Full wwPDB X-ray Structure Validation Report (i)

Mar 17, 2026 – 07:09 PM UTC

PDB ID	:	6LKN / pdb_00006lkn
Title	:	Crystal structure of ATP11C-CDC50A in PtdSer-bound E2P state
Authors	:	Abe, K.; Irie, K.; Nakanishi, H.; Hasegawa, K.
Deposited on	:	2019-12-19
Resolution	:	3.90 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 (i) 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 (i)) were used in the production of this report:

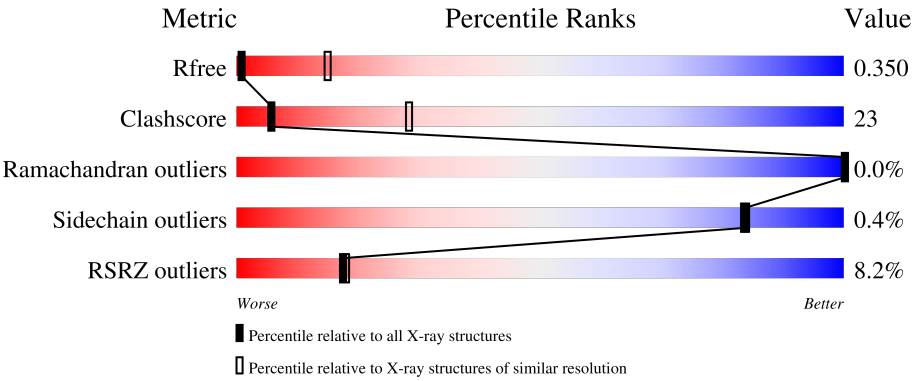
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 Å.

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



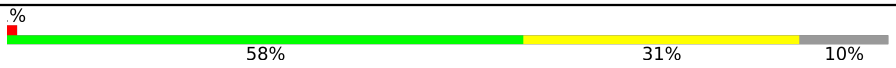
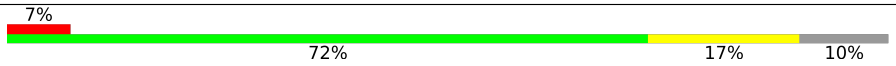
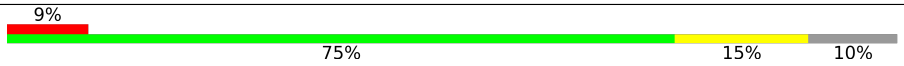
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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 <=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	1129	6% 58% 35% · 6%
1	E	1129	9% 59% 35% · 6%
1	I	1129	7% 66% 27% · 6%
1	M	1129	12% 66% 28% 6%
2	C	361	5% 60% 30% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	361	
2	J	361	
2	N	361	

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
1	BFD	E	409	-	-	X	-
5	NAG	F	405	-	-	X	-
5	NAG	J	404	-	-	X	-
5	NAG	J	405	-	-	X	-
5	NAG	N	405	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 45252 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 Phospholipid-transporting ATPase IG.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	1064	Total	Be	C	F	N	O	S	0	0	0
			8601	1	5556	3	1401	1594	46			
1	E	1064	Total	Be	C	F	N	O	S	0	0	0
			8601	1	5556	3	1401	1594	46			
1	I	1064	Total	Be	C	F	N	O	S	0	0	0
			8601	1	5556	3	1401	1594	46			
1	M	1064	Total	Be	C	F	N	O	S	0	0	0
			8601	1	5556	3	1401	1594	46			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8NB49
A	2	PHE	-	expression tag	UNP Q8NB49
A	3	ARG	-	expression tag	UNP Q8NB49
A	4	ARG	-	expression tag	UNP Q8NB49
A	5	SER	-	expression tag	UNP Q8NB49
A	6	LEU	-	expression tag	UNP Q8NB49
A	7	ASN	-	expression tag	UNP Q8NB49
A	8	ARG	-	expression tag	UNP Q8NB49
A	9	PHE	-	expression tag	UNP Q8NB49
A	111	TRP	CYS	engineered mutation	UNP Q8NB49
E	1	MET	-	initiating methionine	UNP Q8NB49
E	2	PHE	-	expression tag	UNP Q8NB49
E	3	ARG	-	expression tag	UNP Q8NB49
E	4	ARG	-	expression tag	UNP Q8NB49
E	5	SER	-	expression tag	UNP Q8NB49
E	6	LEU	-	expression tag	UNP Q8NB49
E	7	ASN	-	expression tag	UNP Q8NB49
E	8	ARG	-	expression tag	UNP Q8NB49
E	9	PHE	-	expression tag	UNP Q8NB49
E	111	TRP	CYS	engineered mutation	UNP Q8NB49
I	1	MET	-	initiating methionine	UNP Q8NB49

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	2	PHE	-	expression tag	UNP Q8NB49
I	3	ARG	-	expression tag	UNP Q8NB49
I	4	ARG	-	expression tag	UNP Q8NB49
I	5	SER	-	expression tag	UNP Q8NB49
I	6	LEU	-	expression tag	UNP Q8NB49
I	7	ASN	-	expression tag	UNP Q8NB49
I	8	ARG	-	expression tag	UNP Q8NB49
I	9	PHE	-	expression tag	UNP Q8NB49
I	111	TRP	CYS	engineered mutation	UNP Q8NB49
M	1	MET	-	initiating methionine	UNP Q8NB49
M	2	PHE	-	expression tag	UNP Q8NB49
M	3	ARG	-	expression tag	UNP Q8NB49
M	4	ARG	-	expression tag	UNP Q8NB49
M	5	SER	-	expression tag	UNP Q8NB49
M	6	LEU	-	expression tag	UNP Q8NB49
M	7	ASN	-	expression tag	UNP Q8NB49
M	8	ARG	-	expression tag	UNP Q8NB49
M	9	PHE	-	expression tag	UNP Q8NB49
M	111	TRP	CYS	engineered mutation	UNP Q8NB49

- Molecule 2 is a protein called Cell cycle control protein 50A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	324	Total	C	N	O	S	0	0	0
			2613	1696	439	466	12			
2	F	324	Total	C	N	O	S	0	0	0
			2613	1696	439	466	12			
2	J	324	Total	C	N	O	S	0	0	0
			2613	1696	439	466	12			
2	N	324	Total	C	N	O	S	0	0	0
			2613	1696	439	466	12			

There are 8 discrepancies between the modelled and reference sequences:

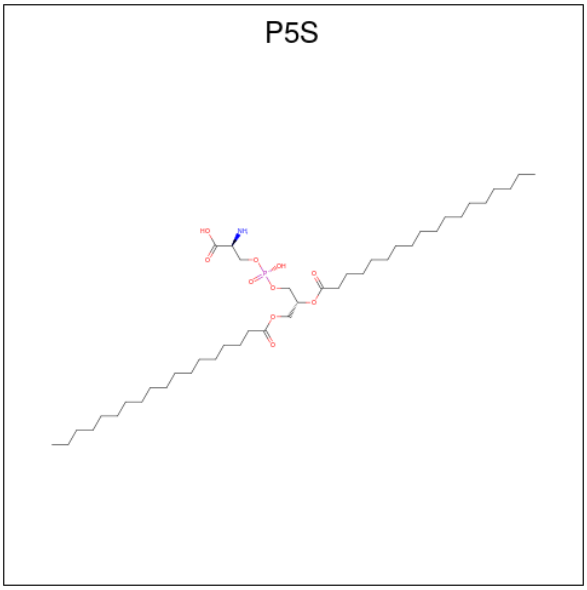
Chain	Residue	Modelled	Actual	Comment	Reference
C	190	GLN	ASN	engineered mutation	UNP Q9NV96
C	292	TRP	SER	engineered mutation	UNP Q9NV96
F	190	GLN	ASN	engineered mutation	UNP Q9NV96
F	292	TRP	SER	engineered mutation	UNP Q9NV96
J	190	GLN	ASN	engineered mutation	UNP Q9NV96
J	292	TRP	SER	engineered mutation	UNP Q9NV96
N	190	GLN	ASN	engineered mutation	UNP Q9NV96

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
N	292	TRP	SER	engineered mutation	UNP Q9NV96

- Molecule 3 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: $C_{42}H_{82}NO_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			11	3	1	6	1		
3	C	1	Total	C	N	O	P	0	0
			54	42	1	10	1		
3	E	1	Total	C	N	O	P	0	0
			11	3	1	6	1		
3	E	1	Total	C	N	O	P	0	0
			11	3	1	6	1		
3	I	1	Total	C	N	O	P	0	0
			11	3	1	6	1		
3	I	1	Total	C	N	O	P	0	0
			11	3	1	6	1		
3	M	1	Total	C	N	O	P	0	0
			11	3	1	6	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

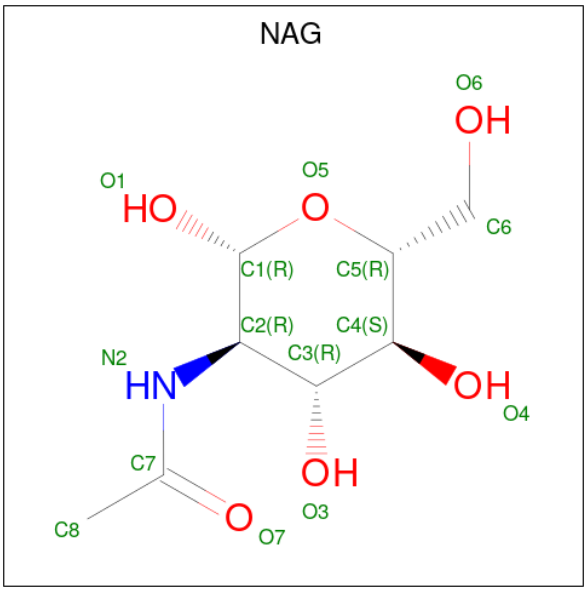
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Mg 1 1	0	0
4	I	1	Total Mg 1 1	0	0
4	M	1	Total Mg 1 1	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



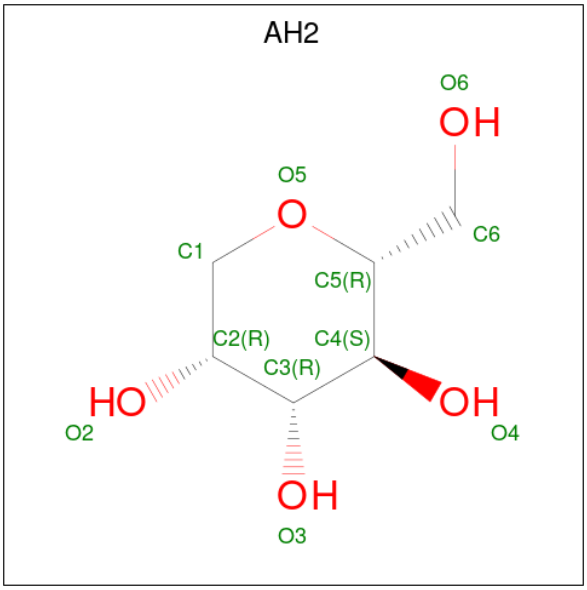
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 13 8 1 4	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 13 8 1 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	1	Total C N O 14 8 1 5	0	0
5	J	1	Total C N O 14 8 1 5	0	0
5	J	1	Total C N O 14 8 1 5	0	0
5	J	1	Total C N O 13 8 1 4	0	0
5	N	1	Total C N O 14 8 1 5	0	0
5	N	1	Total C N O 14 8 1 5	0	0
5	N	1	Total C N O 14 8 1 5	0	0
5	N	1	Total C N O 13 8 1 4	0	0

- Molecule 6 is 1-deoxy-alpha-D-mannopyranose (CCD ID: AH2) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 11 6 5	0	0
6	F	1	Total C O 11 6 5	0	0
6	J	1	Total C O 11 6 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	N	1	Total C O 11 6 5	0	0

- Molecule 7 is water.

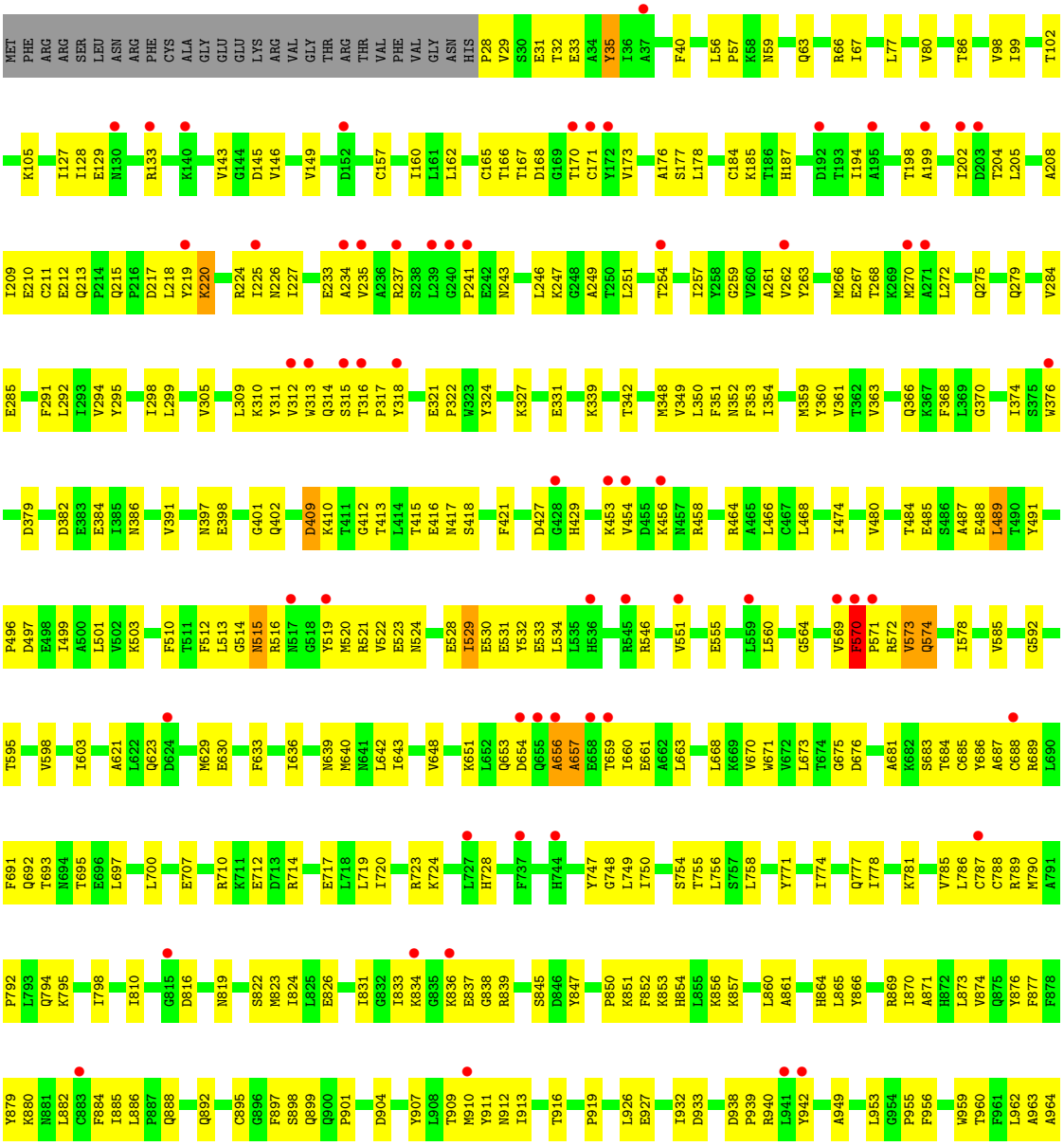
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total O 2 2	0	0
7	E	2	Total O 2 2	0	0
7	I	2	Total O 2 2	0	0
7	M	2	Total O 2 2	0	0

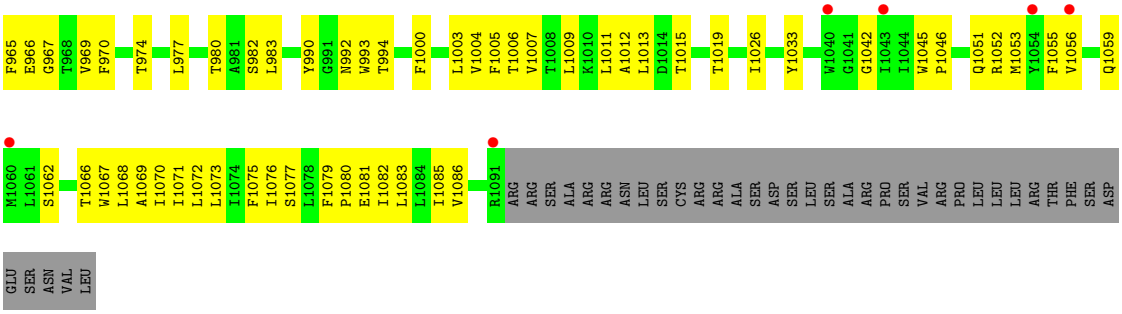
3 Residue-property plots (i)

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: Phospholipid-transporting ATPase IG

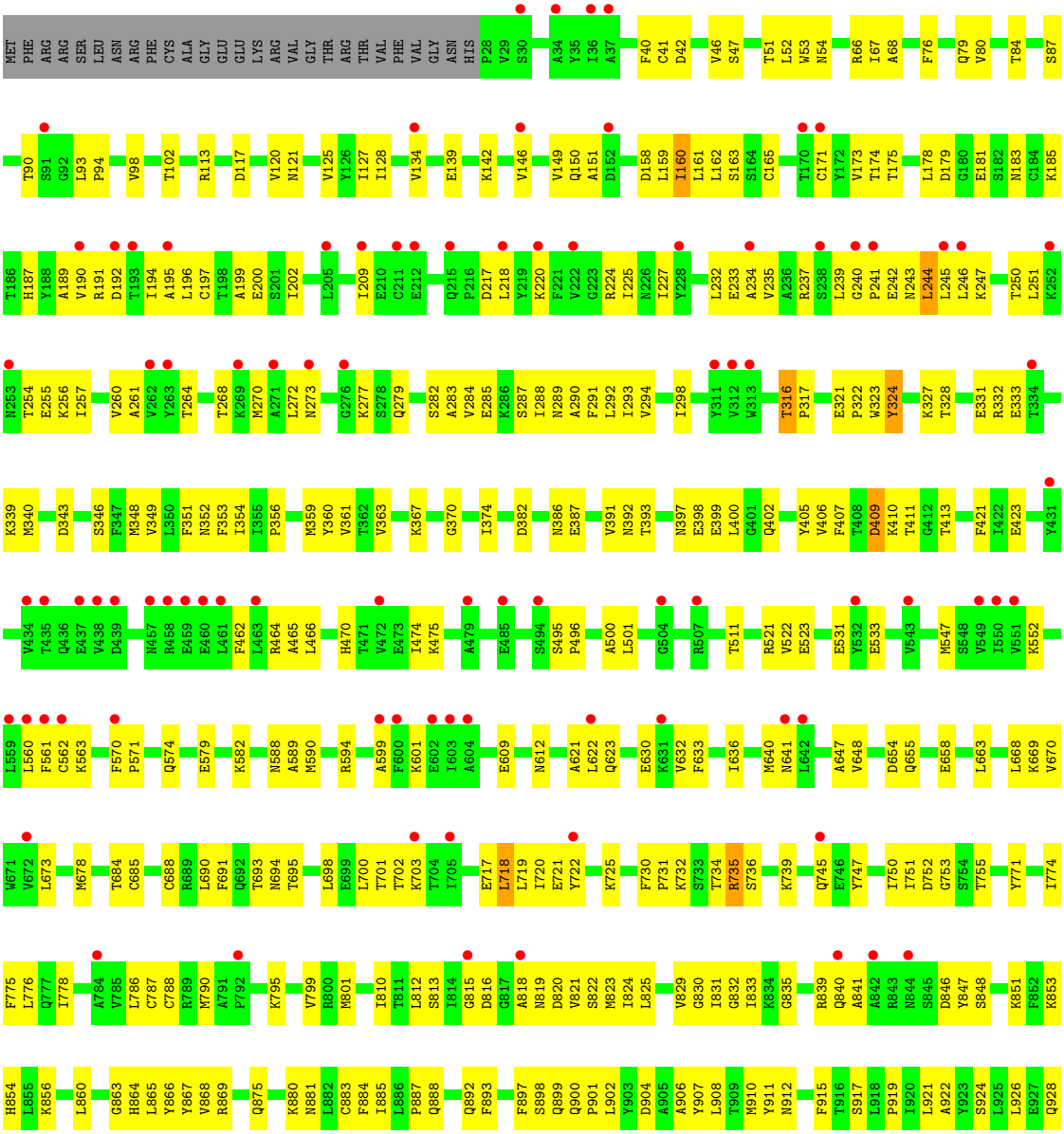
Chain A:

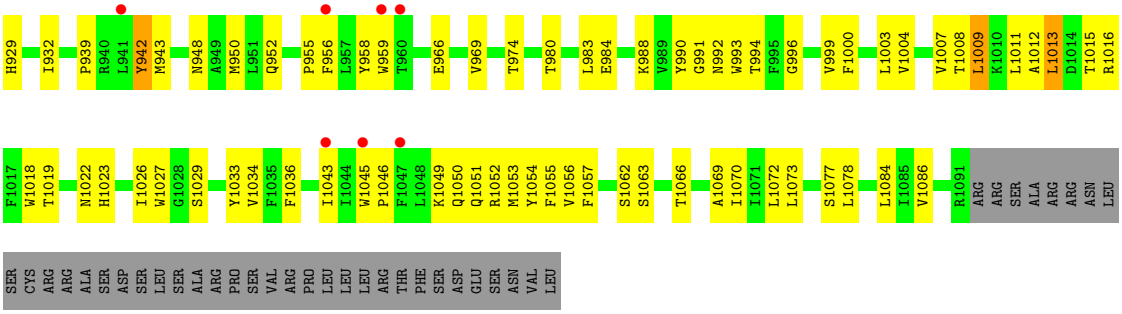




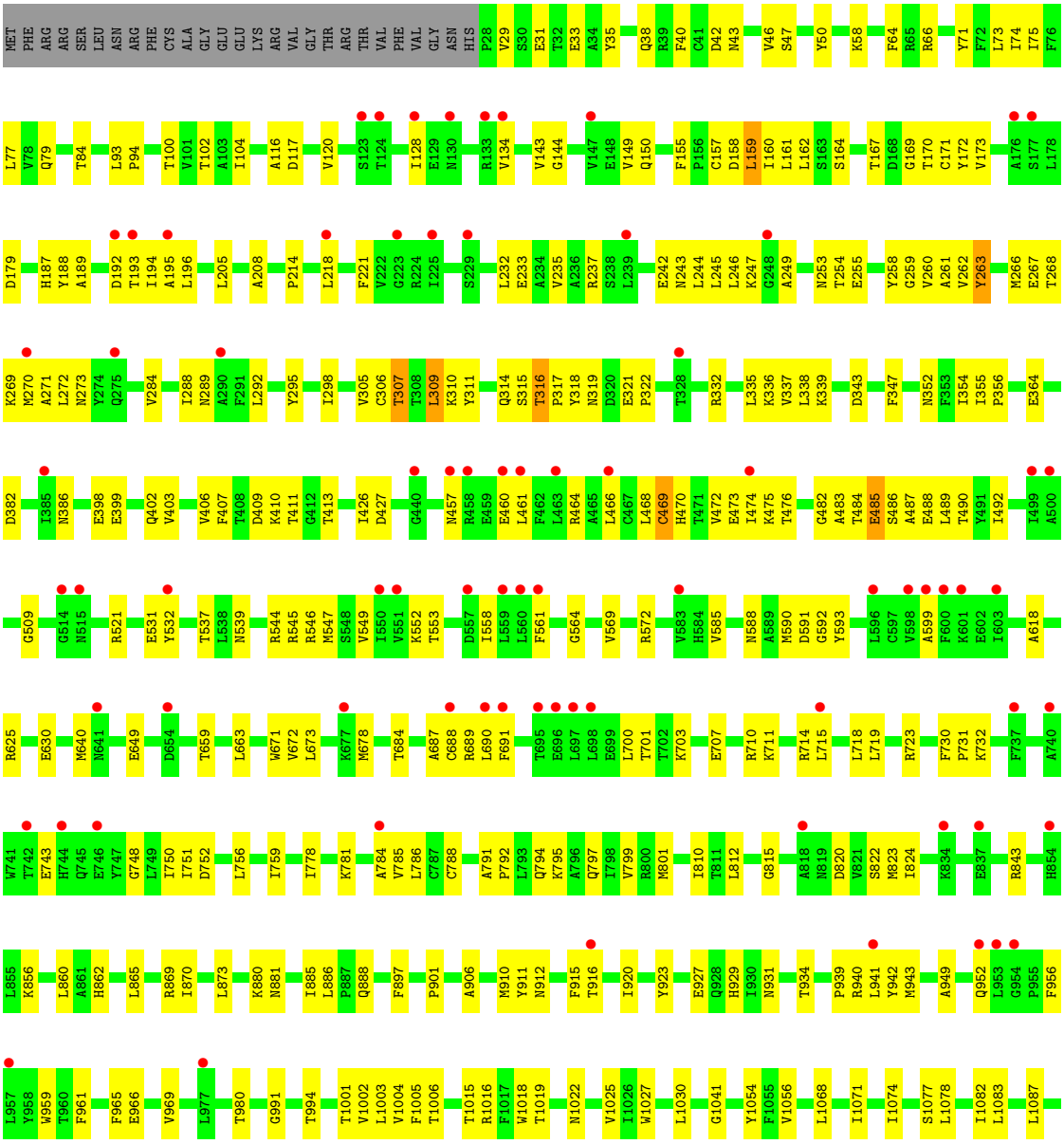
• Molecule 1: Phospholipid-transporting ATPase IG

Chain E:



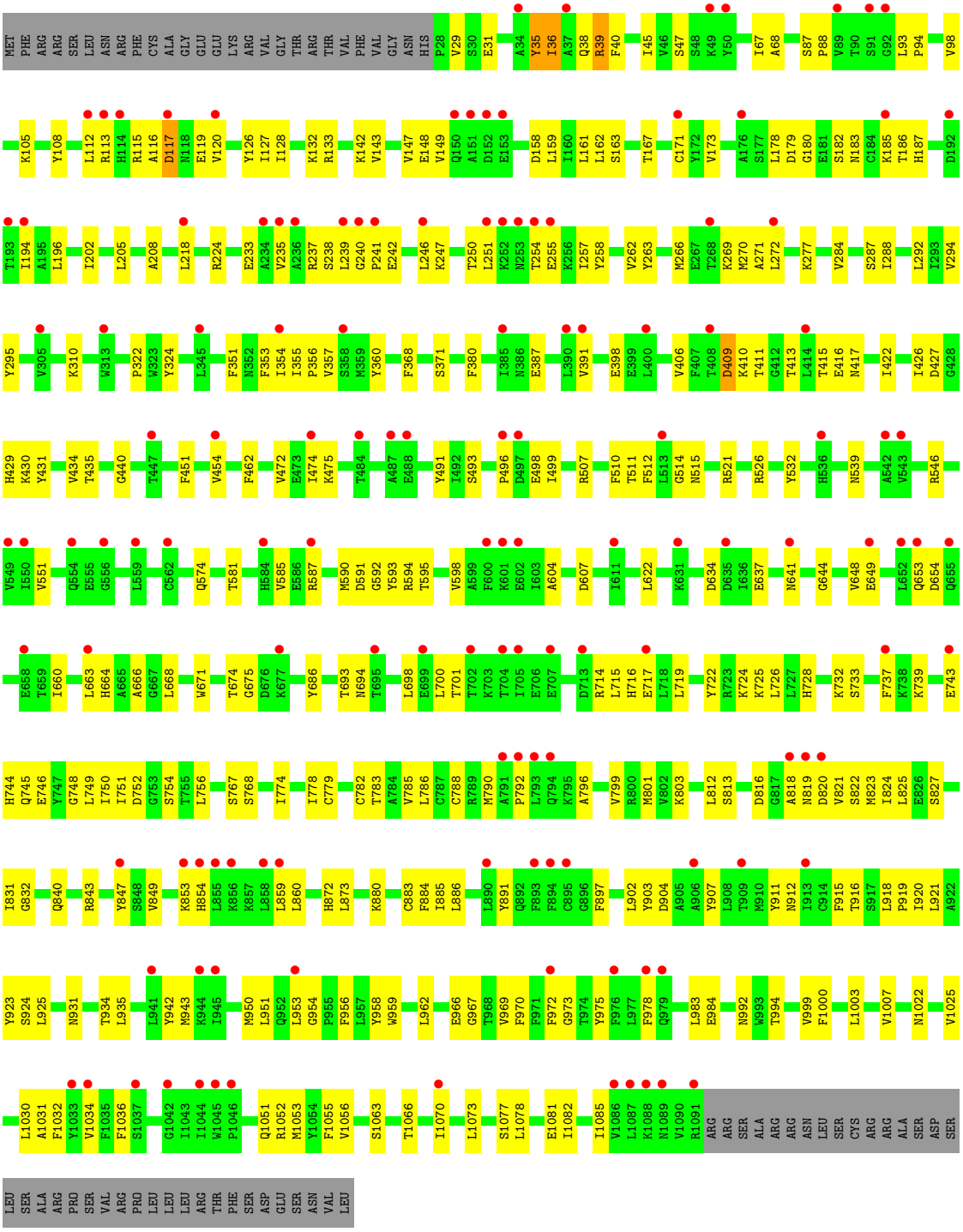


• Molecule 1: Phospholipid-transporting ATPase IG



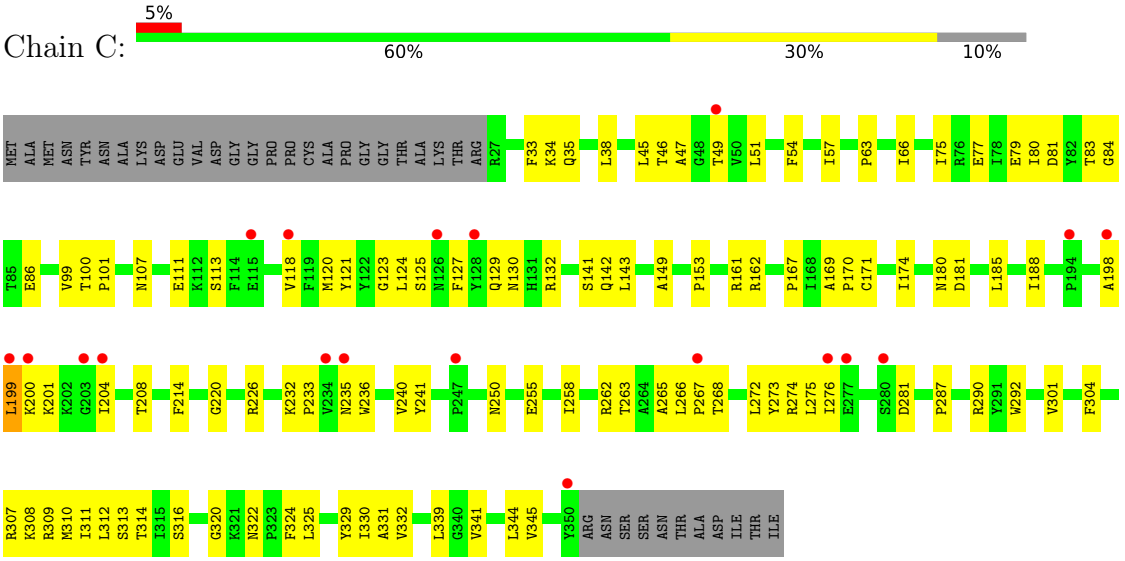
• Molecule 1: Phospholipid-transporting ATPase IG

Chain M:



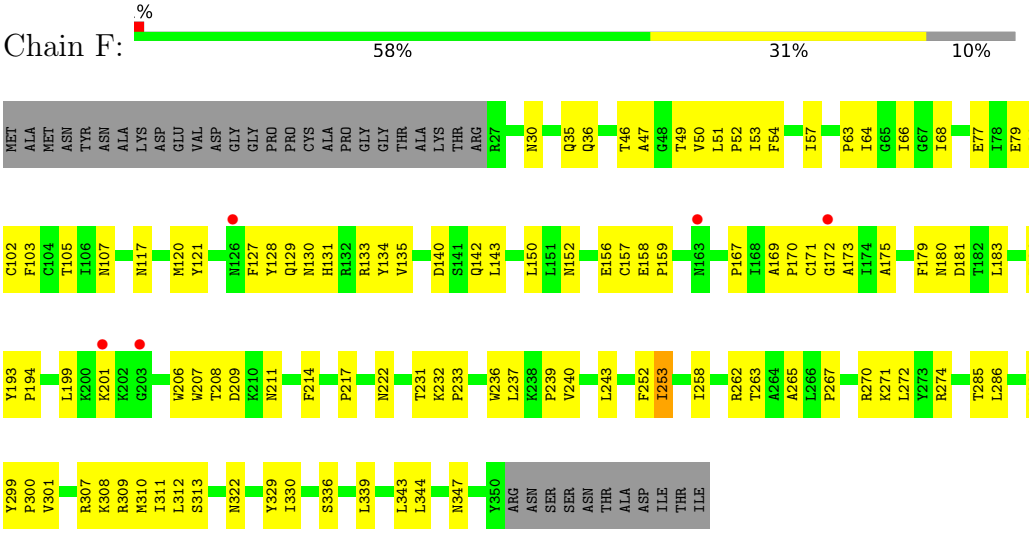
• Molecule 2: Cell cycle control protein 50A

Chain C:



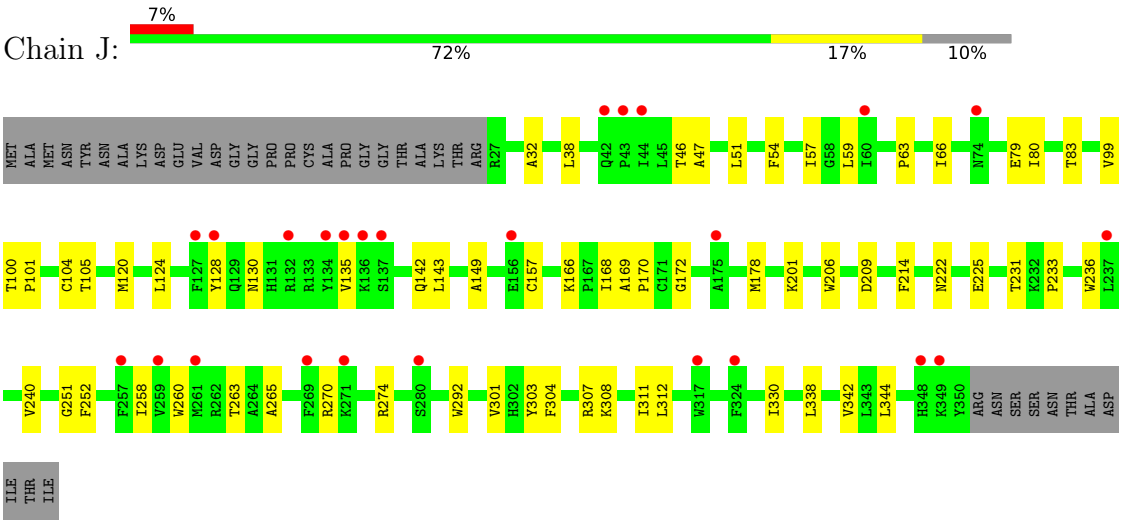
• Molecule 2: Cell cycle control protein 50A

Chain F:



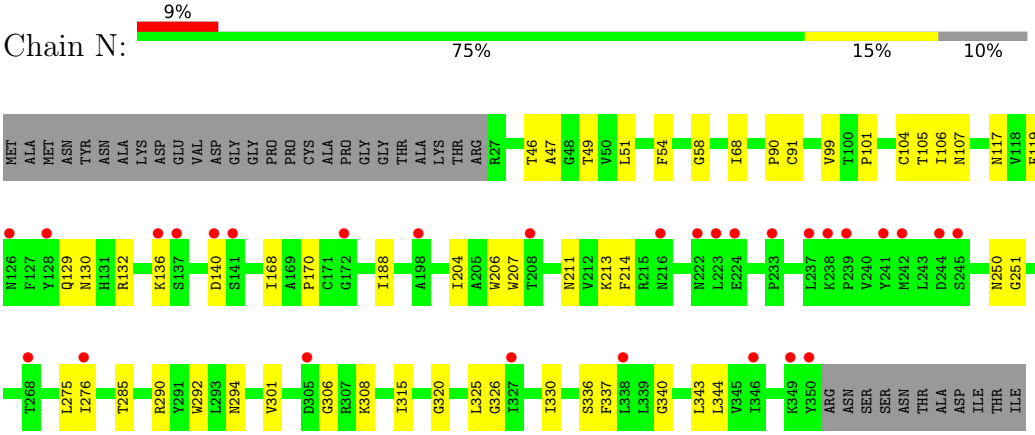
• Molecule 2: Cell cycle control protein 50A

Chain J:



• Molecule 2: Cell cycle control protein 50A

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.46Å 232.83Å 492.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 3.90 49.97 – 3.90	Depositor EDS
% Data completeness (in resolution range)	71.4 (49.97-3.90) 71.3 (49.97-3.90)	Depositor EDS
R_{merge}	1.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.281 , 0.350 0.283 , 0.350	Depositor DCC
R_{free} test set	3779 reflections (3.23%)	wwPDB-VP
Wilson B-factor (Å^2)	98.3	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 105.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	45252	wwPDB-VP
Average B, all atoms (Å^2)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AH2, MG, P5S, BFD, NAG

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	0.30	0/8777	0.77	14/11883 (0.1%)
1	E	0.29	0/8777	0.77	6/11883 (0.1%)
1	I	0.24	0/8777	0.70	4/11883 (0.0%)
1	M	0.23	0/8777	0.67	3/11883 (0.0%)
2	C	0.27	0/2690	0.71	0/3659
2	F	0.28	0/2690	0.75	3/3659 (0.1%)
2	J	0.20	0/2690	0.57	0/3659
2	N	0.21	0/2690	0.55	0/3659
All	All	0.26	0/45868	0.71	30/62168 (0.0%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	512	PHE	N-CA-C	11.28	124.11	110.91
1	I	307	THR	N-CA-C	10.61	122.42	111.07
1	M	454	VAL	N-CA-C	-10.25	102.66	112.29
1	E	195	ALA	N-CA-C	9.89	122.06	111.28
1	A	573	VAL	N-CA-C	7.75	117.86	110.42
1	A	962	LEU	CA-C-N	-7.72	109.94	120.28
1	A	962	LEU	C-N-CA	-7.72	109.94	120.28
1	E	917	SER	N-CA-C	7.64	119.30	110.97
1	A	279	GLN	N-CA-C	7.15	122.12	111.04
2	F	253	ILE	N-CA-C	-6.81	106.17	112.43
1	A	33	GLU	N-CA-C	6.52	118.27	111.03
1	A	215	GLN	CA-C-N	6.37	126.12	119.05
1	A	215	GLN	C-N-CA	6.37	126.12	119.05
1	E	735	ARG	N-CA-C	6.19	119.93	111.39
1	A	313	TRP	N-CA-C	6.08	117.70	111.14
1	A	570	PHE	CA-C-N	6.05	125.76	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	570	PHE	C-N-CA	6.05	125.76	119.05
1	I	487	ALA	N-CA-C	5.99	117.74	109.54
1	A	312	VAL	N-CA-C	5.90	116.08	110.53
1	A	657	ALA	N-CA-C	5.78	117.25	111.07
1	E	160	ILE	N-CA-C	-5.57	99.62	107.75
1	M	185	LYS	N-CA-C	5.47	117.93	110.55
1	A	529	ILE	N-CA-C	5.42	116.15	110.62
1	I	159	LEU	N-CA-C	5.34	117.19	109.07
1	E	244	LEU	N-CA-C	5.08	117.18	108.90
1	A	656	ALA	N-CA-C	5.05	116.86	111.36
1	E	734	THR	N-CA-C	5.03	116.59	108.34
2	F	192	SER	CA-C-N	-5.02	111.25	121.48
2	F	192	SER	C-N-CA	-5.02	111.25	121.48
1	I	263	TYR	N-CA-C	5.02	116.75	111.28

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	8601	0	8587	608	0
1	E	8601	0	8588	444	0
1	I	8601	0	8587	460	0
1	M	8601	0	8588	277	0
2	C	2613	0	2592	108	0
2	F	2613	0	2594	112	0
2	J	2613	0	2592	70	0
2	N	2613	0	2592	88	0
3	A	11	0	5	0	0
3	C	54	0	80	2	0
3	E	22	0	10	1	0
3	I	22	0	10	9	0
3	M	11	0	5	1	0
4	A	1	0	0	0	0
4	E	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	1	0	0	0	0
4	M	1	0	0	0	0
5	C	55	0	50	3	0
5	F	55	0	50	24	0
5	J	55	0	50	20	0
5	N	55	0	49	15	0
6	C	11	0	0	0	0
6	F	11	0	0	0	0
6	J	11	0	0	0	0
6	N	11	0	0	0	0
7	A	2	0	0	0	0
7	E	2	0	0	4	0
7	I	2	0	0	1	0
7	M	2	0	0	1	0
All	All	45252	0	45029	2106	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 23.

All (2106) 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:I:678:MET:HE1	1:I:700:LEU:CD1	1.21	1.65
1:I:214:PRO:HB3	1:I:268:THR:CG2	1.23	1.60
1:I:678:MET:CE	1:I:700:LEU:HD13	1.27	1.60
1:A:28:PRO:CD	1:A:212:GLU:HA	1.15	1.58
1:A:519:TYR:HD2	1:A:532:TYR:CB	0.97	1.58
1:A:519:TYR:CE1	1:A:551:VAL:HG11	1.35	1.58
1:A:519:TYR:CD2	1:A:532:TYR:CB	1.80	1.58
1:I:159:LEU:HB2	1:I:262:VAL:CG2	1.30	1.56
1:I:314:GLN:HE22	3:I:1201:P5S:CB	1.13	1.56
1:A:790:MET:SD	1:A:794:GLN:HB3	1.46	1.55
1:A:28:PRO:HD3	1:A:212:GLU:CA	1.33	1.55
1:I:159:LEU:CB	1:I:262:VAL:HG22	1.34	1.55
1:I:159:LEU:CD1	1:I:262:VAL:HG23	1.33	1.54
1:A:519:TYR:CE1	1:A:551:VAL:CG1	1.90	1.53
2:N:188:ILE:CD1	2:N:292:TRP:CD1	1.90	1.52
1:I:214:PRO:CB	1:I:268:THR:CG2	1.82	1.51
1:M:126:TYR:CE1	1:M:133:ARG:CD	1.95	1.49
2:N:188:ILE:HD12	2:N:292:TRP:CD1	0.99	1.48
1:I:143:VAL:HG13	1:I:263:TYR:CZ	1.47	1.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:126:TYR:CE1	1:M:133:ARG:HD3	1.46	1.46
2:J:292:TRP:CD1	5:J:404:NAG:HO6	1.31	1.45
1:A:654:ASP:OD2	1:A:853:LYS:CB	1.65	1.43
1:I:143:VAL:HG13	1:I:263:TYR:CE2	1.54	1.43
2:N:188:ILE:HD12	2:N:292:TRP:NE1	1.29	1.43
1:A:659:THR:HG21	1:A:852:PHE:CE2	1.55	1.40
1:I:314:GLN:NE2	3:I:1201:P5S:HBA	1.13	1.40
1:I:314:GLN:O	1:I:319:ASN:CB	1.70	1.40
1:A:519:TYR:CD2	1:A:532:TYR:HB3	1.43	1.36
1:A:833:ILE:HG12	1:A:836:LYS:CG	1.54	1.35
2:J:292:TRP:CZ3	5:J:405:NAG:O6	1.70	1.34
1:I:318:TYR:CZ	2:J:128:TYR:HE2	1.43	1.34
1:A:519:TYR:CZ	1:A:551:VAL:HG11	1.62	1.34
2:J:292:TRP:CD1	5:J:404:NAG:C6	2.11	1.33
1:I:214:PRO:CB	1:I:268:THR:HG22	1.49	1.32
1:A:833:ILE:HD11	1:A:836:LYS:CD	1.61	1.31
1:A:28:PRO:CD	1:A:212:GLU:CA	1.90	1.30
2:J:292:TRP:CG	5:J:404:NAG:HO6	1.49	1.30
1:A:569:VAL:C	1:A:571:PRO:HD2	1.58	1.29
1:E:717:GLU:OE1	1:E:774:ILE:HD12	1.29	1.28
1:A:519:TYR:CD2	1:A:532:TYR:HB2	1.52	1.28
1:I:318:TYR:O	1:I:322:PRO:CD	1.80	1.28
1:E:159:LEU:O	1:E:244:LEU:HD23	1.30	1.27
1:I:318:TYR:CE1	2:J:128:TYR:HE2	1.53	1.27
1:I:159:LEU:HD11	1:I:259:GLY:CA	1.65	1.26
1:A:176:ALA:HB3	1:A:837:GLU:OE2	1.36	1.25
1:E:717:GLU:CD	1:E:774:ILE:HD12	1.60	1.25
1:A:28:PRO:N	1:A:212:GLU:HA	1.50	1.25
1:I:159:LEU:HD13	1:I:262:VAL:CG2	1.66	1.25
1:A:28:PRO:CA	1:A:211:CYS:O	1.85	1.25
1:I:158:ASP:O	1:I:262:VAL:HA	1.33	1.25
1:A:413:THR:O	1:A:653:GLN:NE2	1.70	1.24
1:I:143:VAL:CG1	1:I:263:TYR:CZ	2.20	1.24
1:I:159:LEU:CB	1:I:262:VAL:CG2	1.97	1.24
1:A:512:PHE:CZ	1:A:515:ASN:ND2	2.06	1.23
2:J:292:TRP:CD1	5:J:404:NAG:O6	1.91	1.23
2:N:107:ASN:ND2	5:N:405:NAG:H2	1.53	1.23
1:A:29:VAL:HG12	1:A:211:CYS:N	1.51	1.22
1:I:700:LEU:O	1:I:701:THR:CG2	1.86	1.22
1:E:717:GLU:CD	1:E:774:ILE:CD1	2.13	1.21
1:I:310:LYS:HD2	1:I:311:TYR:N	1.53	1.21

