LEU:HD21	2.02	0.42
1:C:186:LEU:HA	1:C:187:PRO:HD3	1.83	0.42
1:D:406:PHE:CD1	1:D:406:PHE:N	2.88	0.42
1:F:333:GLY:O	1:F:336:LEU:HB2	2.20	0.42
1:F:456:LEU:C	1:F:458:CYS:N	2.77	0.42
1:F:459:GLY:O	1:F:460:LEU:C	2.62	0.42
1:A:224:LEU:O	1:A:225:LEU:C	2.62	0.42
1:A:225:LEU:HB3	1:A:228:PHE:CD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ASN:O	1:B:419:ASN:C	2.61	0.42
1:B:449:THR:O	1:B:450:GLN:C	2.62	0.42
1:C:96:HIS:CE1	1:C:212:ILE:HD11	2.54	0.42
1:C:333:GLY:O	1:C:336:LEU:HB2	2.18	0.42
1:C:371:PRO:HB3	1:C:453:ALA:HB2	2.01	0.42
1:D:256:VAL:HG13	1:D:256:VAL:O	2.19	0.42
1:E:84:ARG:NH2	1:E:91:GLU:C	2.77	0.42
1:E:423:ALA:HB1	1:E:479:PHE:CE1	2.54	0.42
1:E:456:LEU:C	1:E:458:CYS:N	2.76	0.42
1:F:229:ASP:OD1	1:F:231:ASP:HB3	2.20	0.42
1:F:488:SER:C	1:F:490:ALA:N	2.76	0.42
1:A:142:ALA:HB3	1:A:152:TYR:HE1	1.85	0.42
1:A:212:ILE:O	1:A:212:ILE:HG23	2.18	0.42
1:A:459:GLY:O	1:A:460:LEU:C	2.62	0.42
1:B:229:ASP:OD1	1:B:231:ASP:HB3	2.19	0.42
1:B:337:GLU:O	1:B:339:LYS:HG2	2.20	0.42
1:C:188:TYR:CG	1:C:263:THR:HB	2.54	0.42
1:C:255:LYS:HE3	1:C:257:GLU:CD	2.44	0.42
1:D:158:LEU:HD11	1:D:332:ILE:HB	2.01	0.42
1:D:263:THR:O	1:D:265:GLY:N	2.53	0.42
1:E:266:ARG:NH1	1:E:266:ARG:HB3	2.34	0.42
1:E:277:GLU:O	1:E:278:GLU:O	2.38	0.42
1:F:142:ALA:HB3	1:F:152:TYR:HE1	1.85	0.42
1:F:293:ARG:CZ	2:F:600:FAD:HM81	2.50	0.42
1:A:194:LEU:HB2	1:A:284:TYR:CD1	2.55	0.42
1:A:389:LYS:NZ	1:A:389:LYS:HB2	2.34	0.42
1:A:391:VAL:HG12	1:A:399:ILE:HD11	2.01	0.42
1:B:142:ALA:HB3	1:B:152:TYR:HE1	1.85	0.42
1:B:212:ILE:HA	1:B:212:ILE:HD12	1.76	0.42
1:B:392:GLU:O	1:B:392:GLU:HG2	2.18	0.42
1:C:30:GLU:HG3	1:C:351:ARG:HA	2.01	0.42
1:C:123:LYS:O	1:C:124:LYS:CB	2.62	0.42
1:C:301:GLY:HA2	1:C:303:GLU:OE2	2.20	0.42
1:D:77:GLY:HA2	1:D:80:LEU:HD12	2.00	0.42
1:D:225:LEU:HB3	1:D:228:PHE:HD2	1.85	0.42
1:E:69:LEU:O	1:E:72:GLN:HB3	2.19	0.42
1:E:142:ALA:HB3	1:E:152:TYR:HE1	1.85	0.42
1:E:344:PRO:HD3	2:E:600:FAD:O2	2.19	0.42
1:E:449:THR:O	1:E:450:GLN:C	2.62	0.42
1:F:80:LEU:O	1:F:83:SER:OG	2.35	0.42
4:F:700:MPD:HM2	4:F:700:MPD:H4	1.89	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ASP:HB2	1:A:153:SER:O	2.20	0.42
1:A:29:LYS:HD2	1:A:123:LYS:HZ2	1.85	0.42
1:A:75:LEU:HB3	4:B:700:MPD:H53	2.02	0.42
1:A:273:SER:HG	1:A:275:ASN:H	1.65	0.42
1:A:411:TRP:C	1:A:414:PRO:HD2	2.45	0.42
1:B:32:ALA:C	1:B:34:TYR:N	2.77	0.42
1:B:219:MET:SD	1:B:253:PRO:HD3	2.60	0.42
1:B:409:LEU:C	1:B:411:TRP:H	2.28	0.42
1:C:41:LEU:HD23	1:C:128:GLU:HB3	2.00	0.42
1:D:142:ALA:HB3	1:D:152:TYR:HE1	1.85	0.42
1:E:76:LEU:CD2	1:F:86:TYR:CD2	3.03	0.42
1:E:251:PHE:CD2	1:E:272:GLN:C	2.97	0.42
1:E:373:THR:HG21	1:E:446:GLY:CA	2.49	0.42
1:E:391:VAL:C	1:E:393:LYS:H	2.27	0.42
1:A:29:LYS:HB2	1:A:29:LYS:HZ2	1.81	0.42
1:A:98:TRP:NE1	1:A:102:ILE:HG13	2.34	0.42
1:A:180:SER:HA	1:A:288:MET:HE3	2.01	0.42
1:C:55:LEU:HD22	1:C:56:GLY:N	2.35	0.42
1:C:340:VAL:HG22	1:C:345:VAL:HG11	2.01	0.42
1:D:405:TYR:CD1	1:D:492:ILE:HG13	2.55	0.42
1:F:161:THR:O	2:F:600:FAD:H8A	2.20	0.42
1:F:164:ARG:O	1:F:293:ARG:HB3	2.19	0.42
1:F:209:LEU:O	1:F:212:ILE:HG22	2.19	0.42
1:A:58:THR:O	1:A:63:GLY:N	2.52	0.42
1:A:410:GLU:O	1:A:414:PRO:HG2	2.20	0.42
1:A:492:ILE:C	1:A:494:GLN:H	2.27	0.42
1:B:38:VAL:CG2	1:B:39:MET:N	2.83	0.42
1:B:163:GLU:OE1	1:B:334:ASP:HB3	2.19	0.42
1:B:309:ILE:O	1:B:311:GLU:N	2.53	0.42
1:C:17:ILE:HD12	1:C:28:ALA:HB2	2.02	0.42
1:C:68:LYS:NZ	1:D:410:GLU:OE2	2.53	0.42
1:C:456:LEU:C	1:C:458:CYS:N	2.78	0.42
1:D:191:GLY:O	1:D:193:THR:CG2	2.67	0.42
1:E:98:TRP:HB3	1:E:189:CYS:HB2	2.02	0.42
1:A:48:PRO:HG2	1:A:167:TYR:CZ	2.56	0.41
1:A:84:ARG:HD2	1:A:90:VAL:O	2.20	0.41
1:A:114:TRP:O	1:A:115:GLY:C	2.60	0.41
1:A:477:GLU:HA	1:B:450:GLN:NE2	2.35	0.41
1:D:376:THR:O	1:D:377:PRO:C	2.62	0.41
1:E:188:TYR:HD2	1:E:264:PRO:HG3	1.85	0.41
1:F:207:GLY:HA2	1:F:245:ILE:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:400:GLU:OE2	1:F:400:GLU:HA	2.20	0.41
1:F:410:GLU:O	1:F:414:PRO:HG2	2.20	0.41
1:A:402:TYR:CD2	1:A:485:THR:HG22	2.55	0.41
1:B:298:ARG:H	1:B:298:ARG:HG2	1.50	0.41
1:D:69:LEU:O	1:D:72:GLN:HB3	2.20	0.41
1:D:391:VAL:HG23	1:D:392:GLU:N	2.34	0.41
1:E:55:LEU:HD23	1:E:127:TYR:CZ	2.55	0.41
1:E:110:GLY:O	1:E:111:SER:C	2.63	0.41
1:F:36:LYS:O	1:F:38:VAL:HG13	2.20	0.41
1:F:167:TYR:CE2	1:F:174:LYS:HG2	2.55	0.41
1:F:397:GLU:HA	1:F:487:ARG:NH2	2.33	0.41
1:A:48:PRO:HB2	1:A:49:LEU:HD22	2.01	0.41
1:A:456:LEU:C	1:A:458:CYS:N	2.78	0.41
1:B:189:CYS:HA	1:B:190:PRO:HD3	1.93	0.41
1:B:225:LEU:HB3	1:B:228:PHE:CD2	2.55	0.41
1:C:236:ILE:HD11	1:C:380:TYR:HB2	2.02	0.41
1:C:319:THR:C	1:C:321:GLU:H	2.28	0.41
1:C:413:ILE:N	1:C:414:PRO:CD	2.83	0.41
1:D:408:PRO:O	1:D:411:TRP:N	2.39	0.41
1:E:333:GLY:O	1:E:336:LEU:HB2	2.20	0.41
1:F:61:ASN:HA	1:F:109:ILE:HD13	2.02	0.41
1:A:70:MET:HE3	1:A:184:PHE:HD1	1.85	0.41
1:A:192:LYS:HB3	1:A:285:ASN:HD22	1.84	0.41
1:A:309:ILE:O	1:A:311:GLU:N	2.53	0.41
1:A:449:THR:O	1:A:450:GLN:C	2.62	0.41
1:A:471:ILE:N	1:B:450:GLN:HE22	2.18	0.41
1:B:108:HIS:CE1	1:B:112:LEU:HD11	2.55	0.41
1:B:456:LEU:C	1:B:458:CYS:N	2.78	0.41
1:D:105:VAL:C	1:D:107:ASN:N	2.76	0.41
1:D:374:VAL:CG1	1:D:376:THR:HG23	2.51	0.41
1:F:191:GLY:O	1:F:193:THR:CG2	2.67	0.41
1:F:260:GLU:H	1:F:266:ARG:HB2	1.85	0.41
1:A:348:GLN:HG3	1:B:469:ILE:CD1	2.50	0.41
1:A:494:GLN:HE21	1:A:494:GLN:HB3	1.63	0.41
1:B:267:LEU:HD23	1:B:287:VAL:CG2	2.50	0.41
1:D:273:SER:CB	1:D:276:SER:HB3	2.51	0.41
1:E:64:CYS:O	1:E:67:LYS:HB3	2.19	0.41
1:E:286:THR:HG22	1:E:287:VAL:N	2.34	0.41
1:F:69:LEU:O	1:F:72:GLN:HB3	2.19	0.41
1:F:391:VAL:HG23	1:F:392:GLU:N	2.34	0.41
1:A:69:LEU:CD1	1:A:105:VAL:HG13	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:TYR:CD2	1:A:413:ILE:HD11	2.55	0.41
1:B:158:LEU:HD11	1:B:332:ILE:HB	2.02	0.41
1:B:258:GLN:O	1:B:258:GLN:HG2	2.21	0.41
1:C:229:ASP:OD1	1:C:231:ASP:HB3	2.21	0.41
1:C:267:LEU:HD13	1:C:285:ASN:O	2.21	0.41
1:D:207:GLY:HA2	1:D:245:ILE:HD11	2.03	0.41
1:D:413:ILE:C	1:D:415:SER:N	2.77	0.41
1:E:208:PHE:CD1	1:E:208:PHE:C	2.99	0.41
1:F:263:THR:CB	1:F:264:PRO:CD	2.98	0.41
1:A:86:TYR:HE2	1:A:414:PRO:CG	2.29	0.41
1:A:94:VAL:HG13	1:B:89:LYS:O	2.20	0.41
1:A:392:GLU:O	1:A:392:GLU:HG2	2.21	0.41
1:A:440:VAL:HG13	1:A:440:VAL:O	2.20	0.41
1:C:215:ASP:CG	1:C:246:LYS:HZ1	2.27	0.41
1:D:272:GLN:HA	1:D:279:ILE:HA	2.02	0.41
1:E:432:ASN:HD22	1:E:463:LYS:HZ3	1.66	0.41
1:A:318:VAL:CG1	1:A:322:GLU:HA	2.51	0.41
1:A:409:LEU:HD12	1:A:409:LEU:O	2.21	0.41
1:B:49:LEU:N	1:B:49:LEU:CD2	2.84	0.41
1:B:472:HIS:HA	1:B:473:PRO:HA	1.92	0.41
1:D:156:ARG:HD3	1:D:330:TYR:HE2	1.86	0.41
1:D:292:GLY:HA2	3:D:601:NAP:PA	2.61	0.41
1:E:236:ILE:HD11	1:E:380:TYR:HB2	2.03	0.41
1:E:376:THR:O	1:E:377:PRO:C	2.63	0.41
1:F:47:THR:O	1:F:49:LEU:N	2.54	0.41
1:F:251:PHE:CE2	1:F:280:ILE:HG23	2.56	0.41
1:F:438:PHE:CE2	1:F:479:PHE:CE1	3.09	0.41
1:F:485:THR:O	1:F:488:SER:O	2.39	0.41
1:A:13:TYR:O	1:A:154:ALA:HA	2.21	0.41
1:A:259:ILE:CD1	1:A:268:ARG:HB2	2.31	0.41
1:A:319:THR:C	1:A:321:GLU:H	2.29	0.41
1:A:385:LEU:HD22	1:A:389:LYS:CG	2.51	0.41
1:A:446:GLY:CA	1:B:474:VAL:HG21	2.50	0.41
1:B:255:LYS:HG2	1:B:256:VAL:N	2.35	0.41
1:B:318:VAL:CG1	1:B:322:GLU:HA	2.51	0.41
1:C:56:GLY:O	1:C:60:VAL:HG23	2.21	0.41
1:C:209:LEU:HD23	1:C:209:LEU:HA	1.94	0.41
1:C:236:ILE:HD11	1:C:380:TYR:CB	2.50	0.41
1:C:397:GLU:HA	1:C:487:ARG:HH22	1.86	0.41
1:C:440:VAL:O	1:C:440:VAL:HG13	2.21	0.41
1:D:103:GLU:O	1:D:107:ASN:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:ASP:CG	1:D:246:LYS:HZ1	2.29	0.41
1:D:236:ILE:HD11	1:D:380:TYR:CB	2.51	0.41
1:D:309:ILE:O	1:D:311:GLU:N	2.54	0.41
1:D:340:VAL:O	1:D:345:VAL:HG21	2.20	0.41
1:D:396:GLU:CD	1:D:396:GLU:C	2.89	0.41
1:D:440:VAL:HB	1:D:479:PHE:HZ	1.85	0.41
1:E:12:ASP:OD1	1:E:153:SER:OG	2.37	0.41
1:F:23:GLY:O	1:F:24:GLY:C	2.64	0.41
1:F:43:PHE:HE2	1:F:45:THR:HA	1.86	0.41
1:F:407:TRP:CG	1:F:418:ASN:HD22	2.38	0.41
1:F:476:ALA:C	1:F:478:VAL:H	2.29	0.41
1:A:55:LEU:HD23	1:A:56:GLY:H	1.86	0.41
1:A:156:ARG:HG3	1:A:156:ARG:NH1	2.35	0.41
1:A:471:ILE:HD13	1:B:373:THR:HG22	2.01	0.41
1:B:172:GLY:CA	1:B:175:GLU:HG2	2.51	0.41
1:C:391:VAL:C	1:C:393:LYS:H	2.29	0.41
1:D:114:TRP:O	1:D:117:ARG:HB2	2.21	0.41
1:D:405:TYR:CE1	1:D:492:ILE:HG13	2.56	0.41
1:E:16:ILE:HG12	1:E:39:MET:HE2	2.02	0.41
1:E:123:LYS:NZ	1:E:123:LYS:CB	2.83	0.41
1:E:456:LEU:C	1:E:458:CYS:H	2.28	0.41
1:F:200:TYR:C	1:F:200:TYR:CD2	2.99	0.41
1:B:250:GLN:O	1:B:273:SER:HA	2.21	0.40
1:C:186:LEU:HA	1:C:186:LEU:HD23	1.95	0.40
1:D:137:PRO:HA	1:D:328:TYR:OH	2.21	0.40
1:D:373:THR:HG21	1:D:446:GLY:CA	2.52	0.40
1:F:49:LEU:HD23	1:F:182:ASP:OD2	2.20	0.40
1:F:133:GLN:O	1:F:140:ILE:HG13	2.21	0.40
1:F:373:THR:HG21	1:F:446:GLY:CA	2.52	0.40
1:C:158:LEU:HD11	1:C:332:ILE:HB	2.03	0.40
1:C:189:CYS:HA	1:C:190:PRO:HD3	1.91	0.40
1:C:255:LYS:O	1:C:270:VAL:N	2.39	0.40
1:E:76:LEU:CD1	4:F:700:MPD:HM3	2.50	0.40
1:E:340:VAL:HG13	1:E:340:VAL:O	2.22	0.40
1:E:342:LEU:O	1:E:345:VAL:HG22	2.21	0.40
1:E:406:PHE:O	1:E:421:CYS:HB2	2.22	0.40
1:A:97:ASP:CG	1:A:100:ARG:HB2	2.46	0.40
1:B:191:GLY:O	1:B:193:THR:CG2	2.67	0.40
1:B:413:ILE:HG12	1:B:414:PRO:HD3	2.02	0.40
1:C:203:LEU:HD22	1:C:240:MET:SD	2.61	0.40
1:C:318:VAL:HG22	1:C:322:GLU:C	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ARG:HG2	1:C:361:SER:O	2.22	0.40
1:C:374:VAL:HG12	1:C:376:THR:HG23	2.03	0.40
1:D:176:TYR:CE1	1:D:258:GLN:HB2	2.56	0.40
1:D:391:VAL:C	1:D:393:LYS:H	2.29	0.40
1:F:112:LEU:O	1:F:113:ASN:C	2.64	0.40
1:F:203:LEU:HD23	1:F:203:LEU:HA	1.93	0.40
1:F:270:VAL:HA	1:F:280:ILE:O	2.21	0.40
1:F:385:LEU:HD22	1:F:389:LYS:CG	2.51	0.40
1:F:392:GLU:HG2	1:F:392:GLU:O	2.20	0.40
1:A:55:LEU:CD2	1:A:56:GLY:N	2.85	0.40
1:A:80:LEU:HD21	1:B:90:VAL:HG21	2.03	0.40
1:B:212:ILE:O	1:B:212:ILE:HG23	2.20	0.40
1:B:342:LEU:O	1:B:345:VAL:HG22	2.22	0.40
1:C:107:ASN:O	1:C:108:HIS:C	2.62	0.40
1:C:399:ILE:O	1:C:399:ILE:CD1	2.68	0.40
1:C:449:THR:O	1:C:450:GLN:C	2.62	0.40
1:D:189:CYS:HA	1:D:190:PRO:HD3	1.91	0.40
1:D:263:THR:HB	1:D:264:PRO:HD3	2.03	0.40
1:D:476:ALA:C	1:D:478:VAL:H	2.29	0.40
1:F:63:GLY:O	1:F:66:PRO:HG2	2.21	0.40
1:F:332:ILE:HD13	1:F:353:LEU:HD22	2.04	0.40
1:F:391:VAL:C	1:F:393:LYS:H	2.29	0.40
1:A:100:ARG:HG3	1:A:100:ARG:NH1	2.37	0.40
1:A:331:ALA:O	1:A:332:ILE:HD12	2.21	0.40
1:B:271:ALA:O	1:B:279:ILE:HG23	2.22	0.40
1:C:156:ARG:HG3	1:C:156:ARG:NH1	2.36	0.40
1:D:9:LYS:C	1:D:11:TYR:H	2.30	0.40
1:D:23:GLY:O	1:D:24:GLY:C	2.64	0.40
1:D:67:LYS:HD2	1:D:68:LYS:N	2.36	0.40
4:D:700:MPD:O4	4:D:700:MPD:C1	2.69	0.40
1:E:391:VAL:C	1:E:393:LYS:N	2.80	0.40
1:E:391:VAL:HG23	1:E:392:GLU:N	2.36	0.40
1:F:164:ARG:HA	1:F:164:ARG:HD2	1.89	0.40
1:F:376:THR:O	1:F:377:PRO:C	2.64	0.40
1:F:409:LEU:O	1:F:409:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/519 (93%)	426 (88%)	51 (10%)	8 (2%)	7	27
1	B	485/519 (93%)	419 (86%)	60 (12%)	6 (1%)	10	34
1	C	430/519 (83%)	373 (87%)	47 (11%)	10 (2%)	5	18
1	D	489/519 (94%)	424 (87%)	51 (10%)	14 (3%)	3	13
1	E	488/519 (94%)	421 (86%)	54 (11%)	13 (3%)	4	15
1	F	484/519 (93%)	417 (86%)	55 (11%)	12 (2%)	4	16
All	All	2861/3114 (92%)	2480 (87%)	318 (11%)	63 (2%)	5	19

