



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 06:16 PM JST

PDB ID : 7XCM
Title : Crystal structure of sulfite MttB structure at 3.2 Å resolution
Authors : Li, J.; Chan, M.K.
Deposited on : 2022-03-24
Resolution : 3.20 Å(reported)

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

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

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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

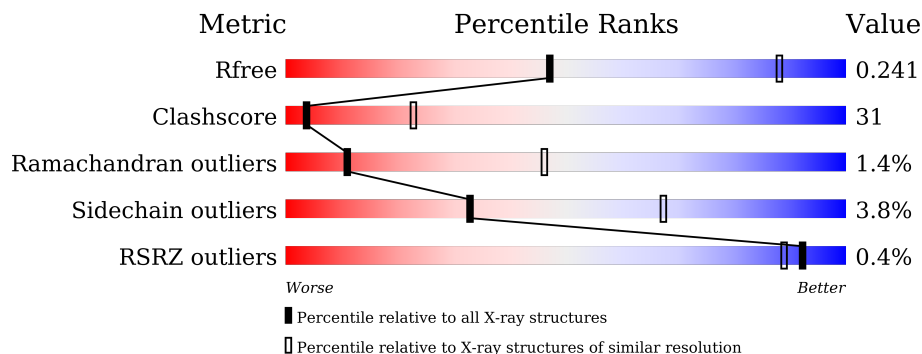
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	503	
1	B	503	
1	C	503	
1	D	503	
1	E	503	
1	F	503	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	C	603	-	-	X	-
4	GOL	D	604	-	-	X	-
4	GOL	F	603	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 22891 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 Trimethylamine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	494	3765	2394	629	720	22	0	0	0
1	B	494	3765	2394	629	720	22	0	0	0
1	C	493	3757	2389	628	719	21	0	0	0
1	D	494	3765	2394	629	720	22	0	0	0
1	E	494	3765	2394	629	720	22	0	0	0
1	F	494	3765	2394	629	720	22	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

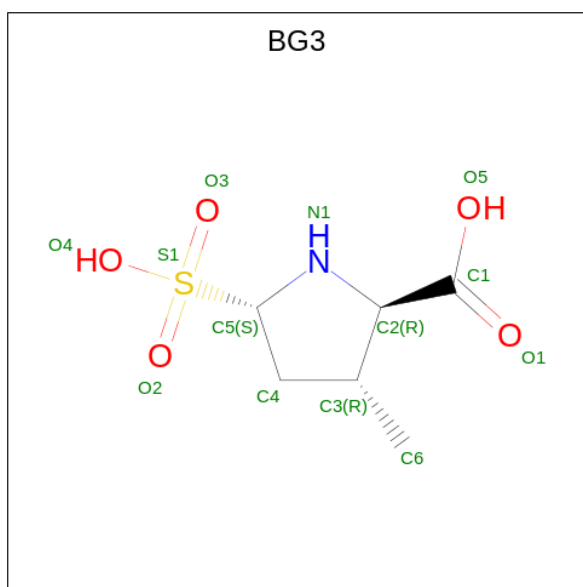
Chain	Residue	Modelled	Actual	Comment	Reference
A	334	LYS	PYL	conflict	UNP A0A0E3QRM4
A	496	GLY	-	expression tag	UNP A0A0E3QRM4
A	497	GLY	-	expression tag	UNP A0A0E3QRM4
A	498	HIS	-	expression tag	UNP A0A0E3QRM4
A	499	HIS	-	expression tag	UNP A0A0E3QRM4
A	500	HIS	-	expression tag	UNP A0A0E3QRM4
A	501	HIS	-	expression tag	UNP A0A0E3QRM4
A	502	HIS	-	expression tag	UNP A0A0E3QRM4
A	503	HIS	-	expression tag	UNP A0A0E3QRM4
B	334	LYS	PYL	conflict	UNP A0A0E3QRM4
B	496	GLY	-	expression tag	UNP A0A0E3QRM4
B	497	GLY	-	expression tag	UNP A0A0E3QRM4
B	498	HIS	-	expression tag	UNP A0A0E3QRM4
B	499	HIS	-	expression tag	UNP A0A0E3QRM4
B	500	HIS	-	expression tag	UNP A0A0E3QRM4
B	501	HIS	-	expression tag	UNP A0A0E3QRM4
B	502	HIS	-	expression tag	UNP A0A0E3QRM4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	503	HIS	-	expression tag	UNP A0A0E3QRM4
C	334	LYS	PYL	conflict	UNP A0A0E3QRM4
C	496	GLY	-	expression tag	UNP A0A0E3QRM4
C	497	GLY	-	expression tag	UNP A0A0E3QRM4
C	498	HIS	-	expression tag	UNP A0A0E3QRM4
C	499	HIS	-	expression tag	UNP A0A0E3QRM4
C	500	HIS	-	expression tag	UNP A0A0E3QRM4
C	501	HIS	-	expression tag	UNP A0A0E3QRM4
C	502	HIS	-	expression tag	UNP A0A0E3QRM4
C	503	HIS	-	expression tag	UNP A0A0E3QRM4
D	334	LYS	PYL	conflict	UNP A0A0E3QRM4
D	496	GLY	-	expression tag	UNP A0A0E3QRM4
D	497	GLY	-	expression tag	UNP A0A0E3QRM4
D	498	HIS	-	expression tag	UNP A0A0E3QRM4
D	499	HIS	-	expression tag	UNP A0A0E3QRM4
D	500	HIS	-	expression tag	UNP A0A0E3QRM4
D	501	HIS	-	expression tag	UNP A0A0E3QRM4
D	502	HIS	-	expression tag	UNP A0A0E3QRM4
D	503	HIS	-	expression tag	UNP A0A0E3QRM4
E	334	LYS	PYL	conflict	UNP A0A0E3QRM4
E	496	GLY	-	expression tag	UNP A0A0E3QRM4
E	497	GLY	-	expression tag	UNP A0A0E3QRM4
E	498	HIS	-	expression tag	UNP A0A0E3QRM4
E	499	HIS	-	expression tag	UNP A0A0E3QRM4
E	500	HIS	-	expression tag	UNP A0A0E3QRM4
E	501	HIS	-	expression tag	UNP A0A0E3QRM4
E	502	HIS	-	expression tag	UNP A0A0E3QRM4
E	503	HIS	-	expression tag	UNP A0A0E3QRM4
F	334	LYS	PYL	conflict	UNP A0A0E3QRM4
F	496	GLY	-	expression tag	UNP A0A0E3QRM4
F	497	GLY	-	expression tag	UNP A0A0E3QRM4
F	498	HIS	-	expression tag	UNP A0A0E3QRM4
F	499	HIS	-	expression tag	UNP A0A0E3QRM4
F	500	HIS	-	expression tag	UNP A0A0E3QRM4
F	501	HIS	-	expression tag	UNP A0A0E3QRM4
F	502	HIS	-	expression tag	UNP A0A0E3QRM4
F	503	HIS	-	expression tag	UNP A0A0E3QRM4

- Molecule 2 is 3-METHYL-5-SULFO-PYRROLIDINE-2-CARBOXYLIC ACID (three-letter code: BG3) (formula: C₆H₁₁NO₅S) (labeled as "Ligand of Interest" by depositor).

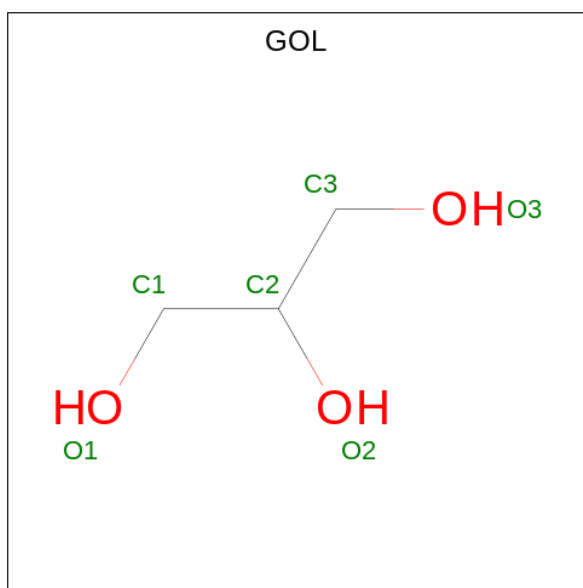


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		
3	F	1	Total	Na	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0

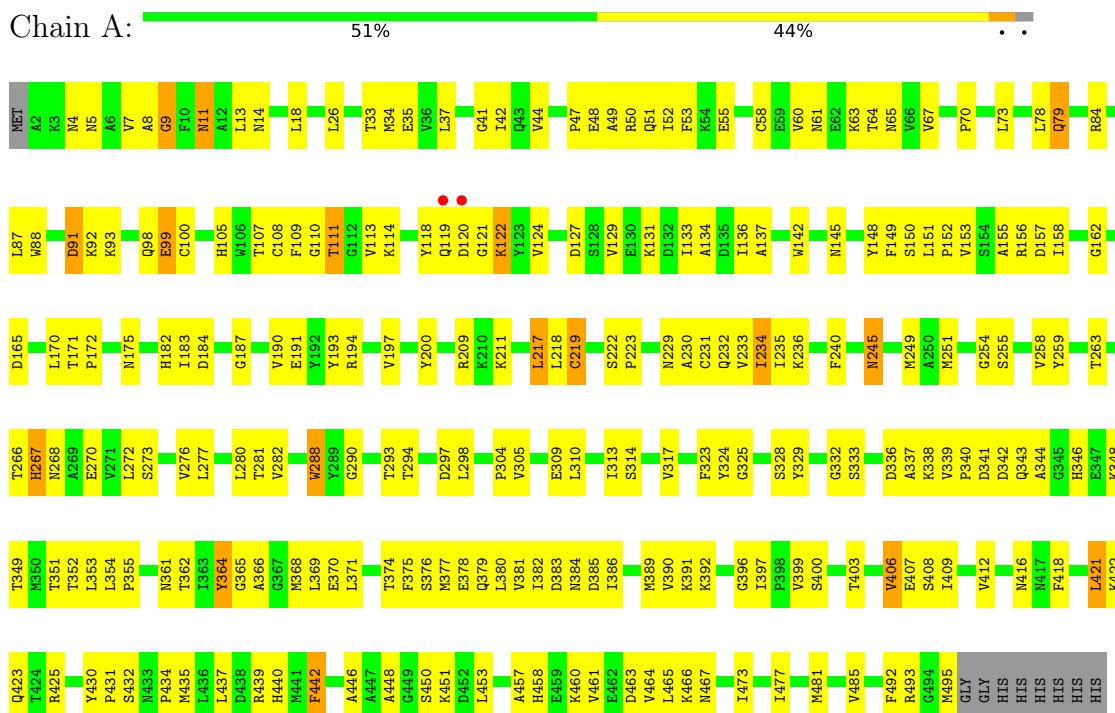
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total 30	O 30	0	0
5	B	28	Total 28	O 28	0	0
5	C	23	Total 23	O 23	0	0
5	D	29	Total 29	O 29	0	0
5	E	25	Total 25	O 25	0	0
5	F	30	Total 30	O 30	0	0

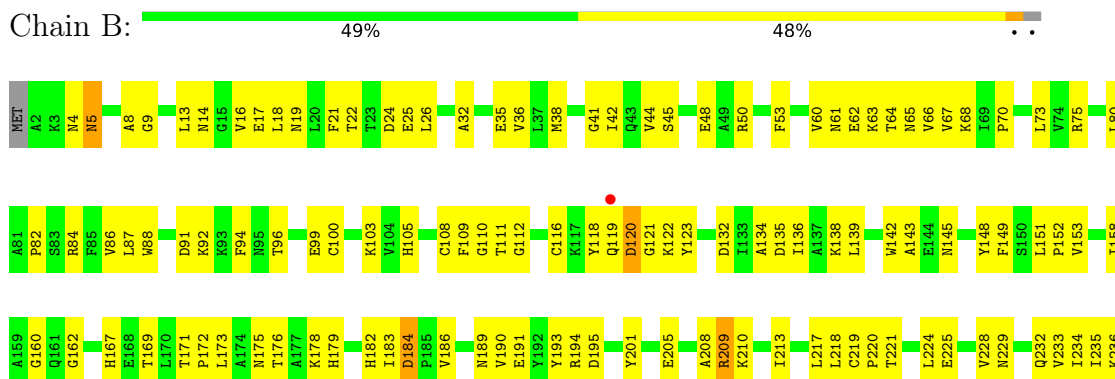
3 Residue-property plots

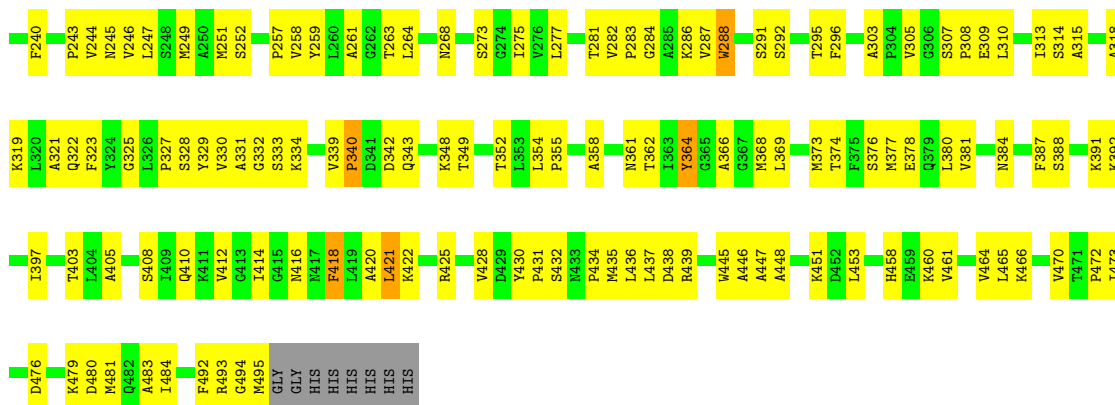
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

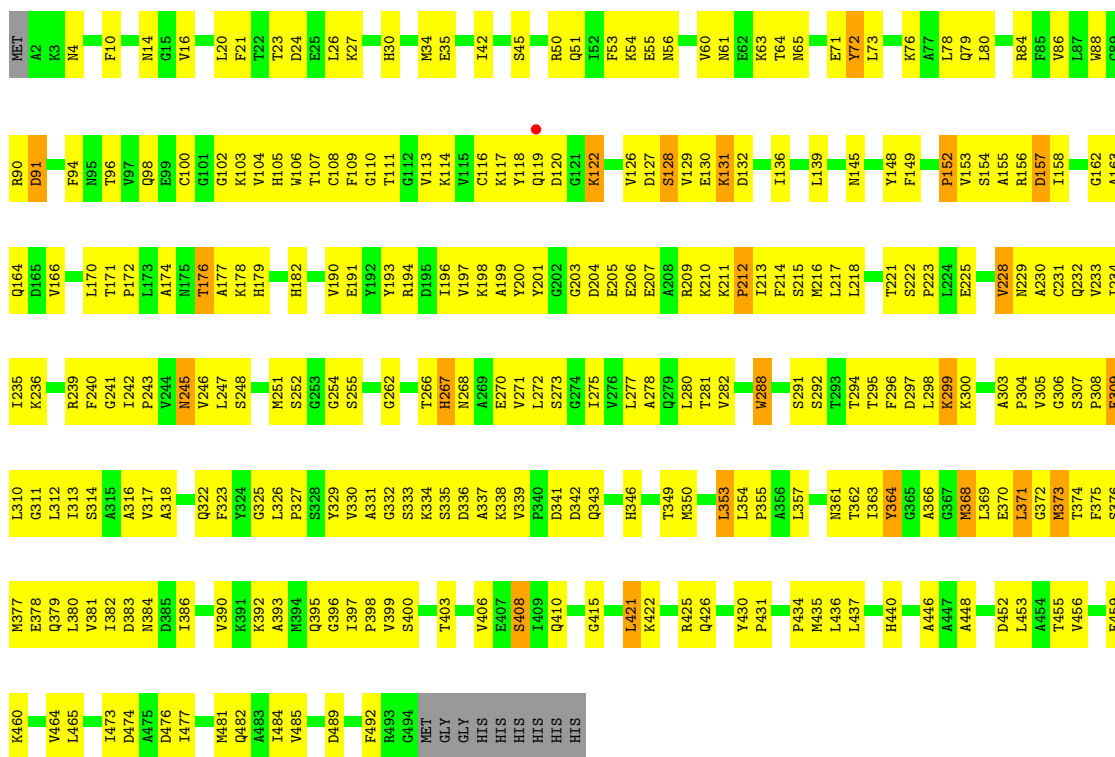


- Molecule 1: Trimethylamine methyltransferase

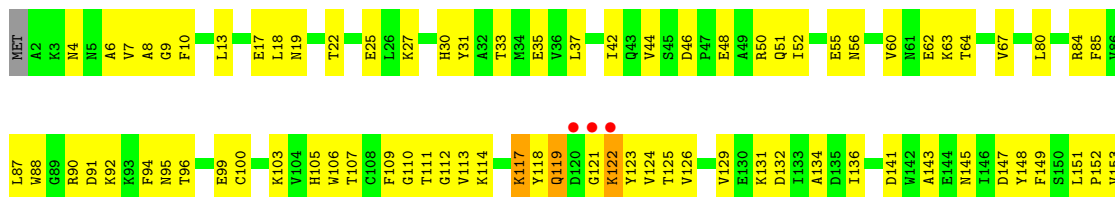


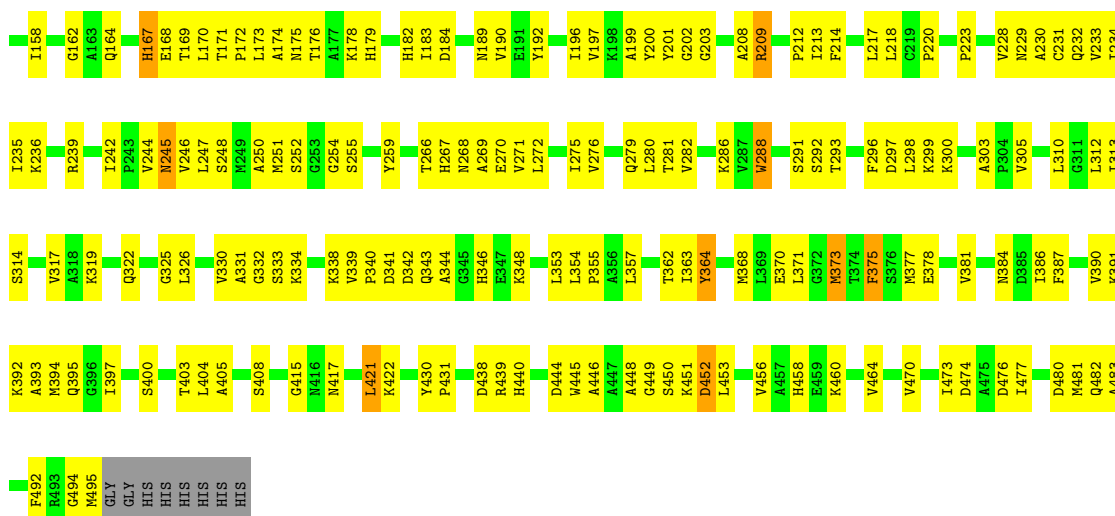


● Molecule 1: Trimethylamine methyltransferase

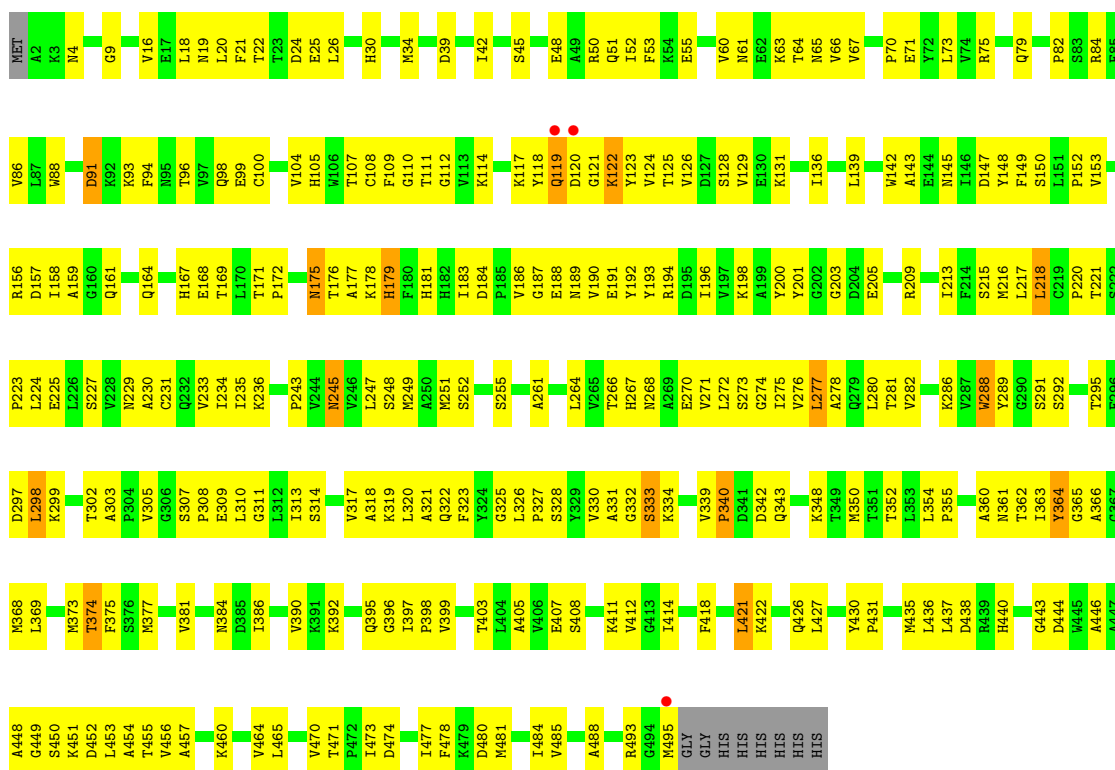
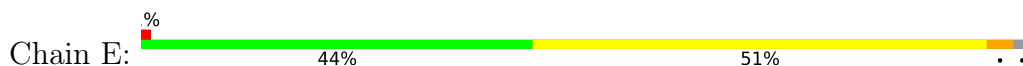


● Molecule 1: Trimethylamine methyltransferase





● Molecule 1: Trimethylamine methyltransferase



● Molecule 1: Trimethylamine methyltransferase



I473	D474	A475	D476	I477	F478	K479	D480	M481	Q482	A483	L484	V485	D486	K487	A488	D489	F492	M495	GLY	GLY	HIS	HIS	HIS	HIS	HIS	HIS																												
V390	K391	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	A360	N361	T362	L363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379	L380	V381	I382	D383	M384	D385	I386	F387	
V317	A318	K319	L320	A321	Q322	F323	G332	S333	K334	A337	K338	V339	P340	D341	D342	Q343	H346	E347	K348	T349	M350	T351	T352	L353	L354	P355	A356	L357	A358	G359	A360	N361	T362	L363	Y364	G365	M368	L369	G372	M373	T374	F375	S376	M377	E378	Q379	L380	V381	I382	D383	M384	D385	I386	F387
G241	I242	N245	V246	L247	S248	M249	A250	M251	S252	Y259	L260	A261	H267	M268	V271	L272	S273	G274	I275	A278	Q279	L280	T281	V282	P283	G284	A285	K286	V287	W288	Y289	G290	S291	S292	T293	T294	T295	F296	D297	L298	K299	K300	G301	T302	A303	P304	V305	G306	S307	P308	E309	L310	G311	
H167	E168	T169	L170	T171	P172	L173	A174	M175	T176	A177	K178	H179	F180	H181	D184	P185	V186	G187	E188	M189	V190	E191	Y192	Y193	R194	D196	I196	V197	K198	A199	Y200	D204	E207	A208	R209	K210	K211	M216	L217	L218	C219	L224	S227	N229	A230	C231	Q232	V233	I234	L235	K236			
K92	R93	F94	E99	V104	H105	M106	T107	C108	F109	G110	T111	G112	V113	K114	V115	C116	K117	Y118	Q119	D120	G121	K122	Y123	V124	T125	V126	D127	S128	V129	E130	K131	D132	I133	A134	D135	I136	D141	W142	M145	I146	D147	Y148	F149	S150	L151	P152	V153	D157	I158	G162	D165	V166		

4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.84Å 174.84Å 300.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.20 19.95 – 3.20	Depositor EDS
% Data completeness (in resolution range)	84.5 (20.00-3.20) 84.5 (19.95-3.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.22Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.167 , 0.243 0.166 , 0.241	Depositor DCC
R_{free} test set	7479 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtrriage
Anisotropy	0.517	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 77.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22891	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BG3, NA, GOL

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	0.34	0/3840	0.61	0/5209
1	B	0.35	0/3840	0.63	0/5209
1	C	0.33	0/3832	0.60	0/5199
1	D	0.34	0/3840	0.62	0/5209
1	E	0.34	0/3840	0.62	0/5209
1	F	0.35	0/3840	0.60	0/5209
All	All	0.34	0/23032	0.61	0/31244

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3765	0	3762	256	0
1	B	3765	0	3762	227	0
1	C	3757	0	3753	274	0
1	D	3765	0	3762	242	0
1	E	3765	0	3762	243	0
1	F	3765	0	3762	288	0
2	A	12	0	10	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	9	2	0
2	C	12	0	10	1	0
2	D	12	0	10	0	0
2	E	12	0	10	0	0
2	F	12	0	10	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	12	0	16	3	0
4	B	12	0	16	3	0
4	C	6	0	8	5	0
4	D	18	0	24	9	0
4	E	12	0	16	0	0
4	F	6	0	8	7	0
5	A	30	0	0	3	0
5	B	28	0	0	1	0
5	C	23	0	0	3	0
5	D	29	0	0	4	0
5	E	25	0	0	3	0
5	F	30	0	0	3	0
All	All	22891	0	22710	1416	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 31.