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:TYR:OH	1:A:551:VAL:HG21	1.32	1.21
1:E:246:LEU:CD2	1:E:268:THR:HG21	1.69	1.21
1:I:472:VAL:O	1:I:475:LYS:NZ	1.73	1.21
1:A:489:LEU:HD11	1:A:503:LYS:NZ	1.55	1.20
1:A:792:PRO:O	1:A:823:MET:CE	1.89	1.20
1:I:318:TYR:CZ	2:J:128:TYR:CE2	2.29	1.20
1:I:214:PRO:CB	1:I:268:THR:HG23	1.56	1.20
1:E:162:LEU:O	1:E:194:ILE:HG23	1.38	1.19
1:I:489:LEU:HD22	1:I:509:GLY:O	1.42	1.19
1:I:700:LEU:HD23	1:I:751:ILE:C	1.67	1.19
1:I:143:VAL:CG1	1:I:263:TYR:CE2	2.25	1.18
1:I:307:THR:O	1:I:310:LYS:HE3	1.37	1.18
1:A:654:ASP:OD2	1:A:853:LYS:HB2	1.01	1.18
1:I:700:LEU:O	1:I:701:THR:HG22	1.01	1.18
1:A:28:PRO:HA	1:A:211:CYS:O	1.39	1.16
1:E:1009:LEU:HD12	1:E:1078:LEU:HD22	1.26	1.16
2:J:292:TRP:NE1	5:J:404:NAG:H62	1.58	1.16
1:A:521:ARG:HD3	1:A:531:GLU:OE2	1.42	1.15
1:I:214:PRO:CA	1:I:268:THR:CG2	2.23	1.15
2:N:107:ASN:HD21	5:N:405:NAG:H2	0.99	1.15
1:I:159:LEU:CD1	1:I:259:GLY:HA3	1.74	1.15
2:J:292:TRP:CH2	5:J:405:NAG:O6	1.98	1.15
1:E:1009:LEU:HD12	1:E:1078:LEU:CD2	1.75	1.15
1:A:833:ILE:CG1	1:A:836:LYS:CG	2.23	1.14
1:A:569:VAL:C	1:A:571:PRO:CD	2.20	1.14
1:E:185:LYS:HD3	1:E:245:LEU:HD11	1.30	1.14
1:I:700:LEU:HD22	1:I:788:CYS:HB3	1.15	1.14
1:I:482:GLY:HA3	1:I:490:THR:HG22	1.19	1.13
1:A:28:PRO:N	1:A:212:GLU:CA	2.04	1.13
1:A:519:TYR:HE1	1:A:551:VAL:CG1	1.39	1.13
1:A:311:TYR:O	1:A:315:SER:HB3	1.46	1.13
1:A:468:LEU:HD13	1:A:519:TYR:OH	1.46	1.13
1:I:160:ILE:HG12	1:I:261:ALA:HB3	1.24	1.13
1:M:715:LEU:O	1:M:719:LEU:HD13	1.43	1.13
1:I:318:TYR:CE1	2:J:128:TYR:CE2	2.37	1.12
1:I:700:LEU:HD23	1:I:752:ASP:N	1.63	1.13
1:M:127:ILE:HD12	1:M:147:VAL:HG22	1.23	1.12
1:I:306:CYS:O	1:I:310:LYS:HG3	1.47	1.12
1:A:310:LYS:HE2	1:A:897:PHE:HB2	1.31	1.12
1:E:655:GLN:CG	1:E:658:GLU:HG2	1.78	1.12
1:M:126:TYR:HE1	1:M:133:ARG:CD	1.44	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:159:LEU:HD11	1:I:259:GLY:HA3	1.14	1.11
1:A:28:PRO:CD	1:A:212:GLU:C	2.24	1.11
1:A:521:ARG:HB3	1:A:531:GLU:CD	1.74	1.11
1:I:678:MET:HE3	1:I:700:LEU:H	1.06	1.11
1:A:833:ILE:CD1	1:A:836:LYS:HD3	1.80	1.10
1:I:47:SER:OG	1:I:117:ASP:CG	1.93	1.10
1:A:572:ARG:NE	1:A:639:ASN:HB2	1.66	1.10
1:E:47:SER:HB2	1:E:117:ASP:OD2	1.49	1.10
1:I:482:GLY:CA	1:I:490:THR:HG22	1.80	1.10
1:A:512:PHE:CE1	1:A:515:ASN:ND2	2.20	1.10
1:A:654:ASP:CG	1:A:853:LYS:HB2	1.76	1.10
1:A:524:ASN:HB2	1:A:530:GLU:OE1	1.51	1.09
2:F:292:TRP:HH2	5:F:405:NAG:C6	1.66	1.09
1:I:159:LEU:CD1	1:I:262:VAL:CG2	2.25	1.09
1:I:314:GLN:NE2	3:I:1201:P5S:CB	1.86	1.09
1:A:28:PRO:N	1:A:211:CYS:C	2.09	1.09
1:A:790:MET:SD	1:A:794:GLN:CB	2.39	1.09
1:I:318:TYR:O	1:I:322:PRO:HD3	1.39	1.09
1:A:833:ILE:CG1	1:A:836:LYS:HG2	1.81	1.09
1:I:489:LEU:CD2	1:I:509:GLY:O	2.00	1.09
1:M:113:ARG:O	1:M:117:ASP:OD1	1.71	1.09
1:A:792:PRO:HG3	1:A:819:ASN:O	1.52	1.09
2:F:143:LEU:HD22	2:F:252:PHE:CE2	1.86	1.09
1:I:690:LEU:HD12	1:I:691:PHE:N	1.68	1.09
1:A:28:PRO:N	1:A:211:CYS:O	1.84	1.08
1:M:47:SER:OG	1:M:843:ARG:CZ	1.99	1.08
1:I:690:LEU:HD11	1:I:691:PHE:CD2	1.87	1.08
1:I:700:LEU:CD2	1:I:751:ILE:C	2.27	1.08
1:A:519:TYR:CE2	1:A:532:TYR:HB3	1.86	1.08
1:A:833:ILE:CD1	1:A:836:LYS:CG	2.32	1.07
1:A:521:ARG:CD	1:A:531:GLU:OE2	2.02	1.07
1:I:310:LYS:HB2	1:I:897:PHE:HB2	1.33	1.07
1:I:160:ILE:CG1	1:I:261:ALA:HB3	1.84	1.07
1:A:570:PHE:N	1:A:571:PRO:CD	2.18	1.07
1:A:654:ASP:OD2	1:A:853:LYS:CA	2.03	1.07
1:A:29:VAL:HG21	1:A:31:GLU:OE2	1.54	1.06
1:A:792:PRO:O	1:A:823:MET:HE3	1.54	1.06
1:I:307:THR:C	1:I:310:LYS:HE3	1.80	1.06
1:E:732:LYS:HG3	1:E:739:LYS:NZ	1.69	1.06
1:I:700:LEU:HD11	1:I:750:ILE:HG23	1.36	1.06
1:E:196:LEU:HD21	1:E:199:ALA:HB3	1.07	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:GLY:O	1:A:836:LYS:HB3	1.54	1.06
1:A:176:ALA:CB	1:A:837:GLU:OE2	2.04	1.05
1:I:318:TYR:O	1:I:322:PRO:HD2	1.51	1.05
1:I:316:THR:HB	1:I:317:PRO:HD3	1.34	1.05
1:A:756:LEU:HD13	1:A:790:MET:HE1	1.36	1.05
2:F:143:LEU:HD22	2:F:252:PHE:HE2	1.15	1.05
2:J:292:TRP:NE1	5:J:404:NAG:C6	2.16	1.04
1:A:519:TYR:CE1	1:A:551:VAL:HG12	1.90	1.04
1:E:163:SER:HB3	1:E:194:ILE:HG22	1.39	1.04
1:E:732:LYS:NZ	1:E:739:LYS:CE	2.20	1.03
1:I:158:ASP:O	1:I:262:VAL:CA	2.06	1.03
1:A:219:TYR:HA	1:A:235:VAL:CG1	1.86	1.03
1:A:570:PHE:N	1:A:571:PRO:HD3	1.72	1.03
1:A:219:TYR:CE2	1:A:235:VAL:O	2.11	1.03
1:A:316:THR:OG1	1:A:317:PRO:HD3	1.58	1.03
1:E:717:GLU:OE2	1:E:774:ILE:HD13	1.58	1.03
1:I:159:LEU:HD11	1:I:259:GLY:C	1.81	1.03
1:A:833:ILE:CD1	1:A:836:LYS:CD	2.33	1.03
1:E:159:LEU:HD11	1:E:261:ALA:H	1.22	1.03
1:E:191:ARG:N	1:E:194:ILE:HD12	1.73	1.03
1:I:159:LEU:CG	1:I:262:VAL:CG2	2.36	1.03
1:I:306:CYS:O	1:I:310:LYS:CG	2.07	1.03
1:A:519:TYR:OH	1:A:551:VAL:CG2	2.07	1.02
1:M:126:TYR:CE1	1:M:133:ARG:CG	2.41	1.02
1:A:31:GLU:HG3	1:A:209:ILE:HG23	1.39	1.02
1:E:732:LYS:HG3	1:E:739:LYS:HZ3	0.86	1.02
1:E:185:LYS:CD	1:E:245:LEU:HD11	1.90	1.01
1:A:792:PRO:O	1:A:823:MET:HE1	1.57	1.01
1:I:167:THR:HB	1:I:473:GLU:O	1.61	1.01
1:I:318:TYR:OH	2:J:128:TYR:CE2	2.12	1.01
1:E:640:MET:SD	1:E:641:ASN:O	2.18	1.01
1:E:732:LYS:HZ2	1:E:739:LYS:HE2	1.23	1.01
1:I:47:SER:OG	1:I:117:ASP:OD2	1.78	1.01
1:I:474:ILE:C	1:I:475:LYS:HD2	1.86	1.00
1:A:519:TYR:HB2	1:A:533:GLU:CA	1.91	1.00
1:M:47:SER:OG	1:M:843:ARG:NH2	1.93	1.00
1:I:310:LYS:HB3	1:I:897:PHE:CG	1.95	1.00
1:I:678:MET:CE	1:I:700:LEU:H	1.75	1.00
1:A:833:ILE:CD1	1:A:836:LYS:HG3	1.89	0.99
1:I:314:GLN:C	1:I:319:ASN:HB2	1.86	0.99
2:N:117:ASN:ND2	2:N:119:PHE:CE2	2.29	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:LEU:CD2	1:E:199:ALA:HB3	1.92	0.99
1:E:246:LEU:HD22	1:E:268:THR:HG21	1.43	0.99
1:M:126:TYR:OH	1:M:133:ARG:HG3	1.60	0.99
1:A:31:GLU:O	1:A:208:ALA:HB1	1.62	0.99
1:A:519:TYR:CE2	1:A:532:TYR:CB	2.45	0.99
1:A:218:LEU:HB2	1:A:267:GLU:HG3	1.40	0.99
1:I:159:LEU:CA	1:I:262:VAL:HG22	1.91	0.99
1:A:311:TYR:O	1:A:315:SER:CB	2.11	0.98
1:E:732:LYS:NZ	1:E:739:LYS:HE3	1.77	0.98
1:M:126:TYR:CD1	1:M:133:ARG:HD3	1.98	0.98
1:I:690:LEU:CD1	1:I:691:PHE:CD2	2.46	0.98
1:I:700:LEU:CD2	1:I:788:CYS:HB3	1.91	0.98
1:A:219:TYR:HA	1:A:235:VAL:HG12	0.98	0.98
2:F:292:TRP:CH2	5:F:405:NAG:H61	1.98	0.98
1:I:214:PRO:HB2	1:I:268:THR:HG22	1.41	0.98
1:A:468:LEU:CD1	1:A:519:TYR:OH	2.10	0.98
1:I:307:THR:O	1:I:310:LYS:CE	2.11	0.98
1:I:485:GLU:HG3	1:I:488:GLU:CD	1.88	0.98
1:A:468:LEU:HD13	1:A:519:TYR:CZ	1.99	0.97
1:E:717:GLU:OE2	1:E:774:ILE:CD1	2.10	0.97
1:A:219:TYR:CA	1:A:235:VAL:HG12	1.92	0.97
1:M:126:TYR:CE1	1:M:133:ARG:HD2	1.96	0.97
1:I:703:LYS:HE3	1:I:714:ARG:HD3	1.47	0.97
1:A:519:TYR:CZ	1:A:551:VAL:CG1	2.33	0.97
1:A:882:LEU:HD12	1:A:963:ALA:HB1	1.46	0.97
1:E:655:GLN:HG3	1:E:658:GLU:HG2	1.43	0.97
1:I:310:LYS:HZ3	1:I:343:ASP:CG	1.73	0.97
2:N:188:ILE:HD12	2:N:292:TRP:HD1	1.19	0.96
1:I:700:LEU:CD1	1:I:750:ILE:HG23	1.94	0.96
1:A:524:ASN:CB	1:A:530:GLU:OE1	2.12	0.96
1:I:143:VAL:HG13	1:I:263:TYR:CE1	2.00	0.96
1:M:126:TYR:HE1	1:M:133:ARG:CG	1.76	0.96
1:E:732:LYS:HZ2	1:E:739:LYS:CE	1.77	0.96
1:I:159:LEU:CG	1:I:259:GLY:HA3	1.94	0.96
2:N:290:ARG:HE	2:N:292:TRP:NE1	1.63	0.96
1:A:512:PHE:CE2	1:A:515:ASN:ND2	2.34	0.96
2:J:292:TRP:HE1	5:J:404:NAG:H62	1.25	0.95
1:A:519:TYR:CZ	1:A:551:VAL:CB	2.49	0.95
1:I:307:THR:CA	1:I:310:LYS:HE3	1.96	0.95
1:E:1009:LEU:CD1	1:E:1078:LEU:HD22	1.97	0.95
1:I:310:LYS:NZ	1:I:343:ASP:OD2	1.99	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:188:ILE:CD1	2:N:292:TRP:NE1	2.08	0.94
1:M:434:VAL:HG23	1:M:440:GLY:O	1.65	0.94
1:A:28:PRO:N	1:A:212:GLU:N	2.15	0.94
1:E:125:VAL:HG13	1:E:127:ILE:HG22	1.50	0.94
1:E:698:LEU:HD11	1:E:719:LEU:HB3	1.50	0.94
1:I:159:LEU:CG	1:I:262:VAL:HG23	1.93	0.94
1:M:247:LYS:HE2	1:M:269:LYS:HA	1.50	0.94
1:M:126:TYR:CE1	1:M:133:ARG:HG3	2.03	0.94
1:A:519:TYR:OH	1:A:551:VAL:HG11	1.67	0.93
2:N:292:TRP:CZ3	5:N:405:NAG:O5	2.22	0.93
1:A:659:THR:HG21	1:A:852:PHE:HE2	1.29	0.93
1:A:659:THR:CG2	1:A:852:PHE:CE2	2.50	0.93
1:E:1003:LEU:O	1:E:1007:VAL:HG22	1.69	0.93
1:E:233:GLU:CD	1:E:244:LEU:H	1.75	0.93
1:I:214:PRO:CA	1:I:268:THR:HG22	1.92	0.93
1:A:519:TYR:HD2	1:A:532:TYR:CA	1.81	0.93
1:I:159:LEU:HD21	1:I:259:GLY:HA3	1.50	0.93
1:A:28:PRO:HD3	1:A:212:GLU:C	1.87	0.93
2:F:292:TRP:HH2	5:F:405:NAG:H61	1.33	0.93
1:A:489:LEU:HD11	1:A:503:LYS:HZ3	1.28	0.92
1:A:464:ARG:NH2	1:A:532:TYR:OH	2.01	0.92
1:E:165:CYS:HG	1:E:197:CYS:HG	0.96	0.92
1:E:233:GLU:OE1	1:E:243:ASN:N	2.02	0.92
1:E:117:ASP:O	1:E:121:ASN:HB2	1.70	0.92
1:I:159:LEU:CD2	1:I:259:GLY:HA3	2.00	0.92
1:A:519:TYR:HB2	1:A:533:GLU:HA	1.47	0.91
1:A:29:VAL:H	1:A:211:CYS:H	1.18	0.91
1:E:233:GLU:CD	1:E:244:LEU:N	2.28	0.91
1:I:159:LEU:HB2	1:I:262:VAL:HG21	1.49	0.91
1:I:314:GLN:O	1:I:319:ASN:HB2	0.74	0.91
2:J:292:TRP:HZ3	5:J:405:NAG:O6	1.21	0.91
1:A:177:SER:HB3	1:A:837:GLU:HG3	1.53	0.91
1:A:833:ILE:HG12	1:A:836:LYS:HG2	0.93	0.91
1:I:700:LEU:HD22	1:I:788:CYS:CB	2.01	0.91
1:M:127:ILE:CD1	1:M:147:VAL:HG22	2.00	0.91
1:A:218:LEU:HB2	1:A:267:GLU:CG	2.00	0.90
1:A:512:PHE:CE1	1:A:520:MET:HG3	2.07	0.90
1:A:833:ILE:CG1	1:A:836:LYS:HG3	1.98	0.90
1:A:833:ILE:HD13	1:A:836:LYS:HG3	1.53	0.90
1:M:126:TYR:CZ	1:M:133:ARG:HG3	2.07	0.90
1:E:233:GLU:OE2	1:E:244:LEU:N	2.04	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:201:LYS:HD3	2:C:201:LYS:H	1.36	0.90
1:I:214:PRO:CA	1:I:268:THR:HG21	2.02	0.90
2:N:107:ASN:HB3	2:N:292:TRP:CE3	2.06	0.90
1:A:128:ILE:HD13	1:A:133:ARG:HA	1.53	0.90
1:A:792:PRO:CG	1:A:819:ASN:O	2.20	0.90
1:I:310:LYS:CB	1:I:897:PHE:HB2	2.02	0.89
1:E:185:LYS:HD3	1:E:245:LEU:CD1	2.03	0.89
2:N:130:ASN:HB3	2:N:265:ALA:HB1	1.53	0.89
2:F:301:VAL:HG21	2:F:308:LYS:HD3	1.51	0.89
1:E:717:GLU:CD	1:E:774:ILE:HD13	1.91	0.89
1:I:678:MET:HE3	1:I:700:LEU:N	1.87	0.89
1:I:700:LEU:C	1:I:701:THR:HG22	1.97	0.89
1:I:157:CYS:HB2	1:I:262:VAL:CG1	2.01	0.89
2:N:290:ARG:HE	2:N:292:TRP:HE1	1.18	0.89
1:E:732:LYS:HZ3	1:E:739:LYS:HE3	1.31	0.89
1:E:1009:LEU:C	1:E:1009:LEU:HD13	1.98	0.89
2:N:290:ARG:CZ	2:N:292:TRP:HZ2	1.86	0.89
1:E:880:LYS:HG2	1:E:1007:VAL:HG11	1.55	0.88
1:E:163:SER:HB3	1:E:194:ILE:CG2	2.03	0.88
1:E:574:GLN:CB	1:E:640:MET:HE1	2.03	0.88
1:A:697:LEU:HA	1:A:747:TYR:HD2	1.38	0.88
1:A:519:TYR:HD2	1:A:532:TYR:HB2	0.88	0.88
1:I:307:THR:HA	1:I:310:LYS:CE	2.04	0.88
2:J:292:TRP:CD1	5:J:404:NAG:H61	2.07	0.88
1:E:158:ASP:O	1:E:159:LEU:HD22	1.74	0.88
1:A:519:TYR:CB	1:A:533:GLU:CA	2.52	0.88
1:I:310:LYS:HB3	1:I:897:PHE:CD1	2.09	0.88
1:A:29:VAL:HG12	1:A:211:CYS:H	1.33	0.88
2:F:292:TRP:CE3	5:F:404:NAG:O6	2.26	0.88
1:E:915:PHE:HZ	1:E:1008:THR:CG2	1.87	0.87
2:J:292:TRP:HZ3	5:J:405:NAG:C6	1.87	0.87
1:E:1009:LEU:HD13	1:E:1009:LEU:O	1.74	0.87
1:A:521:ARG:CG	1:A:531:GLU:OE2	2.23	0.87
1:A:572:ARG:HG2	1:A:640:MET:H	1.38	0.86
1:E:720:ILE:HD12	1:E:778:ILE:HG21	1.56	0.86
1:E:339:LYS:NZ	1:E:343:ASP:CG	2.33	0.86
2:F:292:TRP:CH2	5:F:405:NAG:C6	2.54	0.86
1:I:310:LYS:HD2	1:I:311:TYR:H	1.40	0.86
1:M:183:ASN:HA	1:M:499:ILE:HG13	1.57	0.86
2:N:290:ARG:CZ	2:N:292:TRP:CZ2	2.59	0.86
1:A:489:LEU:HD11	1:A:503:LYS:HZ2	1.40	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:LEU:HD13	1:A:790:MET:CE	2.06	0.86
1:I:143:VAL:HG13	1:I:263:TYR:CD2	2.10	0.86
1:I:159:LEU:HD21	1:I:259:GLY:CA	2.05	0.86
1:I:473:GLU:HA	1:I:475:LYS:HZ3	1.41	0.86
2:N:117:ASN:HD21	2:N:119:PHE:HE2	1.24	0.86
1:A:219:TYR:CD2	1:A:235:VAL:O	2.29	0.85
1:A:512:PHE:HE1	1:A:520:MET:CG	1.89	0.85
1:A:520:MET:O	1:A:522:VAL:HG13	1.76	0.85
1:A:898:SER:O	2:C:132:ARG:NH2	2.08	0.85
1:E:655:GLN:CD	1:E:658:GLU:HG2	2.02	0.85
1:E:127:ILE:HD11	1:E:146:VAL:HG23	1.58	0.85
1:M:115:ARG:O	1:M:119:GLU:HG3	1.76	0.85
1:A:572:ARG:HD3	1:A:639:ASN:HA	1.58	0.85
1:E:162:LEU:O	1:E:194:ILE:CG2	2.24	0.85
1:E:196:LEU:HD21	1:E:199:ALA:CB	2.01	0.85
2:N:90:PRO:CG	5:N:405:NAG:H83	2.07	0.84
1:E:246:LEU:HD22	1:E:268:THR:CG2	2.06	0.84
1:A:31:GLU:HG3	1:A:209:ILE:CG2	2.06	0.84
1:A:519:TYR:CE1	1:A:551:VAL:CB	2.60	0.84
1:E:233:GLU:OE2	1:E:244:LEU:HB3	1.77	0.84
1:E:339:LYS:HZ3	1:E:343:ASP:CG	1.83	0.84
1:A:833:ILE:HD11	1:A:836:LYS:HD3	0.88	0.84
1:E:246:LEU:HD21	1:E:268:THR:HG21	1.58	0.84
1:E:574:GLN:HB3	1:E:640:MET:HE1	1.58	0.84