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	GLY
1	B	263	THR
1	C	263	THR
1	C	276	SER
1	C	278	GLU
1	C	417	ASP
1	D	263	THR
1	D	497	CYS
1	E	261	ALA
1	E	262	GLY
1	E	263	THR
1	E	278	GLU
1	F	58	THR
1	F	59	CYS
1	F	263	THR
1	A	311	GLU
1	B	311	GLU
1	C	260	GLU
1	C	311	GLU
1	D	260	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	273	SER
1	D	311	GLU
1	D	489	GLY
1	D	495	ALA
1	E	115	GLY
1	E	311	GLU
1	E	341	GLU
1	E	488	SER
1	E	496	GLY
1	F	32	ALA
1	F	259	ILE
1	F	311	GLU
1	F	417	ASP
1	F	492	ILE
1	A	33	GLN
1	A	83	SER
1	A	278	GLU
1	B	476	ALA
1	D	91	GLU
1	D	255	LYS
1	D	494	GLN
1	D	496	GLY
1	E	64	CYS
1	E	114	TRP
1	A	404	SER
1	B	93	THR
1	C	490	ALA
1	D	409	LEU
1	F	275	ASN
1	A	263	THR
1	C	273	SER
1	C	275	ASN
1	D	417	ASP
1	F	31	ALA
1	B	259	ILE
1	E	255	LYS
1	F	35	GLY
1	A	473	PRO
1	B	473	PRO
1	C	473	PRO
1	D	473	PRO
1	F	473	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	473	PRO

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	399/426 (94%)	365 (92%)	34 (8%)	10	31
1	B	400/426 (94%)	366 (92%)	34 (8%)	10	31
1	C	401/426 (94%)	363 (90%)	38 (10%)	8	26
1	D	402/426 (94%)	368 (92%)	34 (8%)	10	31
1	E	401/426 (94%)	367 (92%)	34 (8%)	10	31
1	F	399/426 (94%)	366 (92%)	33 (8%)	10	32
All	All	2402/2556 (94%)	2195 (91%)	207 (9%)	10	31

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	38	VAL
1	A	55	LEU
1	A	64	CYS
1	A	76	LEU
1	A	91	GLU
1	A	111	SER
1	A	123	LYS
1	A	133	GLN
1	A	139	ARG
1	A	144	ASN
1	A	151	ILE
1	A	175	GLU
1	A	183	LEU
1	A	193	THR
1	A	212	ILE
1	A	255	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	256	VAL
1	A	263	THR
1	A	267	LEU
1	A	298	ARG
1	A	303	GLU
1	A	318	VAL
1	A	332	ILE
1	A	336	LEU
1	A	340	VAL
1	A	345	VAL
1	A	373	THR
1	A	389	LYS
1	A	404	SER
1	A	409	LEU
1	A	413	ILE
1	A	493	LEU
1	A	494	GLN
1	B	14	ASP
1	B	38	VAL
1	B	40	VAL
1	B	55	LEU
1	B	64	CYS
1	B	76	LEU
1	B	90	VAL
1	B	93	THR
1	B	109	ILE
1	B	121	ARG
1	B	133	GLN
1	B	139	ARG
1	B	144	ASN
1	B	151	ILE
1	B	175	GLU
1	B	183	LEU
1	B	193	THR
1	B	212	ILE
1	B	252	VAL
1	B	268	ARG
1	B	277	GLU
1	B	280	ILE
1	B	298	ARG
1	B	303	GLU
1	B	318	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	332	ILE
1	B	336	LEU
1	B	345	VAL
1	B	373	THR
1	B	389	LYS
1	B	413	ILE
1	B	416	ARG
1	B	474	VAL
1	B	483	SER
1	C	37	LYS
1	C	38	VAL
1	C	45	THR
1	C	51	THR
1	C	55	LEU
1	C	64	CYS
1	C	76	LEU
1	C	83	SER
1	C	111	SER
1	C	118	VAL
1	C	133	GLN
1	C	139	ARG
1	C	144	ASN
1	C	151	ILE
1	C	175	GLU
1	C	183	LEU
1	C	193	THR
1	C	212	ILE
1	C	277	GLU
1	C	279	ILE
1	C	283	GLU
1	C	298	ARG
1	C	303	GLU
1	C	318	VAL
1	C	332	ILE
1	C	336	LEU
1	C	340	VAL
1	C	345	VAL
1	C	373	THR
1	C	389	LYS
1	C	408	PRO
1	C	413	ILE
1	C	417	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	474	VAL
1	C	475	CYS
1	C	483	SER
1	C	494	GLN
1	C	498	CYS
1	D	38	VAL
1	D	49	LEU
1	D	55	LEU
1	D	64	CYS
1	D	76	LEU
1	D	83	SER
1	D	90	VAL
1	D	91	GLU
1	D	111	SER
1	D	133	GLN
1	D	139	ARG
1	D	144	ASN
1	D	151	ILE
1	D	175	GLU
1	D	183	LEU
1	D	193	THR
1	D	212	ILE
1	D	254	ILE
1	D	267	LEU
1	D	270	VAL
1	D	291	ILE
1	D	298	ARG
1	D	303	GLU
1	D	318	VAL
1	D	332	ILE
1	D	336	LEU
1	D	340	VAL
1	D	345	VAL
1	D	373	THR
1	D	389	LYS
1	D	406	PHE
1	D	413	ILE
1	D	487	ARG
1	D	497	CYS
1	E	45	THR
1	E	49	LEU
1	E	52	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	64	CYS
1	E	76	LEU
1	E	84	ARG
1	E	92	GLU
1	E	93	THR
1	E	94	VAL
1	E	95	LYS
1	E	123	LYS
1	E	133	GLN
1	E	139	ARG
1	E	144	ASN
1	E	151	ILE
1	E	175	GLU
1	E	183	LEU
1	E	193	THR
1	E	212	ILE
1	E	254	ILE
1	E	257	GLU
1	E	267	LEU
1	E	298	ARG
1	E	303	GLU
1	E	318	VAL
1	E	332	ILE
1	E	336	LEU
1	E	345	VAL
1	E	373	THR
1	E	389	LYS
1	E	413	ILE
1	E	416	ARG
1	E	493	LEU
1	E	498	CYS
1	F	11	TYR
1	F	30	GLU
1	F	38	VAL
1	F	49	LEU
1	F	52	ARG
1	F	64	CYS
1	F	76	LEU
1	F	91	GLU
1	F	102	ILE
1	F	107	ASN
1	F	133	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	139	ARG
1	F	144	ASN
1	F	151	ILE
1	F	175	GLU
1	F	183	LEU
1	F	193	THR
1	F	212	ILE
1	F	269	VAL
1	F	281	GLU
1	F	298	ARG
1	F	303	GLU
1	F	318	VAL
1	F	332	ILE
1	F	336	LEU
1	F	345	VAL
1	F	373	THR
1	F	389	LYS
1	F	408	PRO
1	F	413	ILE
1	F	416	ARG
1	F	420	LYS
1	F	493	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	113	ASN
1	A	129	ASN
1	A	133	GLN
1	A	138	HIS
1	A	145	ASN
1	A	258	GLN
1	A	285	ASN
1	A	325	ASN
1	A	348	GLN
1	A	418	ASN
1	A	428	ASN
1	A	432	ASN
1	A	439	HIS
1	A	450	GLN
1	A	494	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	78	GLN
1	B	85	ASN
1	B	96	HIS
1	B	108	HIS
1	B	129	ASN
1	B	133	GLN
1	B	145	ASN
1	B	258	GLN
1	B	285	ASN
1	B	325	ASN
1	B	418	ASN
1	B	419	ASN
1	B	428	ASN
1	B	432	ASN
1	B	439	HIS
1	B	450	GLN
1	B	472	HIS
1	B	494	GLN
1	C	81	GLN
1	C	96	HIS
1	C	106	GLN
1	C	107	ASN
1	C	113	ASN
1	C	129	ASN
1	C	133	GLN
1	C	258	GLN
1	C	285	ASN
1	C	325	ASN
1	C	418	ASN
1	C	419	ASN
1	C	428	ASN
1	C	432	ASN
1	C	439	HIS
1	C	450	GLN
1	C	494	GLN
1	D	33	GLN
1	D	96	HIS
1	D	108	HIS
1	D	113	ASN
1	D	129	ASN
1	D	133	GLN
1	D	138	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	145	ASN
1	D	258	GLN
1	D	275	ASN
1	D	285	ASN
1	D	325	ASN
1	D	348	GLN
1	D	418	ASN
1	D	428	ASN
1	D	432	ASN
1	D	439	HIS
1	D	450	GLN
1	E	85	ASN
1	E	96	HIS
1	E	106	GLN
1	E	107	ASN
1	E	113	ASN
1	E	133	GLN
1	E	138	HIS
1	E	258	GLN
1	E	285	ASN
1	E	325	ASN
1	E	418	ASN
1	E	428	ASN
1	E	432	ASN
1	E	439	HIS
1	E	444	ASN
1	E	450	GLN
1	F	61	ASN
1	F	96	HIS
1	F	106	GLN
1	F	129	ASN
1	F	133	GLN
1	F	138	HIS
1	F	145	ASN
1	F	258	GLN
1	F	272	GLN
1	F	275	ASN
1	F	285	ASN
1	F	325	ASN
1	F	418	ASN
1	F	419	ASN
1	F	428	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	432	ASN
1	F	439	HIS
1	F	450	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAP	A	601	-	50,52,52	1.78	8 (16%)	71,80,80	2.74	12 (16%)
4	MPD	F	700	-	7,7,7	0.41	0	9,10,10	0.42	0
4	MPD	A	701	-	7,7,7	0.33	0	9,10,10	0.41	0
2	FAD	F	600	-	58,58,58	1.50	7 (12%)	85,89,89	1.94	8 (9%)
2	FAD	C	600	-	58,58,58	1.86	10 (17%)	85,89,89	1.81	9 (10%)
3	NAP	C	601	-	50,52,52	1.68	7 (14%)	71,80,80	2.69	11 (15%)
4	MPD	B	701	-	7,7,7	0.37	0	9,10,10	0.33	0
3	NAP	D	601	-	50,52,52	1.79	11 (22%)	71,80,80	1.13	4 (5%)
3	NAP	B	601	-	50,52,52	1.70	7 (14%)	71,80,80	2.49	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MPD	B	700	-	7,7,7	0.35	0	9,10,10	0.41	0
4	MPD	D	700	-	7,7,7	0.36	0	9,10,10	0.25	0
2	FAD	E	600	-	58,58,58	1.61	8 (13%)	85,89,89	1.76	7 (8%)
3	NAP	E	601	-	50,52,52	1.47	7 (14%)	71,80,80	1.12	7 (9%)
2	FAD	D	600	-	58,58,58	1.92	12 (20%)	85,89,89	1.80	9 (10%)
3	NAP	F	601	-	50,52,52	1.49	8 (16%)	71,80,80	1.27	6 (8%)
2	FAD	B	600	-	58,58,58	1.70	10 (17%)	85,89,89	1.79	8 (9%)
2	FAD	A	600	-	58,58,58	1.70	9 (15%)	85,89,89	1.83	7 (8%)