All (1416) 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:C:368:MET:HG2	1:C:369:LEU:H	1.22	1.05
1:F:209:ARG:HH12	1:F:241:GLY:HA3	1.21	1.05
1:D:118:TYR:H	4:D:604:GOL:H12	1.23	1.03
1:B:377:MET:HE1	1:B:465:LEU:HD11	1.40	1.00
1:F:136:ILE:HG21	1:F:152:PRO:HG3	1.42	0.98
1:A:63:LYS:HG3	1:A:64:THR:HG23	1.45	0.98
1:B:430:TYR:HB3	1:B:431:PRO:HD3	1.48	0.95
1:F:209:ARG:NH1	1:F:241:GLY:HA3	1.82	0.93
1:B:217:LEU:HD11	1:B:247:LEU:HD22	1.50	0.92
1:D:218:LEU:HD21	1:D:246:VAL:HG22	1.52	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:473:ILE:HG21	1:E:481:MET:HE1	1.51	0.88
1:C:368:MET:HG2	1:C:369:LEU:N	1.88	0.88
1:F:209:ARG:HH12	1:F:241:GLY:CA	1.86	0.87
1:E:334:LYS:HB3	1:E:368:MET:HE1	1.57	0.87
1:A:342:ASP:HB3	1:F:453:LEU:HD23	1.53	0.87
1:C:174:ALA:HA	1:C:473:ILE:HD11	1.54	0.86
1:C:217:LEU:HD23	1:C:218:LEU:N	1.90	0.85
1:A:122:LYS:H	1:A:122:LYS:HD3	1.41	0.85
1:C:61:ASN:HD21	1:C:63:LYS:HE2	1.41	0.84
1:D:421:LEU:HD12	1:D:422:LYS:H	1.43	0.83
1:C:229:ASN:O	1:C:233:VAL:HG23	1.77	0.83
1:D:354:LEU:HB2	1:D:355:PRO:HD3	1.60	0.83
1:D:209:ARG:HB3	1:D:209:ARG:HH11	1.44	0.82
1:D:392:LYS:O	1:D:395:GLN:HB3	1.79	0.81
1:B:251:MET:HE2	1:B:296:PHE:HB2	1.59	0.81
1:E:339:VAL:HG23	1:E:340:PRO:HD2	1.62	0.81
1:C:145:ASN:H	1:C:384:ASN:HD21	1.27	0.81
1:C:210:LYS:O	1:C:211:LYS:HG3	1.81	0.80
1:A:61:ASN:OD1	1:A:63:LYS:HG2	1.82	0.79
1:F:171:THR:HB	1:F:172:PRO:HD3	1.64	0.79
1:A:111:THR:HB	1:A:151:LEU:O	1.83	0.79
1:A:437:LEU:HD22	1:F:343:GLN:HG3	1.64	0.79
1:B:50:ARG:HH21	1:B:65:ASN:ND2	1.79	0.79
1:F:377:MET:HE3	1:F:465:LEU:HD11	1.65	0.79
1:D:473:ILE:HD13	1:D:481:MET:HE1	1.65	0.78
1:C:117:LYS:HB2	4:C:603:GOL:H12	1.64	0.78
1:D:171:THR:HB	1:D:172:PRO:HD3	1.65	0.78
1:F:118:TYR:H	4:F:603:GOL:H31	1.48	0.78
1:C:337:ALA:HB2	1:C:343:GLN:HE21	1.48	0.78
1:E:61:ASN:OD1	1:E:63:LYS:HG2	1.83	0.78
1:B:369:LEU:HD12	1:B:376:SER:HB2	1.66	0.78
1:E:430:TYR:HB3	1:E:431:PRO:HD3	1.65	0.78
1:D:332:GLY:HA3	1:D:363:ILE:CG2	2.13	0.77
1:F:473:ILE:HG21	1:F:481:MET:HE3	1.65	0.77
1:D:218:LEU:HD22	1:D:234:ILE:HG12	1.65	0.77
1:A:309:GLU:O	1:A:313:ILE:HG13	1.84	0.77
1:B:218:LEU:HD22	1:B:234:ILE:HG12	1.67	0.76
1:A:113:VAL:HG23	1:A:114:LYS:HG3	1.67	0.76
1:A:118:TYR:H	4:A:604:GOL:H12	1.50	0.76
1:E:171:THR:HB	1:E:172:PRO:HD3	1.68	0.76
1:E:245:ASN:HA	1:E:288:TRP:HB2	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:LEU:HD11	1:E:234:ILE:HD11	1.66	0.76
1:B:493:ARG:C	1:B:495:MET:H	1.89	0.76
1:C:136:ILE:HG21	1:C:152:PRO:HB3	1.66	0.76
1:B:50:ARG:HH21	1:B:65:ASN:HD21	1.33	0.76
1:F:422:LYS:HA	1:F:425:ARG:NH1	2.01	0.76
1:C:297:ASP:HB2	1:C:304:PRO:HD3	1.66	0.75
1:F:26:LEU:HD13	1:F:323:PHE:CD1	2.21	0.75
1:A:218:LEU:HD12	1:A:230:ALA:HB1	1.67	0.75
1:A:343:GLN:HG3	1:F:437:LEU:HD22	1.68	0.75
1:E:421:LEU:HD12	1:E:422:LYS:N	2.01	0.75
1:E:205:GLU:HG3	1:E:209:ARG:HD2	1.67	0.75
1:F:377:MET:HE2	4:F:603:GOL:H11	1.68	0.75
1:E:318:ALA:O	1:E:322:GLN:HG3	1.87	0.75
1:B:453:LEU:HD22	1:E:343:GLN:HB2	1.68	0.74
1:D:229:ASN:O	1:D:233:VAL:HG23	1.87	0.74
1:F:245:ASN:HA	1:F:288:TRP:HB2	1.69	0.74
1:B:245:ASN:HA	1:B:288:TRP:HB2	1.69	0.74
1:B:4:ASN:HD22	1:C:105:HIS:CE1	2.05	0.74
1:C:453:LEU:HD23	1:D:342:ASP:HB3	1.70	0.74
1:A:4:ASN:HD22	1:D:105:HIS:CE1	2.05	0.73
1:D:63:LYS:HG3	1:D:64:THR:HG23	1.68	0.73
1:A:298:LEU:HD12	1:F:428:VAL:HA	1.70	0.73
1:B:162:GLY:HA2	1:B:492:PHE:HD2	1.53	0.73
1:F:251:MET:CE	1:F:303:ALA:HB2	2.18	0.73
1:B:331:ALA:HB1	1:B:334:LYS:HE3	1.71	0.73
1:C:91:ASP:HB2	1:C:177:ALA:HB1	1.70	0.73
1:F:492:PHE:O	1:F:495:MET:HG2	1.89	0.73
1:B:118:TYR:OH	1:B:121:GLY:HA2	1.88	0.72
1:B:318:ALA:O	1:B:322:GLN:HG3	1.89	0.72
1:C:251:MET:HE2	1:C:296:PHE:HB2	1.70	0.72
1:A:35:GLU:HB2	1:E:84:ARG:CZ	2.18	0.72
1:A:11:ASN:HD22	1:A:11:ASN:H	1.35	0.72
1:C:171:THR:HB	1:C:172:PRO:HD3	1.72	0.72
1:E:339:VAL:CG2	1:E:340:PRO:HD2	2.20	0.72
1:F:251:MET:HE3	1:F:303:ALA:HB2	1.72	0.71
1:A:84:ARG:CB	1:A:99:GLU:HB2	2.21	0.70
1:F:229:ASN:O	1:F:233:VAL:HG23	1.89	0.70
1:B:435:MET:HG2	1:B:436:LEU:CD1	2.21	0.70
1:D:245:ASN:HA	1:D:288:TRP:HB2	1.73	0.70
1:F:250:ALA:HB3	1:F:293:THR:HG23	1.73	0.70
1:B:209:ARG:HH11	1:B:209:ARG:HB3	1.56	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:LYS:HG3	1:B:425:ARG:HH22	1.56	0.70
1:F:117:LYS:HB3	4:F:603:GOL:H12	1.73	0.70
1:F:145:ASN:HB2	1:F:384:ASN:ND2	2.06	0.70
1:A:44:VAL:HB	1:A:50:ARG:HG3	1.73	0.70
1:A:108:CYS:HA	1:A:366:ALA:HB3	1.73	0.70
1:F:53:PHE:O	1:F:58:CYS:HB2	1.92	0.70
1:B:171:THR:HB	1:B:172:PRO:HD3	1.74	0.70
1:D:37:LEU:HD23	1:D:42:ILE:HD11	1.73	0.69
1:A:171:THR:HB	1:A:172:PRO:HD3	1.75	0.69
1:F:174:ALA:HA	1:F:473:ILE:HD11	1.73	0.69
1:F:218:LEU:C	1:F:218:LEU:HD12	2.13	0.69
1:E:251:MET:CE	1:E:303:ALA:HB2	2.22	0.69
1:F:145:ASN:H	1:F:384:ASN:HD21	1.40	0.69
1:D:111:THR:HG21	1:D:184:ASP:OD2	1.92	0.69
1:A:439:ARG:HB2	1:F:300:LYS:HE2	1.74	0.69
1:A:453:LEU:HD23	1:F:342:ASP:HB3	1.75	0.69
1:F:334:LYS:HD3	1:F:368:MET:HE1	1.75	0.69
1:A:386:ILE:O	1:A:390:VAL:HG23	1.92	0.69
1:B:218:LEU:HD12	1:B:219:CYS:N	2.07	0.69
1:D:122:LYS:HD3	1:D:122:LYS:H	1.57	0.69
1:C:311:GLY:HA3	1:C:354:LEU:HD12	1.75	0.69
1:C:406:VAL:HG11	1:D:35:GLU:OE1	1.93	0.69
1:D:421:LEU:HD12	1:D:422:LYS:N	2.08	0.68
1:D:148:TYR:OH	1:D:362:THR:HG21	1.93	0.68
1:D:281:THR:HG22	1:D:282:VAL:HG23	1.75	0.68
1:E:145:ASN:H	1:E:384:ASN:HD21	1.41	0.68
1:E:231:CYS:O	1:E:235:ILE:HG13	1.92	0.68
1:A:148:TYR:OH	1:A:362:THR:HG21	1.92	0.68
1:E:354:LEU:HB2	1:E:355:PRO:HD3	1.73	0.68
1:F:118:TYR:OH	1:F:121:GLY:HA2	1.92	0.68
1:A:473:ILE:HG21	1:A:481:MET:CE	2.23	0.68
1:B:41:GLY:O	1:E:414:ILE:HD11	1.94	0.68
1:D:473:ILE:HG21	1:D:481:MET:HE2	1.76	0.68
1:F:136:ILE:HD12	1:F:375:PHE:CE1	2.29	0.68
1:B:281:THR:HG22	1:B:282:VAL:HG23	1.75	0.68
1:C:430:TYR:HB3	1:C:431:PRO:HD3	1.75	0.68
1:D:117:LYS:HA	4:D:604:GOL:H31	1.76	0.68
1:A:346:HIS:CE1	1:F:386:ILE:HG23	2.28	0.68
1:B:422:LYS:HA	1:B:425:ARG:NH1	2.09	0.68
1:E:186:VAL:HB	1:E:189:ASN:HD22	1.58	0.68
1:A:281:THR:HG22	1:A:282:VAL:HG23	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ASN:ND2	1:D:103:LYS:HB3	2.09	0.67
1:F:354:LEU:HB2	1:F:355:PRO:HD3	1.74	0.67
1:B:435:MET:HG2	1:B:436:LEU:HD13	1.77	0.67
1:D:113:VAL:HG23	1:D:114:LYS:HG3	1.75	0.67
1:D:174:ALA:HA	1:D:473:ILE:HD11	1.75	0.67
1:A:421:LEU:HD12	1:A:422:LYS:N	2.10	0.67
1:F:332:GLY:O	1:F:333:SER:HB3	1.94	0.67
1:B:331:ALA:HB2	1:B:364:TYR:CE1	2.29	0.67
1:D:218:LEU:HD22	1:D:234:ILE:CG1	2.25	0.67
1:F:435:MET:HG2	1:F:436:LEU:HD12	1.76	0.67
1:B:84:ARG:HG2	5:D:717:HOH:O	1.93	0.67
1:E:51:GLN:O	1:E:55:GLU:HG3	1.95	0.67
1:F:136:ILE:CG2	1:F:152:PRO:HG3	2.21	0.67
1:A:349:THR:HA	1:A:352:THR:HG22	1.75	0.67
1:B:61:ASN:OD1	1:B:63:LYS:HG2	1.95	0.67
1:B:21:PHE:HE1	1:E:397:ILE:HG21	1.60	0.67
1:C:190:VAL:HA	1:C:193:TYR:CD2	2.30	0.67
1:A:105:HIS:NE2	1:D:4:ASN:HB2	2.10	0.66
1:A:460:LYS:O	1:A:464:VAL:HG23	1.95	0.66
1:A:477:ILE:HG22	1:A:481:MET:HE2	1.75	0.66
1:C:231:CYS:O	1:C:235:ILE:HG13	1.95	0.66
1:A:354:LEU:HB2	1:A:355:PRO:HD3	1.77	0.66
1:E:108:CYS:HA	1:E:366:ALA:HB3	1.78	0.66
1:C:298:LEU:O	1:C:299:LYS:HG3	1.95	0.66
1:C:304:PRO:HB3	1:D:439:ARG:HD3	1.77	0.66
1:F:460:LYS:O	1:F:464:VAL:HG23	1.94	0.66
1:E:50:ARG:HG2	1:E:60:VAL:HG11	1.77	0.66
1:E:332:GLY:HA3	1:E:363:ILE:HG23	1.77	0.66
1:D:313:ILE:O	1:D:317:VAL:HG23	1.95	0.66
1:F:377:MET:CE	1:F:465:LEU:HD11	2.26	0.66
1:F:189:ASN:HB3	1:F:192:TYR:HD2	1.61	0.66
1:F:190:VAL:HA	1:F:193:TYR:CD2	2.30	0.66
1:C:129:VAL:HG22	1:C:132:ASP:OD2	1.95	0.65
1:F:458:HIS:O	1:F:462:GLU:HG2	1.96	0.65
1:A:134:ALA:HA	1:A:175:ASN:ND2	2.11	0.65
1:E:421:LEU:HD12	1:E:422:LYS:H	1.60	0.65
1:A:148:TYR:HH	1:A:362:THR:HG21	1.61	0.65
1:C:247:LEU:HD21	1:C:292:SER:HB2	1.79	0.65
1:C:354:LEU:HB2	1:C:355:PRO:HD3	1.77	0.65
1:D:473:ILE:HG21	1:D:481:MET:CE	2.26	0.65
1:E:234:ILE:CG2	1:E:278:ALA:HB2	2.27	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:GLY:HA2	1:B:492:PHE:CD2	2.32	0.65
1:C:136:ILE:HG21	1:C:152:PRO:CB	2.26	0.65
1:C:474:ASP:HB3	1:C:477:ILE:HB	1.78	0.65
1:A:222:SER:HA	1:A:270:GLU:OE2	1.97	0.65
1:B:369:LEU:HD12	1:B:376:SER:CB	2.28	0.65
1:C:267:HIS:CE1	1:C:271:VAL:HG21	2.32	0.65
1:D:94:PHE:CE1	1:D:178:LYS:HE2	2.32	0.65
1:F:473:ILE:HG21	1:F:481:MET:CE	2.26	0.65
1:F:477:ILE:HG22	1:F:481:MET:HE2	1.79	0.65
1:A:430:TYR:HB3	1:A:431:PRO:HD3	1.79	0.64
1:B:422:LYS:HG3	1:B:425:ARG:NH2	2.11	0.64
1:C:245:ASN:HA	1:C:288:TRP:HB2	1.79	0.64
1:E:251:MET:HE2	1:E:303:ALA:HB2	1.79	0.64
1:B:190:VAL:HA	1:B:193:TYR:CD2	2.33	0.64
1:B:252:SER:OG	1:B:295:THR:HA	1.96	0.64
1:E:63:LYS:HG3	1:E:64:THR:HG23	1.79	0.64
1:E:63:LYS:HG3	1:E:64:THR:N	2.11	0.64
1:C:331:ALA:HB1	1:C:334:LYS:HE3	1.79	0.64
1:C:369:LEU:HD12	1:C:376:SER:HB2	1.78	0.64
1:D:452:ASP:O	1:D:456:VAL:HG23	1.97	0.64
1:F:348:LYS:HD2	1:F:383:ASP:OD1	1.98	0.64
1:A:309:GLU:OE2	1:F:392:LYS:HE2	1.98	0.64
1:B:42:ILE:HD12	1:B:273:SER:HB3	1.79	0.64
1:C:373:MET:HA	1:C:373:MET:HE2	1.78	0.64
1:D:84:ARG:NH2	1:F:35:GLU:HG3	2.13	0.64
1:C:61:ASN:ND2	1:C:63:LYS:HE2	2.12	0.64
1:D:286:LYS:HE2	5:D:718:HOH:O	1.97	0.64
1:A:473:ILE:HD13	1:A:481:MET:HE3	1.80	0.64
1:E:4:ASN:HD22	1:F:105:HIS:CE1	2.15	0.64
1:F:368:MET:HG2	1:F:369:LEU:N	2.13	0.64
1:B:343:GLN:HG3	1:E:437:LEU:HD22	1.79	0.63
1:C:350:MET:HE2	1:C:354:LEU:HD11	1.78	0.63
1:D:117:LYS:HD2	1:D:126:VAL:HG21	1.79	0.63
1:F:421:LEU:HD12	1:F:422:LYS:H	1.62	0.63
1:C:61:ASN:OD1	1:C:63:LYS:HG2	1.97	0.63
1:C:247:LEU:HD21	1:C:292:SER:CB	2.29	0.63
1:B:434:PRO:HB3	1:B:437:LEU:HD12	1.80	0.63
1:E:247:LEU:HD23	1:E:248:SER:O	1.99	0.63
1:A:170:LEU:HD22	1:A:485:VAL:HG21	1.80	0.63
1:C:53:PHE:CZ	1:C:277:LEU:HB2	2.33	0.63
1:B:119:GLN:HG3	1:B:120:ASP:OD1	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:VAL:CG2	1:B:340:PRO:HD2	2.29	0.63
1:C:162:GLY:HA2	1:C:492:PHE:CD2	2.33	0.63
1:A:42:ILE:HD12	1:A:273:SER:HB3	1.79	0.63
1:A:353:LEU:HD23	1:F:353:LEU:HD23	1.80	0.63
1:B:332:GLY:O	1:B:333:SER:HB3	1.99	0.63
1:D:114:LYS:NZ	1:D:125:THR:HG21	2.14	0.63
1:E:221:THR:HB	1:E:225:GLU:HB2	1.80	0.63
1:D:114:LYS:HZ1	1:D:125:THR:HG21	1.63	0.63
1:B:14:ASN:HD22	1:C:10:PHE:HD2	1.46	0.62
1:C:400:SER:OG	1:C:403:THR:HG23	1.98	0.62
1:E:198:LYS:HE3	1:E:203:GLY:O	1.99	0.62
1:E:381:VAL:CG2	1:E:457:ALA:HB1	2.29	0.62
1:E:348:LYS:O	1:E:352:THR:HG22	1.98	0.62
1:F:136:ILE:HG21	1:F:152:PRO:CG	2.25	0.62
1:C:64:THR:O	1:C:65:ASN:HB2	1.98	0.62
1:C:148:TYR:HB2	1:C:179:HIS:HB3	1.80	0.62
1:E:332:GLY:O	1:E:333:SER:HB3	1.99	0.62
1:C:305:VAL:HG22	1:C:310:LEU:HD22	1.80	0.62
1:C:337:ALA:CB	1:C:343:GLN:HE21	2.12	0.62
1:C:422:LYS:O	1:C:426:GLN:HG3	2.00	0.62
1:A:98:GLN:HG3	1:A:288:TRP:HZ2	1.65	0.62
1:D:105:HIS:O	1:D:362:THR:HA	1.99	0.62
1:A:190:VAL:HA	1:A:193:TYR:CD2	2.34	0.62
1:B:349:THR:HA	1:B:352:THR:HG22	1.82	0.62
1:E:477:ILE:HA	1:E:480:ASP:OD2	2.00	0.62
1:C:460:LYS:O	1:C:464:VAL:HG23	1.99	0.62
1:F:217:LEU:HD23	1:F:218:LEU:N	2.14	0.62
1:A:473:ILE:HD13	1:A:481:MET:CE	2.30	0.62
1:B:251:MET:HE1	1:B:296:PHE:HD1	1.65	0.62
1:D:440:HIS:HB3	1:D:444:ASP:HB2	1.82	0.61
1:A:217:LEU:O	1:A:217:LEU:HD23	2.00	0.61
1:C:435:MET:HG2	1:C:436:LEU:HD12	1.81	0.61
1:F:172:PRO:O	1:F:176:THR:HG22	1.99	0.61
1:B:145:ASN:H	1:B:384:ASN:HD21	1.46	0.61
1:A:191:GLU:HG3	1:A:240:PHE:CZ	2.35	0.61
1:B:319:LYS:HE2	1:B:358:ALA:HB1	1.82	0.61
1:F:42:ILE:CD1	1:F:273:SER:HB3	2.30	0.61
1:F:217:LEU:HD11	1:F:247:LEU:HD13	1.81	0.61
1:A:120:ASP:HB2	1:A:122:LYS:HE2	1.83	0.61
1:E:96:THR:HG23	1:E:105:HIS:CD2	2.36	0.61
1:C:86:VAL:HG13	1:C:88:TRP:HE1	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:THR:HG23	1:D:105:HIS:CD2	2.35	0.61
1:D:109:PHE:HB2	1:D:368:MET:HB2	1.82	0.61
1:B:428:VAL:HG23	1:E:298:LEU:HB3	1.83	0.61
1:E:332:GLY:HA3	1:E:363:ILE:CG2	2.31	0.61
1:F:190:VAL:HG11	1:F:236:LYS:HB3	1.81	0.61
1:F:250:ALA:HB3	1:F:293:THR:CG2	2.30	0.61
1:F:305:VAL:CG2	1:F:334:LYS:HD2	2.31	0.61
1:D:460:LYS:O	1:D:464:VAL:HG23	2.01	0.61
1:A:11:ASN:HD22	1:A:11:ASN:N	1.98	0.61
1:A:235:ILE:HG12	1:A:277:LEU:HD21	1.82	0.61
1:B:305:VAL:O	1:B:310:LEU:HD22	2.00	0.61
1:B:414:ILE:HG23	1:E:224:LEU:O	2.00	0.61
1:C:116:CYS:HB2	1:C:374:THR:HG21	1.83	0.61
1:C:309:GLU:CD	1:D:392:LYS:HE2	2.21	0.61
1:A:313:ILE:O	1:A:317:VAL:HG23	2.01	0.60
1:C:45:SER:HB2	1:C:228:VAL:HG22	1.83	0.60
1:C:122:LYS:H	1:C:122:LYS:HD3	1.65	0.60
1:F:157:ASP:O	1:F:158:ILE:HD13	2.00	0.60
1:F:218:LEU:HD13	1:F:230:ALA:HB1	1.82	0.60
1:B:249:MET:HE1	2:B:601:BG3:H42	1.82	0.60
1:B:309:GLU:O	1:B:313:ILE:HG13	2.01	0.60
1:E:109:PHE:CB	1:E:368:MET:HB2	2.31	0.60
1:D:251:MET:HE2	1:D:296:PHE:HB2	1.82	0.60
1:F:193:TYR:O	1:F:197:VAL:HG23	2.01	0.60
1:A:61:ASN:HD21	1:A:63:LYS:HE2	1.67	0.60
1:D:37:LEU:CD2	1:D:42:ILE:HD11	2.31	0.60
1:B:377:MET:CE	4:B:603:GOL:H32	2.31	0.60
1:D:297:ASP:C	1:D:299:LYS:H	2.05	0.60
1:A:84:ARG:HB3	1:A:99:GLU:HB2	1.81	0.60
1:A:218:LEU:HD23	1:A:218:LEU:H	1.66	0.60
1:B:249:MET:HG2	1:B:292:SER:HB3	1.83	0.60
1:D:339:VAL:HG23	1:D:340:PRO:HD2	1.83	0.60
1:F:118:TYR:N	4:F:603:GOL:H31	2.17	0.60
1:B:75:ARG:NH2	1:F:83:SER:HB3	2.16	0.60
1:F:186:VAL:HB	1:F:189:ASN:ND2	2.16	0.60
1:B:132:ASP:O	1:B:136:ILE:HG12	2.02	0.60
1:E:217:LEU:HD23	1:E:218:LEU:N	2.16	0.60
1:F:70:PRO:HD2	1:F:73:LEU:HD12	1.83	0.60
1:F:107:THR:HG23	1:F:364:TYR:HB2	1.84	0.60
1:F:281:THR:HG22	1:F:282:VAL:HG23	1.84	0.60
1:C:118:TYR:H	4:C:603:GOL:C1	2.14	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:CYS:O	1:D:235:ILE:HG13	2.01	0.60
1:A:70:PRO:HG2	1:A:73:LEU:HG	1.84	0.59
1:B:259:TYR:CD2	1:E:403:THR:HA	2.37	0.59
1:E:289:TYR:HE1	1:E:317:VAL:HG13	1.67	0.59
1:C:305:VAL:HG21	2:C:601:BG3:H62	1.83	0.59
1:F:377:MET:CE	4:F:603:GOL:H11	2.31	0.59
1:B:50:ARG:HG2	1:B:60:VAL:HG11	1.85	0.59
1:D:239:ARG:HA	1:D:282:VAL:HG21	1.84	0.59
1:A:245:ASN:C	1:A:245:ASN:HD22	2.04	0.59
1:A:466:LYS:O	1:A:466:LYS:HG2	2.01	0.59
1:B:70:PRO:HD2	1:B:73:LEU:HD12	1.85	0.59
1:B:305:VAL:HG22	1:B:310:LEU:HD22	1.84	0.59
1:B:473:ILE:HD13	1:B:481:MET:CE	2.33	0.59
1:D:218:LEU:CD2	1:D:234:ILE:HG12	2.33	0.59
1:D:266:THR:O	1:D:270:GLU:HG3	2.02	0.59
1:E:114:LYS:HD2	1:E:125:THR:HG22	1.84	0.59
1:A:391:LYS:HG2	1:D:6:ALA:HB2	1.84	0.59
1:D:162:GLY:HA2	1:D:492:PHE:CD2	2.37	0.59
1:A:11:ASN:N	1:A:11:ASN:ND2	2.50	0.59
1:A:386:ILE:HG23	1:F:346:HIS:CE1	2.37	0.59
1:B:84:ARG:CZ	1:D:35:GLU:HB2	2.32	0.59
1:B:194:ARG:HG2	1:B:194:ARG:HH11	1.66	0.59
1:C:199:ALA:HB3	1:C:481:MET:HG2	1.84	0.59
1:A:266:THR:O	1:A:270:GLU:HG3	2.03	0.59
1:B:44:VAL:HG21	1:B:53:PHE:CE2	2.37	0.59
1:C:73:LEU:HD22	1:C:280:LEU:HD11	1.84	0.59
1:D:158:ILE:HB	1:D:164:GLN:HG3	1.84	0.59
1:E:377:MET:SD	1:E:465:LEU:HD11	2.42	0.59
1:F:234:ILE:HG23	1:F:278:ALA:HB2	1.84	0.59
1:B:473:ILE:HD13	1:B:481:MET:HE2	1.85	0.59
1:C:129:VAL:HG23	1:C:131:LYS:H	1.67	0.59
1:D:136:ILE:HD12	1:D:375:PHE:CE1	2.38	0.59
1:F:320:LEU:O	1:F:323:PHE:HB3	2.03	0.59
1:D:338:LYS:HG3	1:D:370:GLU:HG3	1.85	0.59
1:D:162:GLY:HA2	1:D:492:PHE:HD2	1.67	0.58
1:C:247:LEU:HD23	1:C:248:SER:O	2.03	0.58
1:E:314:SER:HB3	1:E:330:VAL:CG2	2.32	0.58
1:F:170:LEU:HD22	1:F:485:VAL:HG21	1.85	0.58
1:F:421:LEU:HD12	1:F:422:LYS:N	2.18	0.58
1:A:339:VAL:HG23	1:A:340:PRO:HD2	1.86	0.58
1:C:489:ASP:O	1:C:492:PHE:HB3	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:ALA:O	1:D:234:ILE:HG13	2.03	0.58
1:E:105:HIS:CE1	1:F:4:ASN:HD22	2.21	0.58
1:F:192:TYR:O	1:F:196:ILE:HG13	2.03	0.58
1:A:344:ALA:HB3	1:F:342:ASP:OD1	2.03	0.58
1:E:128:SER:O	1:E:156:ARG:HG3	2.03	0.58
1:D:92:LYS:HA	1:D:95:ASN:OD1	2.04	0.58
1:D:217:LEU:C	1:D:217:LEU:HD23	2.24	0.58
1:B:354:LEU:HB2	1:B:355:PRO:HD3	1.84	0.58
1:F:297:ASP:OD1	1:F:299:LYS:HB2	2.04	0.58
1:A:118:TYR:OH	1:A:121:GLY:HA2	2.04	0.58
1:A:392:LYS:HE2	1:F:309:GLU:OE2	2.04	0.58
1:B:148:TYR:OH	1:B:362:THR:HG21	2.03	0.58
1:F:305:VAL:HG22	1:F:334:LYS:HD2	1.85	0.58
1:A:9:GLY:HA3	1:D:17:GLU:HG3	1.86	0.58
1:E:448:ALA:O	1:E:451:LYS:HE3	2.03	0.58
1:F:448:ALA:O	1:F:451:LYS:HE3	2.04	0.58
1:B:460:LYS:O	1:B:464:VAL:HG23	2.03	0.58
1:C:437:LEU:HD22	1:D:343:GLN:HG3	1.85	0.58
1:C:318:ALA:O	1:C:322:GLN:HG3	2.04	0.57
1:F:22:THR:OG1	1:F:25:GLU:HG3	2.03	0.57
1:B:218:LEU:HD22	1:B:234:ILE:CG1	2.33	0.57
1:B:437:LEU:HD22	1:E:343:GLN:HG3	1.84	0.57
1:C:271:VAL:O	1:C:275:ILE:HG13	2.04	0.57
1:D:117:LYS:HB3	4:D:604:GOL:H31	1.86	0.57
1:E:60:VAL:HG22	1:E:67:VAL:HG13	1.86	0.57
1:E:187:GLY:O	1:E:190:VAL:HG23	2.03	0.57
1:A:339:VAL:CG2	1:A:340:PRO:HD2	2.34	0.57
1:E:119:GLN:HB3	1:E:122:LYS:HE3	1.87	0.57
1:E:148:TYR:OH	1:E:362:THR:HG21	2.05	0.57
1:F:94:PHE:HE2	1:F:177:ALA:HB3	1.68	0.57
1:A:245:ASN:HA	1:A:288:TRP:HB2	1.87	0.57
1:C:346:HIS:CE1	1:D:386:ILE:HG23	2.40	0.57
1:A:84:ARG:HB2	1:A:99:GLU:HB2	1.86	0.57
1:B:309:GLU:OE2	1:E:392:LYS:HE2	2.05	0.57
1:C:373:MET:HA	1:C:373:MET:CE	2.35	0.57
1:F:104:VAL:HG22	1:F:360:ALA:O	2.05	0.57
1:A:51:GLN:O	1:A:55:GLU:HG3	2.04	0.57
1:B:80:LEU:HD13	1:B:283:PRO:HB3	1.86	0.57
1:B:314:SER:O	1:B:330:VAL:HG11	2.05	0.57
1:D:109:PHE:CD1	1:D:110:GLY:N	2.73	0.57
1:A:232:GLN:NE2	1:A:236:LYS:HE3	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:458:HIS:HE1	4:F:603:GOL:H32	1.70	0.56
1:B:448:ALA:O	1:B:451:LYS:HE3	2.05	0.56
1:A:98:GLN:HG3	1:A:288:TRP:CZ2	2.40	0.56
1:A:421:LEU:HD12	1:A:422:LYS:H	1.70	0.56
1:B:307:SER:HB2	1:B:308:PRO:HD2	1.87	0.56
1:C:453:LEU:HD22	1:D:343:GLN:HB2	1.86	0.56
1:D:218:LEU:HD13	1:D:230:ALA:HB1	1.87	0.56
1:E:307:SER:HB2	1:E:308:PRO:HD2	1.87	0.56
1:F:111:THR:HG23	1:F:111:THR:O	2.05	0.56
1:B:21:PHE:HE1	1:E:397:ILE:CG2	2.18	0.56
1:C:118:TYR:H	4:C:603:GOL:H12	1.69	0.56
1:A:122:LYS:H	1:A:122:LYS:CD	2.16	0.56
1:D:118:TYR:OH	1:D:121:GLY:HA2	2.06	0.56
1:D:118:TYR:N	4:D:604:GOL:H12	2.07	0.56
1:F:305:VAL:HG23	1:F:310:LEU:HD13	1.87	0.56
1:B:13:LEU:HD23	1:E:20:LEU:C	2.26	0.56
1:E:42:ILE:HD12	1:E:273:SER:HB3	1.88	0.56
1:E:112:GLY:O	1:E:153:VAL:HA	2.06	0.56
1:A:223:PRO:HB3	1:A:255:SER:O	2.06	0.56
1:A:290:GLY:HA2	1:A:329:TYR:O	2.06	0.56
1:E:473:ILE:HD13	1:E:481:MET:CE	2.36	0.56
1:B:173:LEU:HD22	1:B:213:ILE:HD12	1.88	0.56
1:C:216:MET:HE2	1:C:242:ILE:HG21	1.87	0.56
1:F:151:LEU:H	1:F:180:PHE:HE1	1.54	0.56
1:A:8:ALA:HA	5:A:705:HOH:O	2.05	0.56
1:B:251:MET:HE1	1:B:303:ALA:HB2	1.88	0.56
1:B:392:LYS:HG2	1:B:432:SER:HB3	1.87	0.56
1:B:258:VAL:HB	1:E:427:LEU:HD12	1.87	0.55
1:C:245:ASN:C	1:C:245:ASN:HD22	2.10	0.55
1:B:186:VAL:HB	1:B:189:ASN:HD22	1.71	0.55
1:B:342:ASP:HB3	1:E:453:LEU:HD23	1.89	0.55
1:C:473:ILE:HG21	1:C:481:MET:CE	2.36	0.55
1:D:51:GLN:HE21	1:D:55:GLU:HG3	1.71	0.55
1:E:94:PHE:HB3	1:E:178:LYS:HG2	1.89	0.55
1:E:100:CYS:SG	1:E:325:GLY:HA2	2.46	0.55
1:E:190:VAL:HA	1:E:193:TYR:CD2	2.41	0.55
1:E:310:LEU:HD11	1:E:331:ALA:HB3	1.87	0.55
1:F:429:ASP:HB2	5:F:703:HOH:O	2.07	0.55
1:B:387:PHE:O	1:B:391:LYS:HG3	2.06	0.55
1:C:148:TYR:HH	1:C:329:TYR:HE2	1.53	0.55
1:C:201:TYR:OH	1:C:213:ILE:HG23	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:LEU:HD13	1:C:380:LEU:C	2.27	0.55
1:A:111:THR:HG22	1:A:183:ILE:HB	1.88	0.55
1:C:370:GLU:O	1:C:372:GLY:N	2.39	0.55
1:E:143:ALA:HB1	1:E:384:ASN:ND2	2.21	0.55
1:E:368:MET:SD	1:E:369:LEU:N	2.80	0.55
1:F:70:PRO:HG2	1:F:73:LEU:HG	1.87	0.55
1:B:339:VAL:HG23	1:B:340:PRO:HD2	1.88	0.55
1:C:474:ASP:OD2	1:C:477:ILE:HG12	2.06	0.55
1:E:158:ILE:HG22	1:E:158:ILE:O	2.07	0.55
1:E:309:GLU:O	1:E:313:ILE:HG13	2.07	0.55
1:F:210:LYS:HG2	1:F:211:LYS:HG3	1.87	0.55
1:B:64:THR:OG1	1:B:66:VAL:HG23	2.05	0.55
1:E:50:ARG:HG2	1:E:60:VAL:CG1	2.37	0.55
1:F:118:TYR:CZ	1:F:121:GLY:HA2	2.41	0.55
1:C:221:THR:O	1:C:225:GLU:HB2	2.07	0.55
1:D:94:PHE:CD1	1:D:178:LYS:HG2	2.41	0.55
1:D:446:ALA:HA	1:D:450:SER:OG	2.06	0.55
1:E:45:SER:HA	1:E:65:ASN:HD22	1.71	0.55
1:E:136:ILE:HD12	1:E:375:PHE:CE1	2.42	0.55
1:F:142:TRP:HB2	1:F:468:HIS:CD2	2.41	0.55
1:F:339:VAL:HG23	1:F:340:PRO:HD2	1.88	0.55
1:F:435:MET:HG2	1:F:436:LEU:CD1	2.37	0.55
1:D:149:PHE:CZ	1:D:152:PRO:HD3	2.42	0.55
1:E:109:PHE:HB2	1:E:368:MET:HB2	1.88	0.55
1:A:218:LEU:HD13	1:A:234:ILE:HG13	1.89	0.55
1:D:109:PHE:CG	1:D:368:MET:HB2	2.41	0.55
1:A:187:GLY:O	1:A:190:VAL:HG23	2.06	0.55
1:B:18:LEU:HD21	1:E:16:VAL:HG13	1.89	0.55
1:B:158:ILE:HG21	1:B:167:HIS:CD2	2.41	0.55
1:E:407:GLU:HA	5:E:702:HOH:O	2.07	0.55
1:B:305:VAL:HG21	2:B:601:BG3:H62	1.89	0.54
1:C:107:THR:HG23	1:C:364:TYR:HB2	1.90	0.54
1:C:215:SER:HB2	1:C:243:PRO:HB2	1.88	0.54
1:F:85:PHE:CD2	1:F:286:LYS:HB3	2.42	0.54
1:A:118:TYR:HB3	4:A:604:GOL:O1	2.07	0.54
1:B:377:MET:CE	1:B:465:LEU:HD11	2.27	0.54
1:C:236:LYS:HB3	1:C:240:PHE:CE2	2.43	0.54
1:D:190:VAL:HB	1:D:236:LYS:HD3	1.89	0.54
1:E:98:GLN:HG3	1:E:288:TRP:CZ2	2.42	0.54
1:A:258:VAL:HB	1:F:427:LEU:HD13	1.88	0.54
1:A:369:LEU:HD12	1:A:376:SER:HB2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:LEU:HD13	1:B:323:PHE:CD1	2.42	0.54
1:C:182:HIS:HB2	1:C:214:PHE:CE2	2.42	0.54
1:D:167:HIS:C	1:D:169:THR:H	2.11	0.54
1:A:251:MET:HA	1:A:294:THR:O	2.08	0.54
1:C:148:TYR:OH	1:C:362:THR:HG21	2.08	0.54
1:D:109:PHE:CB	1:D:368:MET:HB2	2.37	0.54
1:E:34:MET:SD	1:E:71:GLU:HG3	2.48	0.54
1:E:252:SER:HB2	1:E:295:THR:OG1	2.07	0.54
1:E:305:VAL:HG22	1:E:310:LEU:HD22	1.90	0.54
1:C:114:LYS:O	1:C:374:THR:HA	2.08	0.54
1:C:266:THR:O	1:C:270:GLU:HG3	2.08	0.54
1:C:406:VAL:HG23	5:C:712:HOH:O	2.08	0.54
1:D:42:ILE:N	1:D:42:ILE:HD12	2.22	0.54
1:B:418:PHE:HD1	1:B:418:PHE:H	1.54	0.54
1:C:201:TYR:HH	1:C:213:ILE:HG23	1.73	0.54
1:F:134:ALA:HA	1:F:175:ASN:ND2	2.22	0.54
1:A:100:CYS:SG	1:A:325:GLY:HA2	2.46	0.54
1:C:23:THR:HG22	1:C:27:LYS:HE3	1.89	0.54
1:E:217:LEU:HD11	1:E:247:LEU:HD13	1.89	0.54
1:D:305:VAL:HG22	1:D:310:LEU:HD22	1.89	0.54
1:C:209:ARG:NH1	1:C:241:GLY:HA3	2.22	0.53
1:C:309:GLU:OE2	1:D:392:LYS:HE2	2.08	0.53
1:D:114:LYS:HD2	1:D:125:THR:CG2	2.38	0.53
1:F:217:LEU:HD12	1:F:245:ASN:OD1	2.08	0.53
1:A:149:PHE:CZ	1:A:152:PRO:HD3	2.43	0.53
1:B:221:THR:O	1:B:225:GLU:HB2	2.08	0.53
1:C:312:LEU:HD11	1:D:393:ALA:HA	1.90	0.53
1:D:91:ASP:HB2	1:D:94:PHE:HD2	1.73	0.53
1:F:85:PHE:HB2	1:F:286:LYS:HD3	1.90	0.53
1:F:271:VAL:O	1:F:275:ILE:HG13	2.09	0.53
1:A:109:PHE:HB2	1:A:365:GLY:HA2	1.91	0.53
1:B:380:LEU:C	1:B:380:LEU:HD13	2.28	0.53
1:C:353:LEU:CD1	1:C:357:LEU:HG	2.39	0.53
1:D:94:PHE:CG	1:D:178:LYS:HG2	2.44	0.53
1:E:150:SER:O	1:E:152:PRO:HD3	2.08	0.53
1:F:480:ASP:O	1:F:483:ALA:HB3	2.07	0.53
1:B:494:GLY:O	1:B:495:MET:O	2.26	0.53
1:D:370:GLU:C	1:D:371:LEU:HD12	2.28	0.53
1:E:218:LEU:CD2	1:E:234:ILE:HG12	2.39	0.53
1:A:58:CYS:O	1:A:60:VAL:HG23	2.09	0.53
1:A:137:ALA:HB3	1:A:175:ASN:HB2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:CYS:SG	1:B:325:GLY:HA2	2.48	0.53
1:C:292:SER:HA	1:C:331:ALA:HB2	1.90	0.53
1:D:292:SER:HA	1:D:331:ALA:HB2	1.89	0.53
1:E:201:TYR:OH	1:E:213:ILE:HG23	2.08	0.53
1:E:223:PRO:HB3	1:E:255:SER:O	2.09	0.53
1:E:110:GLY:HA3	1:E:183:ILE:HG13	1.91	0.53
1:B:32:ALA:O	1:B:36:VAL:HG23	2.09	0.53
1:B:446:ALA:C	1:B:448:ALA:H	2.12	0.53
1:C:88:TRP:O	1:C:213:ILE:HA	2.08	0.53
1:C:440:HIS:NE2	1:D:300:LYS:HD2	2.23	0.53
1:D:250:ALA:O	1:D:293:THR:HG23	2.08	0.53
1:E:186:VAL:HB	1:E:189:ASN:ND2	2.22	0.53
1:E:411:LYS:NZ	1:E:421:LEU:HD13	2.23	0.53
1:F:109:PHE:CG	1:F:368:MET:HB2	2.44	0.53
1:F:305:VAL:O	1:F:310:LEU:HD22	2.08	0.53
1:B:218:LEU:HD23	1:B:244:VAL:CG1	2.39	0.53
1:C:90:ARG:N	1:C:177:ALA:O	2.41	0.53
1:C:156:ARG:C	1:C:158:ILE:H	2.13	0.53
1:C:422:LYS:HA	1:C:425:ARG:NH1	2.24	0.53
1:E:386:ILE:O	1:E:390:VAL:HG23	2.08	0.53
1:F:209:ARG:NH1	1:F:209:ARG:HG2	2.23	0.53
1:A:263:THR:CG2	1:A:293:THR:HG21	2.38	0.53
1:D:114:LYS:HE2	1:D:373:MET:CG	2.39	0.53
1:D:214:PHE:O	1:D:242:ILE:HG23	2.09	0.53
1:D:332:GLY:HA3	1:D:363:ILE:HG23	1.91	0.53
1:F:392:LYS:O	1:F:395:GLN:HB3	2.09	0.53
1:A:171:THR:HG23	1:A:175:ASN:HD21	1.74	0.53
1:B:4:ASN:ND2	1:C:103:LYS:HB3	2.23	0.53
1:B:48:GLU:HG2	1:B:235:ILE:HD13	1.91	0.53
1:E:26:LEU:HD13	1:E:323:PHE:CD1	2.43	0.53
1:E:84:ARG:HG3	1:E:84:ARG:HH11	1.73	0.53
1:A:217:LEU:HB2	1:A:245:ASN:HB3	1.90	0.52
1:A:463:ASP:O	1:A:467:ASN:HB2	2.09	0.52
1:E:128:SER:O	1:E:129:VAL:HG13	2.09	0.52
1:F:194:ARG:HG2	1:F:194:ARG:HH11	1.73	0.52
1:E:243:PRO:HG3	1:E:286:LYS:HD2	1.91	0.52
1:E:412:VAL:HG11	1:E:418:PHE:CE1	2.45	0.52
1:F:477:ILE:HG22	1:F:481:MET:CE	2.39	0.52
1:A:403:THR:HB	1:F:261:ALA:HB3	1.91	0.52
1:C:223:PRO:HB3	1:C:255:SER:O	2.10	0.52
1:D:85:PHE:HB2	1:D:286:LYS:HD3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:VAL:CG2	1:D:310:LEU:HD22	2.40	0.52
1:A:377:MET:HE3	1:A:465:LEU:HD11	1.90	0.52
1:C:368:MET:O	1:C:369:LEU:HG	2.10	0.52
1:D:91:ASP:HB2	1:D:94:PHE:CD2	2.43	0.52
1:A:162:GLY:HA2	1:A:492:PHE:CD2	2.45	0.52
1:A:385:ASP:OD1	1:A:435:MET:HB3	2.09	0.52
1:A:78:LEU:HD22	1:A:324:TYR:HB3	1.92	0.52
1:A:107:THR:HG23	1:A:364:TYR:HB2	1.92	0.52
1:A:142:TRP:HZ2	1:A:435:MET:HE1	1.75	0.52
1:B:145:ASN:HB2	1:B:384:ASN:ND2	2.25	0.52
1:B:473:ILE:HG21	1:B:481:MET:HE2	1.92	0.52
1:C:313:ILE:O	1:C:317:VAL:HG23	2.10	0.52
1:F:454:ALA:O	1:F:457:ALA:HB3	2.10	0.52
1:C:299:LYS:O	1:C:300:LYS:HD3	2.10	0.52
1:D:158:ILE:O	1:D:158:ILE:HG22	2.10	0.52
1:F:476:ASP:O	1:F:479:LYS:HB2	2.09	0.52
1:B:167:HIS:C	1:B:169:THR:H	2.13	0.52
1:B:305:VAL:HG23	1:B:310:LEU:HD13	1.92	0.52
1:C:106:TRP:HB2	1:C:145:ASN:O	2.10	0.52
1:D:114:LYS:HE2	1:D:373:MET:HG3	1.91	0.51
1:E:105:HIS:HB3	1:E:147:ASP:OD2	2.11	0.51
1:F:50:ARG:NH2	1:F:65:ASN:ND2	2.58	0.51
1:F:114:LYS:HD2	1:F:125:THR:HG22	1.91	0.51
1:A:217:LEU:HD12	1:A:245:ASN:OD1	2.09	0.51
1:B:377:MET:HE3	4:B:603:GOL:H32	1.92	0.51
1:D:197:VAL:HG12	1:D:208:ALA:HB1	1.91	0.51
1:E:98:GLN:HG3	1:E:288:TRP:HZ2	1.75	0.51
1:A:37:LEU:O	1:A:41:GLY:HA2	2.10	0.51
1:A:406:VAL:HG11	1:F:35:GLU:OE1	2.10	0.51
1:C:245:ASN:C	1:C:245:ASN:ND2	2.64	0.51
1:D:446:ALA:C	1:D:448:ALA:H	2.14	0.51
1:F:267:HIS:CE1	1:F:271:VAL:HG21	2.45	0.51
1:F:299:LYS:O	1:F:301:GLY:N	2.43	0.51
1:B:152:PRO:HG2	1:B:153:VAL:H	1.76	0.51
1:F:77:ALA:O	1:F:279:GLN:HG3	2.10	0.51
1:F:166:VAL:HG12	1:F:485:VAL:HG13	1.92	0.51
1:A:171:THR:HG23	1:A:175:ASN:ND2	2.25	0.51
1:A:442:PHE:CD1	1:A:442:PHE:C	2.84	0.51
1:B:17:GLU:HB3	1:E:19:ASN:HB2	1.93	0.51
1:B:453:LEU:HD23	1:E:342:ASP:HB3	1.93	0.51
1:C:382:ILE:O	1:C:386:ILE:HG13	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:THR:OG1	1:D:147:ASP:HB3	2.10	0.51
1:E:109:PHE:CG	1:E:368:MET:HB2	2.45	0.51
1:A:61:ASN:CG	1:A:63:LYS:HG2	2.31	0.51
1:C:371:LEU:N	1:C:371:LEU:HD12	2.25	0.51
1:E:456:VAL:HG21	5:E:722:HOH:O	2.11	0.51
1:F:151:LEU:HD13	1:F:168:GLU:HB3	1.92	0.51
1:A:48:GLU:HG2	1:A:235:ILE:HD13	1.93	0.51
1:A:51:GLN:NE2	1:A:55:GLU:HG2	2.25	0.51
1:B:418:PHE:N	1:B:418:PHE:CD1	2.79	0.51
1:E:30:HIS:O	1:E:34:MET:HG2	2.11	0.51
1:E:334:LYS:HB3	1:E:368:MET:CE	2.36	0.51
1:B:173:LEU:O	1:B:473:ILE:HD11	2.11	0.51
1:E:446:ALA:HA	1:E:450:SER:OG	2.11	0.51
1:F:310:LEU:HD23	1:F:351:THR:CG2	2.41	0.51
1:F:349:THR:HA	1:F:352:THR:HG22	1.92	0.51
1:A:343:GLN:HG3	1:F:437:LEU:CD2	2.38	0.51
1:B:183:ILE:O	1:B:183:ILE:HG22	2.11	0.51
1:C:369:LEU:HD12	1:C:376:SER:CB	2.41	0.51
1:C:440:HIS:CE1	1:D:300:LYS:HD2	2.45	0.51
1:D:51:GLN:NE2	1:D:55:GLU:HG3	2.26	0.51
1:E:105:HIS:O	1:E:362:THR:HA	2.11	0.51
1:B:22:THR:OG1	1:B:25:GLU:HG3	2.10	0.51
1:C:109:PHE:CD1	1:C:110:GLY:N	2.79	0.51
1:C:338:LYS:NZ	1:D:438:ASP:OD1	2.39	0.51
1:F:118:TYR:HB2	1:F:458:HIS:CE1	2.46	0.51
1:B:275:ILE:HG23	1:B:287:VAL:HG21	1.93	0.50
1:B:327:PRO:HA	1:B:361:ASN:OD1	2.10	0.50
1:C:393:ALA:HA	1:D:312:LEU:HD11	1.93	0.50
1:D:209:ARG:HB3	1:D:209:ARG:NH1	2.19	0.50
1:E:118:TYR:HB2	1:E:123:TYR:CE1	2.46	0.50
1:E:430:TYR:HB3	1:E:431:PRO:CD	2.38	0.50
1:A:354:LEU:CB	1:A:355:PRO:HD3	2.41	0.50
1:A:493:ARG:C	1:A:495:MET:H	2.14	0.50
1:B:205:GLU:HG3	1:B:209:ARG:HD2	1.91	0.50
1:E:118:TYR:HE1	1:E:121:GLY:C	2.15	0.50
1:F:158:ILE:HG21	1:F:167:HIS:HD2	1.75	0.50
1:F:334:LYS:HD3	1:F:368:MET:CE	2.41	0.50
1:A:79:GLN:HG3	1:A:79:GLN:O	2.11	0.50
1:A:131:LYS:O	1:A:134:ALA:HB3	2.11	0.50
1:B:252:SER:HB3	1:B:263:THR:OG1	2.12	0.50
1:F:61:ASN:OD1	1:F:63:LYS:CG	2.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:LEU:HD13	1:F:283:PRO:HB3	1.93	0.50
1:F:119:GLN:HB2	1:F:124:VAL:CG2	2.40	0.50
1:F:248:SER:HB3	1:F:271:VAL:HG23	1.94	0.50
1:A:473:ILE:HG21	1:A:481:MET:HE1	1.91	0.50
1:D:119:GLN:HB2	1:D:124:VAL:HG23	1.93	0.50
1:F:18:LEU:HD13	1:F:357:LEU:HB2	1.93	0.50
1:F:71:GLU:HB2	5:F:705:HOH:O	2.12	0.50
1:A:34:MET:HA	1:A:34:MET:HE2	1.94	0.50
1:C:26:LEU:HD13	1:C:323:PHE:CD1	2.46	0.50
1:D:109:PHE:CG	1:D:110:GLY:N	2.79	0.50
1:F:113:VAL:HG22	1:F:373:MET:CE	2.41	0.50
1:F:422:LYS:O	1:F:426:GLN:HG3	2.11	0.50
1:C:56:ASN:CG	1:C:280:LEU:HD22	2.31	0.50
1:D:271:VAL:O	1:D:275:ILE:HG13	2.11	0.50
1:F:196:ILE:O	1:F:199:ALA:HB3	2.12	0.50
1:F:251:MET:HE1	1:F:303:ALA:HB2	1.92	0.50
1:B:96:THR:HG23	1:B:105:HIS:CD2	2.47	0.50
1:C:117:LYS:CB	4:C:603:GOL:H12	2.38	0.50
1:D:217:LEU:HD23	1:D:218:LEU:N	2.27	0.50
1:E:114:LYS:CB	1:E:374:THR:HG23	2.41	0.50
1:F:90:ARG:HB3	1:F:200:TYR:OH	2.12	0.50
1:A:87:LEU:HD21	1:A:288:TRP:CH2	2.47	0.50
1:A:332:GLY:O	1:A:333:SER:HB3	2.11	0.50
1:A:457:ALA:O	1:A:461:VAL:HG23	2.11	0.50
1:D:131:LYS:O	1:D:131:LYS:HD3	2.12	0.50
1:E:311:GLY:HA3	1:E:354:LEU:HD12	1.93	0.50
1:F:209:ARG:HG2	1:F:209:ARG:HH11	1.77	0.50
1:F:305:VAL:HG11	1:F:368:MET:HE1	1.94	0.50
1:A:13:LEU:HD23	1:F:20:LEU:C	2.32	0.50
1:A:84:ARG:CZ	1:C:35:GLU:HB2	2.42	0.50
1:A:397:ILE:HG22	1:A:399:VAL:HG23	1.93	0.50
1:B:232:GLN:HE21	1:B:236:LYS:HE3	1.76	0.50
1:D:151:LEU:HD22	1:D:182:HIS:CD2	2.47	0.50
1:E:19:ASN:HA	5:E:716:HOH:O	2.11	0.50
1:F:109:PHE:HB2	1:F:365:GLY:HA2	1.93	0.50
1:A:328:SER:H	1:A:361:ASN:HB2	1.77	0.49
1:B:109:PHE:CB	1:B:368:MET:HB2	2.42	0.49
1:C:278:ALA:O	1:C:281:THR:HB	2.12	0.49
1:A:127:ASP:OD1	1:A:156:ARG:NH1	2.45	0.49
1:B:50:ARG:NH2	1:B:65:ASN:HD21	2.08	0.49
1:B:228:VAL:HG23	5:B:708:HOH:O	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:LEU:HA	1:D:343:GLN:OE1	2.12	0.49
1:D:405:ALA:HB1	1:D:408:SER:HB3	1.94	0.49
1:A:170:LEU:CD2	1:A:485:VAL:HG21	2.42	0.49
1:C:395:GLN:O	1:C:395:GLN:HG2	2.12	0.49
1:D:251:MET:HE2	1:D:296:PHE:HA	1.93	0.49
1:F:218:LEU:HD12	1:F:219:CYS:N	2.26	0.49
1:F:368:MET:HG2	1:F:369:LEU:H	1.76	0.49
1:A:84:ARG:NH1	1:C:35:GLU:HB2	2.27	0.49
1:C:201:TYR:OH	1:C:213:ILE:CG2	2.61	0.49
1:C:272:LEU:O	1:C:275:ILE:N	2.46	0.49
1:C:337:ALA:CA	1:C:343:GLN:HE21	2.25	0.49
1:D:143:ALA:O	1:D:178:LYS:NZ	2.46	0.49
1:D:480:ASP:O	1:D:483:ALA:HB3	2.11	0.49
1:E:136:ILE:HG21	1:E:152:PRO:HG3	1.94	0.49
1:A:136:ILE:HD12	1:A:375:PHE:CE1	2.48	0.49
1:A:348:LYS:HE3	1:A:379:GLN:CG	2.41	0.49
1:B:148:TYR:HH	1:B:329:TYR:HE2	1.58	0.49
1:D:117:LYS:HB3	4:D:604:GOL:C3	2.42	0.49
1:D:305:VAL:HG11	1:D:368:MET:HE1	1.94	0.49
1:A:51:GLN:HG3	1:A:55:GLU:OE1	2.13	0.49
1:A:245:ASN:C	1:A:245:ASN:ND2	2.66	0.49
1:B:139:LEU:O	1:B:142:TRP:HB3	2.12	0.49
1:B:430:TYR:HB3	1:B:431:PRO:CD	2.32	0.49
1:B:493:ARG:C	1:B:495:MET:N	2.60	0.49
1:F:169:THR:O	1:F:173:LEU:HD12	2.12	0.49
1:F:305:VAL:HG22	1:F:310:LEU:HD22	1.95	0.49
1:F:368:MET:HE2	1:F:372:GLY:HA2	1.95	0.49
1:A:119:GLN:HG3	1:A:120:ASP:OD1	2.12	0.49
1:A:158:ILE:HG22	1:A:158:ILE:O	2.12	0.49
1:A:435:MET:CE	1:A:460:LYS:HE2	2.42	0.49
1:B:16:VAL:HG22	1:E:20:LEU:CD2	2.42	0.49
1:B:328:SER:O	1:B:361:ASN:HB2	2.12	0.49
1:C:316:ALA:HB2	1:D:397:ILE:CD1	2.43	0.49
1:E:217:LEU:HA	1:E:245:ASN:HB3	1.95	0.49
1:E:478:PHE:HA	1:E:481:MET:HE2	1.95	0.49
1:A:439:ARG:HB2	1:F:300:LYS:HG3	1.94	0.49
1:C:61:ASN:OD1	1:C:64:THR:N	2.46	0.49
1:D:27:LYS:O	1:D:30:HIS:HB3	2.13	0.49
1:D:353:LEU:O	1:D:357:LEU:HG	2.13	0.49
1:D:377:MET:CE	4:D:604:GOL:H32	2.42	0.49
1:E:276:VAL:O	1:E:280:LEU:HG	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:HIS:HE2	1:D:4:ASN:HB2	1.76	0.49
1:A:338:LYS:HG3	1:A:370:GLU:HG3	1.93	0.49
1:B:194:ARG:NH1	1:B:195:ASP:OD1	2.46	0.49
1:C:295:THR:O	1:C:304:PRO:HD2	2.13	0.49
1:E:53:PHE:CZ	1:E:277:LEU:HB2	2.47	0.49
1:F:34:MET:CE	1:F:37:LEU:HD12	2.43	0.49
1:F:119:GLN:HB2	1:F:124:VAL:HG23	1.94	0.49
1:A:148:TYR:HH	1:A:329:TYR:HE2	1.59	0.49
1:A:305:VAL:HG22	1:A:310:LEU:HD22	1.94	0.49
1:B:88:TRP:O	1:B:179:HIS:HB2	2.12	0.49
1:B:405:ALA:HB1	1:B:408:SER:HB3	1.95	0.49
1:F:166:VAL:HG13	1:F:196:ILE:HD11	1.95	0.49
1:A:340:PRO:HD3	1:A:369:LEU:HD11	1.94	0.48
1:B:5:ASN:CG	1:B:5:ASN:O	2.51	0.48
1:B:190:VAL:HG12	1:B:240:PHE:HD2	1.78	0.48
1:B:408:SER:O	1:B:412:VAL:HG23	2.12	0.48
1:B:432:SER:O	1:B:439:ARG:NH1	2.45	0.48
1:C:116:CYS:HB2	1:C:374:THR:CG2	2.43	0.48
1:C:403:THR:HA	1:D:259:TYR:CD2	2.48	0.48
1:C:477:ILE:HG22	1:C:481:MET:HE2	1.95	0.48
1:D:220:PRO:HD2	1:D:247:LEU:O	2.13	0.48
1:E:122:LYS:H	1:E:122:LYS:HD3	1.78	0.48
1:F:42:ILE:HD12	1:F:273:SER:HB3	1.94	0.48
1:A:231:CYS:O	1:A:235:ILE:HG13	2.13	0.48
1:A:493:ARG:C	1:A:495:MET:N	2.64	0.48
1:B:217:LEU:HD23	1:B:217:LEU:C	2.32	0.48
1:B:331:ALA:HB2	1:B:364:TYR:HE1	1.74	0.48
1:C:337:ALA:HB2	1:C:343:GLN:NE2	2.24	0.48
1:E:64:THR:HB	1:E:66:VAL:HG23	1.94	0.48
1:E:94:PHE:CB	1:E:178:LYS:HG2	2.42	0.48
1:E:198:LYS:HG2	1:E:203:GLY:HA2	1.95	0.48
1:F:190:VAL:HB	1:F:236:LYS:HD3	1.94	0.48
1:F:252:SER:O	1:F:296:PHE:HB3	2.13	0.48
1:F:405:ALA:HB1	1:F:408:SER:HB3	1.95	0.48
1:A:442:PHE:C	1:A:442:PHE:HD1	2.16	0.48
1:B:229:ASN:O	1:B:233:VAL:HG23	2.14	0.48
1:C:191:GLU:HG3	1:C:240:PHE:CZ	2.47	0.48
1:D:247:LEU:HD21	1:D:292:SER:HB3	1.96	0.48
1:E:266:THR:HG22	1:E:270:GLU:OE2	2.14	0.48
1:E:350:MET:CE	1:E:354:LEU:HD11	2.43	0.48
1:A:338:LYS:O	1:A:339:VAL:HB	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:VAL:HG22	1:B:67:VAL:HG13	1.95	0.48
1:C:16:VAL:HG13	1:D:18:LEU:HD21	1.96	0.48
1:C:408:SER:OG	1:C:421:LEU:HD21	2.14	0.48
1:D:22:THR:HG23	1:D:25:GLU:OE1	2.13	0.48
1:E:118:TYR:HB2	1:E:123:TYR:HE1	1.78	0.48
1:F:113:VAL:HG22	1:F:373:MET:HE2	1.95	0.48
1:A:435:MET:HE2	1:A:460:LYS:HE2	1.95	0.48
1:B:392:LYS:HE2	1:E:309:GLU:OE2	2.12	0.48
1:C:109:PHE:CG	1:C:110:GLY:N	2.81	0.48
1:C:207:GLU:O	1:C:211:LYS:HB2	2.14	0.48
1:E:104:VAL:O	1:F:4:ASN:ND2	2.47	0.48
1:E:167:HIS:C	1:E:169:THR:H	2.15	0.48
1:F:422:LYS:CA	1:F:425:ARG:NH1	2.75	0.48
1:A:47:PRO:HA	1:A:50:ARG:CZ	2.44	0.48
1:A:458:HIS:HD2	1:A:458:HIS:O	1.97	0.48
1:B:332:GLY:O	1:B:333:SER:CB	2.62	0.48
1:B:377:MET:HE2	4:B:603:GOL:H32	1.95	0.48
1:C:98:GLN:OE1	1:C:362:THR:OG1	2.29	0.48
1:E:234:ILE:HG23	1:E:278:ALA:HB2	1.94	0.48
1:F:291:SER:HB3	1:F:317:VAL:HG11	1.96	0.48
1:B:218:LEU:CD2	1:B:234:ILE:HG12	2.42	0.48
1:C:96:THR:HG23	1:C:105:HIS:CD2	2.49	0.48
1:C:157:ASP:O	1:C:158:ILE:HD13	2.14	0.48
1:C:281:THR:HG22	1:C:282:VAL:HG23	1.96	0.48
1:D:84:ARG:HG3	1:D:84:ARG:HH11	1.78	0.48
1:D:88:TRP:HB2	1:D:212:PRO:O	2.13	0.48
1:E:392:LYS:O	1:E:395:GLN:HB3	2.14	0.48
1:F:339:VAL:CG2	1:F:340:PRO:HD2	2.44	0.48
1:A:453:LEU:HD23	1:F:342:ASP:CB	2.43	0.48
1:B:38:MET:O	1:B:68:LYS:HD3	2.14	0.48
1:B:191:GLU:HG3	1:B:240:PHE:CZ	2.49	0.48
1:C:396:GLY:C	1:C:397:ILE:HD12	2.33	0.48
1:D:90:ARG:HD2	1:D:200:TYR:CE1	2.48	0.48
1:D:174:ALA:CA	1:D:473:ILE:HD11	2.44	0.48
1:D:297:ASP:O	1:D:299:LYS:N	2.41	0.48
1:E:267:HIS:CE1	1:E:291:SER:HB2	2.48	0.48
1:E:289:TYR:CE1	1:E:317:VAL:HG13	2.47	0.48
1:F:333:SER:HG	1:F:387:PHE:HZ	1.58	0.48
1:B:8:ALA:O	1:B:9:GLY:C	2.53	0.48
1:C:305:VAL:CG2	1:C:310:LEU:HD22	2.44	0.48
1:D:107:THR:HG23	1:D:364:TYR:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:442:PHE:CD1	1:F:442:PHE:C	2.87	0.48
1:A:33:THR:O	1:A:37:LEU:HG	2.14	0.47
1:A:194:ARG:HG2	1:A:194:ARG:HH11	1.78	0.47
1:A:380:LEU:HD13	1:A:380:LEU:C	2.35	0.47
1:B:194:ARG:HD2	1:B:205:GLU:OE2	2.13	0.47
1:D:85:PHE:CB	1:D:286:LYS:HD3	2.44	0.47
1:D:173:LEU:HD22	1:D:213:ILE:HD12	1.96	0.47
1:D:319:LYS:HD3	1:D:322:GLN:HE22	1.79	0.47
1:C:45:SER:CB	1:C:228:VAL:HG22	2.43	0.47
1:C:434:PRO:HB3	1:C:437:LEU:HD12	1.96	0.47
1:D:123:TYR:OH	1:D:458:HIS:HB2	2.14	0.47
1:D:251:MET:HE2	1:D:296:PHE:CB	2.44	0.47
1:A:294:THR:HA	1:A:313:ILE:HD12	1.96	0.47
1:B:314:SER:HB2	1:B:355:PRO:HG3	1.96	0.47
1:E:70:PRO:HG2	1:E:73:LEU:HG	1.94	0.47
1:E:94:PHE:CG	1:E:178:LYS:HG2	2.49	0.47
1:F:285:ALA:O	1:F:287:VAL:HG13	2.14	0.47
1:F:311:GLY:HA3	1:F:354:LEU:HD12	1.96	0.47
1:F:319:LYS:HE2	1:F:358:ALA:HB1	1.97	0.47
1:F:353:LEU:O	1:F:357:LEU:HG	2.14	0.47
1:B:109:PHE:CD1	1:B:110:GLY:N	2.82	0.47
1:B:438:ASP:OD2	1:B:445:TRP:HD1	1.97	0.47
1:C:94:PHE:CE1	1:C:178:LYS:HE2	2.49	0.47
1:D:267:HIS:CE1	1:D:271:VAL:HG21	2.49	0.47
1:E:334:LYS:HA	1:E:348:LYS:NZ	2.29	0.47
1:F:296:PHE:CE2	1:F:298:LEU:HD23	2.49	0.47
1:F:297:ASP:C	1:F:299:LYS:N	2.67	0.47
1:B:435:MET:HG2	1:B:436:LEU:HD12	1.96	0.47
1:C:377:MET:CE	1:C:465:LEU:HD11	2.45	0.47
1:D:134:ALA:HA	1:D:175:ASN:ND2	2.30	0.47
1:E:110:GLY:HA2	1:E:111:THR:HA	1.56	0.47
1:F:94:PHE:CE2	1:F:177:ALA:HB3	2.49	0.47
1:F:106:TRP:CZ3	1:F:391:LYS:HE3	2.49	0.47
1:A:378:GLU:O	1:A:381:VAL:HG22	2.14	0.47
1:B:160:GLY:O	1:B:492:PHE:HE2	1.96	0.47
1:D:44:VAL:HG12	1:D:50:ARG:HG3	1.97	0.47
1:D:48:GLU:O	1:D:51:GLN:HB3	2.15	0.47
1:F:483:ALA:O	1:F:486:ASP:HB2	2.14	0.47
1:A:48:GLU:O	1:A:52:ILE:HG13	2.15	0.47
1:A:88:TRP:CD1	1:A:211:LYS:HA	2.50	0.47
1:A:155:ALA:HB1	1:A:158:ILE:HG12	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:ARG:O	1:A:495:MET:HG2	2.15	0.47
1:C:245:ASN:HD22	1:C:246:VAL:N	2.12	0.47
1:F:129:VAL:HG23	1:F:131:LYS:H	1.80	0.47
1:F:234:ILE:CG2	1:F:278:ALA:HB2	2.44	0.47
1:F:318:ALA:O	1:F:322:GLN:HG3	2.14	0.47
1:A:61:ASN:ND2	1:A:63:LYS:HG2	2.29	0.47
1:A:396:GLY:C	1:A:397:ILE:HD12	2.35	0.47
1:C:51:GLN:NE2	1:C:55:GLU:HG3	2.29	0.47
1:C:232:GLN:HE21	1:C:236:LYS:HE3	1.80	0.47
1:C:392:LYS:O	1:C:395:GLN:HB3	2.15	0.47
1:D:46:ASP:HB2	1:D:228:VAL:HG13	1.97	0.47
1:D:310:LEU:HD11	1:D:331:ALA:HB3	1.96	0.47
1:E:117:LYS:HD2	1:E:126:VAL:HG21	1.95	0.47
1:E:230:ALA:O	1:E:234:ILE:HG13	2.15	0.47
1:F:247:LEU:HD23	1:F:247:LEU:C	2.35	0.47
1:A:297:ASP:HB2	1:A:304:PRO:HD3	1.97	0.47
1:A:305:VAL:O	1:A:310:LEU:HD22	2.15	0.47
1:B:315:ALA:O	1:B:318:ALA:HB3	2.14	0.47
1:C:158:ILE:HG22	1:C:158:ILE:O	2.15	0.47
1:C:234:ILE:HG21	1:C:277:LEU:HD12	1.96	0.47
1:C:251:MET:HE2	1:C:296:PHE:CB	2.42	0.47
1:D:373:MET:HE2	1:D:373:MET:HA	1.96	0.47
1:B:18:LEU:HD23	1:B:19:ASN:N	2.30	0.47
1:C:91:ASP:HB2	1:C:177:ALA:CB	2.44	0.47
1:C:107:THR:HG23	1:C:364:TYR:CB	2.44	0.47
1:D:141:ASP:HA	1:D:178:LYS:HE3	1.97	0.47
1:E:470:VAL:HG12	1:E:471:THR:N	2.30	0.47
1:F:475:ALA:O	1:F:479:LYS:HG3	2.15	0.47
1:A:91:ASP:O	1:A:93:LYS:N	2.48	0.46
1:D:162:GLY:CA	1:D:492:PHE:CD2	2.98	0.46
1:D:189:ASN:O	1:D:192:TYR:HB2	2.14	0.46
1:E:297:ASP:C	1:E:299:LYS:H	2.19	0.46
1:F:112:GLY:O	1:F:153:VAL:HA	2.15	0.46
1:F:119:GLN:HG3	1:F:120:ASP:OD1	2.15	0.46
1:B:99:GLU:OE2	1:D:31:TYR:HB3	2.15	0.46
1:B:412:VAL:O	1:B:416:ASN:HB2	2.15	0.46
1:C:20:LEU:C	1:D:13:LEU:HD23	2.36	0.46
1:C:34:MET:SD	1:C:71:GLU:HG3	2.56	0.46
1:D:113:VAL:HG22	1:D:373:MET:HE2	1.96	0.46
1:E:281:THR:HG22	1:E:282:VAL:HG23	1.98	0.46
1:A:259:TYR:CD2	1:F:403:THR:HA	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ASP:O	1:A:386:ILE:HB	2.15	0.46
1:C:355:PRO:HB2	1:C:363:ILE:CD1	2.46	0.46
1:E:94:PHE:CD2	1:E:178:LYS:HG2	2.50	0.46
1:E:122:LYS:HE3	1:E:124:VAL:HG23	1.96	0.46
1:E:229:ASN:O	1:E:233:VAL:HG23	2.15	0.46
1:B:103:LYS:HB3	1:C:4:ASN:ND2	2.30	0.46
1:B:110:GLY:HA2	1:B:111:THR:HA	1.56	0.46
1:C:72:TYR:CD1	1:C:72:TYR:C	2.89	0.46
1:D:56:ASN:CG	1:D:280:LEU:HD22	2.35	0.46
1:D:332:GLY:O	1:D:333:SER:HB3	2.14	0.46
1:E:158:ILE:HG21	1:E:167:HIS:CD2	2.50	0.46
1:E:188:GLU:HA	1:E:236:LYS:HZ2	1.81	0.46
1:F:151:LEU:N	1:F:180:PHE:HE1	2.12	0.46
1:F:231:CYS:O	1:F:235:ILE:HG13	2.15	0.46
1:F:440:HIS:HB3	1:F:444:ASP:HB2	1.98	0.46
1:A:337:ALA:HB2	1:A:343:GLN:CD	2.36	0.46
1:A:371:LEU:N	1:A:371:LEU:HD12	2.31	0.46
1:B:480:ASP:O	1:B:483:ALA:HB3	2.14	0.46
1:D:251:MET:HE2	1:D:296:PHE:CA	2.46	0.46
1:D:297:ASP:OD1	1:D:300:LYS:N	2.47	0.46
1:F:457:ALA:O	1:F:461:VAL:HG23	2.15	0.46
1:A:118:TYR:N	4:A:604:GOL:H12	2.23	0.46
1:A:304:PRO:HB3	1:F:439:ARG:HD3	1.98	0.46
1:C:223:PRO:HG2	1:D:415:GLY:H	1.80	0.46
1:A:119:GLN:CB	1:A:124:VAL:HG21	2.46	0.46
1:A:162:GLY:HA2	1:A:492:PHE:HD2	1.81	0.46
1:B:94:PHE:CE1	1:B:178:LYS:HE2	2.51	0.46
1:C:194:ARG:HD3	1:C:240:PHE:CD1	2.50	0.46
1:C:218:LEU:HD21	1:C:234:ILE:HG12	1.97	0.46
1:D:19:ASN:HA	5:D:711:HOH:O	2.14	0.46
1:E:181:HIS:HA	1:E:215:SER:O	2.16	0.46
1:E:308:PRO:HG2	1:E:309:GLU:OE1	2.16	0.46
1:F:94:PHE:CG	1:F:178:LYS:HG2	2.51	0.46
1:A:61:ASN:ND2	1:A:63:LYS:HE2	2.29	0.46
1:C:209:ARG:HH12	1:C:241:GLY:HA3	1.80	0.46
1:F:40:PRO:HG2	1:F:224:LEU:HD13	1.97	0.46
1:F:141:ASP:O	1:F:178:LYS:HE3	2.16	0.46
1:A:170:LEU:HD22	1:A:485:VAL:CG2	2.45	0.46
1:B:397:ILE:HG21	1:E:21:PHE:HE1	1.81	0.46
1:B:437:LEU:CD2	1:E:343:GLN:HG3	2.46	0.46
1:C:129:VAL:HG22	1:C:132:ASP:CG	2.36	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:SER:CB	1:C:243:PRO:HB2	2.45	0.46
1:E:22:THR:OG1	1:E:25:GLU:HG3	2.16	0.46
1:E:131:LYS:O	1:E:131:LYS:HD3	2.16	0.46
1:E:438:ASP:OD1	1:E:440:HIS:HB2	2.16	0.46
1:F:84:ARG:HB3	1:F:99:GLU:HG3	1.98	0.46
1:A:49:ALA:HB2	1:A:235:ILE:HD11	1.98	0.46
1:C:90:ARG:NH1	1:C:473:ILE:HG12	2.31	0.46
1:E:131:LYS:HD3	1:E:131:LYS:C	2.37	0.46
1:E:192:TYR:O	1:E:196:ILE:HG13	2.15	0.46
1:F:305:VAL:HG13	1:F:334:LYS:HB3	1.98	0.46
1:F:369:LEU:HD12	1:F:376:SER:HB2	1.98	0.46
1:F:447:ALA:C	1:F:449:GLY:H	2.19	0.46
1:A:309:GLU:CD	1:F:392:LYS:HE2	2.37	0.45
1:A:343:GLN:HB2	1:F:453:LEU:HD22	1.97	0.45
1:C:50:ARG:HH21	1:C:65:ASN:ND2	2.14	0.45
1:D:145:ASN:HD22	1:D:387:PHE:HB2	1.81	0.45
1:D:390:VAL:O	1:D:394:MET:HG3	2.16	0.45
1:E:50:ARG:HD3	1:E:65:ASN:HA	1.97	0.45
1:E:218:LEU:HD21	1:E:234:ILE:HG12	1.98	0.45
1:E:328:SER:O	1:E:361:ASN:HB2	2.16	0.45
1:E:422:LYS:O	1:E:426:GLN:HG3	2.17	0.45
1:C:339:VAL:O	1:C:341:ASP:N	2.49	0.45
1:D:107:THR:HG23	1:D:364:TYR:CB	2.47	0.45
1:F:49:ALA:HB2	1:F:235:ILE:HD11	1.97	0.45
1:F:170:LEU:CD2	1:F:485:VAL:HG21	2.45	0.45
1:F:218:LEU:HD21	1:F:234:ILE:HG12	1.98	0.45
1:A:118:TYR:CZ	1:A:121:GLY:HA2	2.51	0.45
1:B:403:THR:HB	1:E:261:ALA:HB3	1.99	0.45
1:D:117:LYS:CA	4:D:604:GOL:H31	2.45	0.45
1:D:190:VAL:HB	1:D:236:LYS:CD	2.46	0.45
1:E:473:ILE:HD13	1:E:481:MET:HE3	1.99	0.45
1:A:145:ASN:ND2	1:A:384:ASN:O	2.48	0.45
1:A:440:HIS:O	1:F:338:LYS:NZ	2.39	0.45
1:B:18:LEU:HD21	1:E:16:VAL:CG1	2.46	0.45
1:C:53:PHE:HZ	1:C:277:LEU:HB2	1.80	0.45
1:C:222:SER:HA	1:C:270:GLU:OE2	2.16	0.45
1:D:303:ALA:HB3	5:D:709:HOH:O	2.16	0.45
1:D:319:LYS:HD3	1:D:322:GLN:NE2	2.31	0.45
1:E:350:MET:HE1	1:E:354:LEU:HD11	1.97	0.45
1:A:60:VAL:HG13	1:A:67:VAL:HG22	1.97	0.45
1:B:118:TYR:HD1	1:B:123:TYR:CE1	2.34	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:CYS:HA	1:C:366:ALA:HB3	1.99	0.45
1:E:91:ASP:HB2	1:E:177:ALA:HB1	1.99	0.45
1:B:112:GLY:O	1:B:153:VAL:HA	2.17	0.45
1:C:332:GLY:HA3	1:C:363:ILE:HG23	1.99	0.45
1:C:375:PHE:CD1	1:C:375:PHE:C	2.89	0.45
1:D:197:VAL:C	1:D:199:ALA:N	2.70	0.45
1:E:42:ILE:HD12	1:E:273:SER:CB	2.46	0.45
1:E:381:VAL:HG23	1:E:457:ALA:HB1	1.97	0.45
1:E:473:ILE:O	1:E:474:ASP:C	2.55	0.45
1:E:493:ARG:C	1:E:495:MET:H	2.20	0.45
1:F:112:GLY:N	1:F:152:PRO:O	2.50	0.45
1:F:296:PHE:CD2	1:F:298:LEU:HD23	2.52	0.45
1:B:428:VAL:HG23	1:E:298:LEU:CB	2.45	0.45
1:B:470:VAL:O	1:B:472:PRO:HD3	2.16	0.45
1:C:79:GLN:HA	1:E:75:ARG:HH11	1.82	0.45
1:C:305:VAL:HG12	1:C:336:ASP:OD1	2.17	0.45
1:F:337:ALA:N	1:F:343:GLN:HE21	2.14	0.45
1:A:412:VAL:HG12	1:A:416:ASN:HB2	1.99	0.45
1:C:247:LEU:HG	1:C:291:SER:CA	2.47	0.45
1:F:190:VAL:HA	1:F:193:TYR:HD2	1.80	0.45
1:A:44:VAL:CB	1:A:50:ARG:HG3	2.45	0.45
1:A:382:ILE:O	1:A:386:ILE:HG13	2.16	0.45
1:B:172:PRO:O	1:B:176:THR:HG22	2.17	0.45
1:B:428:VAL:O	1:E:299:LYS:HE3	2.17	0.45
1:C:111:THR:HG23	1:C:111:THR:O	2.17	0.45
1:C:200:TYR:HA	1:C:477:ILE:CG2	2.47	0.45
1:C:234:ILE:HG21	1:C:277:LEU:CD1	2.47	0.45
1:F:61:ASN:O	1:F:63:LYS:N	2.50	0.45
1:F:110:GLY:HA2	1:F:111:THR:HA	1.61	0.45
1:F:117:LYS:HD2	1:F:126:VAL:HG21	1.99	0.45
1:A:229:ASN:O	1:A:233:VAL:HG23	2.17	0.45
1:B:45:SER:HA	1:B:65:ASN:HD22	1.82	0.45
1:C:128:SER:O	1:C:156:ARG:HG3	2.17	0.45
1:C:262:GLY:HA2	1:D:404:LEU:O	2.17	0.45
1:C:342:ASP:HA	1:D:341:ASP:O	2.17	0.45
1:D:449:GLY:O	1:D:450:SER:C	2.56	0.45
1:E:93:LYS:HE3	1:E:94:PHE:CZ	2.51	0.45
1:E:109:PHE:O	1:E:152:PRO:HA	2.17	0.45
1:E:171:THR:O	1:E:175:ASN:ND2	2.50	0.45
1:E:327:PRO:HA	1:E:361:ASN:OD1	2.17	0.45
1:F:341:ASP:OD1	1:F:343:GLN:HB3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:376:SER:HB3	1:F:379:GLN:HB3	1.98	0.45
1:A:84:ARG:HB3	1:A:99:GLU:HG3	1.99	0.44
1:B:412:VAL:HG21	1:B:418:PHE:CE2	2.52	0.44
1:C:110:GLY:HA2	1:C:111:THR:HA	1.60	0.44
1:C:216:MET:CE	1:C:242:ILE:HG21	2.47	0.44
1:C:336:ASP:HB3	1:C:371:LEU:HG	1.98	0.44
1:D:172:PRO:O	1:D:176:THR:HG22	2.17	0.44
1:D:183:ILE:HG23	1:D:217:LEU:HD13	1.98	0.44
1:D:400:SER:OG	1:D:403:THR:HG23	2.17	0.44
1:E:114:LYS:HB3	1:E:125:THR:CG2	2.47	0.44
1:F:122:LYS:H	1:F:122:LYS:HD3	1.82	0.44
1:A:61:ASN:HD21	1:A:63:LYS:HG2	1.83	0.44
1:B:50:ARG:NH2	1:B:65:ASN:ND2	2.56	0.44
1:B:50:ARG:NH1	1:B:62:GLU:OE2	2.50	0.44
1:C:113:VAL:HG23	1:C:114:LYS:HG3	1.99	0.44
1:C:204:ASP:OD1	1:C:206:GLU:HB2	2.17	0.44
1:C:334:LYS:HD3	1:C:368:MET:HE1	1.98	0.44
1:C:343:GLN:HB2	1:D:453:LEU:HD22	1.98	0.44
1:C:370:GLU:C	1:C:372:GLY:H	2.21	0.44
1:D:430:TYR:HB3	1:D:431:PRO:HD3	1.97	0.44
1:F:421:LEU:O	1:F:425:ARG:HG3	2.16	0.44
1:A:44:VAL:HG21	1:A:67:VAL:HG21	1.99	0.44
1:A:110:GLY:HA2	1:A:111:THR:HA	1.71	0.44
1:B:35:GLU:OE2	1:F:84:ARG:NH1	2.50	0.44
1:B:217:LEU:HA	1:B:245:ASN:HB3	1.99	0.44
1:C:379:GLN:NE2	1:C:383:ASP:OD1	2.48	0.44
1:E:104:VAL:HA	1:E:360:ALA:O	2.16	0.44
1:F:90:ARG:CZ	1:F:473:ILE:HG12	2.48	0.44
1:F:149:PHE:CE1	1:F:152:PRO:HD3	2.52	0.44
1:F:378:GLU:O	1:F:381:VAL:HG22	2.16	0.44
1:A:267:HIS:CD2	1:A:268:ASN:N	2.86	0.44
1:B:190:VAL:HG12	1:B:240:PHE:CD2	2.53	0.44
1:B:251:MET:HE2	1:B:296:PHE:CB	2.39	0.44
1:C:155:ALA:O	1:C:164:GLN:HG3	2.18	0.44
1:D:90:ARG:HH11	1:D:90:ARG:HB3	1.82	0.44
1:D:141:ASP:OD2	1:D:470:VAL:HG22	2.17	0.44
1:E:63:LYS:CG	1:E:64:THR:N	2.78	0.44
1:E:451:LYS:HB3	1:E:455:THR:OG1	2.18	0.44
1:F:305:VAL:HG21	1:F:334:LYS:HD2	1.98	0.44
1:B:84:ARG:NH2	1:D:35:GLU:CD	2.70	0.44
1:C:21:PHE:HE1	1:D:397:ILE:HG21	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:ALA:HA	1:C:343:GLN:NE2	2.32	0.44
1:C:474:ASP:HB3	1:C:477:ILE:CG1	2.48	0.44
1:D:112:GLY:O	1:D:153:VAL:HA	2.18	0.44
1:D:196:ILE:O	1:D:199:ALA:HB3	2.17	0.44
1:E:247:LEU:HG	1:E:291:SER:N	2.32	0.44
1:F:86:VAL:HG13	1:F:88:TRP:HE1	1.83	0.44
1:F:109:PHE:CG	1:F:110:GLY:N	2.86	0.44
1:F:218:LEU:HA	5:F:707:HOH:O	2.17	0.44
1:A:91:ASP:C	1:A:93:LYS:N	2.71	0.44
1:A:197:VAL:O	1:A:200:TYR:HB3	2.17	0.44
1:A:305:VAL:HG12	1:A:336:ASP:OD1	2.18	0.44
1:B:88:TRP:HZ3	1:B:92:LYS:HE2	1.82	0.44
1:C:24:ASP:HB3	1:D:10:PHE:CE1	2.53	0.44
1:C:176:THR:HG23	1:C:176:THR:O	2.17	0.44
1:D:84:ARG:HG3	1:D:84:ARG:NH1	2.33	0.44
1:E:272:LEU:O	1:E:275:ILE:N	2.51	0.44
1:F:109:PHE:CD1	1:F:110:GLY:N	2.86	0.44
1:F:189:ASN:O	1:F:192:TYR:N	2.48	0.44
1:F:485:VAL:O	1:F:488:ALA:HB3	2.17	0.44
1:A:7:VAL:HG12	1:A:8:ALA:O	2.17	0.44
1:B:348:LYS:O	1:B:352:THR:HG22	2.18	0.44
1:C:251:MET:HA	1:C:294:THR:O	2.17	0.44
1:E:220:PRO:CD	1:E:247:LEU:O	2.66	0.44
1:F:90:ARG:NE	1:F:173:LEU:O	2.44	0.44
1:A:408:SER:O	1:A:412:VAL:HG23	2.18	0.44
1:B:458:HIS:O	1:B:461:VAL:HB	2.17	0.44
1:C:100:CYS:SG	1:C:325:GLY:HA2	2.58	0.44
1:C:163:ALA:HB1	1:C:166:VAL:HG23	1.99	0.44
1:C:196:ILE:HG12	1:C:484:ILE:HB	2.00	0.44
1:E:88:TRP:O	1:E:179:HIS:HB2	2.18	0.44
1:E:397:ILE:HG22	1:E:399:VAL:CG2	2.46	0.44
1:F:107:THR:O	1:F:364:TYR:HA	2.17	0.44
1:B:434:PRO:CB	1:B:437:LEU:HD12	2.46	0.44
1:C:246:VAL:O	1:C:271:VAL:HG13	2.17	0.44
1:C:386:ILE:HG23	1:D:346:HIS:CE1	2.53	0.44
1:C:474:ASP:HB3	1:C:477:ILE:CB	2.47	0.44
1:D:119:GLN:HB2	1:D:124:VAL:CG2	2.48	0.44
1:E:48:GLU:O	1:E:52:ILE:HG13	2.18	0.44
1:E:205:GLU:CG	1:E:209:ARG:HD2	2.42	0.44
1:E:321:ALA:HB1	1:E:326:LEU:O	2.18	0.44
1:F:281:THR:HG22	1:F:282:VAL:CG2	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:452:ASP:O	1:F:456:VAL:HG23	2.18	0.44
1:B:42:ILE:HG12	1:B:224:LEU:HB3	1.99	0.43
1:C:145:ASN:N	1:C:384:ASN:HD21	2.05	0.43
1:C:218:LEU:HD13	1:C:230:ALA:HB1	1.99	0.43
1:C:307:SER:HB2	1:C:308:PRO:HD2	2.00	0.43
1:D:100:CYS:SG	1:D:325:GLY:HA2	2.58	0.43
1:D:129:VAL:HG22	1:D:132:ASP:OD2	2.18	0.43
1:F:61:ASN:OD1	1:F:63:LYS:HG2	2.18	0.43
1:F:104:VAL:HA	1:F:360:ALA:O	2.18	0.43
1:A:305:VAL:HG21	2:A:601:BG3:H62	1.99	0.43
1:C:349:THR:O	1:C:353:LEU:HB2	2.18	0.43
1:E:397:ILE:HG22	1:E:399:VAL:HG23	2.00	0.43
1:A:110:GLY:HA3	1:A:183:ILE:HG13	2.00	0.43
1:A:191:GLU:HG3	1:A:240:PHE:HZ	1.82	0.43
1:A:425:ARG:HG3	1:A:425:ARG:HH11	1.83	0.43
1:B:314:SER:HB3	1:B:330:VAL:HB	1.99	0.43
1:C:152:PRO:HG2	1:C:153:VAL:H	1.82	0.43
1:C:390:VAL:O	1:C:393:ALA:HB3	2.17	0.43
1:D:370:GLU:HB3	1:D:373:MET:HB3	1.99	0.43
1:E:396:GLY:O	1:E:398:PRO:HD3	2.18	0.43
1:E:473:ILE:HG21	1:E:481:MET:CE	2.35	0.43
1:F:181:HIS:NE2	1:F:217:LEU:HB2	2.33	0.43
1:F:216:MET:CE	1:F:242:ILE:HG21	2.48	0.43
1:F:353:LEU:HD13	1:F:390:VAL:HG22	1.99	0.43
1:F:445:TRP:CE2	1:F:450:SER:HA	2.53	0.43
1:A:219:CYS:SG	1:A:249:MET:HG3	2.58	0.43
1:A:434:PRO:HB2	1:A:437:LEU:HB2	2.00	0.43
1:C:154:SER:HB3	1:C:164:GLN:NE2	2.34	0.43
1:D:80:LEU:HD12	1:D:279:GLN:HB3	2.00	0.43
1:E:200:TYR:HA	1:E:477:ILE:HG21	2.00	0.43
1:E:411:LYS:HZ3	1:E:421:LEU:HD13	1.82	0.43
1:E:452:ASP:OD1	1:E:455:THR:HG23	2.18	0.43
1:B:151:LEU:HA	1:B:152:PRO:HD2	1.91	0.43
1:B:210:LYS:O	1:B:210:LYS:HG2	2.18	0.43
1:D:248:SER:H	1:D:291:SER:HA	1.83	0.43
1:E:136:ILE:HG22	1:E:149:PHE:HE1	1.83	0.43
1:E:172:PRO:O	1:E:176:THR:HG22	2.18	0.43
1:E:334:LYS:HA	1:E:348:LYS:HZ3	1.83	0.43
1:F:216:MET:HE3	1:F:242:ILE:CG2	2.49	0.43
1:F:305:VAL:HG21	1:F:334:LYS:CD	2.48	0.43
1:F:364:TYR:O	1:F:364:TYR:CD1	2.72	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:O	1:A:276:VAL:HG23	2.19	0.43
1:A:276:VAL:O	1:A:280:LEU:HG	2.19	0.43
1:B:135:ASP:O	1:B:138:LYS:HB3	2.19	0.43
1:B:243:PRO:HG3	1:B:286:LYS:HD2	2.00	0.43
1:C:336:ASP:HA	1:C:371:LEU:H	1.84	0.43
1:D:87:LEU:HD21	1:D:288:TRP:CH2	2.54	0.43
1:D:272:LEU:O	1:D:276:VAL:HG23	2.18	0.43
1:D:297:ASP:C	1:D:299:LYS:N	2.71	0.43
1:D:473:ILE:HG21	1:D:481:MET:HE1	2.00	0.43
1:E:139:LEU:O	1:E:142:TRP:HB3	2.18	0.43
1:E:252:SER:CB	1:E:295:THR:HA	2.48	0.43
1:B:110:GLY:HA3	1:B:183:ILE:HG13	1.99	0.43
1:B:412:VAL:HG21	1:B:418:PHE:CD2	2.53	0.43
1:C:26:LEU:HD13	1:C:323:PHE:CG	2.54	0.43
1:C:88:TRP:CE3	1:C:211:LYS:HG2	2.53	0.43
1:C:129:VAL:HG23	1:C:132:ASP:H	1.84	0.43
1:C:205:GLU:O	1:C:205:GLU:HG3	2.18	0.43
1:A:14:ASN:HA	5:A:717:HOH:O	2.19	0.43
1:B:162:GLY:CA	1:B:492:PHE:CD2	3.00	0.43
1:B:321:ALA:CB	1:B:328:SER:HB3	2.48	0.43
1:C:247:LEU:HG	1:C:291:SER:N	2.33	0.43
1:C:477:ILE:HG22	1:C:481:MET:CE	2.48	0.43
1:D:232:GLN:HE21	1:D:236:LYS:HE3	1.82	0.43
1:D:332:GLY:HA3	1:D:363:ILE:HG22	1.94	0.43
1:E:249:MET:HG2	1:E:292:SER:HB3	2.01	0.43
1:E:473:ILE:HD13	1:E:481:MET:HE1	1.99	0.43
1:F:297:ASP:C	1:F:299:LYS:H	2.22	0.43
1:A:50:ARG:NE	1:A:65:ASN:OD1	2.52	0.43
1:A:91:ASP:C	1:A:93:LYS:H	2.20	0.43
1:A:437:LEU:HA	1:F:343:GLN:OE1	2.19	0.43
1:C:199:ALA:CB	1:C:481:MET:HG2	2.49	0.43
1:C:446:ALA:C	1:C:448:ALA:H	2.22	0.43
1:D:171:THR:HG23	1:D:175:ASN:HD21	1.84	0.43
1:D:179:HIS:HD1	1:D:213:ILE:HA	1.84	0.43
1:D:223:PRO:HB3	1:D:255:SER:O	2.19	0.43
1:D:305:VAL:HG22	1:D:305:VAL:O	2.18	0.43
1:F:54:LYS:HA	1:F:58:CYS:O	2.19	0.43
1:F:85:PHE:CB	1:F:286:LYS:HD3	2.48	0.43
1:F:158:ILE:HG21	1:F:167:HIS:CD2	2.52	0.43
1:F:337:ALA:CA	1:F:343:GLN:NE2	2.82	0.43
1:A:314:SER:HB2	1:A:355:PRO:HG3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LYS:NZ	1:A:368:MET:H	2.17	0.43
1:A:446:ALA:HA	1:A:450:SER:OG	2.19	0.43
1:B:476:ASP:O	1:B:479:LYS:HB2	2.19	0.43
1:C:254:GLY:O	1:D:417:ASN:HA	2.19	0.43
1:C:452:ASP:O	1:C:456:VAL:HG23	2.19	0.43
1:F:53:PHE:C	1:F:58:CYS:HB2	2.38	0.43
1:F:111:THR:HG21	1:F:184:ASP:OD2	2.19	0.43
1:F:128:SER:HA	1:F:132:ASP:OD2	2.19	0.43
1:A:150:SER:HB3	1:A:183:ILE:HD11	2.01	0.42
1:A:389:MET:CE	1:A:432:SER:HB2	2.49	0.42
1:B:21:PHE:CE1	1:E:397:ILE:HG21	2.48	0.42
1:B:420:ALA:O	1:B:421:LEU:C	2.58	0.42
1:C:54:LYS:HB2	1:C:60:VAL:HG21	2.00	0.42
1:C:126:VAL:HG23	1:C:127:ASP:N	2.33	0.42
1:E:247:LEU:HD21	1:E:292:SER:HB3	2.01	0.42
1:F:105:HIS:HB3	1:F:147:ASP:OD2	2.19	0.42
1:F:379:GLN:HG3	1:F:383:ASP:OD2	2.19	0.42
1:A:84:ARG:HH11	1:A:84:ARG:HG3	1.84	0.42
1:A:111:THR:CG2	1:A:183:ILE:HB	2.50	0.42
1:D:8:ALA:O	1:D:9:GLY:C	2.58	0.42
1:D:245:ASN:C	1:D:245:ASN:HD22	2.20	0.42
1:E:84:ARG:HB3	1:E:99:GLU:HG3	2.01	0.42
1:E:111:THR:HG23	1:E:111:THR:O	2.20	0.42
1:F:417:ASN:OD1	1:F:419:LEU:HB2	2.18	0.42
1:F:435:MET:C	1:F:436:LEU:HD12	2.39	0.42
1:A:42:ILE:HD12	1:A:273:SER:CB	2.49	0.42
1:A:44:VAL:HG21	1:A:53:PHE:CD2	2.53	0.42
1:A:194:ARG:HG2	1:A:194:ARG:NH1	2.34	0.42
1:B:194:ARG:HG2	1:B:194:ARG:NH1	2.34	0.42
1:C:251:MET:HE1	1:C:303:ALA:HB2	2.02	0.42
1:C:473:ILE:HG21	1:C:481:MET:HE3	2.00	0.42
1:A:107:THR:HG23	1:A:364:TYR:CB	2.48	0.42
1:A:409:ILE:HA	1:A:418:PHE:HZ	1.84	0.42
1:C:145:ASN:HB2	1:C:384:ASN:ND2	2.34	0.42
1:C:306:GLY:HA3	1:C:335:SER:HA	2.01	0.42
1:E:114:LYS:HB2	1:E:374:THR:HG23	2.00	0.42
1:E:332:GLY:O	1:E:333:SER:CB	2.66	0.42
1:F:189:ASN:O	1:F:190:VAL:C	2.58	0.42
1:A:133:ILE:HG13	1:A:153:VAL:HG23	2.01	0.42
1:A:137:ALA:CB	1:A:175:ASN:HB2	2.48	0.42
1:C:26:LEU:HD23	1:C:26:LEU:HA	1.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:LEU:CD2	1:C:482:GLN:HA	2.49	0.42
1:C:314:SER:HB3	1:C:330:VAL:HB	2.01	0.42
1:D:18:LEU:C	1:D:18:LEU:HD23	2.40	0.42
1:D:90:ARG:HD2	1:D:200:TYR:CZ	2.55	0.42
1:D:111:THR:O	1:D:111:THR:HG23	2.20	0.42
1:E:191:GLU:HG3	1:E:194:ARG:HH21	1.84	0.42
1:E:480:ASP:O	1:E:484:ILE:HG12	2.19	0.42
1:F:107:THR:HG23	1:F:364:TYR:CB	2.48	0.42
1:B:219:CYS:O	1:B:220:PRO:C	2.58	0.42
1:B:422:LYS:HA	1:B:425:ARG:HH12	1.80	0.42
1:C:102:GLY:O	1:C:104:VAL:HG23	2.19	0.42
1:D:445:TRP:CE2	1:D:450:SER:HA	2.54	0.42
1:E:157:ASP:OD1	1:E:157:ASP:N	2.52	0.42
1:E:267:HIS:CE1	1:E:271:VAL:HG21	2.54	0.42
1:F:216:MET:HE3	1:F:242:ILE:HG21	2.01	0.42
1:A:119:GLN:HB3	1:A:124:VAL:HG21	2.01	0.42
1:A:151:LEU:HD22	1:A:182:HIS:CD2	2.54	0.42
1:A:218:LEU:HD11	1:A:234:ILE:HD11	2.00	0.42
1:B:75:ARG:HH22	1:F:83:SER:HB3	1.82	0.42
1:C:397:ILE:HD12	1:C:397:ILE:N	2.35	0.42
1:C:481:MET:HA	1:C:484:ILE:HG12	2.02	0.42
1:E:158:ILE:HG21	1:E:164:GLN:HA	2.00	0.42
1:E:314:SER:HB3	1:E:330:VAL:HG21	2.01	0.42
1:A:109:PHE:CD1	1:A:110:GLY:N	2.88	0.42
1:A:254:GLY:O	1:F:417:ASN:HB2	2.20	0.42
1:A:351:THR:O	1:A:355:PRO:HG2	2.20	0.42
1:B:145:ASN:N	1:B:384:ASN:HD21	2.16	0.42
1:B:195:ASP:HB3	1:B:484:ILE:HD12	2.01	0.42
1:C:42:ILE:HD12	1:C:273:SER:HB3	2.01	0.42
1:D:33:THR:HG23	1:D:269:ALA:HB2	2.01	0.42
1:D:182:HIS:CD2	1:D:184:ASP:H	2.37	0.42
1:D:375:PHE:C	1:D:375:PHE:CD1	2.93	0.42
1:F:53:PHE:CG	1:F:67:VAL:HG11	2.55	0.42
1:F:151:LEU:HD11	1:F:168:GLU:HG2	2.00	0.42
1:F:332:GLY:O	1:F:333:SER:CB	2.61	0.42
1:B:261:ALA:HA	1:B:264:LEU:HD12	2.01	0.42
1:C:139:LEU:HD12	1:C:464:VAL:HG11	2.02	0.42
1:C:337:ALA:O	1:C:369:LEU:HD22	2.20	0.42
1:D:60:VAL:HG22	1:D:67:VAL:HG13	2.02	0.42
1:D:122:LYS:HD3	1:D:122:LYS:N	2.28	0.42
1:D:371:LEU:HD12	1:D:371:LEU:N	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:SER:HB3	1:F:271:VAL:CG2	2.49	0.42
1:F:387:PHE:O	1:F:391:LYS:HG3	2.19	0.42
1:A:26:LEU:HD13	1:A:323:PHE:CD1	2.54	0.42
1:A:182:HIS:CD2	1:A:184:ASP:H	2.38	0.42
1:A:336:ASP:HA	1:A:371:LEU:H	1.85	0.42
1:A:397:ILE:HG21	1:F:21:PHE:HE1	1.85	0.42
1:B:118:TYR:CZ	1:B:121:GLY:HA2	2.54	0.42
1:B:182:HIS:CD2	1:B:184:ASP:H	2.38	0.42
1:B:466:LYS:HG2	1:B:466:LYS:O	2.20	0.42
1:C:455:THR:O	1:C:459:GLU:HG3	2.19	0.42
1:E:107:THR:HG23	1:E:364:TYR:HB2	2.01	0.42
1:E:118:TYR:CE1	1:E:121:GLY:N	2.87	0.42
1:E:460:LYS:O	1:E:464:VAL:HG23	2.20	0.42
1:F:34:MET:HE2	1:F:37:LEU:HD12	2.02	0.42
1:F:90:ARG:HD2	1:F:200:TYR:CE1	2.55	0.42
1:A:209:ARG:CZ	1:A:240:PHE:O	2.68	0.41
1:A:222:SER:HA	1:A:223:PRO:HA	1.80	0.41
1:C:212:PRO:HA	5:C:711:HOH:O	2.19	0.41
1:C:305:VAL:HG22	1:C:334:LYS:HD2	2.02	0.41
1:C:327:PRO:HA	1:C:361:ASN:OD1	2.20	0.41
1:D:171:THR:CB	1:D:172:PRO:HD3	2.44	0.41
1:D:223:PRO:HA	1:D:270:GLU:OE2	2.19	0.41
1:E:109:PHE:CG	1:E:110:GLY:N	2.87	0.41
1:E:218:LEU:HD22	1:E:234:ILE:HG12	2.02	0.41
1:A:122:LYS:HD3	1:A:122:LYS:N	2.20	0.41
1:A:377:MET:CE	1:A:465:LEU:HD11	2.50	0.41
1:B:116:CYS:HB2	1:B:374:THR:HG21	2.02	0.41
1:B:218:LEU:HD21	1:B:246:VAL:HG22	2.02	0.41
1:C:346:HIS:ND1	1:D:386:ILE:HG23	2.35	0.41
1:D:50:ARG:NH1	1:D:62:GLU:OE2	2.53	0.41
1:E:42:ILE:CD1	1:E:273:SER:HB3	2.49	0.41
1:E:435:MET:C	1:E:436:LEU:HD12	2.39	0.41
1:A:129:VAL:HA	1:A:157:ASP:OD1	2.20	0.41
1:A:453:LEU:HD22	1:F:343:GLN:HB2	2.02	0.41
1:A:477:ILE:HD13	1:A:477:ILE:HA	1.91	0.41
1:B:108:CYS:HA	1:B:366:ALA:HB3	2.02	0.41
1:C:76:LYS:HE2	1:C:80:LEU:HD11	2.03	0.41
1:C:235:ILE:O	1:C:239:ARG:HG3	2.20	0.41
1:D:378:GLU:O	1:D:381:VAL:HG22	2.20	0.41
1:E:189:ASN:HB3	1:E:192:TYR:HD2	1.85	0.41
1:E:221:THR:O	1:E:225:GLU:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:SER:HA	1:E:331:ALA:HB2	2.01	0.41
1:F:187:GLY:N	1:F:229:ASN:OD1	2.45	0.41
1:F:294:THR:HG23	1:F:295:THR:O	2.21	0.41
1:A:99:GLU:O	1:A:100:CYS:C	2.57	0.41
1:A:109:PHE:O	1:A:152:PRO:HA	2.21	0.41
1:A:493:ARG:O	1:A:495:MET:N	2.54	0.41
1:B:87:LEU:HD21	1:B:288:TRP:CH2	2.55	0.41
1:B:134:ALA:HA	1:B:175:ASN:ND2	2.35	0.41
1:B:145:ASN:ND2	1:B:384:ASN:O	2.53	0.41
1:C:27:LYS:O	1:C:30:HIS:HB3	2.20	0.41
1:C:106:TRP:CD1	1:C:363:ILE:HB	2.55	0.41
1:D:377:MET:HE1	4:D:604:GOL:H32	2.01	0.41
1:E:274:GLY:O	1:E:277:LEU:HB3	2.20	0.41
1:F:50:ARG:NH1	1:F:62:GLU:OE2	2.53	0.41
1:F:109:PHE:CB	1:F:368:MET:HB2	2.51	0.41
1:F:174:ALA:HA	1:F:473:ILE:CD1	2.46	0.41
1:F:209:ARG:HH11	1:F:209:ARG:CG	2.34	0.41
1:F:267:HIS:CE1	1:F:291:SER:HB2	2.55	0.41
1:A:407:GLU:HG3	5:A:725:HOH:O	2.20	0.41
1:A:448:ALA:O	1:A:451:LYS:HE3	2.20	0.41
1:B:201:TYR:OH	1:B:213:ILE:HG23	2.20	0.41
1:C:78:LEU:CD2	1:C:326:LEU:HD11	2.50	0.41
1:C:170:LEU:CD2	1:C:485:VAL:HG21	2.51	0.41
1:D:201:TYR:HD2	1:D:208:ALA:HB2	1.85	0.41
1:D:344:ALA:O	1:D:348:LYS:HG2	2.20	0.41
1:D:494:GLY:O	1:D:495:MET:C	2.58	0.41
1:A:18:LEU:C	1:A:18:LEU:HD23	2.41	0.41
1:A:343:GLN:CA	1:F:453:LEU:HD22	2.51	0.41
1:B:378:GLU:O	1:B:381:VAL:HG22	2.20	0.41
1:C:311:GLY:CA	1:C:354:LEU:HD12	2.45	0.41
1:D:106:TRP:HZ3	1:D:391:LYS:HE2	1.85	0.41
1:D:110:GLY:HA2	1:D:111:THR:HA	1.58	0.41
1:D:305:VAL:HG21	1:D:334:LYS:HD3	2.03	0.41
1:E:18:LEU:O	1:E:319:LYS:HE3	2.21	0.41
1:F:64:THR:O	1:F:65:ASN:HB2	2.21	0.41
1:A:217:LEU:HD23	1:A:217:LEU:C	2.41	0.41
1:C:90:ARG:HB3	1:C:200:TYR:OH	2.20	0.41
1:C:118:TYR:HB2	4:C:603:GOL:H11	2.02	0.41
1:C:209:ARG:C	1:C:211:LYS:H	2.24	0.41
1:C:332:GLY:O	1:C:333:SER:HB3	2.20	0.41
1:C:410:GLN:HE21	1:C:410:GLN:HB2	1.67	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:ASP:HB2	1:F:177:ALA:HB1	2.03	0.41
1:F:204:ASP:HB3	1:F:207:GLU:HB2	2.01	0.41
1:A:348:LYS:HE3	1:A:379:GLN:HG3	2.02	0.41
1:B:247:LEU:HD12	1:B:291:SER:N	2.36	0.41
1:B:410:GLN:HG2	1:E:39:ASP:OD1	2.20	0.41
1:B:434:PRO:HB2	1:B:437:LEU:HB2	2.01	0.41
1:C:84:ARG:HG3	1:C:84:ARG:HH11	1.85	0.41
1:C:197:VAL:C	1:C:199:ALA:N	2.73	0.41
1:E:9:GLY:N	1:F:16:VAL:O	2.53	0.41
1:E:264:LEU:O	1:E:268:ASN:HB2	2.21	0.41
1:F:92:LYS:HE3	1:F:92:LYS:HB2	1.86	0.41
1:A:44:VAL:HB	1:A:50:ARG:CG	2.46	0.41
1:A:165:ASP:OD2	1:A:193:TYR:OH	2.30	0.41
1:A:370:GLU:OE2	1:F:442:PHE:HB2	2.21	0.41
1:A:437:LEU:HD22	1:F:343:GLN:CG	2.44	0.41
1:B:209:ARG:HH11	1:B:209:ARG:CB	2.30	0.41
1:B:224:LEU:H	1:B:224:LEU:HD23	1.86	0.41
1:B:251:MET:CE	1:B:303:ALA:HB2	2.48	0.41
1:B:328:SER:H	1:B:361:ASN:HB2	1.86	0.41
1:C:14:ASN:HA	5:C:715:HOH:O	2.20	0.41
1:C:105:HIS:O	1:C:362:THR:HA	2.19	0.41
1:C:191:GLU:HG3	1:C:240:PHE:HZ	1.86	0.41
1:C:337:ALA:CA	1:C:343:GLN:NE2	2.84	0.41
1:D:119:GLN:HA	1:D:119:GLN:HE21	1.85	0.41
1:D:247:LEU:HD23	1:D:248:SER:N	2.36	0.41
1:D:252:SER:C	1:D:254:GLY:H	2.24	0.41
1:E:159:ALA:O	1:E:161:GLN:HG2	2.21	0.41
1:E:220:PRO:HB2	1:E:270:GLU:HB3	2.02	0.41
1:E:297:ASP:N	1:E:302:THR:O	2.50	0.41
1:E:305:VAL:HG11	1:E:368:MET:CE	2.51	0.41
1:E:449:GLY:O	1:E:450:SER:HB2	2.21	0.41
1:E:485:VAL:O	1:E:488:ALA:HB3	2.21	0.41
1:F:165:ASP:HA	1:F:168:GLU:OE2	2.21	0.41
1:F:268:ASN:ND2	1:F:289:TYR:OH	2.54	0.41
1:F:318:ALA:O	1:F:321:ALA:HB3	2.21	0.41
1:A:63:LYS:HG3	1:A:64:THR:N	2.35	0.41
1:B:42:ILE:HD12	1:B:273:SER:CB	2.49	0.41
1:C:198:LYS:HG2	1:C:203:GLY:HA2	2.03	0.41
1:C:296:PHE:HD2	1:C:298:LEU:HD23	1.86	0.41
1:D:52:ILE:HA	1:D:55:GLU:OE2	2.21	0.41
1:D:84:ARG:HB3	1:D:99:GLU:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:477:ILE:O	1:D:480:ASP:HB2	2.20	0.41
1:E:82:PRO:C	1:E:84:ARG:H	2.23	0.41
1:E:320:LEU:O	1:E:323:PHE:HB3	2.21	0.41
1:E:477:ILE:HG22	1:E:481:MET:HE2	2.02	0.41
1:F:118:TYR:H	4:F:603:GOL:C3	2.26	0.41
1:F:162:GLY:HA2	1:F:492:PHE:HD2	1.86	0.41
1:F:473:ILE:O	1:F:474:ASP:C	2.58	0.41
1:A:51:GLN:HE21	1:A:55:GLU:HG2	1.83	0.40
1:A:84:ARG:NH2	1:C:35:GLU:OE2	2.54	0.40
1:B:167:HIS:C	1:B:169:THR:N	2.75	0.40
1:C:45:SER:HA	1:C:65:ASN:HD22	1.86	0.40
1:C:378:GLU:O	1:C:381:VAL:HG22	2.20	0.40
1:C:397:ILE:HA	1:C:398:PRO:HD3	1.82	0.40
1:D:7:VAL:HG12	1:D:8:ALA:N	2.35	0.40
1:D:474:ASP:HB3	1:D:477:ILE:HB	2.03	0.40
1:A:473:ILE:HD13	1:A:481:MET:HE1	2.03	0.40
1:B:149:PHE:CZ	1:B:152:PRO:HD3	2.56	0.40
1:B:201:TYR:CE2	1:B:208:ALA:HA	2.56	0.40
1:C:149:PHE:CZ	1:C:152:PRO:HD3	2.56	0.40
1:C:205:GLU:OE1	1:C:205:GLU:HA	2.21	0.40
1:D:117:LYS:HE2	4:D:604:GOL:O3	2.20	0.40
1:D:242:ILE:O	1:D:244:VAL:HG23	2.20	0.40
1:D:275:ILE:HD13	1:D:326:LEU:HD13	2.02	0.40
1:E:452:ASP:OD2	1:E:454:ALA:HB3	2.20	0.40
1:E:481:MET:O	1:E:485:VAL:HG23	2.21	0.40
1:A:84:ARG:HB3	1:A:99:GLU:CB	2.49	0.40
1:A:423:GLN:NE2	1:F:259:TYR:HE2	2.19	0.40
1:A:442:PHE:HE2	1:F:125:THR:OG1	2.03	0.40
1:C:294:THR:HB	1:C:310:LEU:HD13	2.03	0.40
1:C:415:GLY:H	1:D:223:PRO:HG2	1.85	0.40
1:D:343:GLN:O	1:D:344:ALA:C	2.58	0.40
1:E:272:LEU:HD23	1:E:272:LEU:HA	1.96	0.40
1:F:37:LEU:HD23	1:F:37:LEU:HA	1.80	0.40
1:F:148:TYR:OH	1:F:362:THR:HG21	2.20	0.40
1:F:194:ARG:HG2	1:F:194:ARG:NH1	2.36	0.40
1:F:489:ASP:O	1:F:492:PHE:HB3	2.21	0.40
1:A:341:ASP:O	1:F:342:ASP:HA	2.21	0.40
1:A:400:SER:H	1:A:403:THR:HG1	1.66	0.40
1:B:26:LEU:HD13	1:B:323:PHE:CG	2.57	0.40
1:B:73:LEU:HD23	1:B:73:LEU:HA	1.97	0.40
1:B:82:PRO:HD3	1:B:284:GLY:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:PHE:CG	1:B:178:LYS:HG2	2.56	0.40
1:C:130:GLU:HB2	1:C:155:ALA:HB1	2.04	0.40
1:D:314:SER:HB3	1:D:330:VAL:CG2	2.52	0.40
1:E:405:ALA:O	1:E:408:SER:HB3	2.21	0.40
1:F:199:ALA:HB3	1:F:481:MET:HG2	2.03	0.40
1:F:307:SER:HB2	1:F:308:PRO:HD2	2.03	0.40
1:C:84:ARG:HG3	1:C:84:ARG:NH1	2.36	0.40
1:C:94:PHE:CD1	1:C:178:LYS:HE2	2.57	0.40
1:C:209:ARG:O	1:C:212:PRO:HD3	2.22	0.40
1:C:397:ILE:HG22	1:C:399:VAL:HG23	2.03	0.40
1:D:170:LEU:HD22	1:D:482:GLN:HA	2.02	0.40
1:D:448:ALA:O	1:D:451:LYS:HE3	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	492/503 (98%)	434 (88%)	55 (11%)	3 (1%)	25	64
1	B	492/503 (98%)	435 (88%)	52 (11%)	5 (1%)	15	54
1	C	491/503 (98%)	424 (86%)	57 (12%)	10 (2%)	7	38
1	D	492/503 (98%)	424 (86%)	63 (13%)	5 (1%)	15	54
1	E	492/503 (98%)	417 (85%)	64 (13%)	11 (2%)	6	35
1	F	492/503 (98%)	433 (88%)	51 (10%)	8 (2%)	9	43
All	All	2951/3018 (98%)	2567 (87%)	342 (12%)	42 (1%)	11	46