1:I:214:PRO:HA	1:I:268:THR:HG21	1.58	0.84
1:A:220:LYS:HB2	1:A:220:LYS:NZ	1.93	0.84
1:E:190:VAL:C	1:E:194:ILE:HD12	2.01	0.84
1:I:473:GLU:HA	1:I:475:LYS:NZ	1.93	0.84
1:I:678:MET:CE	1:I:700:LEU:CD1	2.10	0.83
1:A:572:ARG:CZ	1:A:639:ASN:CB	2.55	0.83
1:A:468:LEU:HD13	1:A:519:TYR:HH	1.37	0.83
1:A:516:ARG:O	1:A:516:ARG:NE	2.12	0.83
1:A:569:VAL:O	1:A:571:PRO:HD2	1.76	0.83
1:I:159:LEU:HD12	1:I:160:ILE:H	1.43	0.83
1:I:321:GLU:CD	2:J:303:TYR:O	2.21	0.83
1:I:700:LEU:HD11	1:I:750:ILE:CG2	2.09	0.83
1:A:572:ARG:NE	1:A:639:ASN:CB	2.42	0.83
2:N:117:ASN:ND2	2:N:119:PHE:HE2	1.77	0.83
1:A:29:VAL:CG1	1:A:211:CYS:N	2.40	0.83
1:A:574:GLN:O	1:A:578:ILE:HG13	1.78	0.83
1:E:719:LEU:O	1:E:722:TYR:HB3	1.78	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:GLU:C	1:E:243:ASN:HD22	1.87	0.82
1:E:233:GLU:CG	1:E:244:LEU:HB3	2.09	0.82
1:A:519:TYR:CZ	1:A:551:VAL:HG21	2.14	0.82
1:I:307:THR:HA	1:I:310:LYS:HE3	1.58	0.82
1:A:521:ARG:HB3	1:A:531:GLU:OE2	1.79	0.82
2:F:292:TRP:CH2	5:F:405:NAG:O5	2.33	0.82
1:A:464:ARG:CZ	1:A:532:TYR:OH	2.26	0.82
1:I:160:ILE:CG1	1:I:261:ALA:CB	2.58	0.82
1:M:354:ILE:HG13	1:M:885:ILE:HD13	1.62	0.81
1:M:1031:ALA:HA	1:M:1034:VAL:HG22	1.61	0.81
1:A:176:ALA:HB3	1:A:837:GLU:CD	2.05	0.81
1:A:572:ARG:CZ	1:A:639:ASN:HB2	2.08	0.81
1:A:176:ALA:C	1:A:837:GLU:OE2	2.23	0.81
1:I:214:PRO:C	1:I:268:THR:HG22	2.05	0.81
1:E:720:ILE:HG23	1:E:778:ILE:HB	1.60	0.81
1:E:1009:LEU:HD12	1:E:1078:LEU:HD21	1.62	0.81
1:E:127:ILE:HD12	1:E:128:ILE:H	1.45	0.81
1:E:640:MET:CE	1:E:641:ASN:O	2.29	0.81
2:F:80:ILE:HD11	2:F:310:MET:HE2	1.63	0.81
1:I:468:LEU:O	1:I:468:LEU:HD13	1.81	0.81
1:A:31:GLU:CG	1:A:209:ILE:HG23	2.11	0.81
1:I:321:GLU:OE1	2:J:303:TYR:O	1.86	0.81
1:M:126:TYR:HE1	1:M:133:ARG:HD3	0.94	0.81
1:M:127:ILE:HD12	1:M:147:VAL:CG2	2.10	0.80
2:N:292:TRP:HH2	5:N:405:NAG:C4	1.91	0.80
1:A:519:TYR:CD2	1:A:532:TYR:C	2.57	0.80
1:E:185:LYS:CE	1:E:245:LEU:HD11	2.10	0.80
1:I:159:LEU:HD21	1:I:259:GLY:N	1.96	0.80
1:E:1009:LEU:CD1	1:E:1078:LEU:CD2	2.55	0.80
1:I:489:LEU:CD1	1:I:509:GLY:O	2.30	0.80
1:I:690:LEU:CD1	1:I:691:PHE:CG	2.64	0.80
1:I:700:LEU:CD2	1:I:750:ILE:HG12	2.12	0.80
1:I:310:LYS:CB	1:I:897:PHE:CB	2.60	0.79
1:E:233:GLU:CD	1:E:244:LEU:HB3	2.07	0.79
1:E:191:ARG:HB2	1:E:194:ILE:CD1	2.13	0.79
1:I:143:VAL:HG22	1:I:263:TYR:CD2	2.17	0.79
1:I:703:LYS:HB3	1:I:711:LYS:HD2	1.64	0.79
1:E:158:ASP:OD2	1:E:268:THR:OG1	1.98	0.79
1:E:880:LYS:NZ	1:E:912:ASN:OD1	2.15	0.79
1:I:473:GLU:CA	1:I:475:LYS:NZ	2.45	0.79
2:C:80:ILE:HD11	2:C:310:MET:HE2	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:107:ASN:HB3	2:N:292:TRP:CZ3	2.18	0.79
1:A:275:GLN:NE2	1:A:826:GLU:H	1.81	0.79
1:E:233:GLU:HG2	1:E:244:LEU:CB	2.12	0.79
1:A:519:TYR:HE1	1:A:551:VAL:HG12	1.29	0.78
1:E:339:LYS:NZ	1:E:343:ASP:OD2	2.17	0.78
1:A:516:ARG:HE	1:A:516:ARG:C	1.92	0.78
1:E:79:GLN:HB2	1:E:84:THR:HG21	1.65	0.78
1:E:655:GLN:OE1	1:E:658:GLU:HG2	1.83	0.78
2:N:107:ASN:ND2	2:N:292:TRP:CZ3	2.51	0.78
1:E:718:LEU:HD23	1:E:718:LEU:H	1.48	0.78
1:M:47:SER:CB	1:M:843:ARG:CZ	2.62	0.78
1:A:28:PRO:HD3	1:A:212:GLU:CB	2.13	0.78
1:A:697:LEU:HA	1:A:747:TYR:CD2	2.19	0.78
1:A:723:ARG:NH2	1:A:778:ILE:O	2.16	0.77
1:E:732:LYS:CG	1:E:739:LYS:HZ3	1.83	0.77
1:A:519:TYR:HB2	1:A:533:GLU:C	2.08	0.77
1:A:519:TYR:HH	1:A:551:VAL:HG11	1.45	0.77
1:M:237:ARG:NH1	1:M:409:BFD:F2	2.08	0.77
1:M:351:PHE:HA	1:M:885:ILE:HD11	1.65	0.77
1:A:28:PRO:HD2	1:A:212:GLU:C	2.07	0.77
1:A:673:LEU:HD22	1:A:787:CYS:HB2	1.65	0.77
1:A:129:GLU:HB2	1:A:146:VAL:HG22	1.67	0.77
1:I:700:LEU:HD21	1:I:750:ILE:HG12	1.67	0.77
1:A:176:ALA:CA	1:A:837:GLU:OE2	2.32	0.76
1:A:572:ARG:HD3	1:A:639:ASN:CB	2.14	0.76
1:A:177:SER:CB	1:A:837:GLU:HG3	2.15	0.76
2:F:308:LYS:N	2:F:308:LYS:HD2	2.00	0.76
1:I:489:LEU:HD13	1:I:509:GLY:O	1.84	0.76
1:I:700:LEU:HB3	1:I:752:ASP:HB3	1.68	0.76
2:N:290:ARG:NE	2:N:292:TRP:NE1	2.33	0.76
1:A:28:PRO:HD3	1:A:212:GLU:HA	0.82	0.76
1:A:219:TYR:O	1:A:234:ALA:HA	1.85	0.76
1:A:790:MET:SD	1:A:794:GLN:C	2.69	0.76
1:A:1045:TRP:HB3	1:A:1051:GLN:HE21	1.50	0.76
1:A:756:LEU:CD1	1:A:790:MET:HE1	2.14	0.76
1:M:113:ARG:O	1:M:117:ASP:CG	2.29	0.76
1:A:384:GLU:O	1:A:386:ASN:OD1	2.03	0.75
1:A:660:ILE:HD11	1:A:670:VAL:HG21	1.68	0.75
1:A:657:ALA:O	1:A:661:GLU:HB2	1.87	0.75
1:A:522:VAL:O	1:A:529:ILE:O	2.04	0.75
2:F:167:PRO:O	2:F:231:THR:OG1	2.04	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:159:LEU:HD13	1:I:262:VAL:HG23	0.77	0.75
1:I:311:TYR:CE1	1:I:339:LYS:HG2	2.21	0.75
1:I:307:THR:OG1	1:I:347:PHE:CD2	2.37	0.75
2:N:91:CYS:HA	2:N:104:CYS:HB2	1.68	0.75
2:N:290:ARG:NH2	2:N:292:TRP:CZ2	2.55	0.75
1:A:673:LEU:HD13	1:A:798:ILE:HD12	1.69	0.74
2:C:75:ILE:HD11	2:C:316:SER:HB3	1.69	0.74
1:A:792:PRO:CB	1:A:819:ASN:O	2.36	0.74
1:I:143:VAL:HG11	1:I:263:TYR:CE2	2.22	0.74
1:I:157:CYS:HB2	1:I:262:VAL:HG12	1.69	0.74
1:I:700:LEU:CD1	1:I:750:ILE:HG12	2.17	0.74
2:C:170:PRO:HD2	2:C:233:PRO:HD3	1.69	0.74
1:E:655:GLN:HB3	1:E:853:LYS:HG3	1.70	0.74
1:A:657:ALA:O	1:A:661:GLU:CB	2.36	0.74
1:A:519:TYR:OH	1:A:551:VAL:CG1	2.31	0.74
1:I:314:GLN:NE2	3:I:1201:P5S:CA	2.51	0.74
2:N:107:ASN:HD22	2:N:292:TRP:HZ3	1.34	0.74
1:E:159:LEU:CD1	1:E:261:ALA:H	2.00	0.74
1:I:688:CYS:SG	1:I:690:LEU:HG	2.27	0.74
1:A:1056:VAL:HG22	2:C:262:ARG:HH22	1.52	0.73
1:A:1072:LEU:HD11	2:C:332:VAL:HG21	1.68	0.73
1:E:717:GLU:OE2	1:E:774:ILE:HG21	1.87	0.73
1:A:512:PHE:HE1	1:A:520:MET:HG3	1.46	0.73
1:E:159:LEU:HD11	1:E:261:ALA:N	2.03	0.73
2:N:292:TRP:HZ3	5:N:405:NAG:O5	1.69	0.73
1:E:246:LEU:CD2	1:E:268:THR:CG2	2.57	0.73
2:J:143:LEU:HD11	2:J:214:PHE:HD1	1.54	0.73
1:A:654:ASP:OD2	1:A:853:LYS:HA	1.88	0.73
2:C:201:LYS:H	2:C:201:LYS:CD	2.01	0.73
2:N:107:ASN:ND2	5:N:405:NAG:C2	2.43	0.73
2:N:290:ARG:NE	2:N:292:TRP:HE1	1.86	0.73
5:F:405:NAG:C7	5:F:405:NAG:H5	2.19	0.72
1:I:160:ILE:HG13	1:I:261:ALA:CB	2.18	0.72
1:I:472:VAL:C	1:I:475:LYS:NZ	2.47	0.72
1:E:233:GLU:HG2	1:E:244:LEU:HB3	1.70	0.72
1:I:315:SER:HA	1:I:319:ASN:HB3	1.72	0.72
1:I:678:MET:HE1	1:I:700:LEU:HD12	1.62	0.72
5:F:405:NAG:H5	5:F:405:NAG:O7	1.89	0.72
1:A:653:GLN:NE2	1:A:836:LYS:HE2	2.03	0.72
1:A:834:LYS:HE2	1:A:839:ARG:NE	2.05	0.72
1:E:233:GLU:OE2	1:E:244:LEU:CA	2.38	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ARG:CB	1:A:531:GLU:OE2	2.38	0.72
1:A:911:TYR:OH	1:A:1004:VAL:HG21	1.90	0.72
1:I:700:LEU:HD21	1:I:751:ILE:N	2.05	0.72
1:I:475:LYS:HD2	1:I:475:LYS:N	2.03	0.71
1:I:700:LEU:HD21	1:I:751:ILE:C	2.13	0.71
1:M:179:ASP:O	1:M:237:ARG:NH2	2.23	0.71
1:I:315:SER:HA	1:I:319:ASN:HD22	1.54	0.71
1:M:47:SER:HB3	1:M:843:ARG:NE	2.05	0.71
1:A:574:GLN:HA	1:A:574:GLN:HE21	1.56	0.71
1:E:246:LEU:HD22	1:E:268:THR:CB	2.19	0.71
1:I:703:LYS:CE	1:I:714:ARG:HD3	2.19	0.71
1:A:519:TYR:CZ	1:A:551:VAL:HB	2.24	0.71
1:A:569:VAL:CA	1:A:571:PRO:HD2	2.20	0.71
1:E:351:PHE:HA	1:E:885:ILE:HD11	1.73	0.71
1:I:158:ASP:O	1:I:262:VAL:HG13	1.89	0.71
1:A:521:ARG:CB	1:A:531:GLU:CD	2.59	0.71
1:E:574:GLN:HB2	1:E:640:MET:HE1	1.73	0.71
1:A:512:PHE:CD1	1:A:515:ASN:ND2	2.59	0.71
1:A:572:ARG:CD	1:A:639:ASN:CB	2.69	0.71
1:E:732:LYS:HZ3	1:E:739:LYS:CE	1.95	0.71
1:E:992:ASN:HA	2:F:265:ALA:HB2	1.73	0.71
1:A:712:GLU:HG3	1:A:771:TYR:CZ	2.26	0.71
1:I:564:GLY:HA3	1:I:569:VAL:HG21	1.73	0.70
2:N:301:VAL:HG23	2:N:306:GLY:HA3	1.73	0.70
1:A:574:GLN:HG2	1:A:642:LEU:HB2	1.71	0.70
1:A:653:GLN:HE22	1:A:836:LYS:HE2	1.55	0.70
1:E:185:LYS:HE2	1:E:245:LEU:HD11	1.71	0.70
1:I:315:SER:HA	1:I:319:ASN:CB	2.20	0.70
1:A:856:LYS:O	1:A:860:LEU:HB2	1.92	0.70
1:A:572:ARG:HD3	1:A:639:ASN:CA	2.21	0.70
1:A:700:LEU:HD13	1:A:749:LEU:HD12	1.71	0.70
1:E:655:GLN:HG3	1:E:658:GLU:CG	2.19	0.70
1:A:792:PRO:HB3	1:A:819:ASN:O	1.92	0.70
1:E:915:PHE:CZ	1:E:1008:THR:CG2	2.74	0.70
1:I:411:THR:O	7:I:1301:HOH:O	2.10	0.70
1:M:47:SER:HB2	1:M:117:ASP:OD2	1.90	0.70
1:M:962:LEU:O	1:M:966:GLU:HG2	1.92	0.70
1:A:370:GLY:O	1:A:866:TYR:OH	2.09	0.70
1:A:1069:ALA:HB2	2:C:325:LEU:HD21	1.73	0.70
1:E:179:ASP:O	1:E:237:ARG:NH2	2.25	0.70
1:E:640:MET:SD	1:E:641:ASN:N	2.65	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:498:GLU:N	1:M:498:GLU:OE1	2.23	0.70
1:A:28:PRO:CD	1:A:213:GLN:N	2.54	0.70
2:C:199:LEU:HD23	2:C:199:LEU:H	1.56	0.70
1:I:128:ILE:HD13	1:I:134:VAL:HG22	1.74	0.70
1:I:700:LEU:HD11	1:I:750:ILE:HG12	1.74	0.70
1:E:47:SER:HB2	1:E:117:ASP:CG	2.17	0.70
1:I:750:ILE:HD11	1:I:788:CYS:HB2	1.74	0.70
1:A:904:ASP:HB3	1:A:907:TYR:HB2	1.73	0.69
1:I:316:THR:HB	1:I:317:PRO:CD	2.17	0.69
1:A:833:ILE:HG12	1:A:836:LYS:HG3	1.58	0.69
1:E:185:LYS:HD2	1:E:241:PRO:HB2	1.75	0.69
1:A:29:VAL:CG2	1:A:31:GLU:OE2	2.36	0.69
1:A:29:VAL:O	1:A:210:GLU:HA	1.93	0.69
1:E:655:GLN:CG	1:E:658:GLU:CG	2.65	0.69
1:I:482:GLY:HA3	1:I:490:THR:CG2	2.10	0.69
1:I:956:PHE:HA	1:I:959:TRP:CD1	2.27	0.69
1:I:167:THR:CB	1:I:473:GLU:O	2.39	0.69
1:I:218:LEU:HD12	1:I:235:VAL:HG13	1.74	0.69
2:J:292:TRP:NE1	5:J:404:NAG:O6	2.18	0.69
1:M:973:GLY:HA3	1:M:1073:LEU:HD21	1.75	0.69
1:A:311:TYR:HA	1:A:315:SER:HB2	1.74	0.69
1:A:657:ALA:O	1:A:661:GLU:CG	2.41	0.69
1:I:314:GLN:HE22	3:I:1201:P5S:HB	1.46	0.69
1:I:316:THR:CB	1:I:317:PRO:HD3	2.16	0.69
1:I:473:GLU:C	1:I:475:LYS:HZ2	2.01	0.69
1:M:904:ASP:OD1	1:M:1052:ARG:NH1	2.26	0.69
2:N:99:VAL:HG12	2:N:101:PRO:HD2	1.73	0.69
1:A:28:PRO:HD3	1:A:213:GLN:N	2.08	0.69
1:I:678:MET:HE2	1:I:700:LEU:HB2	1.74	0.69
2:N:188:ILE:CG1	2:N:292:TRP:CD1	2.73	0.69
1:A:409:BFD:OD1	1:A:410:LYS:N	2.26	0.68
1:E:233:GLU:OE2	1:E:244:LEU:CB	2.41	0.68
1:M:36:ILE:C	1:M:36:ILE:HD12	2.18	0.68
1:A:519:TYR:CZ	1:A:551:VAL:CG2	2.72	0.68
1:A:884:PHE:HA	1:A:1003:LEU:HD11	1.75	0.68
1:A:410:LYS:HE2	1:A:681:ALA:HA	1.75	0.68
1:E:158:ASP:OD1	1:E:247:LYS:N	2.26	0.68
1:E:67:ILE:HG13	1:E:292:LEU:HD11	1.74	0.68
1:I:214:PRO:C	1:I:268:THR:CG2	2.66	0.68
1:M:491:TYR:OH	1:M:514:GLY:O	2.10	0.68
1:A:598:VAL:HG13	1:A:643:ILE:HG13	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:153:PRO:HG2	2:C:161:ARG:HG2	1.75	0.68
1:E:1009:LEU:CD1	1:E:1009:LEU:C	2.67	0.68
1:I:700:LEU:HD23	1:I:752:ASP:CA	2.22	0.68
1:E:1049:LYS:O	1:E:1051:GLN:NE2	2.25	0.68
1:A:468:LEU:CD1	1:A:519:TYR:CZ	2.72	0.68
2:C:220:GLY:O	2:C:226:ARG:NH2	2.27	0.68
2:F:66:ILE:HB	2:F:330:ILE:HD11	1.76	0.68
1:M:31:GLU:HB3	1:M:208:ALA:HB1	1.75	0.68
1:M:604:ALA:HB3	1:M:607:ASP:HB2	1.76	0.68
1:M:126:TYR:CD1	1:M:133:ARG:CD	2.68	0.67
1:M:916:THR:O	1:M:920:ILE:HG12	1.93	0.67
1:A:513:LEU:O	1:A:515:ASN:OD1	2.11	0.67
2:F:292:TRP:CZ2	5:F:405:NAG:H61	2.29	0.67
1:I:310:LYS:CD	1:I:311:TYR:N	2.47	0.67
1:E:178:LEU:HD13	1:E:246:LEU:HB2	1.76	0.67
1:M:235:VAL:HG23	1:M:241:PRO:HD3	1.76	0.67
1:I:335:LEU:HD13	1:I:338:LEU:HB2	1.75	0.67
1:A:756:LEU:CD1	1:A:790:MET:CE	2.71	0.67
1:I:310:LYS:HD2	1:I:310:LYS:C	2.18	0.67
2:C:204:ILE:HG12	2:C:255:GLU:HB3	1.76	0.67
1:E:185:LYS:CD	1:E:245:LEU:CD1	2.67	0.67
1:I:311:TYR:HE1	1:I:339:LYS:HG2	1.59	0.67
1:M:911:TYR:O	1:M:915:PHE:HD1	1.77	0.67
1:E:113:ARG:NH1	1:E:392:ASN:O	2.28	0.67
1:E:233:GLU:CD	1:E:244:LEU:CB	2.67	0.67
1:E:240:GLY:N	1:E:241:PRO:HD3	2.10	0.67
1:A:572:ARG:CZ	1:A:639:ASN:HB3	2.24	0.67
1:M:47:SER:HB2	1:M:117:ASP:CG	2.19	0.67
1:A:31:GLU:O	1:A:208:ALA:CB	2.41	0.66
1:A:171:CYS:SG	1:A:257:ILE:HG12	2.35	0.66
1:A:656:ALA:HB1	1:A:688:CYS:SG	2.34	0.66
1:I:485:GLU:HG3	1:I:488:GLU:CG	2.25	0.66
1:A:572:ARG:CD	1:A:639:ASN:HB2	2.26	0.66
1:E:718:LEU:HD23	1:E:718:LEU:N	2.09	0.66
2:J:166:LYS:HD3	2:J:231:THR:HG22	1.77	0.66
1:E:127:ILE:HD11	1:E:146:VAL:CG2	2.26	0.66
1:I:307:THR:OG1	1:I:347:PHE:HD2	1.79	0.66
2:C:199:LEU:HD23	2:C:199:LEU:N	2.11	0.66
1:E:915:PHE:HZ	1:E:1008:THR:HG23	1.61	0.66
1:M:983:LEU:HD11	1:M:1066:THR:HG23	1.76	0.66
1:A:29:VAL:HG12	1:A:211:CYS:CB	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:CYS:SG	1:A:254:THR:HG21	2.36	0.66
1:A:572:ARG:NH1	1:A:639:ASN:HB3	2.10	0.66
1:E:718:LEU:H	1:E:718:LEU:CD2	2.08	0.66
2:C:185:LEU:HD11	2:C:312:LEU:HD21	1.78	0.65
1:I:700:LEU:N	1:I:700:LEU:HD12	2.10	0.65
2:J:292:TRP:CG	5:J:404:NAG:O6	2.30	0.65
2:N:188:ILE:CG1	2:N:292:TRP:HD1	2.09	0.65