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
3	NAP	A	601	-	1/1/12/12	6/35/67/67	0/5/5/5
4	MPD	F	700	-	-	1/5/5/5	-
4	MPD	A	701	-	-	0/5/5/5	-
2	FAD	F	600	-	-	5/34/50/50	0/6/6/6
2	FAD	C	600	-	-	8/34/50/50	0/6/6/6
3	NAP	C	601	-	1/1/12/12	14/35/67/67	0/5/5/5
4	MPD	B	701	-	-	0/5/5/5	-
3	NAP	D	601	-	-	12/35/67/67	0/5/5/5
3	NAP	B	601	-	1/1/12/12	6/35/67/67	0/5/5/5
4	MPD	B	700	-	-	1/5/5/5	-
4	MPD	D	700	-	-	1/5/5/5	-
2	FAD	E	600	-	-	5/34/50/50	0/6/6/6
3	NAP	E	601	-	-	10/35/67/67	0/5/5/5
2	FAD	D	600	-	-	8/34/50/50	0/6/6/6
3	NAP	F	601	-	-	15/35/67/67	0/5/5/5
2	FAD	B	600	-	-	9/34/50/50	0/6/6/6
2	FAD	A	600	-	-	9/34/50/50	0/6/6/6

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	FAD	P-O3P	6.36	1.66	1.59
3	A	601	NAP	O4B-C4B	6.00	1.58	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	FAD	C4X-N5	5.99	1.43	1.30
2	C	600	FAD	P-O3P	5.90	1.65	1.59
2	C	600	FAD	C4X-N5	5.50	1.42	1.30
3	C	601	NAP	O4B-C4B	5.40	1.57	1.45
2	B	600	FAD	P-O3P	5.30	1.65	1.59
2	A	600	FAD	C4X-N5	5.29	1.42	1.30
2	A	600	FAD	P-O3P	5.20	1.65	1.59
2	E	600	FAD	C4X-N5	5.17	1.41	1.30
2	B	600	FAD	C4X-N5	4.95	1.41	1.30
3	F	601	NAP	C2N-N1N	4.94	1.40	1.35
2	C	600	FAD	C9-C8	4.86	1.46	1.39
2	C	600	FAD	PA-O3P	4.80	1.64	1.59
3	B	601	NAP	O4B-C4B	4.74	1.55	1.45
3	D	601	NAP	C2N-N1N	4.68	1.40	1.35
2	F	600	FAD	C4X-N5	4.61	1.40	1.30
2	F	600	FAD	C9-C8	4.52	1.45	1.39
2	A	600	FAD	PA-O3P	4.29	1.64	1.59
2	B	600	FAD	C9-C8	4.21	1.45	1.39
3	D	601	NAP	C4N-C3N	4.18	1.45	1.39
3	A	601	NAP	C2N-N1N	4.08	1.39	1.35
3	C	601	NAP	C4N-C3N	4.01	1.45	1.39
3	A	601	NAP	C6N-N1N	3.97	1.44	1.35
2	E	600	FAD	P-O3P	3.97	1.63	1.59
3	C	601	NAP	C6N-N1N	3.95	1.44	1.35
3	B	601	NAP	C2B-C1B	-3.95	1.43	1.53
2	E	600	FAD	C9-C8	3.94	1.45	1.39
3	F	601	NAP	C6N-N1N	3.93	1.44	1.35
3	B	601	NAP	C4N-C3N	3.90	1.45	1.39
2	D	600	FAD	PA-O3P	3.89	1.63	1.59
2	D	600	FAD	C9-C8	3.89	1.44	1.39
2	C	600	FAD	C9A-N10	3.81	1.47	1.41
3	A	601	NAP	C4N-C3N	3.78	1.45	1.39
3	B	601	NAP	C6N-N1N	3.77	1.43	1.35
2	D	600	FAD	O4B-C1B	3.75	1.50	1.42
3	C	601	NAP	C2N-N1N	3.74	1.39	1.35
2	B	600	FAD	C4A-N3A	3.73	1.41	1.34
3	D	601	NAP	O4B-C4B	3.73	1.53	1.45
3	F	601	NAP	C4N-C3N	3.70	1.45	1.39
3	D	601	NAP	C6N-N1N	3.69	1.43	1.35
3	C	601	NAP	P2B-O2B	3.61	1.65	1.59
3	B	601	NAP	C2N-N1N	3.59	1.38	1.35
2	D	600	FAD	C4A-N3A	3.58	1.41	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	601	NAP	C6N-N1N	3.56	1.43	1.35
3	E	601	NAP	C4N-C3N	3.52	1.44	1.39
3	E	601	NAP	O4B-C4B	3.51	1.52	1.45
2	D	600	FAD	C9A-C5X	3.49	1.46	1.41
2	A	600	FAD	C9-C8	3.48	1.44	1.39
2	C	600	FAD	C6-C5X	3.44	1.45	1.40
2	D	600	FAD	C9A-N10	3.39	1.47	1.41
3	E	601	NAP	C2N-N1N	3.39	1.38	1.35
2	C	600	FAD	C4A-N3A	3.30	1.40	1.34
2	E	600	FAD	C10-N1	3.28	1.39	1.33
3	D	601	NAP	C3N-C7N	3.27	1.55	1.50
2	A	600	FAD	C4A-N3A	3.24	1.40	1.34
2	B	600	FAD	C9A-C5X	3.23	1.46	1.41
3	A	601	NAP	C3B-C2B	-3.22	1.46	1.53
3	D	601	NAP	O4B-C1B	3.19	1.49	1.42
2	E	600	FAD	C9A-C5X	3.18	1.46	1.41
2	E	600	FAD	C4A-N3A	3.17	1.40	1.34
2	F	600	FAD	C4A-N3A	3.15	1.40	1.34
3	D	601	NAP	C5A-N7A	-3.10	1.33	1.39
3	A	601	NAP	P2B-O2B	3.09	1.64	1.59
2	F	600	FAD	P-O3P	3.09	1.62	1.59
3	C	601	NAP	C4A-N3A	3.03	1.40	1.34
2	B	600	FAD	PA-O3P	3.02	1.62	1.59
2	E	600	FAD	C9A-N10	2.99	1.46	1.41
3	F	601	NAP	C4A-N3A	2.97	1.40	1.34
2	F	600	FAD	C9A-N10	2.80	1.46	1.41
3	B	601	NAP	C4A-N3A	2.73	1.39	1.34
3	D	601	NAP	C4A-N3A	2.72	1.39	1.34
2	B	600	FAD	C10-N1	2.70	1.38	1.33
2	F	600	FAD	C10-N1	2.67	1.38	1.33
2	F	600	FAD	C9A-C5X	2.65	1.45	1.41
3	A	601	NAP	C4A-N3A	2.61	1.39	1.34
3	E	601	NAP	O4B-C1B	2.61	1.48	1.42
3	F	601	NAP	P2B-O2B	2.58	1.64	1.59
2	A	600	FAD	C9A-C5X	2.57	1.45	1.41
2	C	600	FAD	C9A-C5X	2.55	1.45	1.41
2	A	600	FAD	C6-C5X	2.55	1.43	1.40
3	B	601	NAP	C3B-C2B	-2.54	1.47	1.53
2	A	600	FAD	O4B-C1B	2.53	1.47	1.42
2	C	600	FAD	C10-N1	2.52	1.38	1.33
2	B	600	FAD	C10-N10	2.46	1.42	1.37
3	E	601	NAP	C4A-N3A	2.43	1.39	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAD	C9A-N10	2.41	1.45	1.41
3	D	601	NAP	C2A-N1A	2.34	1.38	1.33
3	C	601	NAP	C2A-N3A	2.34	1.38	1.33
3	A	601	NAP	C2B-C1B	-2.32	1.47	1.53
2	E	600	FAD	C4'-C3'	2.31	1.57	1.53
2	D	600	FAD	C6-C5X	2.28	1.43	1.40
3	E	601	NAP	C2B-C1B	-2.27	1.47	1.53
3	D	601	NAP	C2B-C1B	-2.24	1.47	1.53
3	F	601	NAP	C2A-N3A	2.14	1.37	1.33
3	D	601	NAP	C5A-C4A	2.13	1.42	1.39
3	F	601	NAP	C5A-C4A	2.13	1.42	1.39
2	B	600	FAD	C2A-N1A	2.12	1.37	1.33
2	D	600	FAD	C10-N1	2.10	1.37	1.33
2	D	600	FAD	C2A-N1A	2.09	1.37	1.33
2	C	600	FAD	C1'-N10	2.03	1.52	1.47
3	F	601	NAP	C5A-N7A	-2.03	1.35	1.39
2	A	600	FAD	C5B-C4B	2.03	1.57	1.51
2	D	600	FAD	C4'-C3'	2.00	1.56	1.53

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NAP	C5B-C4B-C3B	15.76	171.93	115.21
3	B	601	NAP	C5B-C4B-C3B	15.08	169.49	115.21
3	C	601	NAP	C5B-C4B-C3B	14.93	168.96	115.21
2	F	600	FAD	O2A-PA-O3P	-11.78	75.42	107.27
2	D	600	FAD	O2A-PA-O3P	-11.39	76.49	107.27
2	A	600	FAD	O2A-PA-O3P	-11.38	76.52	107.27
2	C	600	FAD	O2A-PA-O3P	-11.24	76.88	107.27
2	B	600	FAD	O2A-PA-O3P	-10.42	79.11	107.27
2	E	600	FAD	O2A-PA-O3P	-10.23	79.61	107.27
3	A	601	NAP	O4B-C4B-C5B	-8.84	81.03	109.33
3	B	601	NAP	O4B-C4B-C5B	-8.09	83.43	109.33
3	C	601	NAP	O4B-C4B-C5B	-8.04	83.59	109.33
2	E	600	FAD	O3P-PA-O1A	-7.59	87.89	110.70
2	F	600	FAD	O3P-PA-O1A	-7.49	88.17	110.70
2	B	600	FAD	O3P-PA-O1A	-7.39	88.47	110.70
2	C	600	FAD	O3P-PA-O1A	-7.13	89.24	110.70
3	C	601	NAP	O4B-C1B-C2B	-7.07	94.42	106.59
2	D	600	FAD	O3P-PA-O1A	-6.87	90.03	110.70
2	A	600	FAD	O3P-PA-O1A	-6.85	90.11	110.70
3	A	601	NAP	O4B-C4B-C3B	-6.45	92.35	105.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NAP	O4B-C1B-C2B	-6.32	95.71	106.59
3	C	601	NAP	C3B-C2B-C1B	-5.73	91.83	102.81
3	C	601	NAP	O4B-C4B-C3B	-5.67	93.89	105.15
3	B	601	NAP	O4B-C1B-C2B	-5.44	97.22	106.59
3	B	601	NAP	O4B-C4B-C3B	-4.87	95.49	105.15
3	A	601	NAP	C3B-C2B-C1B	-4.38	94.42	102.81
2	A	600	FAD	O2A-PA-O1A	4.28	132.34	112.44
2	C	600	FAD	O2A-PA-O1A	4.25	132.19	112.44
2	E	600	FAD	O2A-PA-O1A	4.17	131.86	112.44
2	F	600	FAD	O2A-PA-O1A	4.16	131.78	112.44
2	D	600	FAD	O2A-PA-O1A	4.14	131.72	112.44
2	F	600	FAD	O4B-C4B-C5B	4.14	122.59	109.33
3	C	601	NAP	O5B-C5B-C4B	-4.13	94.93	108.99
2	B	600	FAD	O2A-PA-O1A	4.09	131.48	112.44
3	F	601	NAP	C6N-N1N-C2N	-3.77	118.67	121.88
3	F	601	NAP	O3-PA-O1A	-3.75	99.41	110.70
3	E	601	NAP	C6N-N1N-C2N	-3.52	118.88	121.88
3	C	601	NAP	C2B-C1B-N9A	3.50	119.52	113.75
2	A	600	FAD	O5B-C5B-C4B	3.50	120.90	108.99
2	B	600	FAD	O5B-C5B-C4B	3.46	120.77	108.99
3	C	601	NAP	O2B-C2B-C1B	3.39	121.97	110.05
2	F	600	FAD	O5B-C5B-C4B	3.38	120.51	108.99
3	A	601	NAP	O5B-C5B-C4B	-3.31	97.73	108.99
3	A	601	NAP	C6N-N1N-C2N	-3.31	119.06	121.88
3	D	601	NAP	O4B-C1B-C2B	-3.21	101.07	106.59
3	E	601	NAP	O4B-C4B-C5B	-3.19	99.11	109.33
3	F	601	NAP	O4B-C1B-N9A	-3.09	102.15	108.09
2	F	600	FAD	O4B-C1B-N9A	3.07	113.98	108.09
3	C	601	NAP	C6N-N1N-C2N	-3.05	119.29	121.88
3	B	601	NAP	C3B-C2B-C1B	-3.02	97.03	102.81
3	B	601	NAP	C6N-N1N-C2N	-3.00	119.33	121.88
3	D	601	NAP	C6N-N1N-C2N	-2.92	119.39	121.88
3	A	601	NAP	O2B-C2B-C1B	2.92	120.31	110.05
2	E	600	FAD	O3P-P-O1P	-2.86	102.11	110.70
2	D	600	FAD	O5B-C5B-C4B	2.83	118.63	108.99
3	A	601	NAP	C2B-C1B-N9A	2.81	118.38	113.75
3	B	601	NAP	O5B-C5B-C4B	-2.68	99.87	108.99
3	A	601	NAP	O3-PA-O1A	-2.60	102.88	110.70
2	D	600	FAD	O3P-P-O1P	-2.56	103.00	110.70
2	D	600	FAD	C4X-C10-N10	2.56	120.15	116.48
2	B	600	FAD	C4X-C10-N10	2.53	120.11	116.48
3	F	601	NAP	O4B-C1B-C2B	-2.48	102.32	106.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	601	NAP	C2A-N1A-C6A	2.44	122.74	118.73
3	D	601	NAP	O2B-C2B-C1B	2.43	118.59	110.05
2	A	600	FAD	C4X-C10-N10	2.42	119.95	116.48
2	B	600	FAD	O3P-P-O1P	-2.42	103.41	110.70
3	B	601	NAP	O2B-C2B-C1B	2.41	118.54	110.05
2	D	600	FAD	O2B-C2B-C3B	2.40	119.51	111.82
3	B	601	NAP	O3-PA-O1A	-2.40	103.49	110.70
3	F	601	NAP	O2A-PA-O1A	2.39	123.56	112.44
3	C	601	NAP	C2A-N1A-C6A	2.38	122.64	118.73
3	A	601	NAP	C2A-N1A-C6A	2.38	122.63	118.73
2	C	600	FAD	C4X-C10-N10	2.36	119.87	116.48
2	E	600	FAD	C4A-N9A-C8A	-2.35	103.27	105.74
3	F	601	NAP	C2A-N1A-C6A	2.33	122.56	118.73
2	C	600	FAD	O4B-C1B-N9A	2.32	112.55	108.09
3	B	601	NAP	C2A-N1A-C6A	2.31	122.52	118.73
2	B	600	FAD	O2B-C2B-C3B	2.30	119.18	111.82
2	F	600	FAD	C4X-C10-N10	2.27	119.73	116.48
3	C	601	NAP	O3-PA-O1A	-2.25	103.95	110.70
2	A	600	FAD	O4B-C4B-C5B	2.22	116.45	109.33
3	A	601	NAP	N3A-C2A-N1A	-2.21	125.24	128.58
3	B	601	NAP	C2B-C1B-N9A	2.20	117.37	113.75
2	D	600	FAD	O4B-C1B-N9A	2.19	112.30	108.09
3	E	601	NAP	O4B-C1B-C2B	-2.18	102.84	106.59
3	E	601	NAP	O4B-C4B-C3B	-2.17	100.84	105.15
2	C	600	FAD	C3B-C2B-C1B	2.14	105.52	101.46
2	C	600	FAD	O2A-PA-O5B	2.14	117.25	107.57
2	C	600	FAD	O3P-P-O1P	-2.12	104.33	110.70
3	E	601	NAP	O4B-C1B-N9A	2.12	112.15	108.09
2	C	600	FAD	O2B-C2B-C3B	2.11	118.59	111.82
2	E	600	FAD	C5'-C4'-C3'	-2.11	108.24	112.22
2	F	600	FAD	C4B-O4B-C1B	-2.11	104.81	109.47
2	B	600	FAD	C5'-C4'-C3'	-2.09	108.28	112.22
3	D	601	NAP	C2A-N1A-C6A	2.07	122.14	118.73
3	E	601	NAP	C4D-O4D-C1D	2.07	111.82	109.92
2	D	600	FAD	O5'-C5'-C4'	2.06	114.85	109.36
2	E	600	FAD	C4X-C10-N10	2.05	119.41	116.48
2	A	600	FAD	O2B-C2B-C3B	2.02	118.29	111.82