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	371	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	421	LEU
1	F	62	GLU
1	C	421	LEU
1	D	202	GLY
1	D	298	LEU
1	E	227	SER
1	E	298	LEU
1	F	119	GLN
1	F	227	SER
1	F	300	LYS
1	A	9	GLY
1	A	92	LYS
1	B	340	PRO
1	B	421	LEU
1	C	157	ASP
1	C	176	THR
1	C	299	LYS
1	D	421	LEU
1	E	168	GLU
1	E	340	PRO
1	C	119	GLN
1	D	168	GLU
1	E	119	GLN
1	E	175	ASN
1	B	257	PRO
1	C	128	SER
1	E	179	HIS
1	E	333	SER
1	F	157	ASP
1	A	234	ILE
1	B	143	ALA
1	B	447	ALA
1	C	368	MET
1	C	152	PRO
1	F	151	LEU
1	F	365	GLY
1	D	203	GLY
1	E	443	GLY
1	C	212	PRO
1	F	40	PRO
1	E	365	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	405/412 (98%)	388 (96%)	17 (4%)	30	65
1	B	405/412 (98%)	390 (96%)	15 (4%)	34	68
1	C	404/412 (98%)	387 (96%)	17 (4%)	30	65
1	D	405/412 (98%)	391 (96%)	14 (4%)	36	69
1	E	405/412 (98%)	389 (96%)	16 (4%)	31	66
1	F	405/412 (98%)	391 (96%)	14 (4%)	36	69
All	All	2429/2472 (98%)	2336 (96%)	93 (4%)	33	67