1:A:218:LEU:CB	1:A:267:GLU:HG3	2.20	0.65
1:A:275:GLN:NE2	1:A:822:SER:O	2.29	0.65
2:N:90:PRO:CG	5:N:405:NAG:C8	2.74	0.65
1:E:732:LYS:HB2	1:E:736:SER:HB3	1.76	0.65
1:I:310:LYS:CB	1:I:897:PHE:CG	2.74	0.65
1:I:489:LEU:HD22	1:I:509:GLY:C	2.18	0.65
1:M:663:LEU:HG	1:M:668:LEU:HD12	1.79	0.65
1:E:821:VAL:HB	1:E:841:ALA:HB1	1.79	0.65
1:A:211:CYS:HG	1:A:263:TYR:HH	1.44	0.65
1:E:159:LEU:O	1:E:244:LEU:CD2	2.25	0.65
1:E:161:LEU:HD13	1:E:257:ILE:HG23	1.79	0.65
1:E:409:BFD:F2	7:E:1302:HOH:O	2.03	0.65
2:F:201:LYS:HA	2:F:274:ARG:HD2	1.77	0.65
1:I:473:GLU:C	1:I:475:LYS:NZ	2.55	0.65
2:N:130:ASN:HB3	2:N:265:ALA:CB	2.25	0.65
2:N:188:ILE:CD1	2:N:292:TRP:HD1	1.81	0.65
2:N:290:ARG:NH2	2:N:292:TRP:HZ2	1.93	0.65
1:A:220:LYS:HB2	1:A:220:LYS:HZ2	1.61	0.65
1:E:125:VAL:CG1	1:E:127:ILE:HG22	2.25	0.65
1:E:254:THR:HG22	1:E:255:GLU:H	1.62	0.65
1:A:318:TYR:HA	1:A:321:GLU:HG2	1.79	0.64
1:I:690:LEU:HD12	1:I:690:LEU:C	2.22	0.64
2:N:292:TRP:CH2	5:N:405:NAG:O5	2.50	0.64
1:A:519:TYR:HB2	1:A:534:LEU:N	2.12	0.64
1:A:659:THR:HG21	1:A:852:PHE:CZ	2.28	0.64
2:F:170:PRO:HA	2:F:252:PHE:CZ	2.32	0.64
1:I:159:LEU:HB2	1:I:262:VAL:HG22	0.68	0.64
1:E:233:GLU:HG2	1:E:244:LEU:HB2	1.78	0.64
1:I:795:LYS:HB3	1:I:823:MET:HG3	1.79	0.64
1:A:572:ARG:NH2	1:A:639:ASN:HD22	1.95	0.64
1:I:31:GLU:HB3	1:I:208:ALA:HB1	1.79	0.64
1:M:953:LEU:HD12	1:M:954:GLY:H	1.63	0.64
2:N:90:PRO:HG2	5:N:405:NAG:H83	1.79	0.64
1:E:574:GLN:HB3	1:E:640:MET:CE	2.28	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:309:LEU:HD22	1:I:309:LEU:N	2.11	0.64
2:C:124:LEU:HD22	2:C:308:LYS:HD2	1.78	0.64
1:M:984:GLU:HG2	1:M:1063:SER:HB2	1.79	0.64
1:A:560:LEU:HB2	1:A:603:ILE:HD11	1.79	0.64
1:A:723:ARG:NH1	1:A:777:GLN:O	2.31	0.64
2:C:169:ALA:HB3	2:C:170:PRO:HD3	1.80	0.64
2:J:338:LEU:O	2:J:342:VAL:HG23	1.97	0.64
1:I:482:GLY:N	1:I:490:THR:HG22	2.11	0.64
1:A:32:THR:HB	1:A:35:TYR:HD2	1.62	0.64
1:I:29:VAL:HB	1:I:263:TYR:OH	1.97	0.64
1:A:63:GLN:OE1	1:A:102:THR:OG1	2.17	0.63
2:C:142:GLN:NE2	2:C:171:CYS:SG	2.70	0.63
1:M:202:ILE:HG23	1:M:205:LEU:HD12	1.80	0.63
1:A:29:VAL:HG12	1:A:211:CYS:CA	2.27	0.63
2:C:200:LYS:O	2:C:275:LEU:HD23	1.99	0.63
1:I:171:CYS:SG	1:I:172:TYR:N	2.71	0.63
2:N:107:ASN:CB	2:N:292:TRP:CE3	2.81	0.63
1:A:992:ASN:HB2	2:C:265:ALA:HB2	1.80	0.63
2:C:201:LYS:HD3	2:C:201:LYS:N	2.09	0.63
1:I:306:CYS:O	1:I:310:LYS:HG2	1.97	0.63
1:A:295:TYR:HH	1:A:959:TRP:HH2	1.43	0.63
2:C:80:ILE:O	2:C:80:ILE:HD12	1.99	0.63
1:M:239:LEU:HD21	1:M:496:PRO:HB3	1.79	0.63
1:A:31:GLU:HB3	1:A:209:ILE:H	1.62	0.63
1:A:869:ARG:NH1	1:A:927:GLU:O	2.31	0.63
2:C:174:ILE:H	2:C:174:ILE:HD12	1.64	0.63
1:E:47:SER:CB	1:E:117:ASP:OD2	2.38	0.63
1:I:700:LEU:HD11	1:I:750:ILE:C	2.24	0.63
1:I:707:GLU:HB2	1:I:710:ARG:HB2	1.80	0.63
1:A:519:TYR:CG	1:A:533:GLU:C	2.77	0.63
1:I:307:THR:O	1:I:310:LYS:CD	2.46	0.63
1:M:831:ILE:HD11	1:M:849:VAL:HG22	1.81	0.63
1:A:202:ILE:HG23	1:A:205:LEU:HD12	1.81	0.63
1:A:413:THR:C	1:A:653:GLN:NE2	2.54	0.63
1:A:663:LEU:HG	1:A:668:LEU:HD12	1.79	0.63
1:A:993:TRP:CZ3	1:A:1052:ARG:HB2	2.34	0.63
1:E:189:ALA:O	1:E:194:ILE:HG21	1.99	0.63
1:E:892:GLN:HE22	1:E:900:GLN:N	1.97	0.63
2:F:143:LEU:HD22	2:F:252:PHE:CZ	2.33	0.63
1:M:163:SER:HB3	1:M:257:ILE:HA	1.81	0.63
1:E:354:ILE:HG23	1:E:885:ILE:HG21	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:710:ARG:O	1:I:714:ARG:HB2	1.99	0.63
1:I:218:LEU:HD12	1:I:235:VAL:CG1	2.28	0.62
1:I:723:ARG:H	1:I:723:ARG:HD2	1.64	0.62
1:M:746:GLU:O	1:M:783:THR:N	2.32	0.62
2:N:107:ASN:CB	2:N:292:TRP:CZ3	2.81	0.62
1:E:233:GLU:CG	1:E:244:LEU:CB	2.75	0.62
1:M:178:LEU:HA	1:M:818:ALA:HB3	1.81	0.62
1:M:992:ASN:CB	2:N:265:ALA:HB2	2.29	0.62
2:N:132:ARG:O	2:N:136:LYS:HB3	1.99	0.62
1:I:159:LEU:HD22	1:I:262:VAL:HG21	1.81	0.62
1:A:524:ASN:N	1:A:530:GLU:OE1	2.32	0.62
1:M:953:LEU:HD12	1:M:954:GLY:N	2.14	0.62
1:E:668:LEU:HD22	1:E:943:MET:HE2	1.82	0.62
2:F:292:TRP:HH2	5:F:405:NAG:C5	2.11	0.62
1:I:214:PRO:HB3	1:I:268:THR:HG23	0.63	0.62
1:A:822:SER:HB2	1:A:823:MET:HE2	1.81	0.62
1:E:242:GLU:O	1:E:243:ASN:ND2	2.28	0.62
1:E:1051:GLN:HG2	2:F:140:ASP:OD2	2.00	0.62
2:F:307:ARG:C	2:F:308:LYS:HD2	2.24	0.62
1:I:158:ASP:O	1:I:262:VAL:CB	2.48	0.62
1:I:940:ARG:HG3	1:I:941:LEU:H	1.65	0.62
1:A:217:ASP:O	1:A:218:LEU:HB3	2.00	0.61
1:E:254:THR:HG22	1:E:255:GLU:N	2.16	0.61
1:E:574:GLN:H	1:E:640:MET:HE3	1.65	0.61
1:I:468:LEU:HD13	1:I:468:LEU:C	2.24	0.61
1:A:208:ALA:O	1:A:225:ILE:HG13	2.01	0.61
1:I:170:THR:OG1	1:I:473:GLU:OE2	2.18	0.61
1:M:254:THR:HB	1:M:257:ILE:HD11	1.82	0.61
1:A:351:PHE:HA	1:A:885:ILE:HD11	1.81	0.61
1:A:750:ILE:HD12	1:A:786:LEU:HD13	1.81	0.61
1:E:159:LEU:HG	1:E:260:VAL:H	1.65	0.61
1:A:519:TYR:CE1	1:A:551:VAL:HB	2.35	0.61
1:A:816:ASP:OD2	1:A:837:GLU:CB	2.49	0.61
2:C:107:ASN:ND2	5:C:406:NAG:O5	2.33	0.61
2:J:292:TRP:HH2	5:J:405:NAG:O6	1.77	0.61
2:F:170:PRO:HA	2:F:252:PHE:HZ	1.66	0.61
1:E:409:BFD:HB3	1:E:815:GLY:HA2	1.81	0.61
1:A:28:PRO:HD2	1:A:213:GLN:N	2.15	0.61
2:C:75:ILE:HG23	2:C:314:THR:HG23	1.82	0.61
2:J:169:ALA:HB3	2:J:170:PRO:HD3	1.83	0.61
1:A:519:TYR:OH	1:A:551:VAL:CB	2.49	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ARG:HB2	1:A:529:ILE:HD11	1.83	0.60
1:A:1059:GLN:O	1:A:1062:SER:OG	2.19	0.60
2:F:102:CYS:SG	2:F:103:PHE:N	2.74	0.60
2:F:140:ASP:HA	2:F:143:LEU:HG	1.83	0.60
2:J:292:TRP:HD1	5:J:404:NAG:H61	1.58	0.60
1:I:310:LYS:NZ	1:I:311:TYR:HB2	2.16	0.60
2:C:130:ASN:HB3	2:C:265:ALA:HA	1.84	0.60
1:E:655:GLN:HG3	1:E:655:GLN:O	2.01	0.60
1:E:906:ALA:O	1:E:910:MET:HB3	2.01	0.60
2:N:250:ASN:HD22	2:N:251:GLY:H	1.49	0.60
1:A:519:TYR:CD1	1:A:533:GLU:C	2.78	0.60
1:A:523:GLU:HA	1:A:528:GLU:O	2.01	0.60
1:M:47:SER:CB	1:M:843:ARG:NE	2.64	0.60
1:M:413:THR:N	1:M:816:ASP:OD2	2.33	0.60
1:M:435:THR:H	1:M:440:GLY:HA3	1.66	0.60
1:A:524:ASN:H	1:A:530:GLU:CD	2.09	0.60
1:A:574:GLN:HE21	1:A:574:GLN:CA	2.14	0.60
1:E:904:ASP:OD1	1:E:1052:ARG:NH1	2.34	0.60
1:A:218:LEU:HD22	1:A:267:GLU:CD	2.26	0.60
1:A:512:PHE:CD2	1:A:515:ASN:ND2	2.70	0.60
1:A:657:ALA:HB1	1:A:661:GLU:HG3	1.84	0.60
1:A:747:TYR:CG	1:A:748:GLY:N	2.69	0.60
1:E:952:GLN:O	1:E:956:PHE:HE2	1.85	0.60
1:I:466:LEU:HD23	1:I:470:HIS:ND1	2.17	0.60
1:A:879:TYR:HA	1:A:959:TRP:CZ3	2.36	0.60
1:I:310:LYS:HZ2	1:I:311:TYR:HB2	1.67	0.60
1:E:405:TYR:HE1	1:E:669:LYS:HB2	1.67	0.60
1:M:904:ASP:HB3	1:M:907:TYR:HB2	1.84	0.60
1:A:219:TYR:O	1:A:235:VAL:N	2.35	0.60
1:A:966:GLU:HB3	1:A:970:PHE:CZ	2.36	0.60
1:E:730:PHE:N	1:E:731:PRO:CD	2.64	0.60
1:M:970:PHE:CD2	1:M:1003:LEU:HD12	2.36	0.60
1:A:529:ILE:HG13	1:A:531:GLU:HG2	1.84	0.59
1:I:157:CYS:HB2	1:I:262:VAL:HG13	1.83	0.59
1:I:179:ASP:O	1:I:237:ARG:NH1	2.36	0.59
1:I:1083:LEU:O	1:I:1087:LEU:HD23	2.01	0.59
1:E:191:ARG:HB2	1:E:194:ILE:HD12	1.84	0.59
1:E:966:GLU:OE1	1:E:1077:SER:HB3	2.01	0.59
5:F:405:NAG:H83	5:F:405:NAG:C1	2.32	0.59
1:M:410:LYS:HD3	1:M:411:THR:HG23	1.84	0.59
1:M:426:ILE:HG22	1:M:430:LYS:HB2	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:720:ILE:CD1	1:E:778:ILE:HG21	2.32	0.59
1:A:516:ARG:HD3	1:E:202:ILE:HG21	1.84	0.59
1:E:922:ALA:HB1	1:E:1022:ASN:OD1	2.02	0.59
1:I:159:LEU:CD1	1:I:160:ILE:H	2.14	0.59
1:I:159:LEU:HD11	1:I:260:VAL:N	2.17	0.59
1:I:314:GLN:CD	3:I:1201:P5S:CB	2.71	0.59
1:M:36:ILE:HG23	1:M:36:ILE:O	2.03	0.59
1:M:782:CYS:SG	1:M:783:THR:N	2.76	0.59
1:A:165:CYS:SG	1:A:166:THR:N	2.75	0.59
1:A:519:TYR:CB	1:A:533:GLU:C	2.75	0.59
1:A:284:VAL:HG11	1:A:870:ILE:HD11	1.83	0.59
1:E:851:LYS:HD3	1:E:854:HIS:CG	2.37	0.59
1:I:307:THR:HA	1:I:310:LYS:HE2	1.84	0.59
1:A:1083:LEU:HD21	2:C:339:LEU:HD21	1.82	0.59
1:E:316:THR:HG23	1:E:317:PRO:HD3	1.85	0.59
1:I:700:LEU:CD2	1:I:751:ILE:CA	2.80	0.59
1:A:1053:MET:HB2	1:A:1056:VAL:HG21	1.84	0.59
1:I:235:VAL:HG13	1:I:235:VAL:O	2.02	0.59
2:J:168:ILE:HG22	2:J:170:PRO:HD2	1.85	0.59
1:M:886:LEU:HD23	1:M:967:GLY:HA3	1.83	0.59
1:A:956:PHE:HA	1:A:959:TRP:HD1	1.67	0.59
1:E:562:CYS:SG	1:E:563:LYS:N	2.74	0.59
1:E:655:GLN:OE1	1:E:658:GLU:CG	2.49	0.59
1:E:332:ARG:O	1:E:333:GLU:HG2	2.03	0.59
1:I:158:ASP:O	1:I:262:VAL:CG1	2.50	0.59
1:I:1068:LEU:HD13	1:I:1071:ILE:HD11	1.84	0.59
2:C:124:LEU:HD22	2:C:308:LYS:CD	2.33	0.58
1:E:654:ASP:O	1:E:853:LYS:HB2	2.03	0.58
1:E:68:ALA:HB2	1:E:292:LEU:HD22	1.84	0.58
1:E:980:THR:OG1	2:F:322:ASN:HB2	2.03	0.58
1:M:698:LEU:HD12	1:M:715:LEU:HD11	1.85	0.58
1:E:162:LEU:C	1:E:194:ILE:HG23	2.23	0.58
1:M:972:PHE:HA	1:M:975:TYR:CE1	2.39	0.58
2:N:107:ASN:HD21	5:N:405:NAG:C2	1.93	0.58
1:A:519:TYR:CD2	1:A:532:TYR:CA	2.66	0.58
1:A:992:ASN:CB	2:C:265:ALA:HB2	2.32	0.58
1:A:178:LEU:HD22	1:A:246:LEU:HD22	1.85	0.58
1:A:980:THR:OG1	2:C:322:ASN:HB2	2.03	0.58
1:E:994:THR:HG22	1:E:1056:VAL:HG13	1.86	0.58
1:I:266:MET:HA	1:I:269:LYS:HG2	1.86	0.58
1:M:39:ARG:HB3	1:M:39:ARG:HH11	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:LYS:NZ	1:E:343:ASP:CB	2.67	0.58
1:I:310:LYS:HB3	1:I:897:PHE:CB	2.31	0.58
1:I:585:VAL:HA	1:I:588:ASN:OD1	2.04	0.58
2:J:143:LEU:CD1	2:J:214:PHE:HD1	2.15	0.58
1:E:242:GLU:C	1:E:243:ASN:ND2	2.60	0.58
1:E:282:SER:HB2	1:E:399:GLU:OE1	2.04	0.58
1:I:160:ILE:HG13	1:I:261:ALA:HB2	1.84	0.58
1:I:266:MET:HA	1:I:269:LYS:HZ3	1.68	0.58
2:J:292:TRP:CD1	5:J:404:NAG:H62	2.06	0.58
2:N:207:TRP:CD1	2:N:211:ASN:HD22	2.21	0.58
1:A:220:LYS:NZ	1:A:220:LYS:CB	2.66	0.58
1:A:895:CYS:O	1:A:897:PHE:N	2.35	0.58
2:N:188:ILE:CD1	2:N:292:TRP:HE1	2.12	0.58
1:E:98:VAL:HG22	1:E:361:VAL:HG13	1.85	0.58
2:J:178:MET:HG2	2:J:260:TRP:CD1	2.38	0.58
1:M:235:VAL:HG21	1:M:246:LEU:HD21	1.86	0.58
1:A:29:VAL:HG13	1:A:31:GLU:HG2	1.85	0.58
1:E:171:CYS:HG	1:E:187:HIS:CE1	2.19	0.58
1:E:409:BFD:F3	7:E:1301:HOH:O	2.06	0.58
1:I:160:ILE:HG12	1:I:261:ALA:CB	2.14	0.58
1:I:354:ILE:HG21	1:I:885:ILE:HG21	1.85	0.58
2:N:124:LEU:HD22	2:N:308:LYS:HE3	1.86	0.58
1:A:220:LYS:HB2	1:A:220:LYS:HZ3	1.69	0.57
1:A:994:THR:HG22	1:A:1056:VAL:HG13	1.85	0.57
1:I:295:TYR:HA	1:I:298:ILE:HD12	1.86	0.57
1:I:315:SER:HA	1:I:319:ASN:ND2	2.18	0.57
1:M:935:LEU:HD11	1:M:942:TYR:HB3	1.86	0.57
1:E:244:LEU:HD13	1:E:244:LEU:C	2.28	0.57
1:E:630:GLU:HA	1:E:633:PHE:HB3	1.85	0.57
1:I:700:LEU:HD21	1:I:751:ILE:CA	2.34	0.57
1:M:820:ASP:O	1:M:824:ILE:HG12	2.04	0.57
1:A:218:LEU:HD22	1:A:267:GLU:OE1	2.03	0.57
1:A:514:GLY:C	1:A:515:ASN:OD1	2.47	0.57
1:A:1081:GLU:O	1:A:1085:ILE:HG12	2.04	0.57
1:E:466:LEU:O	1:E:470:HIS:HB2	2.04	0.57
1:I:690:LEU:HD12	1:I:691:PHE:CB	2.34	0.57
1:A:489:LEU:HG	1:A:489:LEU:O	2.03	0.57
1:E:185:LYS:HE2	1:E:245:LEU:HD21	1.87	0.57
1:E:720:ILE:HD12	1:E:778:ILE:CG2	2.30	0.57
2:F:80:ILE:HD12	2:F:80:ILE:O	2.04	0.57
1:I:403:VAL:HA	1:I:810:ILE:HB	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:PHE:CZ	1:A:520:MET:HG3	2.39	0.57
2:C:99:VAL:HG12	2:C:101:PRO:HD2	1.86	0.57
1:I:309:LEU:HD22	1:I:309:LEU:H	1.68	0.57
1:I:544:ARG:HD2	1:I:546:ARG:NH1	2.20	0.57
2:J:206:TRP:HB3	2:J:209:ASP:OD1	2.04	0.57
1:E:640:MET:HE1	1:E:641:ASN:O	2.05	0.57
1:I:307:THR:HG23	1:I:310:LYS:CE	2.34	0.57
1:I:588:ASN:HD22	1:I:593:TYR:HB2	1.69	0.57
1:M:585:VAL:HG22	1:M:595:THR:HG21	1.86	0.57
1:E:983:LEU:HD21	1:E:990:TYR:CD1	2.39	0.57
1:I:403:VAL:HG21	1:I:812:LEU:HB2	1.85	0.57
1:I:472:VAL:O	1:I:472:VAL:HG13	2.04	0.57
1:I:690:LEU:HD11	1:I:691:PHE:HD2	1.60	0.57
1:A:519:TYR:HD1	1:A:534:LEU:CA	2.18	0.57
1:E:185:LYS:HE2	1:E:245:LEU:CD1	2.34	0.57
1:E:400:LEU:HB2	1:E:863:GLY:HA2	1.86	0.57
1:M:972:PHE:HA	1:M:975:TYR:CD1	2.39	0.57
1:A:598:VAL:HG22	1:A:643:ILE:HD11	1.86	0.57
2:C:132:ARG:NH1	3:C:401:P5S:O15	2.38	0.57
2:C:235:ASN:HD22	5:C:402:NAG:H61	1.69	0.57
1:M:35:TYR:CD2	1:M:35:TYR:N	2.73	0.57
1:A:171:CYS:HB2	1:A:187:HIS:CE1	2.39	0.57
1:A:421:PHE:HB2	1:A:648:VAL:HG12	1.87	0.57
1:E:974:THR:HG21	1:E:999:VAL:HG12	1.87	0.57
2:F:47:ALA:HB2	2:F:347:ASN:HD22	1.70	0.57
1:M:380:PHE:HB3	1:M:854:HIS:CG	2.40	0.57
1:A:311:TYR:O	1:A:315:SER:HB2	2.00	0.56
1:M:912:ASN:HA	1:M:915:PHE:CE1	2.40	0.56
1:E:76:PHE:O	1:E:80:VAL:HG13	2.04	0.56
1:E:898:SER:HG	2:F:131:HIS:HE2	1.49	0.56
2:F:253:ILE:O	2:F:253:ILE:HG12	2.04	0.56
1:I:485:GLU:CD	1:I:488:GLU:OE2	2.48	0.56