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	NAP	C4B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
3	B	601	NAP	C4B
3	C	601	NAP	C4B

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C5B-O5B-PA-O2A
2	B	600	FAD	C5B-O5B-PA-O2A
2	B	600	FAD	O4B-C4B-C5B-O5B
2	C	600	FAD	C5B-O5B-PA-O2A
2	C	600	FAD	C4B-C5B-O5B-PA
2	D	600	FAD	C5B-O5B-PA-O2A
2	D	600	FAD	O4B-C4B-C5B-O5B
2	D	600	FAD	C2B-C1B-N9A-C8A
2	E	600	FAD	C5B-O5B-PA-O2A
2	E	600	FAD	C4B-C5B-O5B-PA
2	F	600	FAD	C5B-O5B-PA-O2A
3	A	601	NAP	O4D-C1D-N1N-C2N
3	A	601	NAP	O4D-C1D-N1N-C6N
3	B	601	NAP	C4D-C5D-O5D-PN
3	C	601	NAP	C5D-O5D-PN-O3
3	C	601	NAP	C2D-C1D-N1N-C6N
3	C	601	NAP	C2N-C3N-C7N-O7N
3	C	601	NAP	C2N-C3N-C7N-N7N
3	D	601	NAP	O4D-C4D-C5D-O5D
3	D	601	NAP	O4D-C1D-N1N-C2N
3	D	601	NAP	C2D-C1D-N1N-C2N
3	E	601	NAP	C5D-O5D-PN-O3
3	E	601	NAP	C5D-O5D-PN-O2N
3	E	601	NAP	O4D-C1D-N1N-C6N
3	E	601	NAP	C2N-C3N-C7N-O7N
3	E	601	NAP	C2N-C3N-C7N-N7N
3	F	601	NAP	C5D-O5D-PN-O3
3	F	601	NAP	C5D-O5D-PN-O1N
3	F	601	NAP	C5D-O5D-PN-O2N
3	F	601	NAP	O4D-C1D-N1N-C2N
3	F	601	NAP	C2D-C1D-N1N-C2N
3	F	601	NAP	C2N-C3N-C7N-O7N
3	F	601	NAP	C2N-C3N-C7N-N7N
3	E	601	NAP	C4N-C3N-C7N-O7N
3	E	601	NAP	C4N-C3N-C7N-N7N
3	C	601	NAP	C4N-C3N-C7N-O7N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	601	NAP	C4N-C3N-C7N-N7N
3	F	601	NAP	C4N-C3N-C7N-N7N
3	F	601	NAP	C4N-C3N-C7N-O7N
2	F	600	FAD	O4B-C4B-C5B-O5B
3	A	601	NAP	C3B-C4B-C5B-O5B
3	B	601	NAP	C3D-C4D-C5D-O5D
3	D	601	NAP	C3D-C4D-C5D-O5D
2	B	600	FAD	C3B-C4B-C5B-O5B
2	D	600	FAD	C3B-C4B-C5B-O5B
2	F	600	FAD	C3B-C4B-C5B-O5B
3	A	601	NAP	O4B-C4B-C5B-O5B
3	C	601	NAP	O4B-C4B-C5B-O5B
3	C	601	NAP	O4D-C4D-C5D-O5D
3	F	601	NAP	O4D-C4D-C5D-O5D
2	D	600	FAD	C2B-C1B-N9A-C4A
3	D	601	NAP	C3B-C2B-O2B-P2B
2	C	600	FAD	O4B-C4B-C5B-O5B
3	B	601	NAP	O4B-C4B-C5B-O5B
3	B	601	NAP	O4D-C4D-C5D-O5D
3	C	601	NAP	C3D-C4D-C5D-O5D
2	A	600	FAD	O4B-C4B-C5B-O5B
2	B	600	FAD	C2B-C1B-N9A-C8A
3	B	601	NAP	C2B-O2B-P2B-O1X
2	B	600	FAD	C4B-C5B-O5B-PA
3	D	601	NAP	C1B-C2B-O2B-P2B
2	C	600	FAD	C3B-C4B-C5B-O5B
3	A	601	NAP	PA-O3-PN-O5D
3	C	601	NAP	PA-O3-PN-O5D
3	E	601	NAP	C3B-C2B-O2B-P2B
2	A	600	FAD	C2B-C1B-N9A-C8A
3	F	601	NAP	C3D-C4D-C5D-O5D
2	C	600	FAD	C2B-C1B-N9A-C8A
2	A	600	FAD	P-O3P-PA-O1A
2	B	600	FAD	P-O3P-PA-O1A
2	C	600	FAD	P-O3P-PA-O1A
2	D	600	FAD	P-O3P-PA-O1A
2	E	600	FAD	P-O3P-PA-O1A
2	F	600	FAD	P-O3P-PA-O1A
4	B	700	MPD	O2-C2-C3-C4
4	F	700	MPD	O2-C2-C3-C4
2	A	600	FAD	C2'-C1'-N10-C10
3	C	601	NAP	C5D-O5D-PN-O1N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C4B-C5B-O5B-PA
2	D	600	FAD	C4B-C5B-O5B-PA
3	E	601	NAP	C4D-C5D-O5D-PN
3	D	601	NAP	PN-O3-PA-O2A
2	A	600	FAD	C2B-C1B-N9A-C4A
2	B	600	FAD	C2B-C1B-N9A-C4A
3	D	601	NAP	C2B-O2B-P2B-O2X
3	C	601	NAP	C2D-C1D-N1N-C2N
3	D	601	NAP	C2D-C1D-N1N-C6N
3	F	601	NAP	C2D-C1D-N1N-C6N
2	E	600	FAD	O4B-C4B-C5B-O5B
3	C	601	NAP	O4D-C1D-N1N-C2N
3	C	601	NAP	O4D-C1D-N1N-C6N
3	D	601	NAP	O4D-C1D-N1N-C6N
3	E	601	NAP	O4D-C1D-N1N-C2N
3	F	601	NAP	O4D-C1D-N1N-C6N
3	F	601	NAP	C2B-O2B-P2B-O1X
3	D	601	NAP	C4D-C5D-O5D-PN
2	C	600	FAD	O4B-C1B-N9A-C8A
2	A	600	FAD	O4B-C1B-N9A-C8A
3	B	601	NAP	C3B-C2B-O2B-P2B
2	A	600	FAD	P-O3P-PA-O2A
2	B	600	FAD	P-O3P-PA-O2A
2	C	600	FAD	P-O3P-PA-O2A
2	D	600	FAD	P-O3P-PA-O2A
2	E	600	FAD	P-O3P-PA-O2A
2	F	600	FAD	P-O3P-PA-O2A
4	D	700	MPD	O2-C2-C3-C4
2	B	600	FAD	O4B-C1B-N9A-C8A
3	F	601	NAP	C2B-O2B-P2B-O2X
3	A	601	NAP	PA-O3-PN-O2N
3	D	601	NAP	PN-O3-PA-O1A

There are no ring outliers.

16 monomers are involved in 52 short contacts:

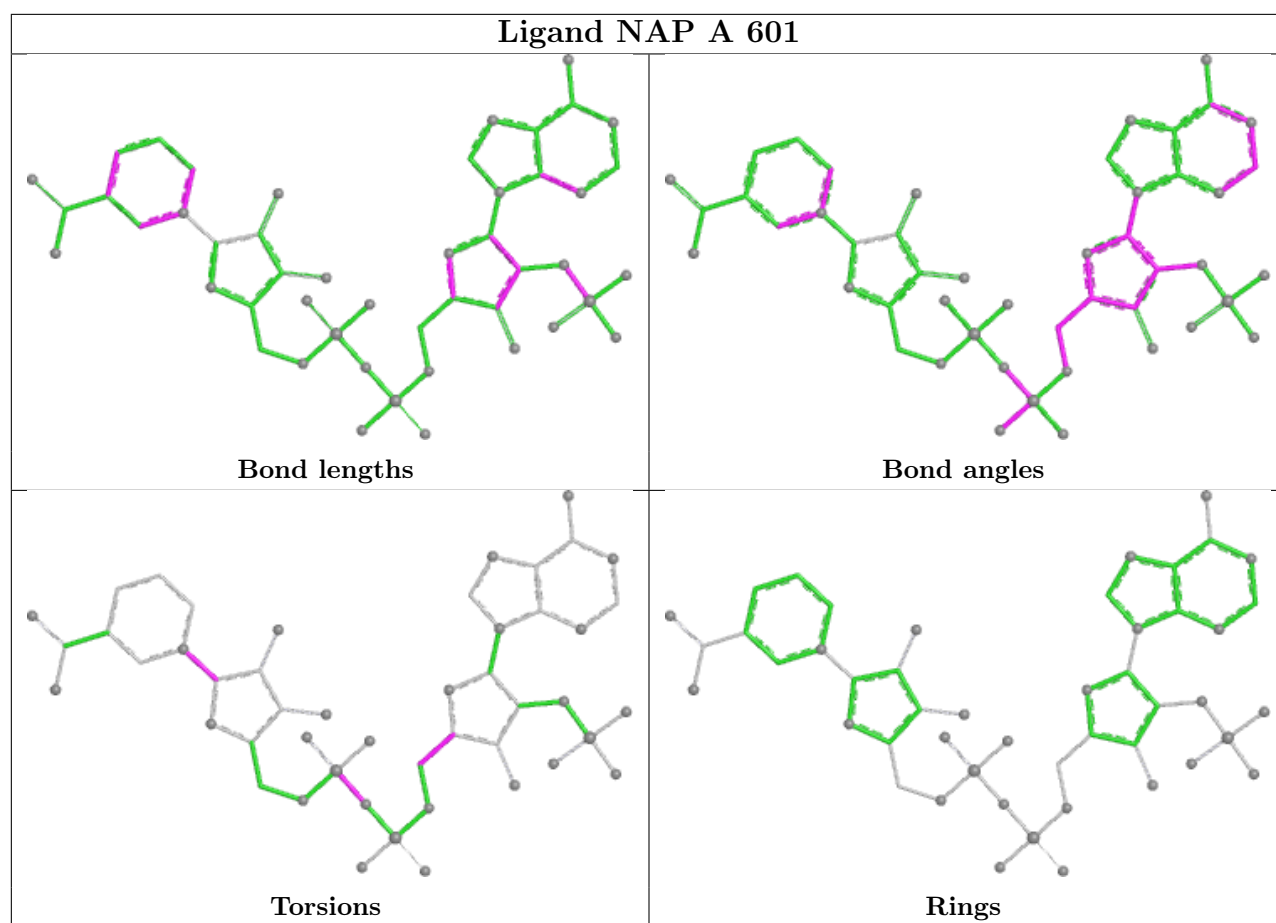
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	NAP	1	0
4	F	700	MPD	5	0
4	A	701	MPD	2	0
2	F	600	FAD	10	0
3	C	601	NAP	1	0

Continued on next page...