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	11	ASN
1	A	79	GLN
1	A	91	ASP
1	A	99	GLU
1	A	111	THR
1	A	122	LYS
1	A	217	LEU
1	A	219	CYS
1	A	245	ASN
1	A	267	HIS
1	A	288	TRP
1	A	364	TYR
1	A	374	THR
1	A	406	VAL
1	A	421	LEU
1	A	442	PHE
1	B	5	ASN
1	B	24	ASP
1	B	86	VAL
1	B	91	ASP
1	B	120	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	122	LYS
1	B	184	ASP
1	B	209	ARG
1	B	268	ASN
1	B	277	LEU
1	B	288	TRP
1	B	364	TYR
1	B	373	MET
1	B	388	SER
1	B	418	PHE
1	C	72	TYR
1	C	91	ASP
1	C	120	ASP
1	C	122	LYS
1	C	131	LYS
1	C	228	VAL
1	C	245	ASN
1	C	252	SER
1	C	267	HIS
1	C	268	ASN
1	C	288	TRP
1	C	309	GLU
1	C	353	LEU
1	C	364	TYR
1	C	373	MET
1	C	408	SER
1	C	476	ASP
1	D	117	LYS
1	D	119	GLN
1	D	122	LYS
1	D	167	HIS
1	D	209	ARG
1	D	245	ASN
1	D	268	ASN
1	D	288	TRP
1	D	364	TYR
1	D	373	MET
1	D	375	PHE
1	D	384	ASN
1	D	452	ASP
1	D	476	ASP
1	E	24	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	79	GLN
1	E	86	VAL
1	E	91	ASP
1	E	120	ASP
1	E	122	LYS
1	E	184	ASP
1	E	216	MET
1	E	218	LEU
1	E	245	ASN
1	E	277	LEU
1	E	288	TRP
1	E	364	TYR
1	E	373	MET
1	E	374	THR
1	E	444	ASP
1	F	24	ASP
1	F	58	CYS
1	F	91	ASP
1	F	116	CYS
1	F	120	ASP
1	F	122	LYS
1	F	245	ASN
1	F	249	MET
1	F	268	ASN
1	F	288	TRP
1	F	342	ASP
1	F	364	TYR
1	F	373	MET
1	F	476	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	51	GLN
1	A	79	GLN
1	A	175	ASN
1	A	182	HIS
1	A	232	GLN
1	A	245	ASN
1	A	268	ASN
1	A	322	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	384	ASN
1	A	395	GLN
1	A	410	GLN
1	A	423	GLN
1	A	458	HIS
1	B	14	ASN
1	B	65	ASN
1	B	79	GLN
1	B	105	HIS
1	B	161	GLN
1	B	167	HIS
1	B	175	ASN
1	B	182	HIS
1	B	189	ASN
1	B	232	GLN
1	B	245	ASN
1	B	268	ASN
1	B	322	GLN
1	B	384	ASN
1	B	410	GLN
1	C	51	GLN
1	C	65	ASN
1	C	79	GLN
1	C	105	HIS
1	C	175	ASN
1	C	232	GLN
1	C	245	ASN
1	C	268	ASN
1	C	322	GLN
1	C	379	GLN
1	C	384	ASN
1	C	410	GLN
1	D	11	ASN
1	D	51	GLN
1	D	56	ASN
1	D	79	GLN
1	D	105	HIS
1	D	119	GLN
1	D	161	GLN
1	D	175	ASN
1	D	182	HIS
1	D	232	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	245	ASN
1	D	268	ASN
1	D	322	GLN
1	D	384	ASN
1	D	410	GLN
1	D	458	HIS
1	E	65	ASN
1	E	79	GLN
1	E	105	HIS
1	E	175	ASN
1	E	182	HIS
1	E	189	ASN
1	E	245	ASN
1	E	268	ASN
1	E	322	GLN
1	E	384	ASN
1	E	410	GLN
1	F	65	ASN
1	F	79	GLN
1	F	105	HIS
1	F	175	ASN
1	F	182	HIS
1	F	232	GLN
1	F	245	ASN
1	F	268	ASN
1	F	322	GLN
1	F	384	ASN
1	F	395	GLN
1	F	410	GLN
1	F	426	GLN
1	F	440	HIS
1	F	458	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	C	603	-	5,5,5	0.31	0	5,5,5	0.81	0
4	GOL	D	605	-	5,5,5	0.33	0	5,5,5	0.50	0
4	GOL	E	604	-	5,5,5	0.33	0	5,5,5	0.95	0
4	GOL	D	603	-	5,5,5	0.29	0	5,5,5	0.49	0
4	GOL	B	603	-	5,5,5	0.27	0	5,5,5	0.80	0
2	BG3	D	601	1	8,12,13	1.06	0	11,18,20	1.54	4 (36%)
4	GOL	A	603	-	5,5,5	0.34	0	5,5,5	0.34	0
4	GOL	B	604	-	5,5,5	0.36	0	5,5,5	0.72	0
2	BG3	E	601	1	8,12,13	1.19	0	11,18,20	1.47	4 (36%)
4	GOL	D	604	-	5,5,5	0.30	0	5,5,5	0.78	0
2	BG3	C	601	1	8,12,13	1.39	1 (12%)	11,18,20	1.42	3 (27%)
4	GOL	F	603	-	5,5,5	0.30	0	5,5,5	1.28	1 (20%)
2	BG3	F	601	1	8,12,13	1.09	0	11,18,20	1.35	3 (27%)
4	GOL	E	603	-	5,5,5	0.32	0	5,5,5	0.48	0
2	BG3	B	601	1	8,12,13	1.59	1 (12%)	11,18,20	1.46	3 (27%)
2	BG3	A	601	1	8,12,13	1.37	1 (12%)	11,18,20	1.51	2 (18%)
4	GOL	A	604	-	5,5,5	0.28	0	5,5,5	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	603	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	605	-	-	4/4/4/4	-
4	GOL	E	604	-	-	0/4/4/4	-
4	GOL	D	603	-	-	2/4/4/4	-
4	GOL	B	603	-	-	3/4/4/4	-
2	BG3	D	601	1	-	1/1/20/22	0/1/1/1
4	GOL	A	603	-	-	4/4/4/4	-
4	GOL	B	604	-	-	4/4/4/4	-
2	BG3	E	601	1	-	1/1/20/22	0/1/1/1
4	GOL	D	604	-	-	2/4/4/4	-
2	BG3	C	601	1	-	0/1/20/22	0/1/1/1
4	GOL	F	603	-	-	1/4/4/4	-
2	BG3	F	601	1	-	1/1/20/22	0/1/1/1
4	GOL	E	603	-	-	2/4/4/4	-
2	BG3	B	601	1	-	1/1/20/22	0/1/1/1
2	BG3	A	601	1	-	1/1/20/22	0/1/1/1
4	GOL	A	604	-	-	4/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	BG3	C3-C2	-3.28	1.51	1.55
2	C	601	BG3	C3-C2	-2.51	1.52	1.55
2	A	601	BG3	C3-C2	-2.37	1.52	1.55