2:J:143:LEU:HD11	2:J:214:PHE:CD1	2.38	0.56
1:M:726:LEU:HD23	1:M:743:GLU:HG2	1.85	0.56
1:A:994:THR:HG22	1:A:1056:VAL:CG1	2.35	0.56
1:M:732:LYS:HD3	1:M:733:SER:H	1.70	0.56
1:A:32:THR:OG1	1:A:35:TYR:HB2	2.06	0.56
1:A:833:ILE:HG13	1:A:850:PRO:HA	1.87	0.56
1:A:870:ILE:HA	1:A:873:LEU:HB3	1.88	0.56
1:E:919:PRO:HB3	1:E:1026:ILE:HG12	1.87	0.56
1:I:489:LEU:CG	1:I:509:GLY:O	2.54	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:750:ILE:HD12	1:I:786:LEU:HD13	1.86	0.56
1:E:158:ASP:CG	1:E:246:LEU:HA	2.31	0.56
1:E:992:ASN:OD1	2:F:263:THR:OG1	2.22	0.56
1:M:147:VAL:HG12	1:M:148:GLU:N	2.20	0.56
1:E:339:LYS:NZ	1:E:343:ASP:HB2	2.21	0.56
1:I:47:SER:OG	1:I:117:ASP:OD1	2.23	0.56
1:I:170:THR:HG21	1:I:473:GLU:HG3	1.87	0.56
1:I:314:GLN:HE22	3:I:1201:P5S:HBA	0.40	0.56
1:I:474:ILE:N	1:I:475:LYS:HZ2	2.03	0.56
1:I:690:LEU:HD12	1:I:691:PHE:CA	2.35	0.56
1:A:31:GLU:CB	1:A:209:ILE:H	2.18	0.56
1:A:322:PRO:HB3	1:A:324:TYR:CE1	2.40	0.56
1:A:512:PHE:CE1	1:A:520:MET:CG	2.73	0.56
1:I:588:ASN:HA	1:I:591:ASP:HB2	1.87	0.56
1:M:126:TYR:CZ	1:M:133:ARG:CG	2.76	0.56
1:M:266:MET:O	1:M:270:MET:HG2	2.05	0.56
1:M:353:PHE:HA	1:M:356:PRO:HB3	1.88	0.56
1:I:116:ALA:O	1:I:120:VAL:HG12	2.06	0.56
1:I:915:PHE:CE2	1:I:1004:VAL:HG23	2.41	0.56
1:A:692:GLN:HB3	1:A:695:THR:HG23	1.87	0.55
1:E:353:PHE:HB3	1:E:881:ASN:OD1	2.06	0.55
1:I:966:GLU:HG2	1:I:1077:SER:HB3	1.87	0.55
1:I:700:LEU:HD11	1:I:750:ILE:O	2.06	0.55
1:M:98:VAL:HG21	1:M:357:VAL:HB	1.88	0.55
1:M:724:LYS:HA	1:M:728:HIS:HB2	1.87	0.55
1:A:29:VAL:HG13	1:A:210:GLU:HA	1.87	0.55
1:A:171:CYS:HB2	1:A:187:HIS:HE1	1.71	0.55
1:A:412:GLY:HA3	1:A:816:ASP:CG	2.31	0.55
1:E:942:TYR:CG	1:E:943:MET:N	2.74	0.55
1:E:1072:LEU:HD22	2:F:329:TYR:CD1	2.42	0.55
1:I:592:GLY:HA3	1:I:687:ALA:HB2	1.88	0.55
1:I:700:LEU:HD11	1:I:750:ILE:CB	2.37	0.55
1:E:392:ASN:HB2	1:E:846:ASP:HA	1.87	0.55
2:F:142:GLN:NE2	2:F:169:ALA:O	2.40	0.55
2:N:290:ARG:HH21	2:N:292:TRP:NE1	2.03	0.55
1:A:719:LEU:CD1	1:A:720:ILE:HD12	2.36	0.55
1:M:272:LEU:HG	1:M:792:PRO:HB3	1.88	0.55
1:A:217:ASP:OD1	1:A:218:LEU:N	2.39	0.55
2:F:181:ASP:HB3	2:F:298:ASN:H	1.71	0.55
1:I:309:LEU:H	1:I:309:LEU:CD2	2.19	0.55
1:I:923:TYR:HA	1:I:927:GLU:HB2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1078:LEU:HB3	1:M:1082:ILE:HD13	1.88	0.55
1:A:167:THR:CG2	1:E:196:LEU:HD13	2.37	0.55
1:A:464:ARG:NE	1:A:532:TYR:OH	2.40	0.55
1:A:546:ARG:HA	1:A:564:GLY:HA2	1.88	0.55
1:A:959:TRP:CZ3	1:A:963:ALA:HB2	2.42	0.55
1:E:127:ILE:CD1	1:E:146:VAL:HG23	2.34	0.55
1:E:522:VAL:O	1:E:523:GLU:HG3	2.07	0.55
1:I:539:ASN:HD22	1:I:547:MET:HB2	1.72	0.55
1:A:723:ARG:NH1	1:A:778:ILE:HA	2.22	0.55
2:C:181:ASP:N	2:C:181:ASP:OD1	2.40	0.55
1:E:409:BFD:F3	7:E:1302:HOH:O	2.08	0.55
1:E:983:LEU:H	1:E:983:LEU:HD23	1.72	0.55
1:I:33:GLU:HB2	1:I:205:LEU:HA	1.89	0.55
1:M:126:TYR:OH	1:M:133:ARG:CG	2.44	0.55
1:M:880:LYS:HZ2	1:M:1007:VAL:HG11	1.72	0.55
5:F:405:NAG:C7	5:F:405:NAG:C5	2.85	0.55
1:M:272:LEU:HD22	1:M:822:SER:H	1.72	0.55
2:F:292:TRP:CZ3	5:F:405:NAG:O5	2.60	0.54
1:A:834:LYS:HE3	1:A:839:ARG:NH2	2.23	0.54
1:E:695:THR:O	1:E:695:THR:HG23	2.07	0.54
1:I:150:GLN:HA	1:I:255:GLU:O	2.06	0.54
1:M:594:ARG:O	1:M:648:VAL:HG22	2.08	0.54
1:E:159:LEU:H	1:E:244:LEU:CD2	2.20	0.54
1:E:816:ASP:OD1	7:E:1301:HOH:O	2.18	0.54
2:F:240:VAL:O	2:F:243:LEU:HD22	2.08	0.54
1:M:843:ARG:HD2	1:M:843:ARG:C	2.33	0.54
1:M:883:CYS:O	1:M:1003:LEU:HD11	2.07	0.54
2:N:290:ARG:NE	2:N:292:TRP:CE2	2.75	0.54
2:C:125:SER:HA	2:C:268:THR:HG22	1.90	0.54
1:I:162:LEU:C	1:I:194:ILE:HG23	2.33	0.54
1:M:162:LEU:O	1:M:194:ILE:HG13	2.08	0.54
1:A:515:ASN:OD1	1:A:515:ASN:N	2.39	0.54
1:E:860:LEU:HD11	1:E:939:PRO:HB3	1.89	0.54
1:I:407:PHE:CE2	1:I:799:VAL:HG22	2.42	0.54
1:A:1055:PHE:CB	2:C:208:THR:HG21	2.37	0.54
2:C:83:THR:HG21	2:C:307:ARG:HD2	1.89	0.54
1:I:473:GLU:CA	1:I:475:LYS:HZ3	2.13	0.54
1:A:176:ALA:O	1:A:837:GLU:HG2	2.07	0.54
1:A:522:VAL:O	1:A:530:GLU:HB2	2.08	0.54
1:I:318:TYR:OH	2:J:128:TYR:CZ	2.27	0.54
1:M:149:VAL:HB	1:M:258:TYR:HE2	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:859:LEU:C	1:M:859:LEU:HD12	2.33	0.54
1:A:29:VAL:HG22	1:A:31:GLU:HG2	1.88	0.54
1:A:225:ILE:O	1:A:225:ILE:HG12	2.06	0.54
1:E:813:SER:OG	1:E:824:ILE:HA	2.08	0.54
1:E:983:LEU:HD12	1:E:1066:THR:HG23	1.89	0.54
1:I:337:VAL:HG23	1:I:338:LEU:H	1.73	0.54
2:N:90:PRO:CD	5:N:405:NAG:H83	2.36	0.54
2:N:107:ASN:ND2	2:N:292:TRP:CH2	2.74	0.54
1:A:67:ILE:HB	1:A:292:LEU:HD23	1.89	0.54
1:I:161:LEU:HD11	1:I:187:HIS:CD2	2.43	0.54
2:J:301:VAL:HG11	2:J:308:LYS:HE2	1.90	0.54
1:A:31:GLU:CD	1:A:209:ILE:HG23	2.32	0.54
1:A:40:PHE:HB3	1:A:143:VAL:HG21	1.90	0.54
1:A:831:ILE:HD13	1:A:847:TYR:HB2	1.89	0.54
1:I:311:TYR:CE2	1:I:336:LYS:HG3	2.43	0.54
1:M:716:HIS:HA	1:M:719:LEU:HD22	1.89	0.54
1:A:29:VAL:N	1:A:211:CYS:H	1.97	0.53
1:A:218:LEU:HD21	1:A:246:LEU:HD23	1.90	0.53
1:A:359:MET:HE1	1:A:874:VAL:HG23	1.90	0.53
1:E:367:LYS:O	1:E:397:ASN:ND2	2.41	0.53
1:E:926:LEU:HD11	1:E:1019:THR:HG21	1.90	0.53
1:E:1012:ALA:O	1:E:1015:THR:HG22	2.08	0.53
1:E:1045:TRP:HB2	1:E:1046:PRO:HD3	1.89	0.53
1:I:1002:VAL:O	1:I:1006:THR:OG1	2.20	0.53
2:J:142:GLN:HA	2:J:149:ALA:HB1	1.89	0.53
1:M:714:ARG:O	1:M:717:GLU:HG3	2.08	0.53
1:A:519:TYR:CD1	1:A:534:LEU:CA	2.91	0.53
1:E:294:VAL:O	1:E:298:ILE:HG12	2.09	0.53
1:E:353:PHE:HB2	1:E:885:ILE:HD12	1.90	0.53
1:E:254:THR:HG21	1:E:257:ILE:CD1	2.38	0.53
1:E:869:ARG:HD3	1:E:924:SER:O	2.09	0.53
1:I:46:VAL:HG21	1:I:270:MET:HE2	1.90	0.53
2:J:222:ASN:HD21	2:J:225:GLU:HB3	1.73	0.53
1:M:422:ILE:O	1:M:507:ARG:NH1	2.41	0.53
1:M:796:ALA:HB2	1:M:823:MET:SD	2.48	0.53
2:N:204:ILE:HG23	2:N:275:LEU:HD22	1.89	0.53
2:C:46:THR:H	2:C:49:THR:HG22	1.73	0.53
1:E:192:ASP:N	1:E:192:ASP:OD1	2.40	0.53
1:E:233:GLU:OE1	1:E:244:LEU:N	2.40	0.53
1:E:673:LEU:HD12	1:E:795:LYS:HE2	1.88	0.53
1:E:915:PHE:HD1	1:E:1029:SER:HB3	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:128:TYR:CE1	2:F:267:PRO:HB3	2.44	0.53
1:I:873:LEU:HD13	1:I:920:ILE:HG21	1.90	0.53
1:A:29:VAL:HG12	1:A:210:GLU:C	2.30	0.53
1:E:354:ILE:O	1:E:356:PRO:HD3	2.09	0.53
2:F:81:ASP:HA	2:F:309:ARG:HB3	1.91	0.53
1:I:144:GLY:N	1:I:263:TYR:CE1	2.76	0.53
1:I:856:LYS:O	1:I:860:LEU:HB2	2.07	0.53
1:A:211:CYS:SG	1:A:263:TYR:OH	2.59	0.53
1:A:774:ILE:HA	1:A:777:GLN:HB2	1.90	0.53
1:E:864:HIS:CG	1:E:942:TYR:CE1	2.96	0.53
2:J:124:LEU:HD22	2:J:308:LYS:HE3	1.91	0.53
1:M:725:LYS:HE2	1:M:732:LYS:HG2	1.90	0.53
2:N:290:ARG:HH21	2:N:292:TRP:HE1	1.56	0.53
1:A:384:GLU:C	1:A:386:ASN:OD1	2.52	0.53
1:A:410:LYS:CE	1:A:681:ALA:HA	2.37	0.53
1:A:573:VAL:O	1:A:578:ILE:HD11	2.09	0.53
2:C:232:LYS:HZ3	2:C:240:VAL:HG12	1.73	0.53
1:E:173:VAL:HG23	1:E:250:THR:O	2.09	0.53
1:E:752:ASP:OD1	1:E:755:THR:OG1	2.19	0.53
1:E:992:ASN:N	2:F:263:THR:O	2.42	0.53
2:F:285:THR:HG22	2:F:286:LEU:HD12	1.90	0.53
1:M:147:VAL:HG12	1:M:148:GLU:H	1.74	0.53
1:A:177:SER:HA	1:A:837:GLU:HG2	1.89	0.53
1:A:723:ARG:NH1	1:A:781:LYS:HB3	2.23	0.53
1:I:544:ARG:NH2	1:I:569:VAL:HG13	2.24	0.53
1:M:472:VAL:HG21	1:M:491:TYR:CE1	2.43	0.53
2:N:168:ILE:HG22	2:N:170:PRO:HD2	1.90	0.53
1:A:374:ILE:HD11	1:A:391:VAL:HG23	1.91	0.53
1:A:569:VAL:CA	1:A:571:PRO:CD	2.85	0.53
1:A:938:ASP:OD1	1:A:940:ARG:HG3	2.09	0.53
1:E:284:VAL:O	1:E:287:SER:OG	2.23	0.53
2:F:51:LEU:HD21	2:F:344:LEU:HD12	1.91	0.53
1:M:147:VAL:HB	1:M:258:TYR:CD1	2.43	0.53
1:A:237:ARG:NE	1:A:789:ARG:HA	2.24	0.53
1:E:128:ILE:HD12	1:E:134:VAL:HG22	1.90	0.53
1:E:893:PHE:HA	1:E:897:PHE:HE1	1.74	0.53
1:E:939:PRO:O	1:E:943:MET:N	2.39	0.53
1:E:1073:LEU:O	1:E:1077:SER:OG	2.22	0.53
2:F:121:TYR:HD1	2:F:272:LEU:HA	1.73	0.53
1:I:292:LEU:HD11	1:I:355:ILE:HG23	1.90	0.53
1:I:911:TYR:CG	1:I:912:ASN:N	2.77	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:218:LEU:HD22	1:M:271:ALA:HB1	1.90	0.53
1:A:384:GLU:HB2	1:A:386:ASN:CG	2.33	0.52
1:E:668:LEU:HD23	1:E:668:LEU:H	1.74	0.52
1:I:102:THR:HG22	1:I:364:GLU:HG3	1.90	0.52
1:I:599:ALA:CB	1:I:640:MET:HE3	2.39	0.52
1:I:703:LYS:HB3	1:I:711:LYS:CD	2.37	0.52
2:J:292:TRP:CH2	5:J:405:NAG:HO6	1.66	0.52
1:M:117:ASP:OD1	1:M:117:ASP:N	2.41	0.52
1:A:176:ALA:CB	1:A:837:GLU:CD	2.73	0.52
1:A:218:LEU:HG	1:A:218:LEU:O	2.09	0.52
2:C:33:PHE:HA	2:C:38:LEU:HD11	1.90	0.52
1:A:310:LYS:CE	1:A:897:PHE:HB2	2.21	0.52
1:A:966:GLU:HG2	1:A:1006:THR:HG21	1.90	0.52
1:E:393:THR:OG1	1:E:846:ASP:HB3	2.09	0.52
1:I:410:LYS:HD3	1:I:411:THR:HG23	1.92	0.52
1:I:700:LEU:CD1	1:I:750:ILE:CG2	2.76	0.52
1:M:539:ASN:ND2	1:M:546:ARG:O	2.43	0.52
1:A:295:TYR:OH	1:A:959:TRP:HH2	1.92	0.52
1:A:1051:GLN:OE1	1:A:1051:GLN:N	2.42	0.52
2:F:117:ASN:OD1	2:F:117:ASN:N	2.43	0.52
2:F:292:TRP:CE3	5:F:404:NAG:C6	2.92	0.52
1:I:75:ILE:HG12	1:I:352:ASN:HD21	1.74	0.52
1:I:743:GLU:OE2	1:I:781:LYS:NZ	2.42	0.52
2:N:90:PRO:HG2	5:N:405:NAG:C8	2.38	0.52
1:A:29:VAL:CG1	1:A:211:CYS:H	2.12	0.52
1:A:512:PHE:HE1	1:A:520:MET:CB	2.22	0.52
1:E:196:LEU:HD11	1:E:199:ALA:CB	2.39	0.52
1:I:35:TYR:HD1	1:I:38:GLN:HE22	1.57	0.52
1:M:39:ARG:CB	1:M:39:ARG:NH1	2.73	0.52
1:M:287:SER:HB2	1:M:951:LEU:HD13	1.91	0.52
2:N:68:ILE:HD12	2:N:325:LEU:HG	1.92	0.52
1:A:723:ARG:CZ	1:A:778:ILE:HA	2.40	0.52
1:A:884:PHE:HA	1:A:1003:LEU:CD1	2.40	0.52
1:A:888:GLN:O	1:A:892:GLN:NE2	2.42	0.52
1:E:736:SER:CB	1:E:739:LYS:HZ1	2.20	0.52
2:F:150:LEU:HD22	2:F:217:PRO:HG2	1.92	0.52
2:F:179:PHE:HA	2:F:299:TYR:CE2	2.45	0.52
1:I:354:ILE:O	1:I:356:PRO:HD3	2.10	0.52
1:I:483:ALA:O	1:I:484:THR:C	2.51	0.52
1:A:209:ILE:HD12	1:A:224:ARG:O	2.10	0.52
1:A:592:GLY:HA3	1:A:687:ALA:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:382:ASP:OD2	1:E:386:ASN:ND2	2.42	0.52
1:I:164:SER:HB2	1:I:169:GLY:HA2	1.92	0.52
1:I:678:MET:SD	1:I:750:ILE:HD13	2.50	0.52
1:I:700:LEU:HD11	1:I:750:ILE:CG1	2.38	0.52
2:J:143:LEU:HD22	2:J:252:PHE:CD2	2.45	0.52
1:A:105:LYS:HE3	1:A:368:PHE:CG	2.45	0.52
1:A:510:PHE:HA	1:A:523:GLU:O	2.10	0.52
1:E:720:ILE:CG2	1:E:778:ILE:HB	2.38	0.52
1:I:473:GLU:CA	1:I:475:LYS:HZ2	2.20	0.52
2:N:188:ILE:HD13	2:N:292:TRP:NE1	2.18	0.52
1:A:792:PRO:HG3	1:A:819:ASN:C	2.33	0.52
1:A:919:PRO:HB3	1:A:1026:ILE:HG12	1.91	0.52
1:E:277:LYS:HE3	1:E:279:GLN:HB2	1.91	0.52
1:E:339:LYS:C	1:E:339:LYS:HD3	2.35	0.52
2:F:64:ILE:O	2:F:68:ILE:HG12	2.10	0.52
1:I:270:MET:O	1:I:273:ASN:ND2	2.43	0.52
1:M:722:TYR:HA	1:M:725:LYS:HZ3	1.74	0.52
1:M:884:PHE:HA	1:M:1003:LEU:HD21	1.92	0.52
1:A:266:MET:O	1:A:270:MET:HG2	2.09	0.51
1:A:327:LYS:HG2	1:A:331:GLU:HA	1.91	0.51
1:A:512:PHE:HA	1:A:522:VAL:HG12	1.92	0.51
1:E:835:GLY:H	1:E:839:ARG:HD2	1.75	0.51
1:E:915:PHE:CD1	1:E:1029:SER:HB3	2.45	0.51
1:I:690:LEU:HD13	1:I:691:PHE:CD2	2.44	0.51
1:I:715:LEU:O	1:I:719:LEU:HB2	2.11	0.51
2:J:51:LEU:HD21	2:J:344:LEU:HD12	1.91	0.51
1:A:324:TYR:HE2	2:C:127:PHE:CZ	2.27	0.51
1:A:816:ASP:OD2	1:A:837:GLU:HB2	2.10	0.51
1:E:185:LYS:HG3	1:E:241:PRO:HD2	1.92	0.51
2:F:159:PRO:HG2	2:F:173:ALA:HB2	1.92	0.51
1:I:284:VAL:O	1:I:288:ILE:HG13	2.10	0.51
1:I:310:LYS:HE2	1:I:347:PHE:HE2	1.75	0.51
1:A:860:LEU:HD21	1:A:939:PRO:HB3	1.92	0.51
1:E:688:CYS:SG	1:E:690:LEU:HD23	2.50	0.51
1:E:820:ASP:O	1:E:824:ILE:HG12	2.10	0.51
1:I:214:PRO:HA	1:I:268:THR:CG2	2.16	0.51
1:I:690:LEU:HD12	1:I:691:PHE:CG	2.46	0.51
1:I:700:LEU:CD1	1:I:700:LEU:N	2.73	0.51
2:N:250:ASN:HD22	2:N:251:GLY:N	2.08	0.51
2:C:162:ARG:HG2	2:C:167:PRO:HA	1.93	0.51
1:E:533:GLU:HG3	1:E:552:LYS:HG2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:932:ILE:HD11	2:F:36:GLN:HG2	1.93	0.51
1:I:100:THR:O	1:I:104:ILE:N	2.43	0.51
1:I:382:ASP:OD2	1:I:386:ASN:ND2	2.44	0.51
1:I:1041:GLY:HA2	1:I:1054:TYR:HB3	1.92	0.51
1:M:824:ILE:O	1:M:827:SER:OG	2.24	0.51
1:E:570:PHE:HB3	1:E:571:PRO:HD3	1.92	0.51
1:E:812:LEU:HA	1:E:829:VAL:HG12	1.91	0.51
2:F:179:PHE:HA	2:F:299:TYR:HE2	1.75	0.51
1:M:39:ARG:HB3	1:M:39:ARG:NH1	2.25	0.51
1:M:45:ILE:HD12	1:M:843:ARG:HH12	1.75	0.51
1:A:837:GLU:OE1	1:A:837:GLU:HA	2.10	0.51
1:A:880:LYS:NZ	1:A:912:ASN:OD1	2.41	0.51
2:C:301:VAL:HG12	2:C:304:PHE:CZ	2.45	0.51
1:E:159:LEU:HD12	1:E:260:VAL:HB	1.93	0.51