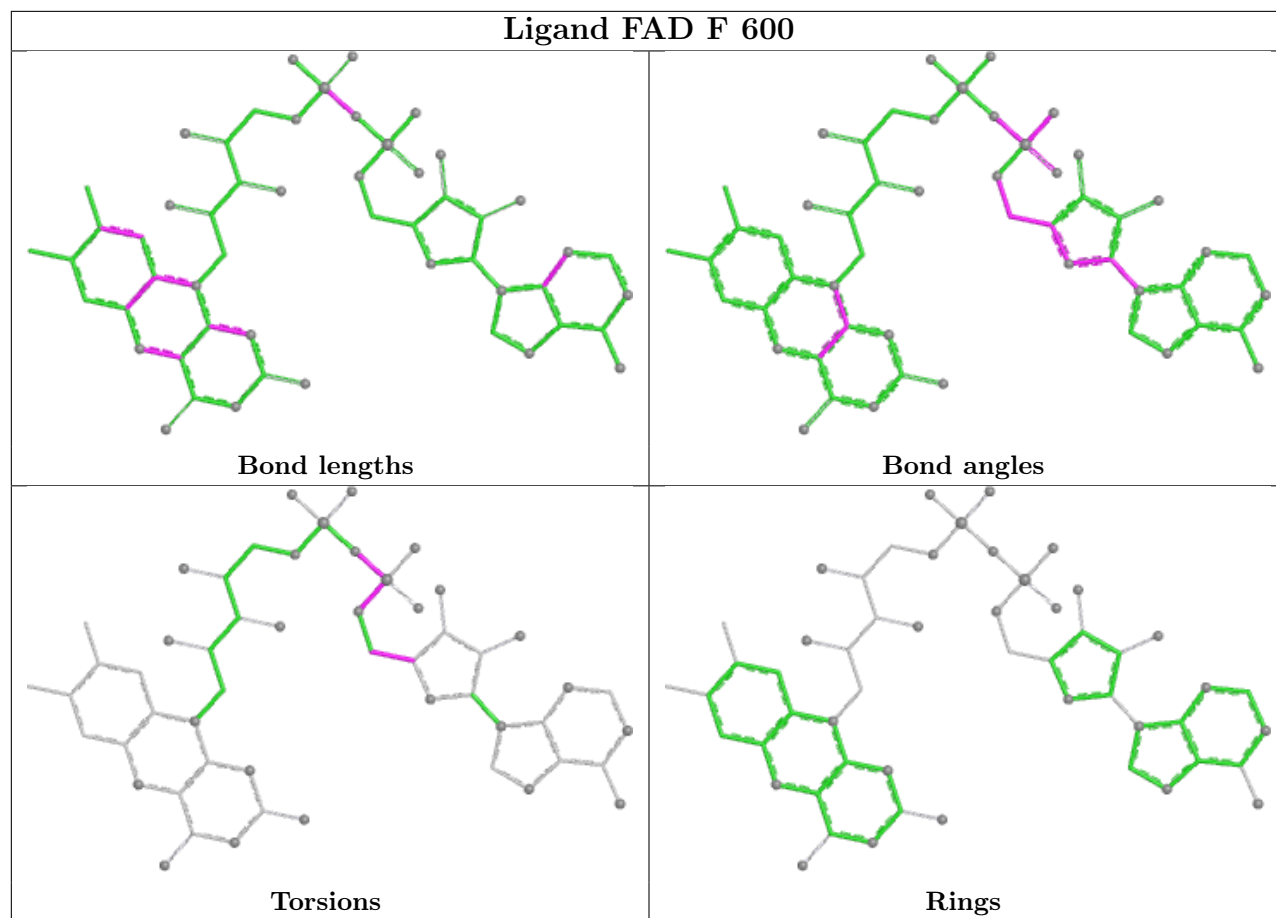
Continued from previous page...

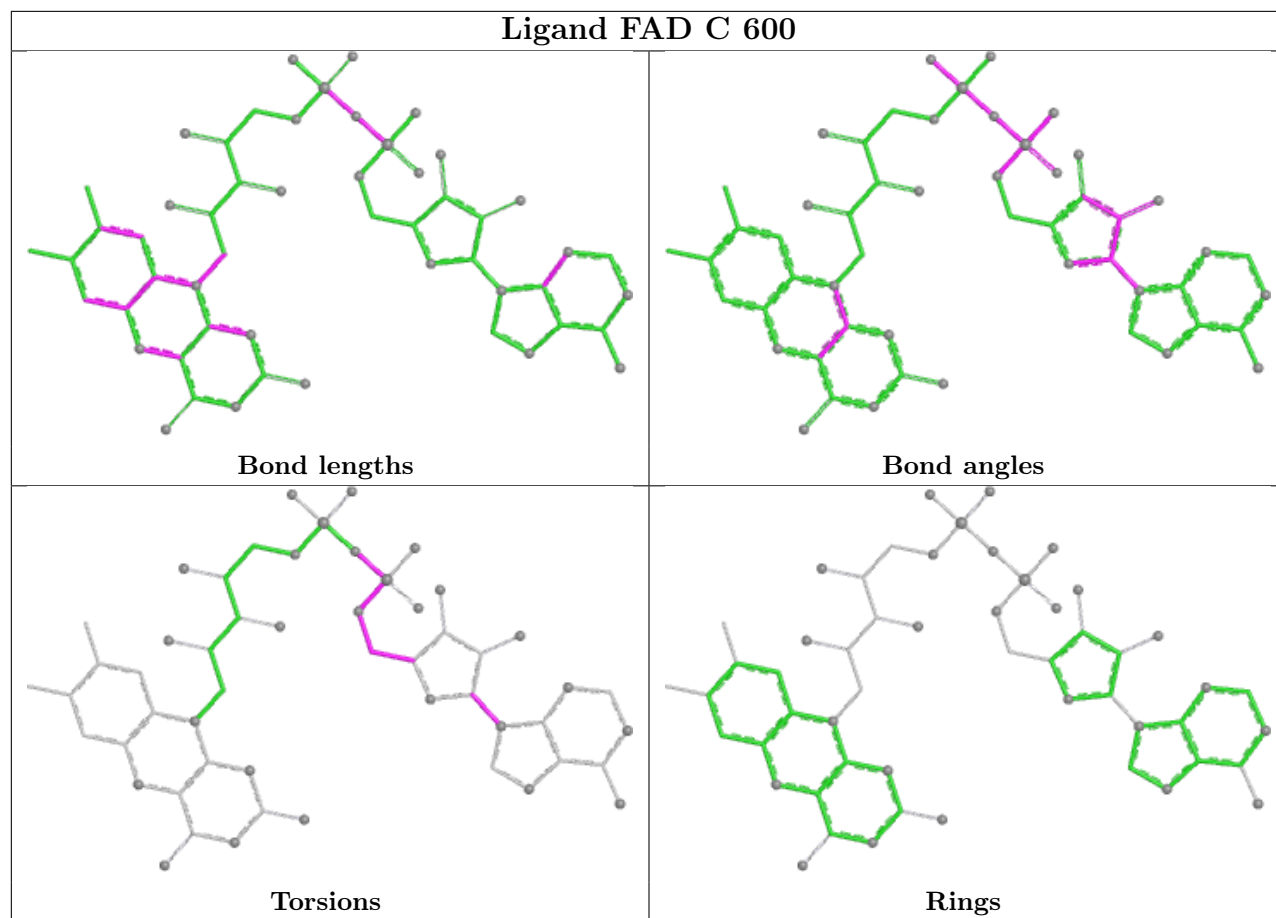
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	701	MPD	3	0
3	D	601	NAP	4	0
3	B	601	NAP	6	0
4	B	700	MPD	2	0
4	D	700	MPD	3	0
2	E	600	FAD	4	0
3	E	601	NAP	2	0
2	D	600	FAD	5	0
3	F	601	NAP	1	0
2	B	600	FAD	1	0
2	A	600	FAD	2	0

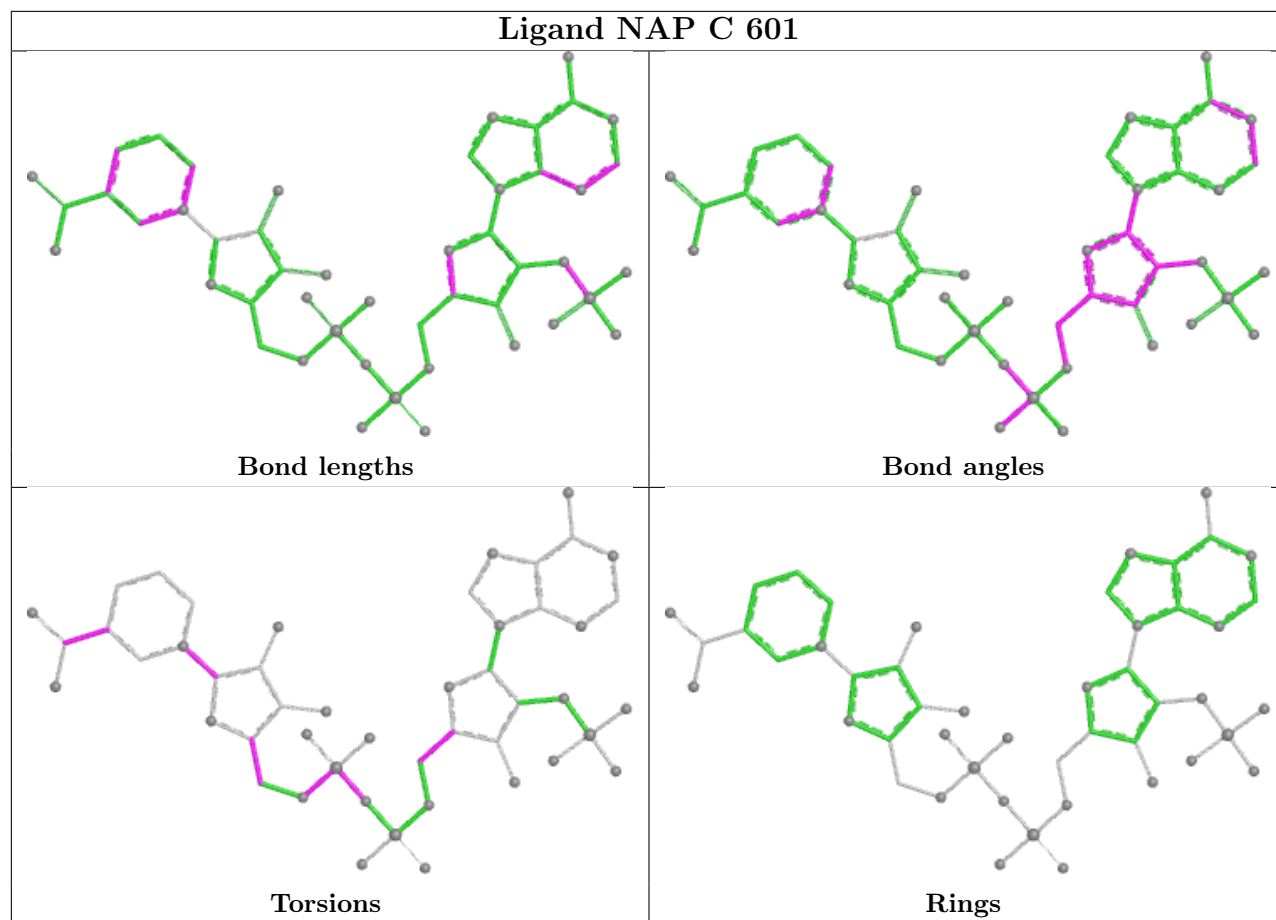
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