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	BG3	C2-N1-C5	-2.66	97.98	106.43
2	D	601	BG3	C6-C3-C4	-2.61	108.21	113.05
2	A	601	BG3	C2-N1-C5	-2.52	98.42	106.43
2	C	601	BG3	C2-N1-C5	-2.50	98.47	106.43
2	E	601	BG3	C2-N1-C5	-2.47	98.57	106.43
2	B	601	BG3	C2-N1-C5	-2.46	98.61	106.43
2	A	601	BG3	C6-C3-C4	-2.42	108.56	113.05
2	E	601	BG3	O3-S1-O2	-2.32	107.37	116.52
2	F	601	BG3	C3-C2-N1	2.30	110.00	104.03
2	B	601	BG3	C6-C3-C4	-2.29	108.80	113.05
2	E	601	BG3	C6-C3-C4	-2.26	108.87	113.05
2	D	601	BG3	C2-N1-C5	-2.24	99.29	106.43
2	C	601	BG3	C6-C3-C4	-2.24	108.91	113.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	BG3	O3-S1-O2	-2.19	107.88	116.52
2	D	601	BG3	C3-C2-N1	2.16	109.62	104.03
2	C	601	BG3	O3-S1-O2	-2.13	108.10	116.52
2	F	601	BG3	C6-C3-C4	-2.12	109.12	113.05
2	B	601	BG3	C3-C2-N1	2.11	109.49	104.03
2	E	601	BG3	C3-C2-N1	2.10	109.48	104.03
4	F	603	GOL	C3-C2-C1	-2.09	103.57	111.70