1:E:225:ILE:HG23	1:E:227:ILE:HG12	1.92	0.51
1:E:324:TYR:CE1	2:F:127:PHE:CZ	2.99	0.51
1:E:678:MET:N	1:E:788:CYS:SG	2.84	0.51
1:E:812:LEU:HG	1:E:829:VAL:HG11	1.92	0.51
2:F:199:LEU:HB2	2:F:274:ARG:HG2	1.91	0.51
1:I:266:MET:SD	1:I:266:MET:C	2.94	0.51
1:A:177:SER:N	1:A:837:GLU:OE2	2.43	0.51
1:A:354:ILE:HG12	1:A:885:ILE:HG21	1.93	0.51
1:A:489:LEU:CD1	1:A:503:LYS:HZ3	2.13	0.51
1:A:657:ALA:HA	1:A:661:GLU:HG2	1.92	0.51
1:A:790:MET:HE3	1:A:798:ILE:HD11	1.92	0.51
1:A:876:TYR:CE2	1:A:1011:LEU:HB2	2.46	0.51
1:E:875:GLN:HG3	1:E:955:PRO:HG3	1.91	0.51
1:E:1045:TRP:CE3	1:E:1051:GLN:HA	2.46	0.51
1:I:159:LEU:CD1	1:I:259:GLY:C	2.71	0.51
1:I:221:PHE:O	1:I:232:LEU:HA	2.10	0.51
1:I:310:LYS:HD2	1:I:311:TYR:CA	2.38	0.51
1:I:700:LEU:CD1	1:I:700:LEU:H	2.24	0.51
1:I:856:LYS:O	1:I:860:LEU:CB	2.58	0.51
1:M:472:VAL:HG21	1:M:491:TYR:CD1	2.46	0.51
1:E:191:ARG:HB2	1:E:194:ILE:HD11	1.92	0.51
2:F:233:PRO:HG2	2:F:236:TRP:CD1	2.45	0.51
1:I:270:MET:SD	1:I:270:MET:C	2.94	0.51
1:A:700:LEU:O	1:A:755:THR:OG1	2.27	0.51
1:E:601:LYS:HB2	1:E:641:ASN:HA	1.92	0.51
1:E:993:TRP:CZ3	1:E:1052:ARG:HB3	2.46	0.51
2:F:207:TRP:CD1	2:F:211:ASN:HD22	2.29	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:485:GLU:HG3	1:I:488:GLU:OE2	2.10	0.51
1:M:574:GLN:NE2	1:M:641:ASN:O	2.41	0.51
1:M:749:LEU:H	1:M:749:LEU:HD23	1.75	0.51
1:M:992:ASN:HB2	2:N:265:ALA:HB2	1.92	0.51
1:A:453:LYS:HG3	1:A:454:VAL:N	2.26	0.50
1:A:519:TYR:CD1	1:A:534:LEU:N	2.79	0.50
1:E:175:THR:O	1:E:175:THR:OG1	2.29	0.50
1:M:725:LYS:HE2	1:M:732:LYS:CG	2.41	0.50
1:M:958:TYR:O	1:M:962:LEU:HB2	2.11	0.50
1:M:1032:PHE:O	1:M:1036:PHE:HB3	2.10	0.50
1:A:496:PRO:HA	1:A:499:ILE:HB	1.93	0.50
1:A:524:ASN:N	1:A:530:GLU:CD	2.69	0.50
1:E:730:PHE:N	1:E:731:PRO:HD3	2.25	0.50
1:E:1055:PHE:CD2	2:F:208:THR:HG21	2.46	0.50
2:F:292:TRP:HH2	5:F:405:NAG:O6	1.93	0.50
1:I:671:TRP:CG	1:I:785:VAL:HG22	2.45	0.50
1:A:886:LEU:HD23	1:A:967:GLY:HA3	1.93	0.50
2:C:77:GLU:HB2	2:C:313:SER:HB3	1.93	0.50
1:E:179:ASP:N	1:E:179:ASP:OD1	2.41	0.50
1:I:318:TYR:CE1	2:J:128:TYR:CD2	2.98	0.50
1:I:880:LYS:HE3	1:I:911:TYR:HE2	1.76	0.50
2:J:79:GLU:HB3	2:J:311:ILE:HG23	1.93	0.50
1:A:66:ARG:HD3	1:A:360:TYR:CZ	2.46	0.50
1:A:834:LYS:HB2	1:A:839:ARG:HG3	1.93	0.50
1:E:51:THR:HG23	1:E:53:TRP:H	1.76	0.50
1:E:178:LEU:HD13	1:E:246:LEU:CB	2.42	0.50
1:E:413:THR:HG22	1:E:833:ILE:HG21	1.93	0.50
1:E:579:GLU:HA	1:E:582:LYS:HE3	1.93	0.50
1:I:464:ARG:HD3	1:I:561:PHE:HB2	1.94	0.50
1:I:678:MET:CE	1:I:700:LEU:HB2	2.41	0.50
1:M:237:ARG:NH1	1:M:409:BFD:F3	2.30	0.50
2:N:90:PRO:HG3	5:N:405:NAG:C8	2.41	0.50
1:A:412:GLY:O	1:A:836:LYS:CB	2.44	0.50
2:C:233:PRO:HG2	2:C:236:TRP:HB2	1.94	0.50
1:E:983:LEU:HD21	1:E:990:TYR:CG	2.45	0.50
2:F:30:ASN:OD1	2:F:35:GLN:HG3	2.12	0.50
2:F:292:TRP:CD2	5:F:404:NAG:O6	2.59	0.50
1:M:272:LEU:HD23	1:M:823:MET:HE3	1.92	0.50
1:A:484:THR:CG2	1:A:487:ALA:O	2.59	0.50
1:A:519:TYR:HD1	1:A:534:LEU:HB2	1.75	0.50
1:A:574:GLN:CA	1:A:574:GLN:NE2	2.73	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:LYS:HZ3	1:A:1003:LEU:HD21	1.77	0.50
1:A:904:ASP:OD2	1:A:1052:ARG:HD2	2.12	0.50
2:C:185:LEU:CD1	2:C:312:LEU:HD21	2.41	0.50
1:I:869:ARG:NH1	1:I:927:GLU:O	2.45	0.50
1:A:520:MET:O	1:A:521:ARG:C	2.52	0.50
1:E:406:VAL:HG13	1:E:670:VAL:HA	1.93	0.50
1:E:1054:TYR:HE2	2:F:208:THR:HB	1.76	0.50
2:F:53:ILE:O	2:F:57:ILE:HG12	2.12	0.50
2:F:292:TRP:CH2	5:F:405:NAG:C5	2.93	0.50
1:I:143:VAL:CG2	1:I:263:TYR:CD2	2.93	0.50
1:I:247:LYS:HD3	1:I:269:LYS:HE3	1.94	0.50
1:I:271:ALA:O	1:I:272:LEU:C	2.54	0.50
1:I:546:ARG:HD2	1:I:630:GLU:HB2	1.94	0.50
1:I:700:LEU:H	1:I:700:LEU:HD12	1.77	0.50
1:M:47:SER:HB3	1:M:843:ARG:CD	2.41	0.50
2:N:58:GLY:HA3	2:N:337:PHE:HB2	1.92	0.50
1:A:1082:ILE:O	1:A:1086:VAL:HG23	2.11	0.50
1:E:158:ASP:HB2	1:E:264:THR:O	2.11	0.50
1:E:339:LYS:HZ1	1:E:343:ASP:HB2	1.77	0.50
1:I:700:LEU:HD21	1:I:750:ILE:CG1	2.39	0.50
1:M:1022:ASN:HA	1:M:1025:VAL:HG22	1.92	0.50
1:A:305:VAL:O	1:A:309:LEU:HB2	2.12	0.50
1:A:398:GLU:HA	1:A:866:TYR:HB3	1.93	0.50
1:A:480:VAL:HG23	1:I:486:SER:HB3	1.93	0.50
1:E:171:CYS:HB2	1:E:254:THR:OG1	2.11	0.50
1:E:685:CYS:HB3	1:E:691:PHE:HD2	1.76	0.50
2:F:232:LYS:HB3	2:F:239:PRO:HG3	1.94	0.50
1:I:42:ASP:OD1	1:I:43:ASN:N	2.45	0.50
1:I:730:PHE:O	1:I:732:LYS:N	2.45	0.50
1:M:105:LYS:HG3	1:M:368:PHE:CE2	2.47	0.50
1:A:299:LEU:HD21	1:A:348:MET:HG2	1.92	0.49
1:A:397:ASN:ND2	1:A:847:TYR:OH	2.44	0.49
1:A:904:ASP:HB3	1:A:907:TYR:CB	2.41	0.49
3:C:401:P5S:H42A	3:C:401:P5S:C17	2.42	0.49
1:E:159:LEU:N	1:E:244:LEU:CD2	2.75	0.49
1:E:609:GLU:O	1:E:612:ASN:ND2	2.42	0.49
1:E:904:ASP:HB2	1:E:1053:MET:HE3	1.94	0.49
1:E:1015:THR:HG23	1:E:1016:ARG:N	2.27	0.49
2:F:131:HIS:CD2	2:F:133:ARG:HG2	2.46	0.49
2:F:222:ASN:OD1	2:F:222:ASN:N	2.45	0.49
1:I:310:LYS:HZ3	1:I:343:ASP:CB	2.25	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:354:ILE:HA	1:I:881:ASN:HB3	1.93	0.49
1:M:182:SER:HA	1:M:417:ASN:HD21	1.76	0.49
1:M:966:GLU:OE1	1:M:1077:SER:OG	2.25	0.49
2:N:188:ILE:HD11	2:N:292:TRP:CD1	2.26	0.49
1:A:149:VAL:HG22	1:A:251:LEU:HD22	1.94	0.49
1:A:348:MET:O	1:A:352:ASN:N	2.44	0.49
1:A:724:LYS:H	1:A:724:LYS:HD2	1.78	0.49
1:I:678:MET:CE	1:I:700:LEU:N	2.59	0.49
1:M:127:ILE:HB	1:M:147:VAL:HG13	1.94	0.49
1:M:1052:ARG:H	1:M:1052:ARG:HE	1.58	0.49
1:A:480:VAL:HG23	1:I:486:SER:CA	2.43	0.49
1:A:851:LYS:HG3	1:A:854:HIS:HB2	1.94	0.49
1:A:856:LYS:O	1:A:860:LEU:CB	2.60	0.49
1:E:285:GLU:O	1:E:288:ILE:HG22	2.12	0.49
1:I:690:LEU:CD1	1:I:690:LEU:C	2.86	0.49
1:I:723:ARG:HH21	1:I:778:ILE:CD1	2.24	0.49
1:M:38:GLN:HG3	1:M:142:LYS:HE3	1.94	0.49
1:M:994:THR:HG22	1:M:1056:VAL:HG22	1.95	0.49
1:A:574:GLN:HG2	1:A:642:LEU:CB	2.42	0.49
1:A:880:LYS:HD3	1:A:1007:VAL:HG11	1.93	0.49
1:E:51:THR:HG22	1:E:54:ASN:OD1	2.13	0.49
1:E:139:GLU:OE1	1:E:139:GLU:N	2.45	0.49
1:E:865:LEU:O	1:E:869:ARG:HG3	2.12	0.49
1:E:1023:HIS:O	1:E:1027:TRP:HB2	2.12	0.49
2:F:135:VAL:HG22	2:F:263:THR:HG21	1.94	0.49
1:I:171:CYS:HB2	1:I:254:THR:HG21	1.94	0.49
1:I:309:LEU:N	1:I:309:LEU:CD2	2.75	0.49
1:I:703:LYS:HE3	1:I:714:ARG:CD	2.32	0.49
1:I:723:ARG:HH21	1:I:778:ILE:HD13	1.77	0.49
1:I:1022:ASN:HA	1:I:1025:VAL:HG22	1.95	0.49
1:M:872:HIS:HB3	1:M:923:TYR:OH	2.12	0.49
1:A:237:ARG:NH1	1:A:789:ARG:H	2.09	0.49
1:A:484:THR:HG21	1:A:487:ALA:O	2.11	0.49
1:A:911:TYR:OH	1:A:1033:TYR:HB2	2.12	0.49
1:E:574:GLN:CB	1:E:640:MET:CE	2.83	0.49
2:F:156:GLU:C	2:F:158:GLU:H	2.20	0.49
1:I:678:MET:CE	1:I:700:LEU:CB	2.90	0.49
1:A:291:PHE:CZ	1:A:956:PHE:HD2	2.30	0.49
1:A:353:PHE:HB2	1:A:885:ILE:HD12	1.94	0.49
1:A:519:TYR:HH	1:A:551:VAL:CG1	2.16	0.49
1:E:402:GLN:O	1:E:810:ILE:HD13	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:117:ASP:O	1:I:120:VAL:CG1	2.61	0.49
1:I:314:GLN:NE2	3:I:1201:P5S:HB	2.08	0.49
1:A:555:GLU:OE1	1:A:555:GLU:N	2.46	0.49
1:A:1079:PHE:CZ	2:C:339:LEU:HD22	2.47	0.49
2:C:266:LEU:HD22	2:C:267:PRO:HD2	1.95	0.49
1:E:327:LYS:NZ	1:E:328:THR:O	2.34	0.49
1:E:948:ASN:O	1:E:950:MET:HG3	2.12	0.49
1:I:468:LEU:C	1:I:468:LEU:CD1	2.86	0.49
1:A:480:VAL:HG23	1:I:486:SER:HA	1.95	0.49
1:A:489:LEU:HD12	1:A:491:TYR:OH	2.13	0.49
1:A:519:TYR:CD1	1:A:534:LEU:HA	2.47	0.49
1:A:572:ARG:HD3	1:A:639:ASN:HB3	1.94	0.49
1:A:912:ASN:O	1:A:916:THR:OG1	2.24	0.49
1:E:387:GLU:OE1	1:E:839:ARG:NH2	2.38	0.49
1:E:898:SER:OG	2:F:131:HIS:NE2	2.43	0.49
2:F:170:PRO:HD2	2:F:233:PRO:HG3	1.95	0.49
1:I:117:ASP:O	1:I:120:VAL:HG13	2.12	0.49
1:I:310:LYS:O	1:I:314:GLN:HB2	2.12	0.49
1:I:475:LYS:N	1:I:475:LYS:CD	2.73	0.49
1:I:700:LEU:CD2	1:I:752:ASP:N	2.50	0.49
1:I:1019:THR:HG23	1:I:1022:ASN:H	1.77	0.49
1:M:247:LYS:HZ1	1:M:818:ALA:HB2	1.77	0.49
1:M:294:VAL:HG21	1:M:959:TRP:HH2	1.78	0.49
1:M:434:VAL:HG23	1:M:440:GLY:C	2.34	0.49
1:E:360:TYR:HA	1:E:363:VAL:HG12	1.94	0.49
1:E:868:VAL:HG11	1:E:929:HIS:CD2	2.48	0.49
1:E:911:TYR:HE2	1:E:1004:VAL:HG21	1.76	0.49
2:F:339:LEU:O	2:F:343:LEU:HB2	2.13	0.49
1:I:159:LEU:O	1:I:245:LEU:N	2.22	0.49
1:I:162:LEU:HB2	1:I:258:TYR:C	2.38	0.49
1:I:406:VAL:HG23	1:I:812:LEU:HD22	1.94	0.49
1:I:649:GLU:N	1:I:649:GLU:OE1	2.46	0.49
1:M:415:THR:HA	1:M:653:GLN:HB2	1.94	0.49
1:M:430:LYS:O	1:M:430:LYS:HD3	2.13	0.49
1:M:719:LEU:HD23	1:M:778:ILE:HG12	1.93	0.49
1:M:992:ASN:HB3	2:N:265:ALA:HB2	1.93	0.49
1:E:942:TYR:CD1	1:E:942:TYR:C	2.88	0.49
1:I:307:THR:CA	1:I:310:LYS:CE	2.71	0.49
1:I:398:GLU:H	1:I:398:GLU:CD	2.20	0.49
1:I:942:TYR:CG	1:I:943:MET:N	2.80	0.49
2:J:292:TRP:HZ3	5:J:405:NAG:HO6	0.50	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:671:TRP:CD2	1:M:785:VAL:HG22	2.48	0.49
2:N:290:ARG:NH2	2:N:292:TRP:HE1	2.11	0.49
1:A:63:GLN:OE1	1:A:99:ILE:HA	2.13	0.48
1:A:220:LYS:CB	1:A:220:LYS:HZ3	2.26	0.48
1:A:956:PHE:HA	1:A:959:TRP:CD1	2.47	0.48
1:E:465:ALA:HA	1:E:501:LEU:HD12	1.95	0.48
1:M:277:LYS:HB2	1:M:825:LEU:HB3	1.95	0.48
1:A:225:ILE:O	1:A:225:ILE:HG23	2.13	0.48
1:A:522:VAL:O	1:A:529:ILE:C	2.55	0.48
1:A:795:LYS:HD3	1:A:823:MET:HG3	1.95	0.48
1:A:824:ILE:HG12	1:A:845:SER:HA	1.95	0.48
1:A:834:LYS:HE2	1:A:839:ARG:HE	1.76	0.48
1:A:456:LYS:HD2	1:A:456:LYS:O	2.13	0.48
1:A:520:MET:N	1:A:520:MET:SD	2.86	0.48
2:C:273:TYR:O	2:C:274:ARG:HD3	2.13	0.48
1:E:594:ARG:HB2	1:E:648:VAL:CG2	2.44	0.48
1:I:233:GLU:HG2	1:I:244:LEU:H	1.78	0.48
1:A:314:GLN:HB3	1:A:318:TYR:HB2	1.94	0.48
1:A:630:GLU:HA	1:A:633:PHE:CE1	2.49	0.48
2:C:121:TYR:HE1	2:C:272:LEU:HD12	1.78	0.48
2:C:199:LEU:N	2:C:199:LEU:CD2	2.75	0.48
1:E:256:LYS:O	1:E:257:ILE:HD12	2.13	0.48
2:F:270:ARG:HD3	2:F:311:ILE:HD12	1.95	0.48
1:I:159:LEU:CA	1:I:262:VAL:CG2	2.70	0.48
1:A:574:GLN:O	1:A:578:ILE:CG1	2.57	0.48
1:A:629:MET:O	1:A:633:PHE:HD1	1.97	0.48
1:E:127:ILE:HD12	1:E:128:ILE:N	2.21	0.48
1:E:632:VAL:O	1:E:636:ILE:HG23	2.14	0.48
2:F:180:ASN:HD21	2:F:298:ASN:HB3	1.77	0.48
1:I:46:VAL:HG21	1:I:270:MET:CE	2.42	0.48
1:M:956:PHE:HA	1:M:959:TRP:NE1	2.29	0.48
2:N:290:ARG:NH2	2:N:292:TRP:CE2	2.81	0.48
1:A:167:THR:HG23	1:E:196:LEU:HD13	1.96	0.48
2:C:81:ASP:OD2	2:C:83:THR:HG22	2.13	0.48
2:C:113:SER:HB2	2:C:287:PRO:HA	1.96	0.48
2:C:121:TYR:HD1	2:C:272:LEU:HA	1.79	0.48
2:C:123:GLY:O	2:C:124:LEU:HD23	2.13	0.48
1:E:465:ALA:HB1	1:E:501:LEU:HB3	1.96	0.48
2:F:206:TRP:CD1	2:F:208:THR:HG23	2.48	0.48
1:M:737:PHE:CE1	1:M:739:LYS:HB2	2.48	0.48
1:A:31:GLU:CG	1:A:209:ILE:CG2	2.82	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:GLN:O	1:A:810:ILE:HD13	2.13	0.48
1:A:1066:THR:O	1:A:1070:ILE:HG23	2.13	0.48
1:E:812:LEU:HD12	1:E:829:VAL:HG21	1.95	0.48
1:E:926:LEU:CD1	1:E:1019:THR:HG21	2.44	0.48
2:F:237:LEU:HB2	5:F:401:NAG:H82	1.95	0.48
1:I:310:LYS:CD	1:I:310:LYS:C	2.86	0.48
2:J:201:LYS:HA	2:J:274:ARG:HD2	1.95	0.48
1:M:912:ASN:HA	1:M:915:PHE:HE1	1.76	0.48
2:C:180:ASN:HD21	5:C:402:NAG:C1	2.26	0.48
1:E:865:LEU:HD11	1:E:928:GLN:HB3	1.96	0.48
1:E:880:LYS:C	1:E:880:LYS:HD3	2.38	0.48
1:I:143:VAL:HG13	1:I:263:TYR:CD1	2.45	0.48
1:M:108:TYR:O	1:M:112:LEU:HD13	2.14	0.48
1:A:401:GLY:HA3	1:A:864:HIS:N	2.28	0.48
1:I:162:LEU:HD21	1:I:260:VAL:HG23	1.96	0.48
1:I:700:LEU:HG	1:I:751:ILE:HA	1.95	0.48
1:I:718:LEU:HG	1:I:719:LEU:HD22	1.96	0.48
2:N:290:ARG:NH2	2:N:292:TRP:NE1	2.62	0.48
1:A:160:ILE:HG12	1:A:261:ALA:HB3	1.96	0.48
1:A:790:MET:SD	1:A:794:GLN:O	2.72	0.48
2:C:129:GLN:HG2	2:C:263:THR:HA	1.96	0.48
1:E:254:THR:HG21	1:E:257:ILE:HD11	1.96	0.48
1:E:321:GLU:N	1:E:322:PRO:HD2	2.29	0.48
1:E:840:GLN:OE1	1:E:840:GLN:N	2.47	0.48
1:E:991:GLY:O	1:E:994:THR:OG1	2.29	0.48
1:E:1011:LEU:HD12	1:E:1011:LEU:O	2.14	0.48
1:E:1043:ILE:O	1:E:1046:PRO:HD2	2.14	0.48
1:I:305:VAL:O	1:I:309:LEU:HD23	2.13	0.48
1:I:310:LYS:CB	1:I:897:PHE:CD1	2.91	0.48
1:M:310:LYS:HD3	1:M:897:PHE:HB2	1.96	0.48
1:A:157:CYS:SG	1:A:262:VAL:HG13	2.54	0.47
1:A:464:ARG:HH21	1:A:532:TYR:HH	1.60	0.47
1:A:834:LYS:CE	1:A:839:ARG:CZ	2.92	0.47
1:A:876:TYR:HE2	1:A:1011:LEU:HB2	1.78	0.47
1:A:1055:PHE:HB2	2:C:208:THR:HG21	1.96	0.47
1:E:290:ALA:O	1:E:293:ILE:HB	2.15	0.47
1:E:900:GLN:NE2	1:E:901:PRO:O	2.47	0.47
1:E:966:GLU:O	1:E:969:VAL:HG12	2.14	0.47
2:F:157:CYS:SG	2:F:171:CYS:HB2	2.54	0.47