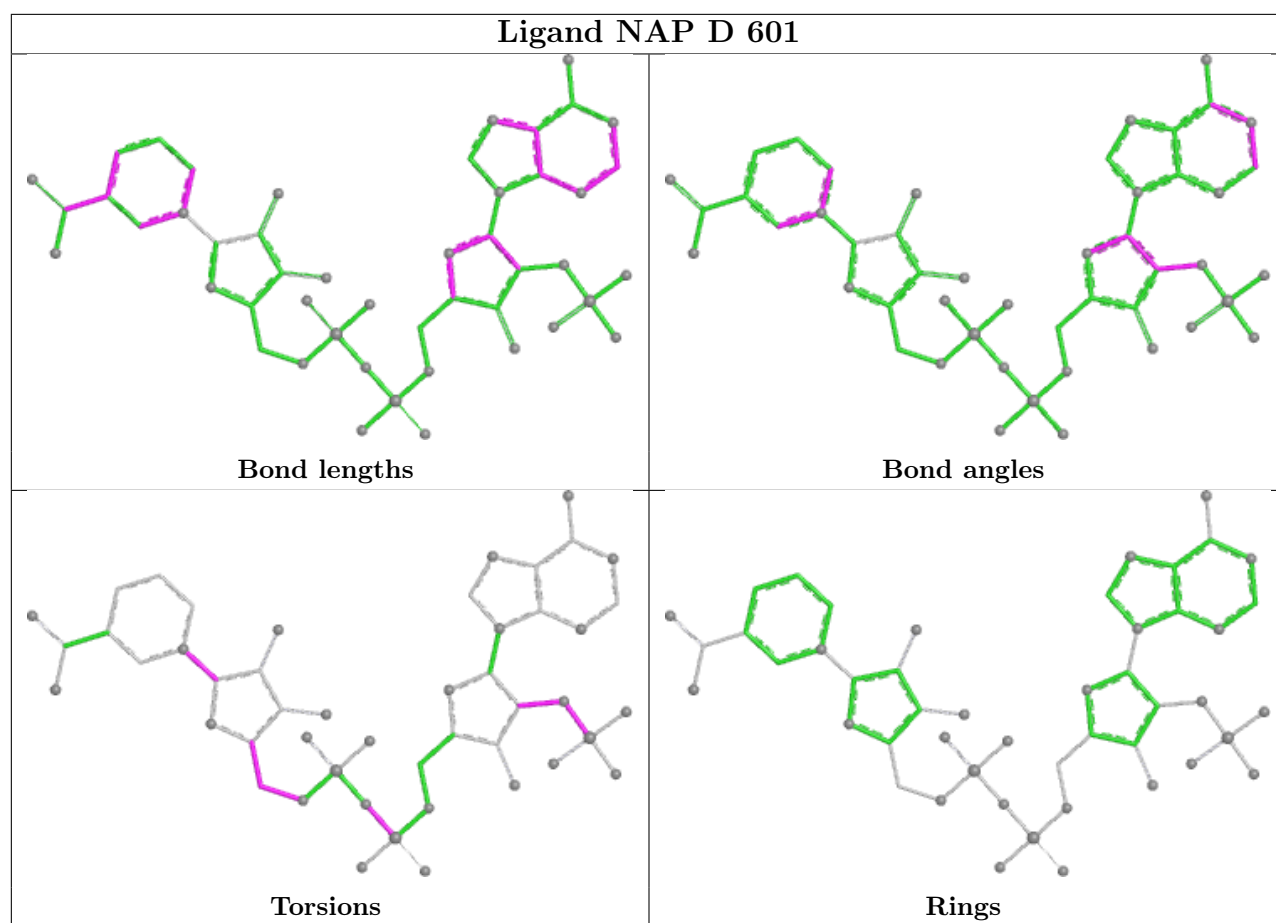


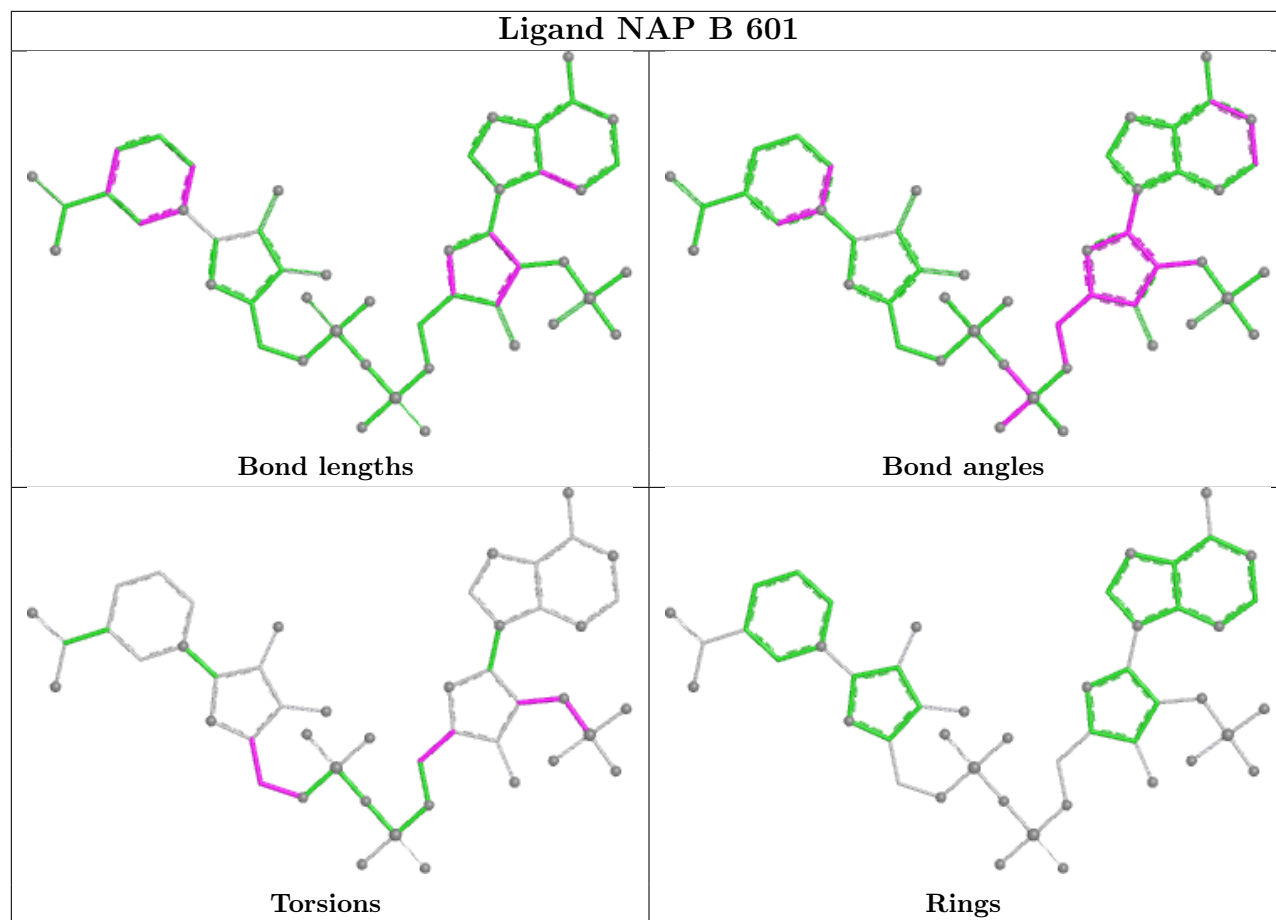
Ligand FAD F 600

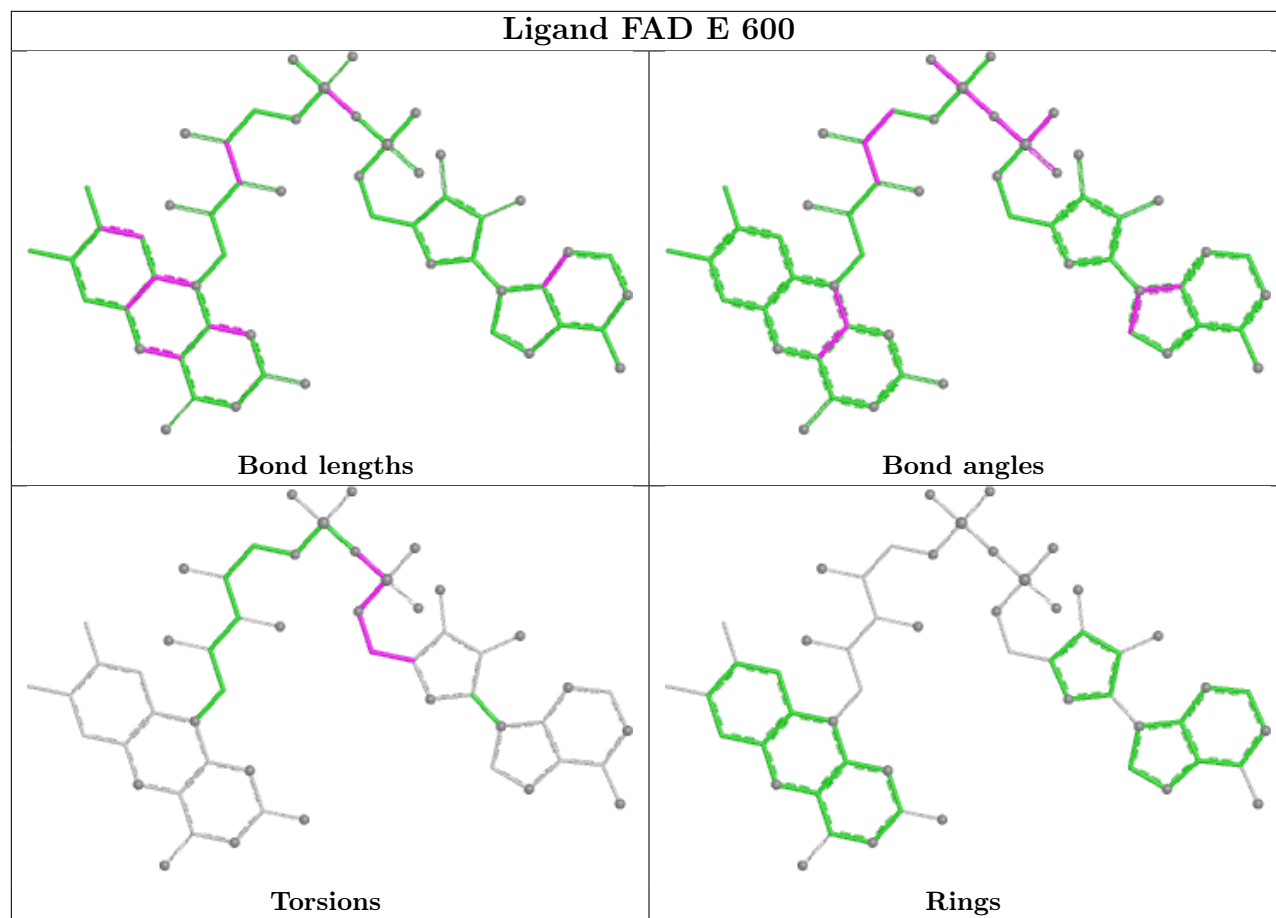


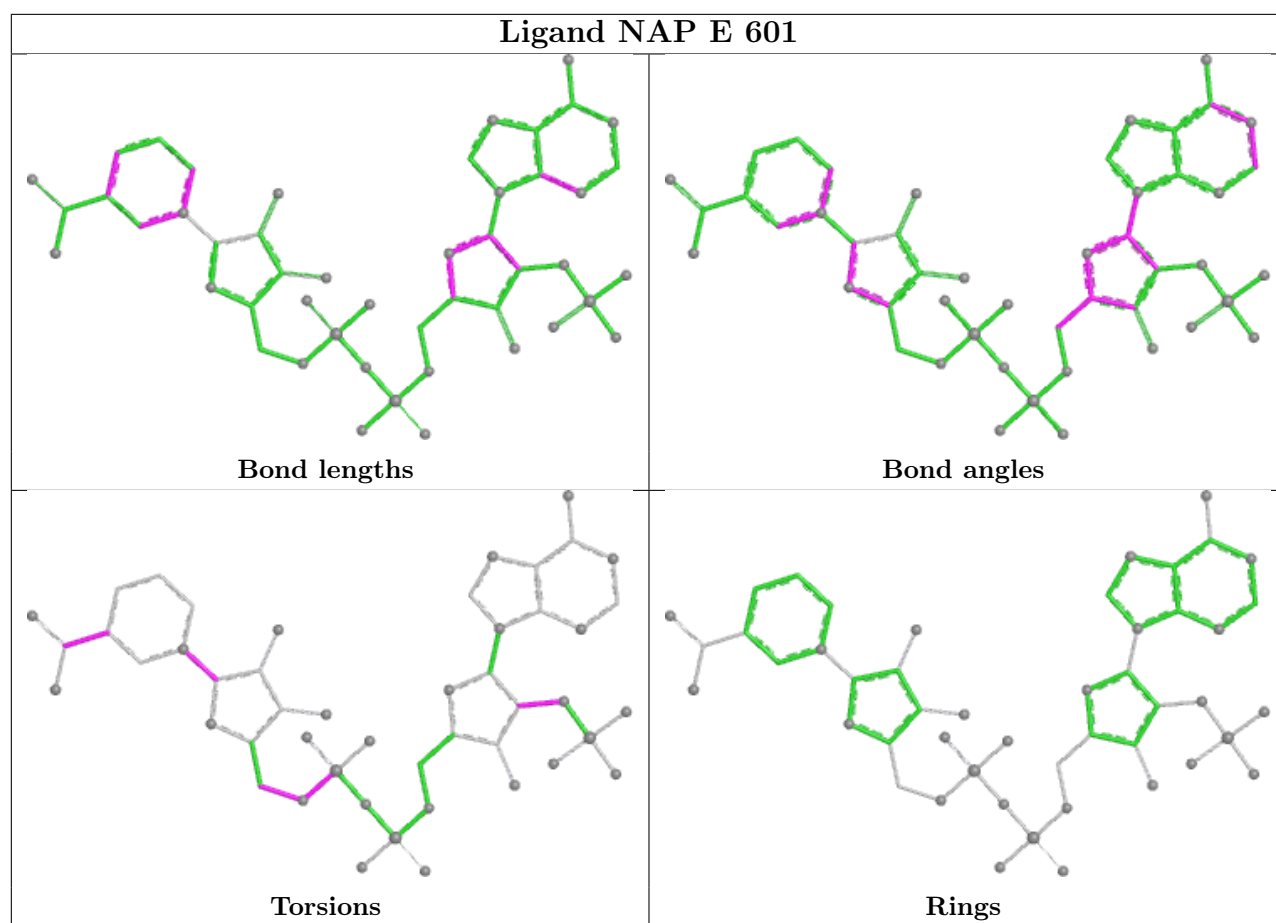


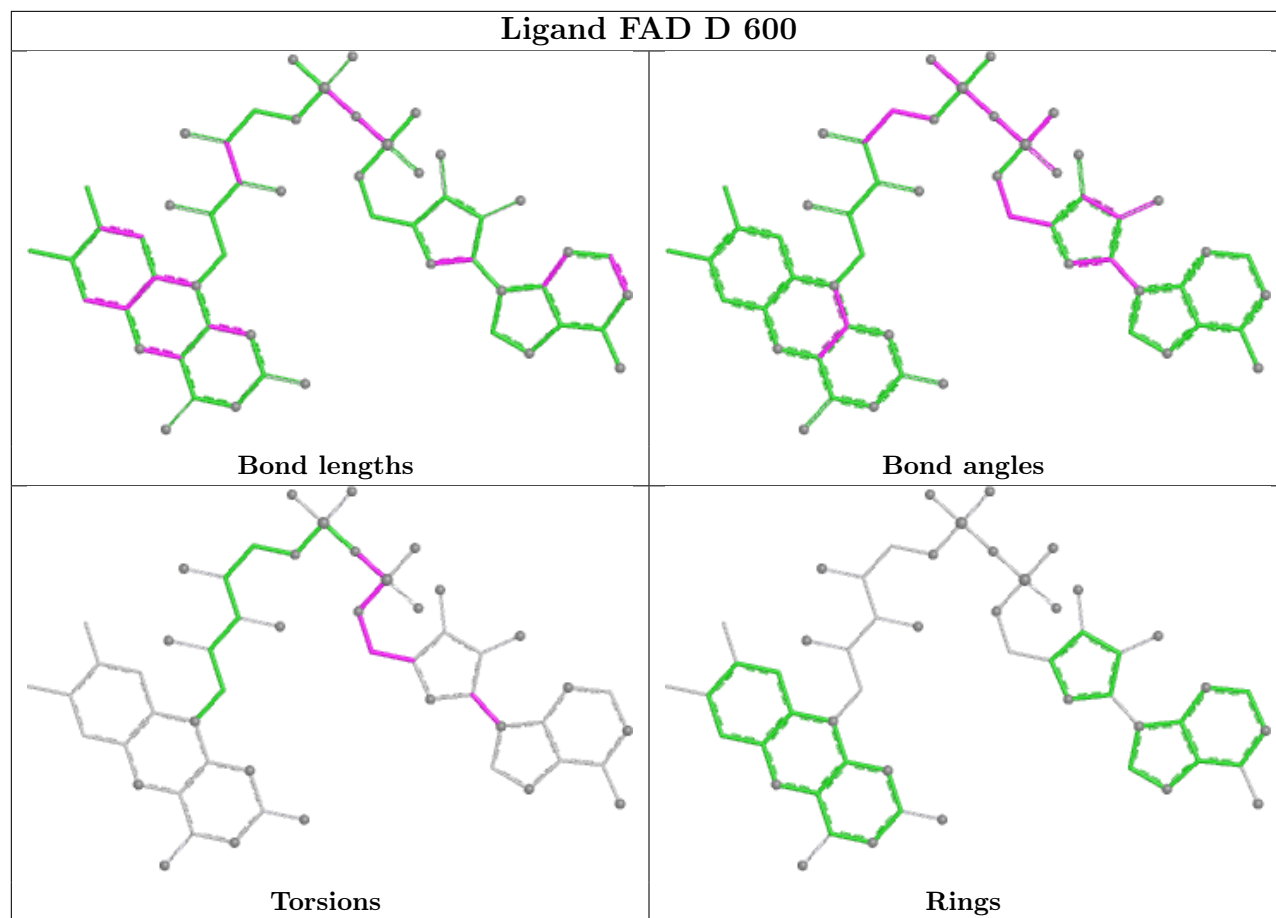


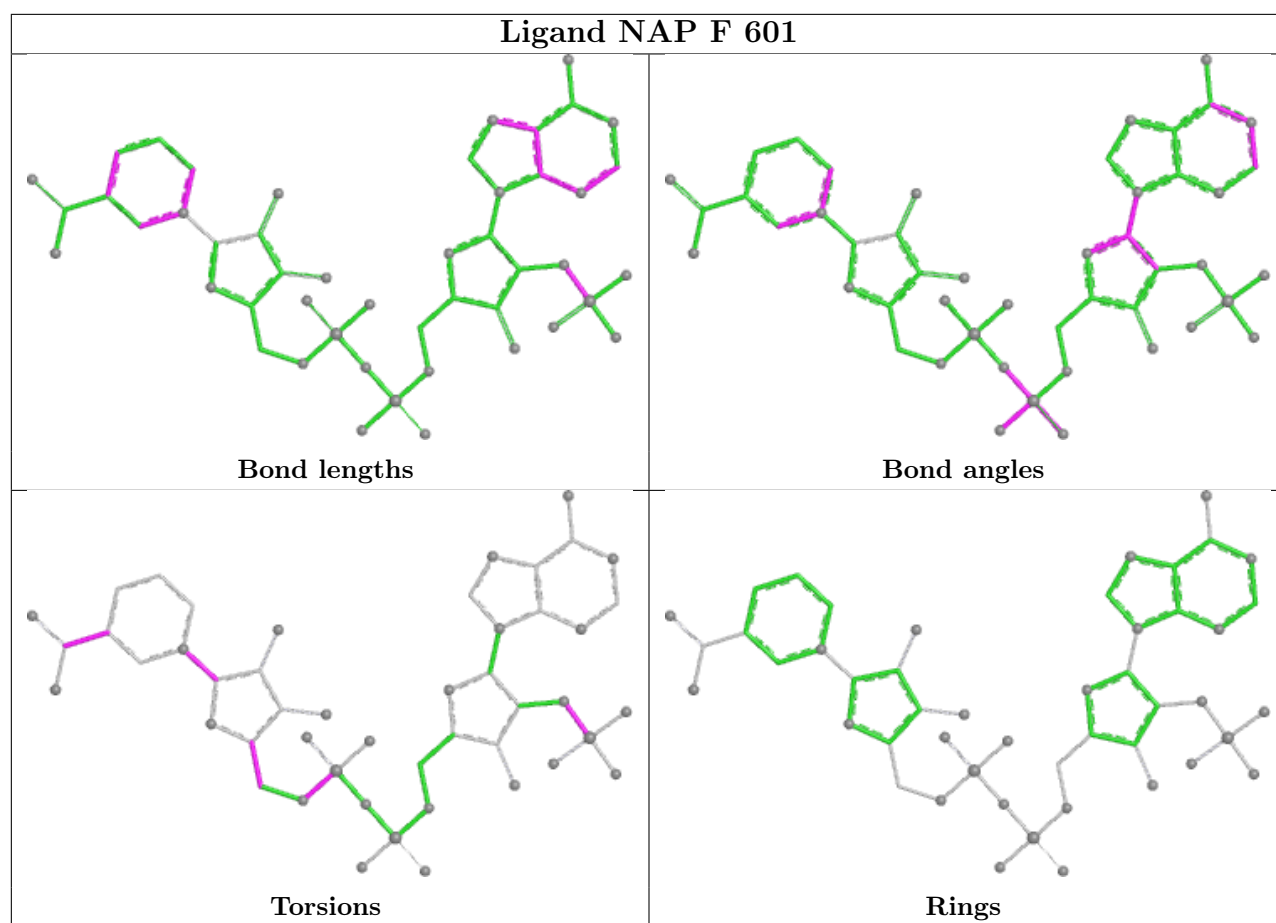




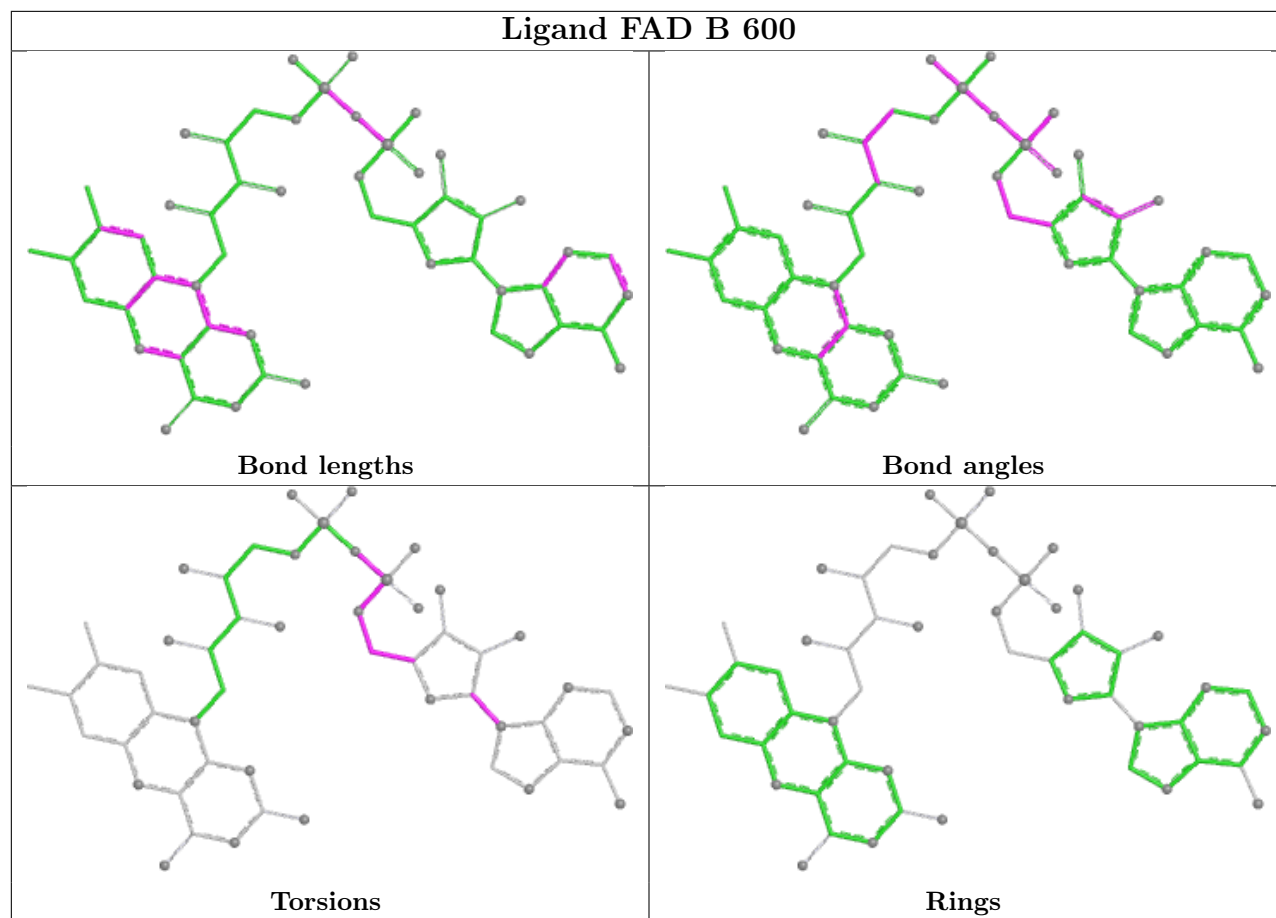


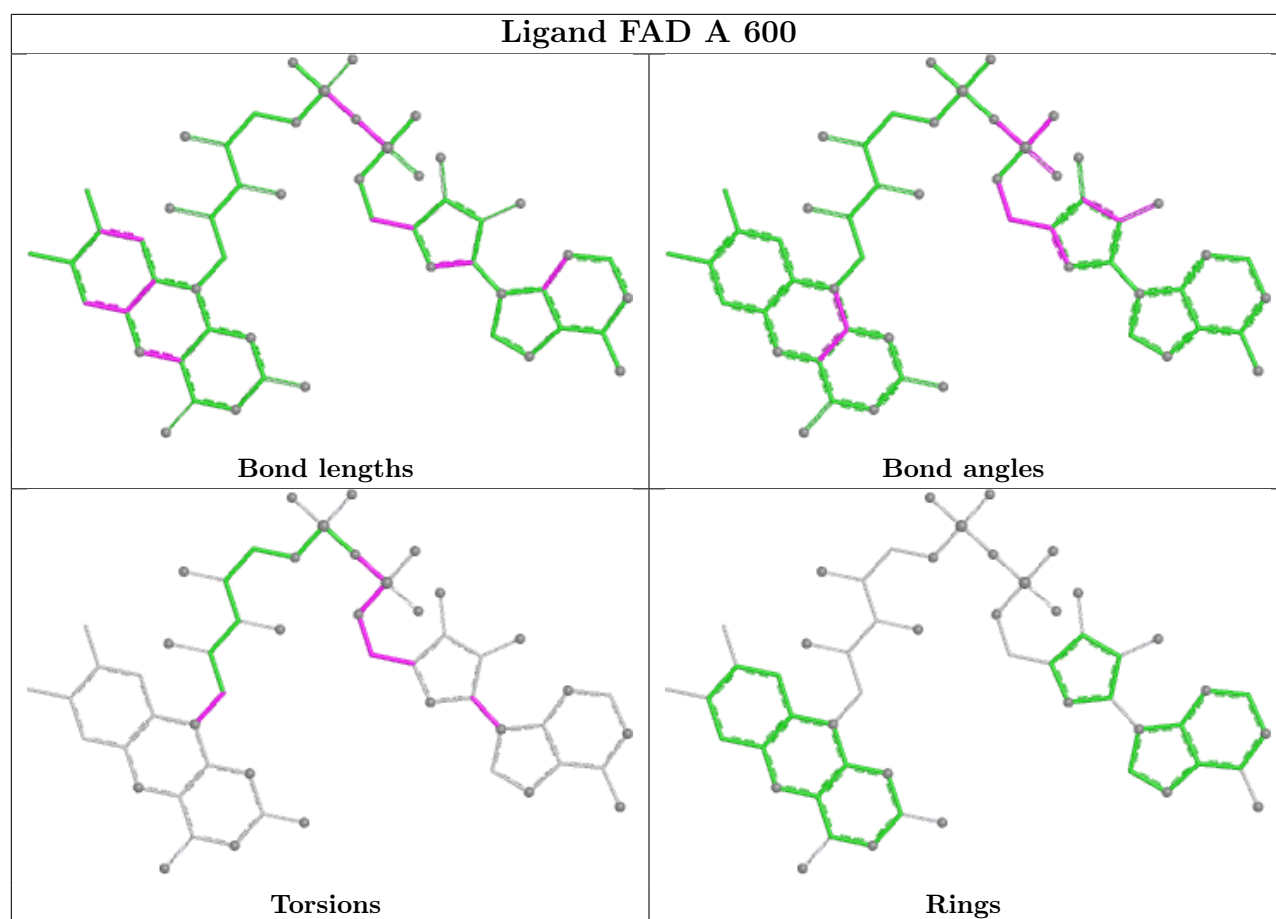






Ligand FAD B 600





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	487/519 (93%)	-0.10	0 100 100	25, 51, 70, 83	0
1	B	487/519 (93%)	-0.13	1 (0%) 91 88	26, 51, 69, 93	0
1	C	490/519 (94%)	0.01	3 (0%) 85 80	31, 55, 75, 102	0
1	D	491/519 (94%)	-0.08	1 (0%) 91 88	26, 52, 73, 107	0
1	E	490/519 (94%)	0.06	4 (0%) 82 75	32, 59, 82, 105	0
1	F	486/519 (93%)	-0.01	1 (0%) 91 88	29, 57, 77, 91	0
All	All	2931/3114 (94%)	-0.04	10 (0%) 90 86	25, 54, 75, 107	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	495	ALA	2.7
1	E	20	GLY	2.6
1	C	132	GLY	2.5
1	E	496	GLY	2.2
1	C	347	ILE	2.2
1	D	495	ALA	2.2
1	C	499	GLY	2.1
1	E	280	ILE	2.0
1	F	259	ILE	2.0
1	B	93	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