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	BG3	O1-C1-C2-C3
2	D	601	BG3	O1-C1-C2-C3
2	E	601	BG3	O1-C1-C2-C3
4	A	603	GOL	O1-C1-C2-C3
4	A	603	GOL	C1-C2-C3-O3
4	A	603	GOL	O2-C2-C3-O3
4	A	604	GOL	O1-C1-C2-C3
4	B	603	GOL	O1-C1-C2-C3
4	B	604	GOL	O1-C1-C2-C3
4	B	604	GOL	C1-C2-C3-O3
4	D	603	GOL	O1-C1-C2-C3
4	D	605	GOL	O1-C1-C2-C3
4	D	605	GOL	C1-C2-C3-O3
4	D	605	GOL	O1-C1-C2-O2
4	D	605	GOL	O2-C2-C3-O3
4	E	603	GOL	O1-C1-C2-O2
4	A	604	GOL	C1-C2-C3-O3
4	C	603	GOL	O1-C1-C2-C3
4	C	603	GOL	C1-C2-C3-O3
4	D	603	GOL	C1-C2-C3-O3
4	E	603	GOL	O1-C1-C2-C3
4	A	603	GOL	O1-C1-C2-O2
4	A	604	GOL	O1-C1-C2-O2
4	A	604	GOL	O2-C2-C3-O3
4	B	603	GOL	O1-C1-C2-O2
4	C	603	GOL	O2-C2-C3-O3
4	C	603	GOL	O1-C1-C2-O2
4	B	604	GOL	O1-C1-C2-O2
4	B	604	GOL	O2-C2-C3-O3
4	F	603	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