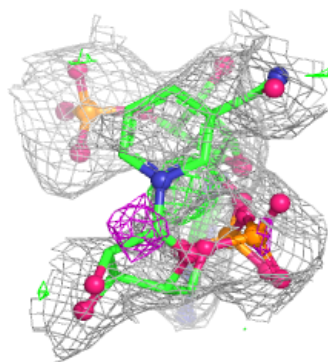
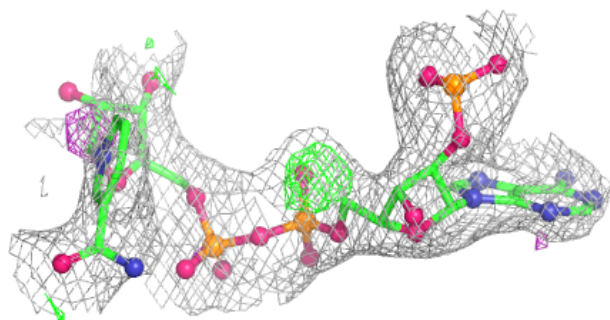
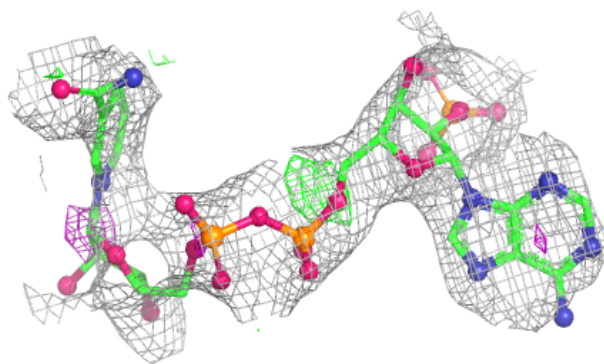
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MPD	A	701	8/8	0.71	0.20	76,78,79,79	0
3	NAP	F	601	48/48	0.74	0.15	83,108,119,120	0
3	NAP	E	601	48/48	0.77	0.14	73,104,121,121	0
4	MPD	B	701	8/8	0.77	0.15	58,60,61,62	0
3	NAP	C	601	48/48	0.83	0.12	80,95,101,102	0
3	NAP	D	601	48/48	0.85	0.12	26,68,87,87	0
3	NAP	A	601	48/48	0.86	0.12	68,86,102,104	0
3	NAP	B	601	48/48	0.86	0.13	63,86,104,105	0
4	MPD	B	700	8/8	0.91	0.12	34,38,39,44	0
2	FAD	E	600	53/53	0.91	0.12	54,59,83,84	0
4	MPD	D	700	8/8	0.91	0.11	39,41,43,43	0
2	FAD	D	600	53/53	0.92	0.10	25,49,70,70	0
2	FAD	F	600	53/53	0.92	0.12	52,60,62,64	0
2	FAD	B	600	53/53	0.94	0.09	35,45,50,52	0
2	FAD	C	600	53/53	0.95	0.08	20,40,61,62	0
2	FAD	A	600	53/53	0.95	0.08	25,35,44,47	0
4	MPD	F	700	8/8	0.95	0.08	34,35,37,37	0

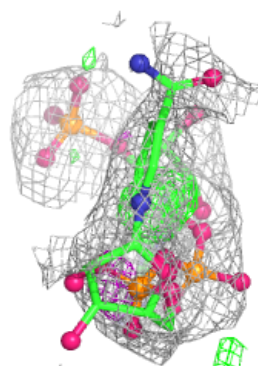
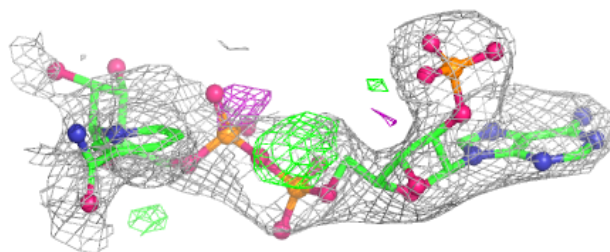
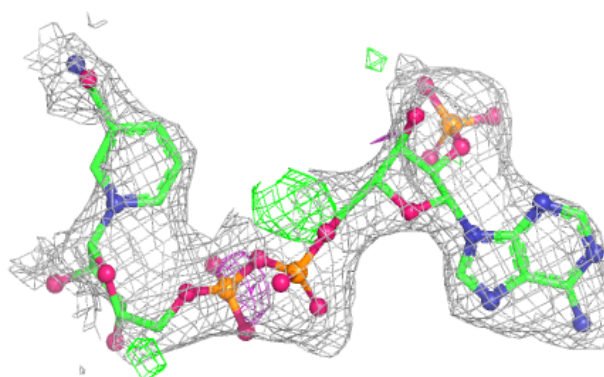
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP F 601:

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

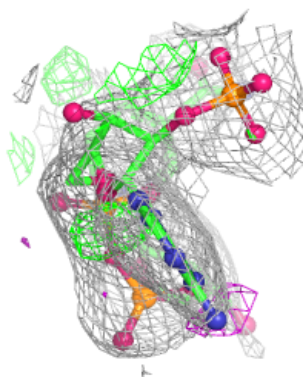
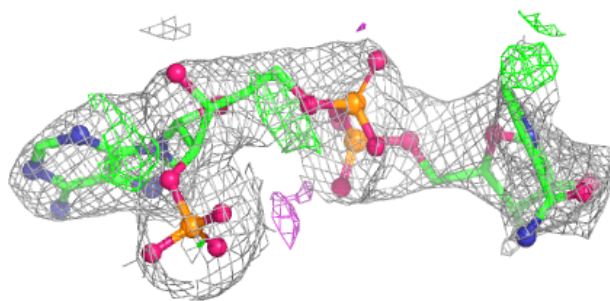
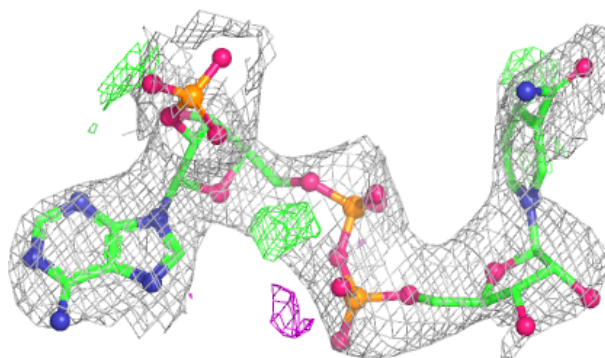
**Electron density around NAP E 601:**

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

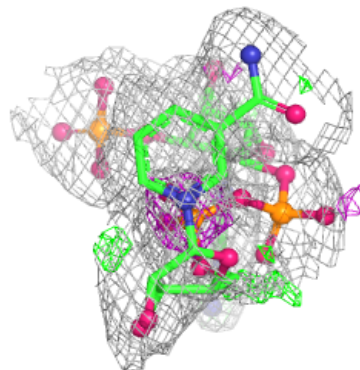
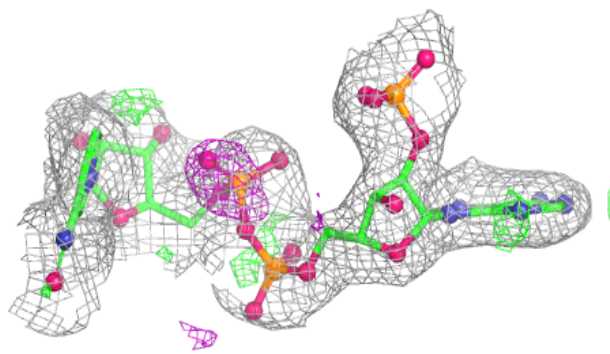
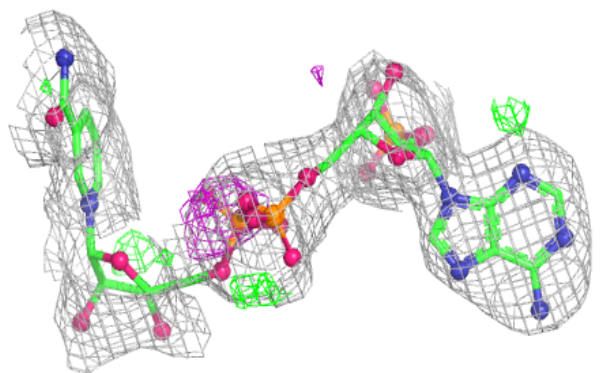


Electron density around NAP C 601:

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

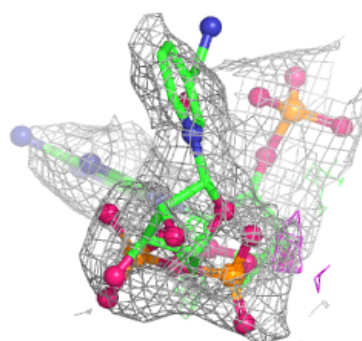
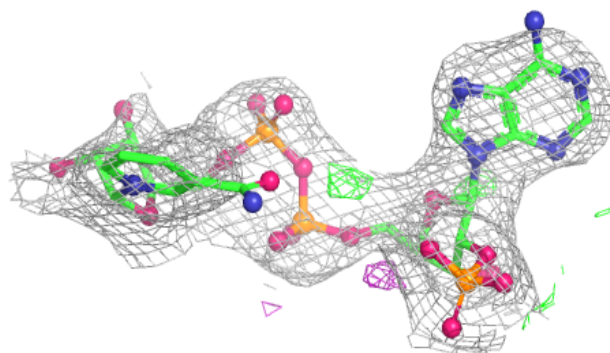
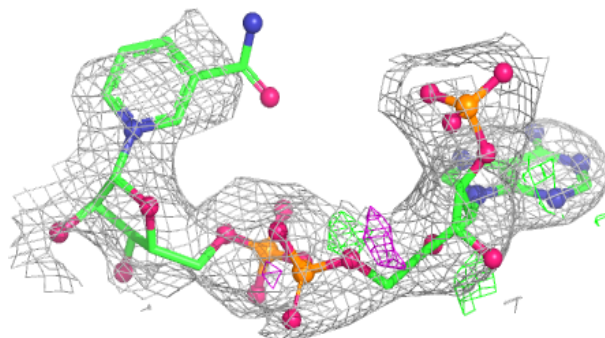
**Electron density around NAP D 601:**

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

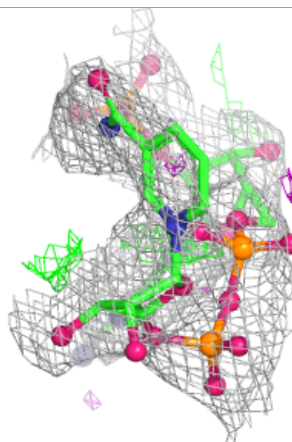
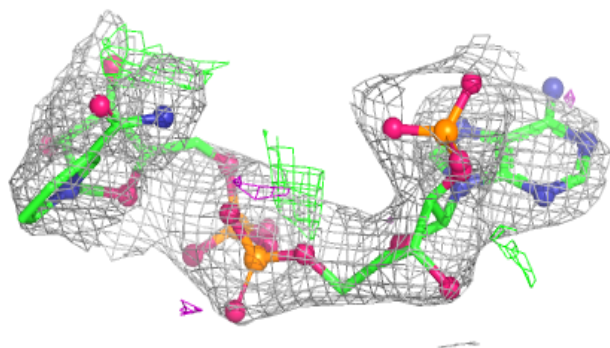
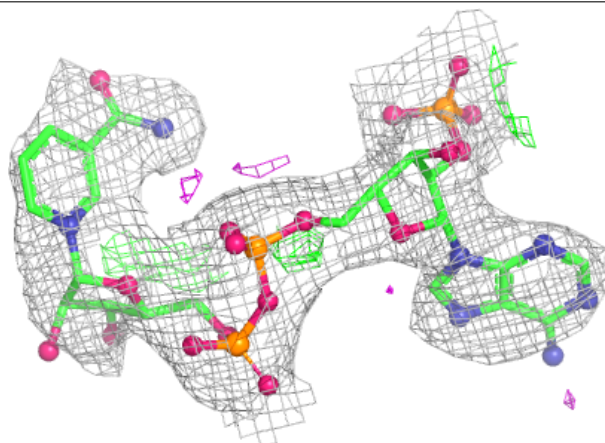


Electron density around NAP A 601:

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

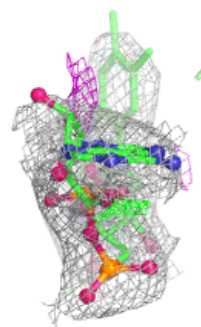
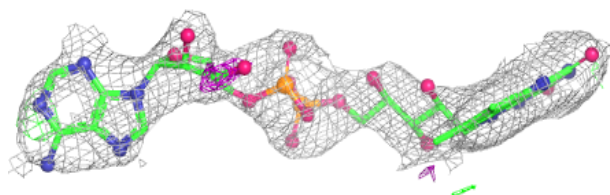
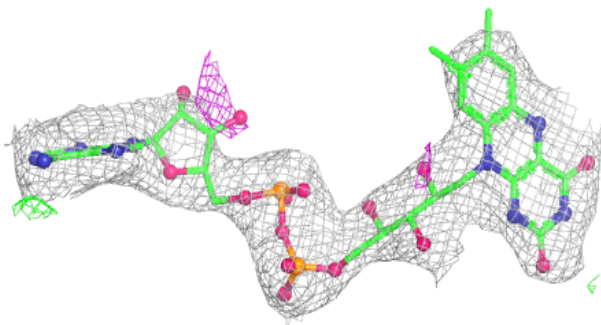
**Electron density around NAP B 601:**

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

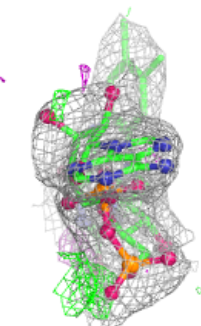
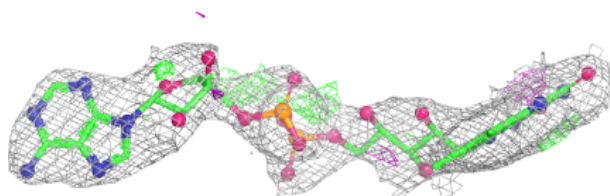
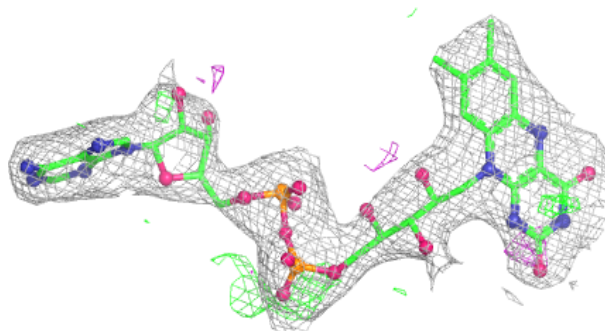


Electron density around FAD E 600:

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

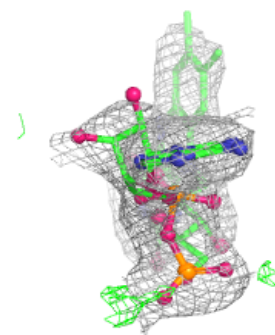
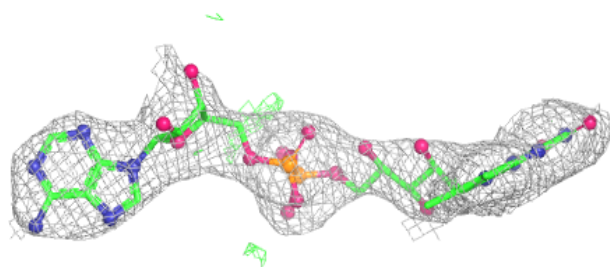
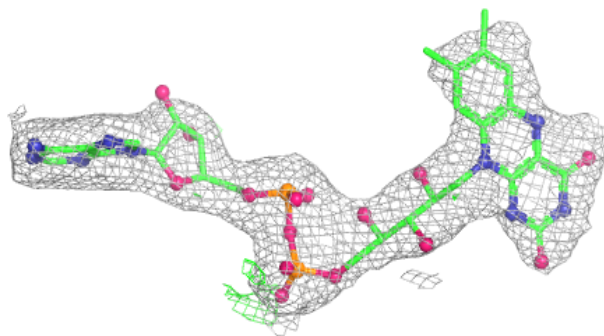
**Electron density around FAD D 600:**

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

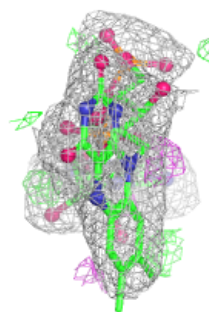
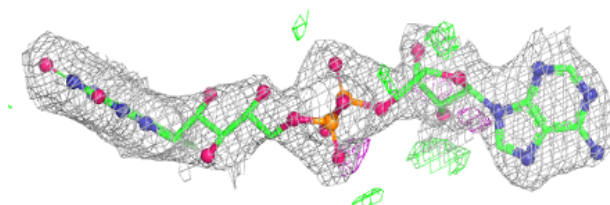
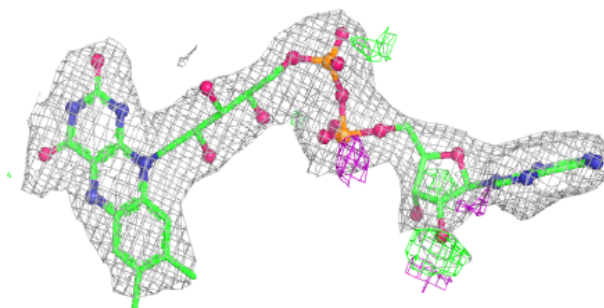


Electron density around FAD F 600:

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

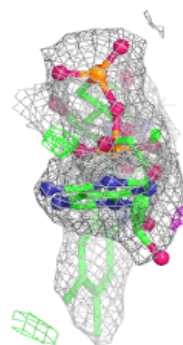
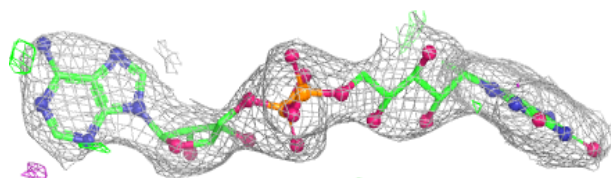
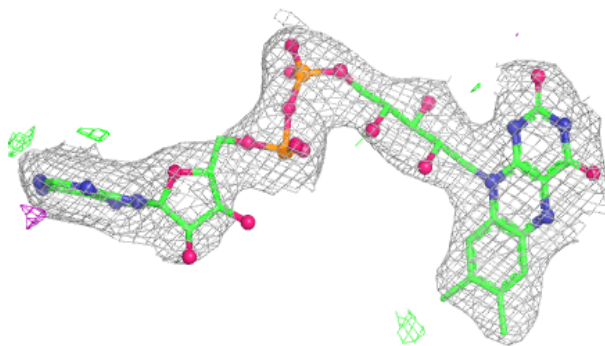
**Electron density around FAD B 600:**

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

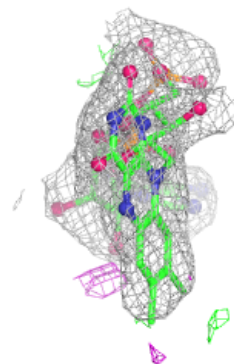
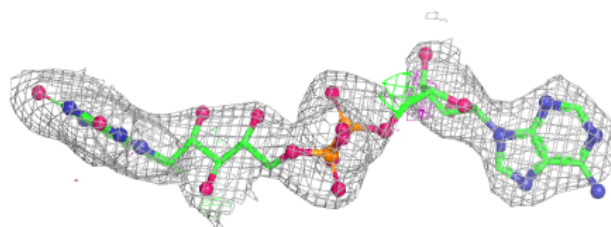
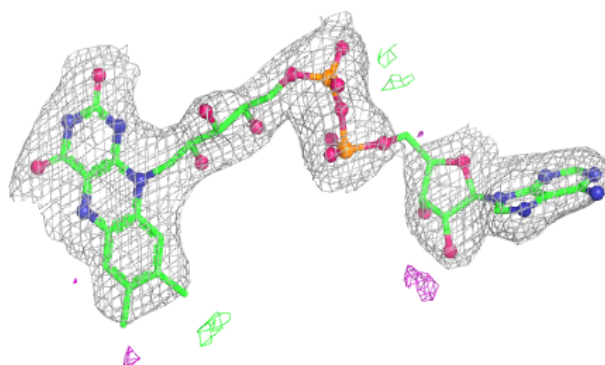


Electron density around FAD C 600:

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

**Electron density around FAD A 600:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.