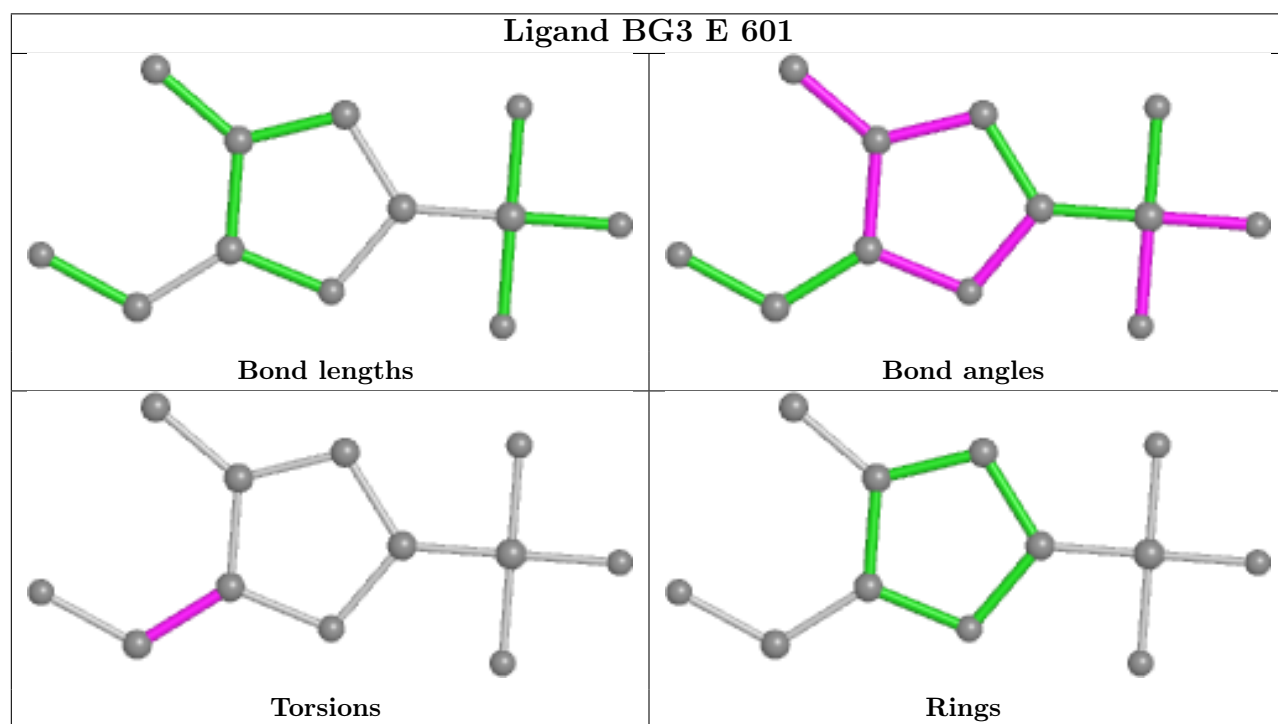
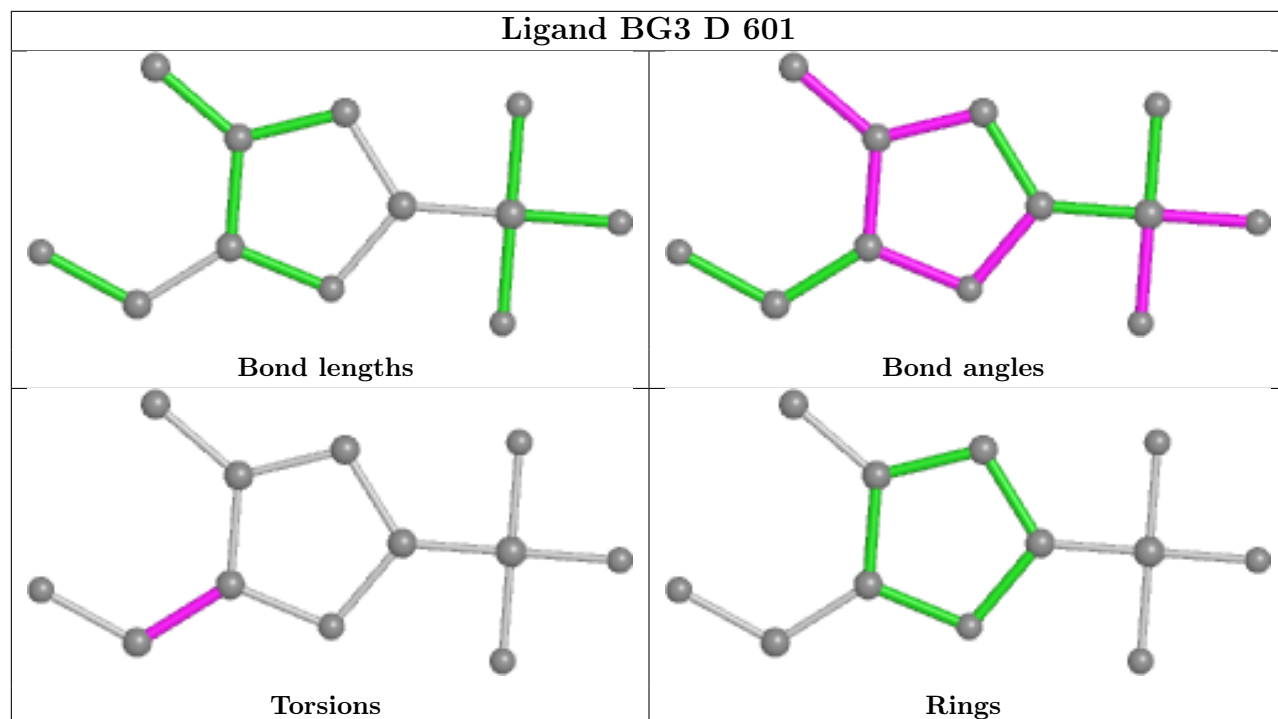
Mol	Chain	Res	Type	Atoms
2	F	601	BG3	O1-C1-C2-C3
4	D	604	GOL	O2-C2-C3-O3
4	B	603	GOL	C1-C2-C3-O3
4	D	604	GOL	C1-C2-C3-O3
2	B	601	BG3	O1-C1-C2-C3

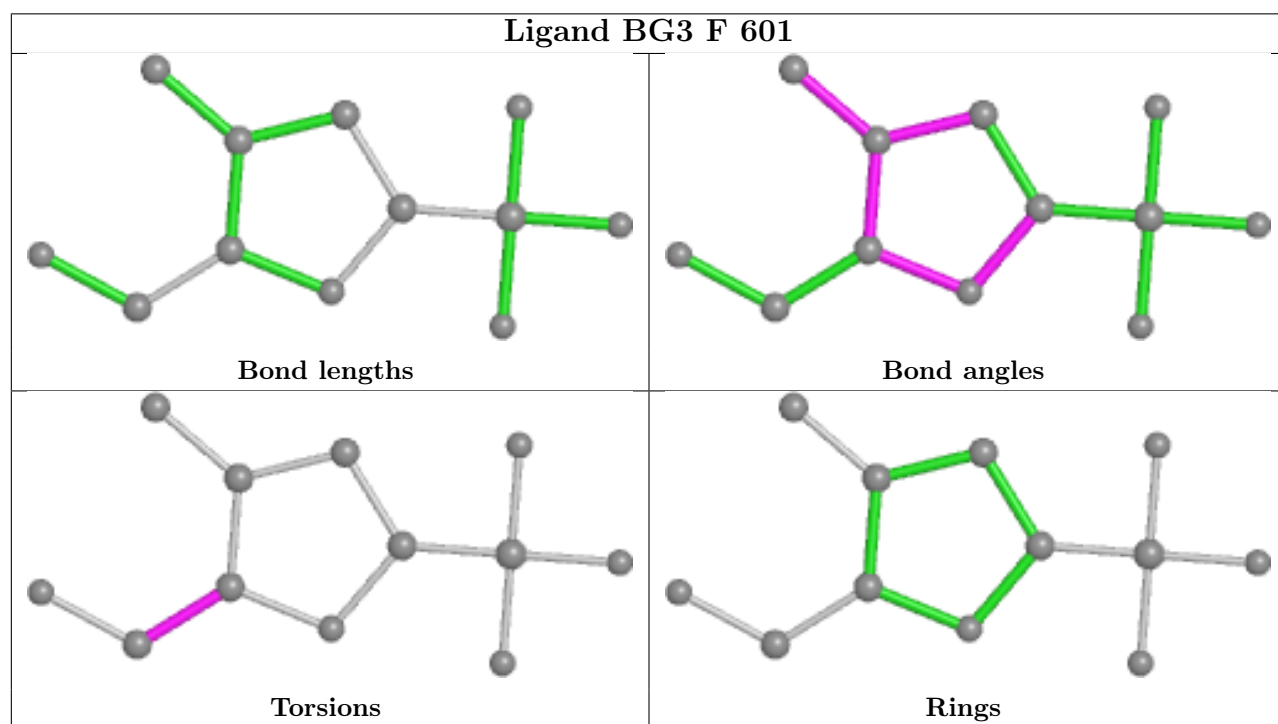
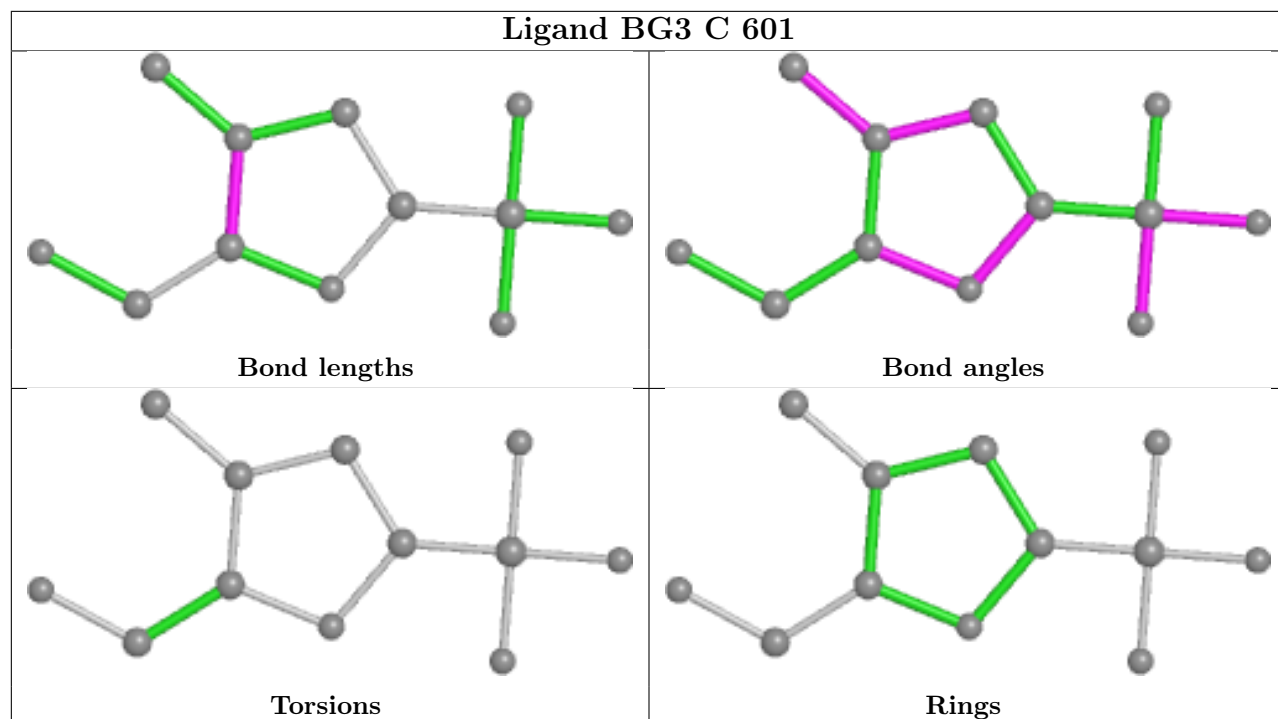
There are no ring outliers.

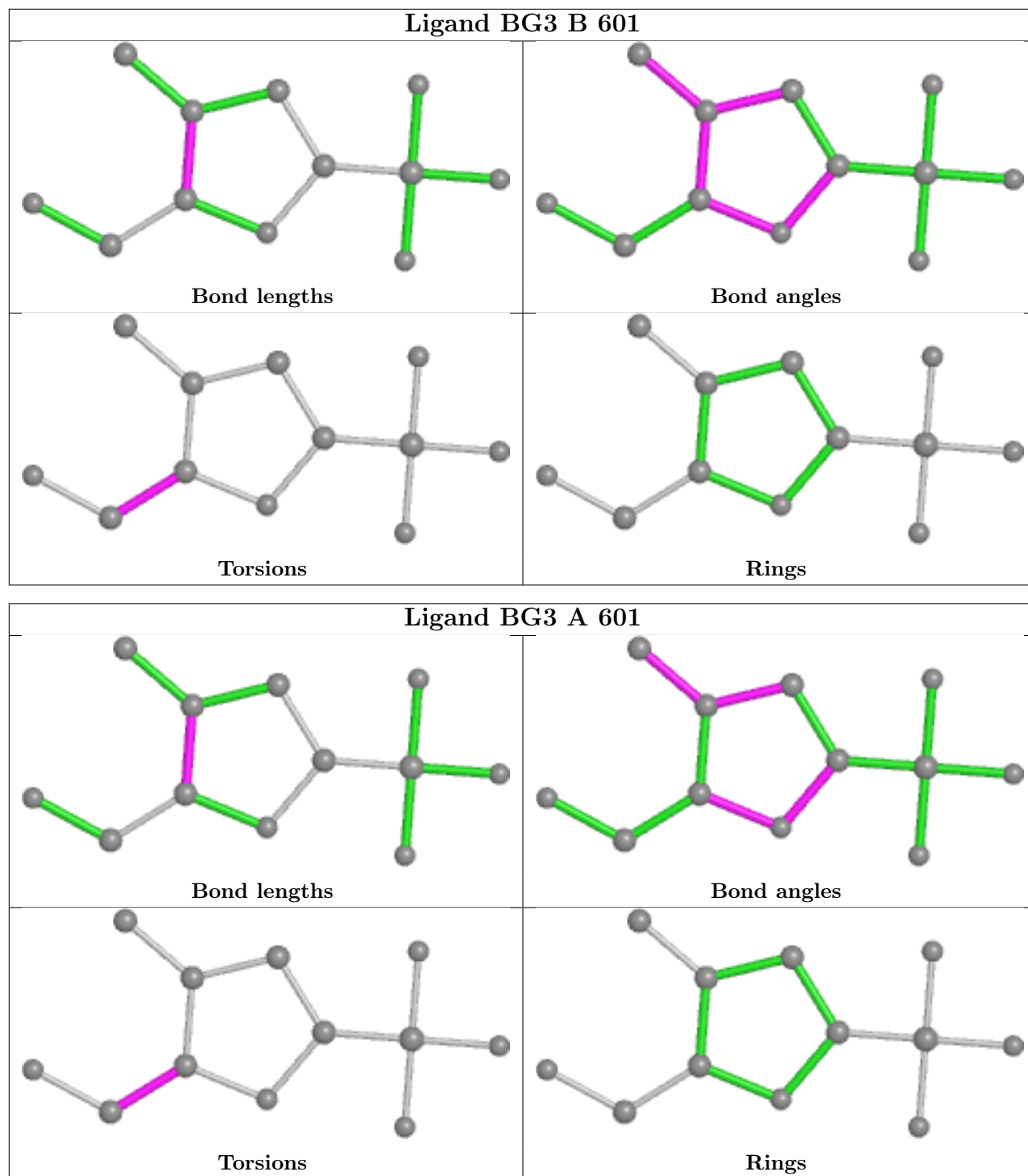
8 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	603	GOL	5	0
4	B	603	GOL	3	0
4	D	604	GOL	9	0
2	C	601	BG3	1	0
4	F	603	GOL	7	0
2	B	601	BG3	2	0
2	A	601	BG3	1	0
4	A	604	GOL	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	494/503 (98%)	-0.79	2 (0%) 92 89	22, 47, 74, 132	0
1	B	494/503 (98%)	-0.85	1 (0%) 95 94	19, 44, 70, 132	0
1	C	493/503 (98%)	-0.62	1 (0%) 95 94	27, 61, 96, 134	0
1	D	494/503 (98%)	-0.76	3 (0%) 89 83	19, 50, 80, 123	0
1	E	494/503 (98%)	-0.77	3 (0%) 89 83	18, 48, 80, 132	0
1	F	494/503 (98%)	-0.73	1 (0%) 95 94	22, 52, 87, 115	0
All	All	2963/3018 (98%)	-0.75	11 (0%) 92 89	18, 50, 85, 134	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	ASP	3.2
1	E	119	GLN	2.7
1	E	120	ASP	2.6
1	F	495	MET	2.5
1	E	495	MET	2.5
1	D	121	GLY	2.5
1	D	120	ASP	2.4
1	B	119	GLN	2.3
1	A	119	GLN	2.2
1	C	119	GLN	2.2
1	D	122	LYS	2.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

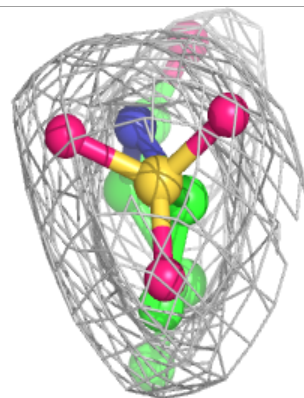
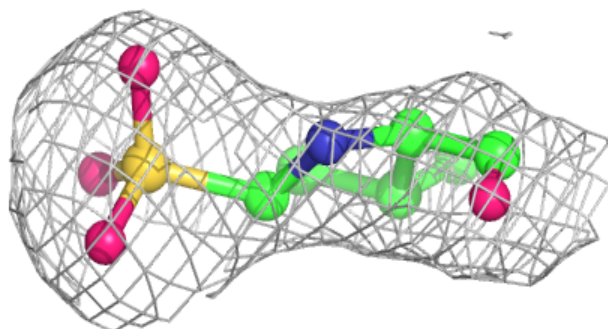
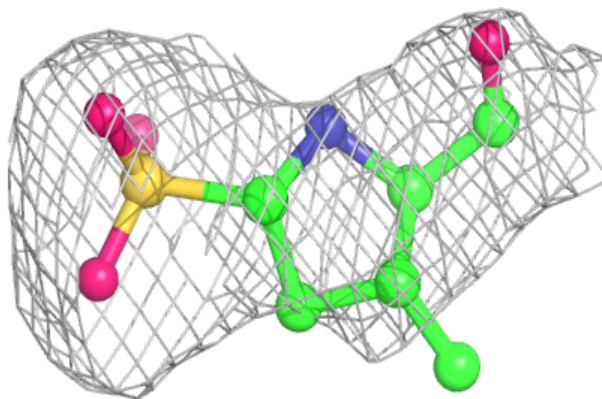
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	D	605	6/6	0.88	0.26	53,76,80,86	0
4	GOL	B	604	6/6	0.89	0.36	28,57,64,65	0
4	GOL	A	603	6/6	0.91	0.30	38,68,70,71	0
4	GOL	F	603	6/6	0.91	0.17	46,53,64,65	0
3	NA	B	602	1/1	0.92	0.07	44,44,44,44	0
4	GOL	D	604	6/6	0.92	0.18	43,63,69,70	0
4	GOL	D	603	6/6	0.93	0.36	29,74,81,92	0
4	GOL	A	604	6/6	0.93	0.12	42,64,72,80	0
3	NA	F	602	1/1	0.93	0.08	50,50,50,50	0
4	GOL	C	603	6/6	0.93	0.19	63,67,74,76	0
4	GOL	E	604	6/6	0.94	0.14	50,62,71,73	0
3	NA	C	602	1/1	0.94	0.07	56,56,56,56	0
2	BG3	C	601	12/13	0.95	0.24	68,99,106,108	0
2	BG3	D	601	12/13	0.95	0.19	37,70,83,91	0
4	GOL	B	603	6/6	0.95	0.14	30,60,65,72	0
3	NA	D	602	1/1	0.95	0.08	73,73,73,73	0
3	NA	A	602	1/1	0.95	0.06	63,63,63,63	0
3	NA	E	602	1/1	0.96	0.09	62,62,62,62	0
2	BG3	E	601	12/13	0.96	0.19	44,69,77,80	0
2	BG3	F	601	12/13	0.96	0.15	48,72,80,82	0
2	BG3	A	601	12/13	0.96	0.19	58,75,85,91	0
4	GOL	E	603	6/6	0.97	0.27	43,51,59,66	0
2	BG3	B	601	12/13	0.98	0.14	32,65,72,85	0

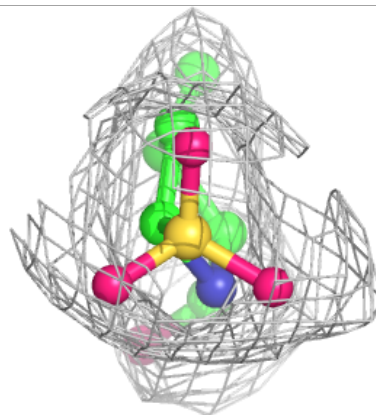
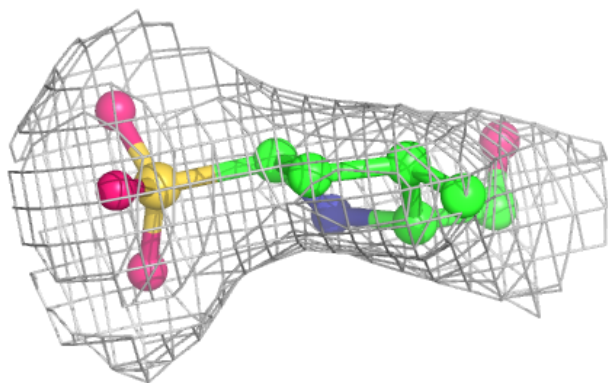
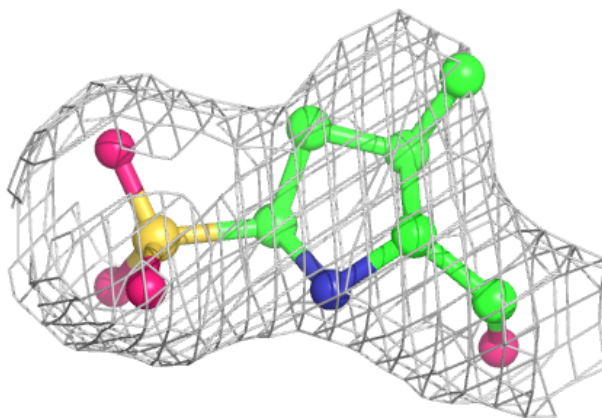
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BG3 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)

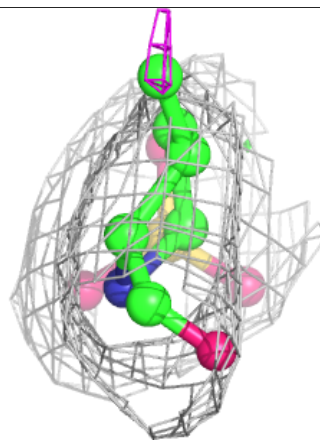
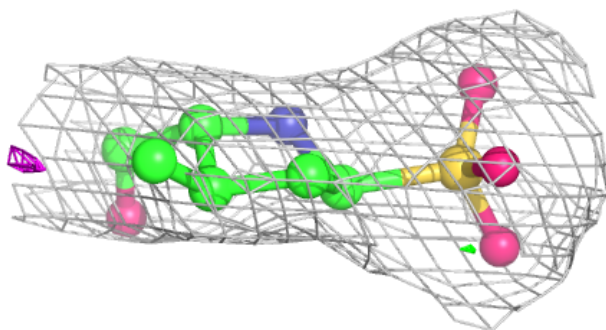
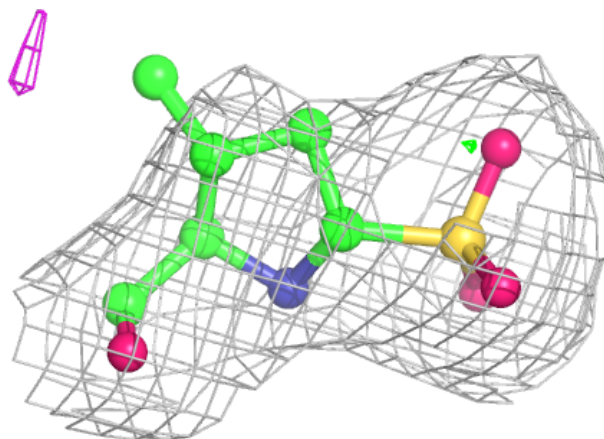
**Electron density around BG3 D 601:**

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



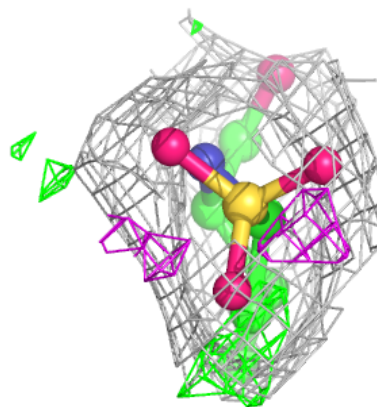
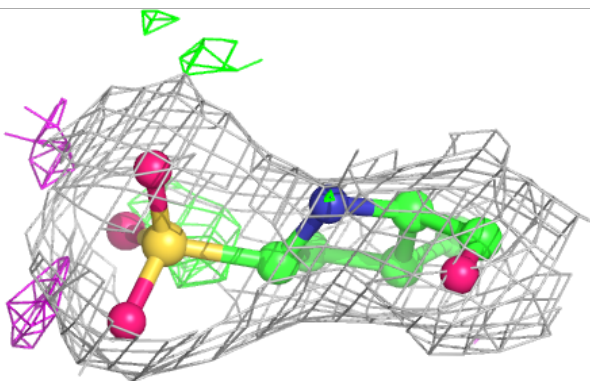
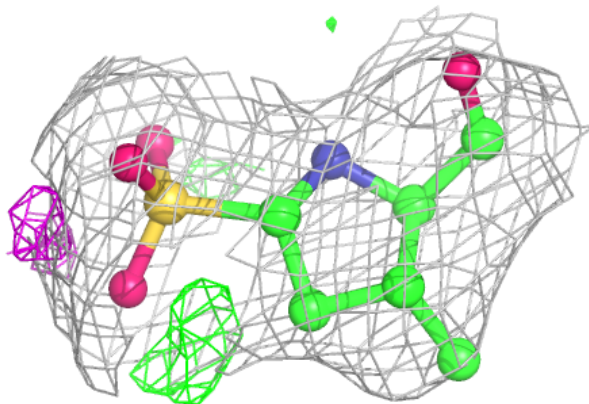
Electron density around BG3 E 601:

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



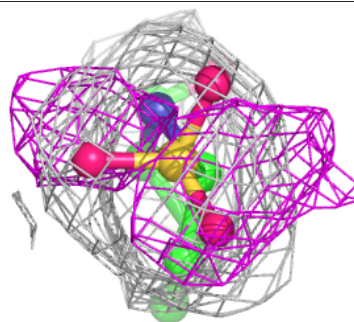
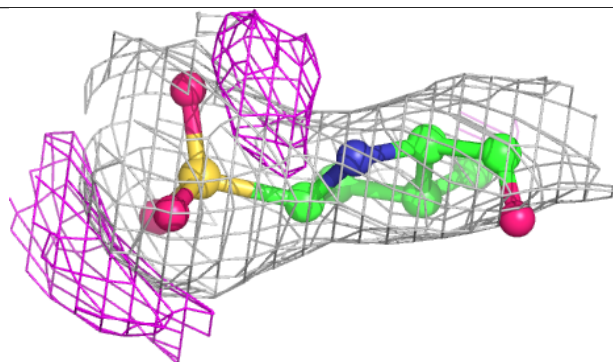
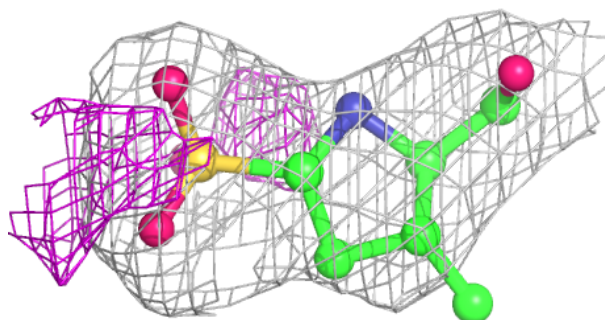
Electron density around BG3 F 601:

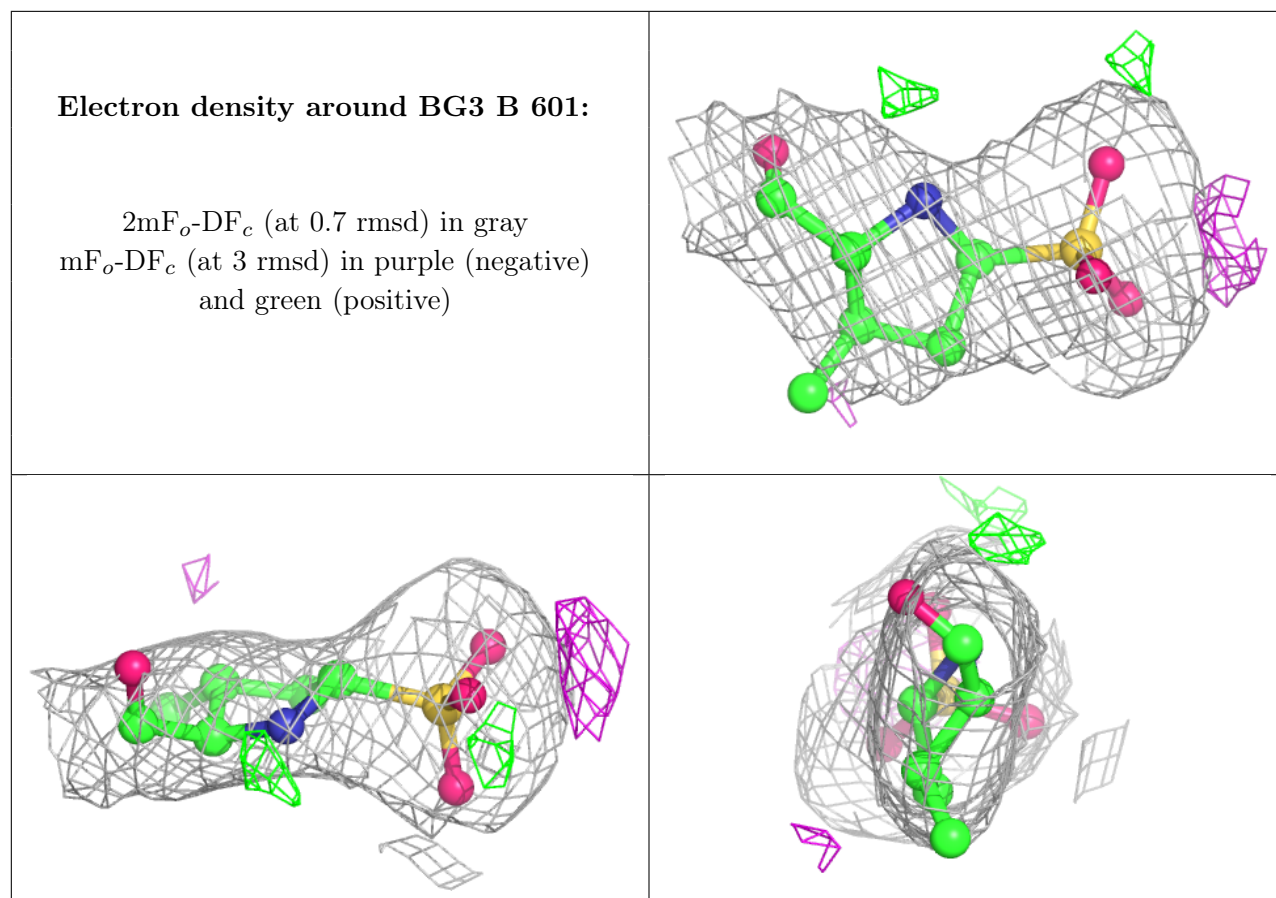
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BG3 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.