1:I:187:HIS:HB3	1:I:242:GLU:O	2.14	0.47
1:M:284:VAL:HB	1:M:398:GLU:HG3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1030:LEU:O	1:M:1034:VAL:HG13	2.14	0.47
1:A:966:GLU:CG	1:A:1077:SER:HB3	2.44	0.47
1:E:753:GLY:N	1:E:788:CYS:O	2.47	0.47
2:F:231:THR:OG1	2:F:232:LYS:N	2.45	0.47
2:F:292:TRP:HH2	5:F:405:NAG:O5	1.85	0.47
1:M:622:LEU:O	1:M:622:LEU:HD23	2.15	0.47
1:M:749:LEU:HD12	1:M:751:ILE:HD11	1.96	0.47
1:A:382:ASP:HB3	1:A:386:ASN:ND2	2.30	0.47
1:A:572:ARG:HG2	1:A:640:MET:N	2.19	0.47
1:A:621:ALA:HB1	1:A:623:GLN:HE22	1.79	0.47
1:E:1063:SER:O	1:E:1066:THR:OG1	2.32	0.47
1:I:66:ARG:HA	1:I:289:ASN:HD21	1.79	0.47
1:I:426:ILE:HG12	1:I:427:ASP:H	1.79	0.47
1:M:598:VAL:HG22	1:M:644:GLY:O	2.14	0.47
1:M:660:ILE:HG23	1:M:664:HIS:CE1	2.50	0.47
1:A:384:GLU:C	1:A:386:ASN:H	2.20	0.47
1:A:497:ASP:N	1:A:497:ASP:OD1	2.47	0.47
2:C:142:GLN:OE1	2:C:149:ALA:O	2.32	0.47
1:E:240:GLY:H	1:E:241:PRO:HD3	1.79	0.47
1:E:464:ARG:HG2	1:E:547:MET:SD	2.55	0.47
1:E:908:LEU:O	1:E:912:ASN:HB2	2.14	0.47
1:I:961:PHE:O	1:I:965:PHE:HB2	2.14	0.47
1:M:593:TYR:CD1	1:M:649:GLU:HG2	2.50	0.47
1:A:480:VAL:CG2	1:I:486:SER:HA	2.45	0.47
1:A:671:TRP:CD2	1:A:785:VAL:HG22	2.50	0.47
1:A:750:ILE:HA	1:A:786:LEU:O	2.14	0.47
2:C:232:LYS:HB3	2:C:233:PRO:HD2	1.95	0.47
1:I:314:GLN:NE2	3:I:1201:P5S:N	2.62	0.47
1:M:233:GLU:HG2	1:M:242:GLU:H	1.80	0.47
1:M:475:LYS:H	1:M:475:LYS:HD3	1.79	0.47
1:M:873:LEU:HD13	1:M:924:SER:HB3	1.97	0.47
1:A:184:CYS:SG	1:A:185:LYS:N	2.87	0.47
1:A:1053:MET:HB2	1:A:1056:VAL:CG2	2.44	0.47
1:E:40:PHE:CZ	1:E:142:LYS:HA	2.50	0.47
1:E:323:TRP:HH2	2:F:300:PRO:O	1.96	0.47
1:I:71:TYR:O	1:I:74:ILE:HG22	2.13	0.47
2:J:292:TRP:CE2	5:J:404:NAG:O6	2.67	0.47
1:M:31:GLU:OE2	1:M:224:ARG:NH2	2.47	0.47
1:M:674:THR:O	1:M:788:CYS:HA	2.14	0.47
1:A:211:CYS:SG	1:A:212:GLU:N	2.87	0.47
1:A:756:LEU:CD1	1:A:790:MET:HE3	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:GLN:HG2	2:C:132:ARG:NH2	2.29	0.47
1:A:966:GLU:HG2	1:A:1077:SER:HB3	1.96	0.47
2:C:301:VAL:HG12	2:C:304:PHE:HZ	1.80	0.47
1:E:410:LYS:HG3	1:E:684:THR:HG21	1.96	0.47
1:E:464:ARG:C	1:E:464:ARG:HD3	2.39	0.47
1:E:717:GLU:OE2	1:E:774:ILE:CG2	2.58	0.47
1:I:307:THR:CG2	1:I:310:LYS:HE3	2.45	0.47
1:I:410:LYS:HE2	1:I:684:THR:HG21	1.97	0.47
1:I:797:GLN:HG2	1:I:801:MET:HE2	1.96	0.47
2:J:301:VAL:HG21	2:J:308:LYS:HD3	1.96	0.47
1:M:532:TYR:CE1	1:M:551:VAL:HG22	2.50	0.47
1:M:634:ASP:HA	1:M:637:GLU:HG2	1.96	0.47
1:A:384:GLU:C	1:A:386:ASN:N	2.71	0.47
2:C:322:ASN:OD1	2:C:324:PHE:HB3	2.15	0.47
1:E:397:ASN:HB3	1:E:866:TYR:CD2	2.49	0.47
1:E:750:ILE:HD12	1:E:786:LEU:HD13	1.97	0.47
1:E:915:PHE:CZ	1:E:1008:THR:HG21	2.48	0.47
2:F:63:PRO:HA	2:F:66:ILE:HG22	1.95	0.47
1:M:891:TYR:CD1	1:M:902:LEU:HD23	2.50	0.47
2:N:54:PHE:CD1	2:N:336:SER:HB2	2.49	0.47
1:I:730:PHE:N	1:I:731:PRO:HD2	2.29	0.47
1:M:744:HIS:O	1:M:745:GLN:HG2	2.15	0.47
1:M:918:LEU:HB2	1:M:919:PRO:HD3	1.96	0.47
1:A:354:ILE:CG1	1:A:885:ILE:HG21	2.45	0.47
1:A:382:ASP:OD1	1:A:851:LYS:HE2	2.15	0.47
2:C:232:LYS:HE3	2:C:233:PRO:HD2	1.95	0.47
1:E:98:VAL:O	1:E:102:THR:OG1	2.23	0.47
1:E:159:LEU:HD13	1:E:264:THR:OG1	2.15	0.47
2:F:120:MET:HE2	2:F:312:LEU:HD11	1.97	0.47
1:I:284:VAL:HG11	1:I:870:ILE:HD13	1.96	0.47
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.84	0.46
1:A:519:TYR:CE2	1:A:532:TYR:HB2	2.26	0.46
1:A:519:TYR:CG	1:A:533:GLU:N	2.75	0.46
1:A:574:GLN:NE2	1:A:574:GLN:N	2.63	0.46
1:E:339:LYS:HD3	1:E:340:MET:N	2.30	0.46
1:I:949:ALA:HA	1:I:952:GLN:HG2	1.97	0.46
1:M:387:GLU:N	1:M:387:GLU:OE1	2.48	0.46
1:A:386:ASN:OD1	1:A:386:ASN:N	2.47	0.46
1:A:514:GLY:C	1:A:515:ASN:CG	2.82	0.46
1:A:953:LEU:HD23	1:A:953:LEU:H	1.80	0.46
5:F:405:NAG:C1	5:F:405:NAG:C8	2.93	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:241:PRO:HG3	1:M:246:LEU:HD13	1.96	0.46
2:N:290:ARG:CZ	2:N:292:TRP:CE2	2.97	0.46
1:A:570:PHE:H	1:A:571:PRO:HD3	1.69	0.46
1:E:196:LEU:HD11	1:E:199:ALA:HB2	1.97	0.46
1:E:234:ALA:O	1:E:241:PRO:HA	2.15	0.46
1:E:407:PHE:HB3	1:E:673:LEU:HD12	1.96	0.46
1:E:776:LEU:HD11	1:E:801:MET:SD	2.56	0.46
1:E:1050:GLN:CD	1:E:1052:ARG:HD3	2.40	0.46
1:M:435:THR:N	1:M:440:GLY:HA3	2.29	0.46
1:M:668:LEU:HD21	1:M:943:MET:HG2	1.98	0.46
2:N:326:GLY:O	2:N:330:ILE:HG12	2.15	0.46
1:A:671:TRP:CG	1:A:785:VAL:HG22	2.51	0.46
1:M:801:MET:HE2	1:M:801:MET:HA	1.98	0.46
1:E:200:GLU:HG3	1:E:200:GLU:O	2.14	0.46
1:E:405:TYR:CE1	1:E:669:LYS:HB2	2.49	0.46
1:E:695:THR:HG1	1:E:747:TYR:HD2	1.57	0.46
1:E:893:PHE:HA	1:E:897:PHE:CE1	2.50	0.46
1:M:515:ASN:C	1:M:515:ASN:HD22	2.24	0.46
2:N:129:GLN:HB3	2:N:265:ALA:HA	1.97	0.46
1:A:177:SER:CA	1:A:837:GLU:CG	2.93	0.46
1:A:275:GLN:HE21	1:A:826:GLU:HB2	1.81	0.46
1:A:294:VAL:O	1:A:298:ILE:HG12	2.16	0.46
1:A:692:GLN:HG3	1:A:693:THR:H	1.80	0.46
1:A:888:GLN:HE21	1:A:901:PRO:HA	1.80	0.46
1:A:1070:ILE:HG13	1:A:1071:ILE:N	2.29	0.46
1:E:270:MET:O	1:E:273:ASN:HB2	2.16	0.46
1:I:188:TYR:CG	1:I:189:ALA:N	2.84	0.46
2:J:240:VAL:HG22	2:J:251:GLY:HA2	1.98	0.46
1:M:700:LEU:HD13	1:M:751:ILE:HG13	1.98	0.46
2:N:46:THR:H	2:N:49:THR:HG22	1.81	0.46
1:A:247:LYS:HG2	1:A:268:THR:HG21	1.97	0.46
1:A:267:GLU:CD	1:A:267:GLU:C	2.84	0.46
1:A:519:TYR:O	1:A:532:TYR:HB2	2.15	0.46
1:E:406:VAL:HG23	1:E:812:LEU:HD23	1.96	0.46
1:E:588:ASN:OD1	1:E:589:ALA:N	2.48	0.46
1:I:158:ASP:HA	1:I:246:LEU:HA	1.96	0.46
1:I:159:LEU:CD2	1:I:262:VAL:HG21	2.46	0.46
1:I:956:PHE:HA	1:I:959:TRP:NE1	2.31	0.46
2:J:104:CYS:SG	2:J:105:THR:N	2.89	0.46
2:J:130:ASN:HB3	2:J:265:ALA:HA	1.97	0.46
1:M:966:GLU:HA	1:M:969:VAL:HG12	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1069:ALA:O	1:A:1073:LEU:HD23	2.15	0.46
1:E:751:ILE:O	1:E:787:CYS:HA	2.15	0.46
2:F:107:ASN:OD1	5:F:405:NAG:C1	2.64	0.46
1:I:315:SER:CA	1:I:319:ASN:HB3	2.44	0.46
1:I:723:ARG:H	1:I:723:ARG:CD	2.26	0.46
1:I:906:ALA:O	1:I:910:MET:CB	2.64	0.46
1:M:163:SER:HA	1:M:194:ILE:HG21	1.97	0.46
1:M:173:VAL:HG23	1:M:250:THR:C	2.41	0.46
1:M:238:SER:O	1:M:240:GLY:N	2.46	0.46
1:M:272:LEU:N	1:M:272:LEU:HD12	2.31	0.46
1:M:750:ILE:HB	1:M:786:LEU:HD13	1.97	0.46
1:A:176:ALA:C	1:A:837:GLU:HG2	2.41	0.46
1:A:382:ASP:OD1	1:A:851:LYS:CE	2.64	0.46
1:A:521:ARG:HB2	1:A:529:ILE:CD1	2.44	0.46
1:A:939:PRO:HA	1:A:942:TYR:HB3	1.97	0.46
2:F:294:ASN:ND2	5:F:404:NAG:H2	2.30	0.46
1:M:68:ALA:HB3	1:M:360:TYR:CE2	2.51	0.46
1:M:767:SER:OG	1:M:768:SER:N	2.49	0.46
1:E:185:LYS:HE2	1:E:245:LEU:CD2	2.46	0.46
1:E:191:ARG:H	1:E:194:ILE:HB	1.81	0.46
1:E:832:GLY:O	1:E:848:SER:HA	2.16	0.46
2:F:77:GLU:HB3	2:F:313:SER:HB2	1.96	0.46
1:I:307:THR:HG23	1:I:310:LYS:NZ	2.30	0.46
1:I:314:GLN:C	1:I:319:ASN:CB	2.66	0.46
1:I:537:THR:HA	1:I:549:VAL:HG11	1.98	0.46
1:M:415:THR:OG1	1:M:416:GLU:N	2.49	0.46
2:N:290:ARG:CZ	2:N:292:TRP:HE1	2.28	0.46
2:C:54:PHE:CE2	2:C:339:LEU:HD23	2.51	0.45
2:F:170:PRO:HB2	2:F:175:ALA:CB	2.46	0.45
1:I:159:LEU:HD21	1:I:258:TYR:C	2.40	0.45
1:I:820:ASP:N	1:I:820:ASP:OD1	2.49	0.45
1:I:1015:THR:HG21	1:I:1018:TRP:CE2	2.52	0.45
2:N:292:TRP:CH2	5:N:405:NAG:C4	2.81	0.45
2:N:340:GLY:HA2	2:N:343:LEU:HD12	1.98	0.45
1:A:198:THR:HG22	1:A:204:THR:OG1	2.16	0.45
1:A:376:TRP:HB2	2:C:34:LYS:HE2	1.99	0.45
1:A:1045:TRP:HB2	1:A:1046:PRO:HD3	1.98	0.45
2:C:46:THR:OG1	2:C:47:ALA:N	2.49	0.45
1:E:40:PHE:CE2	1:E:42:ASP:HA	2.51	0.45
1:E:240:GLY:N	1:E:241:PRO:CD	2.79	0.45
1:E:398:GLU:O	1:E:399:GLU:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:457:ASN:HA	1:I:460:GLU:HB3	1.99	0.45
1:I:940:ARG:HG3	1:I:941:LEU:N	2.29	0.45
1:M:873:LEU:HD22	1:M:924:SER:HB2	1.99	0.45
1:A:366:GLN:HG2	1:A:870:ILE:HG22	1.97	0.45
1:A:861:ALA:O	1:A:865:LEU:HG	2.17	0.45
2:C:66:ILE:HB	2:C:330:ILE:HD11	1.98	0.45
1:E:1015:THR:HG21	1:E:1018:TRP:CZ2	2.52	0.45
1:I:723:ARG:HD2	1:I:723:ARG:N	2.30	0.45
1:I:886:LEU:HD12	1:I:886:LEU:HA	1.74	0.45
1:M:47:SER:HB3	1:M:843:ARG:CZ	2.36	0.45
1:E:246:LEU:HD22	1:E:268:THR:HB	1.98	0.45
1:E:640:MET:CG	1:E:641:ASN:H	2.30	0.45
1:E:787:CYS:SG	1:E:790:MET:HE3	2.57	0.45
1:E:907:TYR:OH	1:E:1033:TYR:HE1	1.99	0.45
2:F:181:ASP:OD1	2:F:181:ASP:N	2.49	0.45
1:I:159:LEU:HG	1:I:160:ILE:N	2.32	0.45
2:J:46:THR:OG1	2:J:47:ALA:N	2.49	0.45
1:M:751:ILE:HG22	1:M:752:ASP:H	1.80	0.45
1:A:173:VAL:CG1	1:A:249:ALA:HB1	2.47	0.45
1:A:176:ALA:C	1:A:837:GLU:CD	2.84	0.45
1:A:384:GLU:HB2	1:A:386:ASN:ND2	2.32	0.45
1:A:412:GLY:O	1:A:836:LYS:HE3	2.16	0.45
1:A:653:GLN:NE2	1:A:836:LYS:CE	2.71	0.45
1:A:724:LYS:HD2	1:A:724:LYS:N	2.31	0.45
2:C:79:GLU:HB3	2:C:311:ILE:HG23	1.97	0.45
1:E:174:THR:OG1	1:E:181:GLU:O	2.34	0.45
2:F:152:ASN:O	2:F:152:ASN:ND2	2.49	0.45
1:I:179:ASP:OD1	1:I:179:ASP:N	2.50	0.45
1:M:732:LYS:HD3	1:M:733:SER:N	2.31	0.45
1:A:524:ASN:CA	1:A:530:GLU:OE1	2.65	0.45
1:A:574:GLN:CG	1:A:642:LEU:HB2	2.42	0.45
1:A:719:LEU:HD11	1:A:720:ILE:HD12	1.98	0.45
1:A:1012:ALA:O	1:A:1015:THR:HG22	2.16	0.45
1:I:544:ARG:NH1	1:I:545:ARG:O	2.50	0.45
1:M:671:TRP:CH2	1:M:779:CYS:HB3	2.51	0.45
2:N:214:PHE:CD2	2:N:258:ILE:HD12	2.52	0.45
1:A:29:VAL:CG1	1:A:211:CYS:CB	2.95	0.45
1:A:529:ILE:CG1	1:A:531:GLU:HG2	2.45	0.45
2:C:188:ILE:HD11	2:C:292:TRP:CD1	2.52	0.45
1:I:159:LEU:CG	1:I:160:ILE:N	2.80	0.45
1:M:701:THR:HG21	1:M:752:ASP:HB3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ASP:HB3	1:A:429:HIS:ND1	2.32	0.45
1:E:220:LYS:HA	1:E:234:ALA:HA	1.99	0.45
1:E:245:LEU:HD22	1:E:245:LEU:N	2.31	0.45
1:E:702:THR:HG23	1:E:703:LYS:HG2	1.99	0.45
1:E:822:SER:HB2	1:E:823:MET:HE2	1.99	0.45
1:I:319:ASN:C	1:I:322:PRO:HD2	2.41	0.45
1:I:457:ASN:HB2	1:I:461:LEU:HG	1.99	0.45
1:M:426:ILE:H	1:M:430:LYS:HB3	1.82	0.45
1:M:832:GLY:N	1:M:847:TYR:O	2.50	0.45
1:A:235:VAL:HA	1:A:241:PRO:HD3	1.99	0.45
1:A:512:PHE:CE1	1:A:520:MET:HB3	2.52	0.45
1:A:707:GLU:HB2	1:A:710:ARG:HB2	1.99	0.45
1:A:926:LEU:HD13	1:A:1019:THR:HG21	1.98	0.45
1:A:1072:LEU:HB2	2:C:329:TYR:HE1	1.81	0.45
1:E:812:LEU:HA	1:E:829:VAL:CG1	2.46	0.45
1:I:931:ASN:HB2	1:I:934:THR:HG22	1.99	0.45
2:J:83:THR:HG21	2:J:307:ARG:HD2	1.98	0.45
1:A:218:LEU:HD13	1:A:267:GLU:HG3	1.99	0.45
1:A:415:THR:OG1	1:A:416:GLU:N	2.50	0.45
1:A:418:SER:C	1:A:651:LYS:HZ2	2.25	0.45
1:A:512:PHE:HE1	1:A:520:MET:HB3	1.82	0.45
1:A:521:ARG:CB	1:A:529:ILE:HD11	2.47	0.45
1:A:683:SER:OG	1:A:684:THR:N	2.50	0.45
2:C:63:PRO:HA	2:C:66:ILE:HG22	1.99	0.45
2:C:118:VAL:CG2	2:C:276:ILE:HB	2.47	0.45
1:E:717:GLU:OE1	1:E:717:GLU:HA	2.16	0.45
1:E:1000:PHE:O	1:E:1003:LEU:HG	2.17	0.45
1:M:903:TYR:CD1	1:M:1000:PHE:CE2	3.05	0.45
1:A:574:GLN:NE2	1:A:574:GLN:H	2.13	0.44
1:A:982:SER:OG	2:C:320:GLY:N	2.44	0.44
1:E:407:PHE:CE2	1:E:799:VAL:HG22	2.52	0.44
1:E:590:MET:HE3	1:E:693:THR:HG22	1.98	0.44
2:F:188:ILE:HG13	2:F:292:TRP:HD1	0.98	0.44
2:F:214:PHE:CD2	2:F:258:ILE:HD12	2.52	0.44
1:I:214:PRO:HG2	1:I:267:GLU:HB2	1.99	0.44
2:J:59:LEU:O	2:J:63:PRO:HG3	2.17	0.44
1:M:171:CYS:HB2	1:M:251:LEU:HD21	2.00	0.44
1:M:911:TYR:O	1:M:915:PHE:CD1	2.66	0.44
1:A:29:VAL:CG1	1:A:31:GLU:HG2	2.47	0.44
1:A:788:CYS:SG	1:A:789:ARG:N	2.90	0.44
1:A:1072:LEU:CD1	2:C:332:VAL:HG21	2.44	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:370:GLY:O	1:E:866:TYR:OH	2.27	0.44
1:I:40:PHE:HB3	1:I:143:VAL:HG21	1.99	0.44
1:I:552:LYS:HB3	1:I:558:ILE:HG23	1.98	0.44
1:I:700:LEU:CD1	1:I:750:ILE:O	2.66	0.44
1:M:254:THR:HG22	1:M:255:GLU:H	1.81	0.44
1:M:590:MET:HB3	1:M:693:THR:HA	2.00	0.44
2:N:290:ARG:NE	2:N:292:TRP:CZ2	2.84	0.44
1:A:685:CYS:HB3	1:A:691:PHE:CE1	2.52	0.44
1:A:697:LEU:HD22	1:A:747:TYR:CD2	2.53	0.44
1:A:714:ARG:O	1:A:717:GLU:HG2	2.17	0.44
1:A:949:ALA:O	1:A:955:PRO:HG3	2.18	0.44
1:E:40:PHE:O	1:E:41:CYS:HB3	2.17	0.44
1:I:50:TYR:HD1	1:I:58:LYS:HD3	1.83	0.44
1:I:159:LEU:CD2	1:I:262:VAL:CG2	2.92	0.44
1:M:426:ILE:O	1:M:427:ASP:C	2.60	0.44
1:A:516:ARG:HE	1:A:516:ARG:CA	2.29	0.44
1:E:120:VAL:HG12	1:E:120:VAL:O	2.16	0.44
1:E:209:ILE:HD12	1:E:224:ARG:O	2.17	0.44
1:E:856:LYS:O	1:E:860:LEU:HB2	2.18	0.44
2:F:140:ASP:OD1	2:F:140:ASP:N	2.41	0.44
1:I:672:VAL:C	1:I:673:LEU:HD23	2.43	0.44
1:E:217:ASP:O	1:E:218:LEU:HG	2.17	0.44
1:E:409:BFD:F3	1:E:411:THR:OG1	2.25	0.44
2:F:50:VAL:O	2:F:53:ILE:HB	2.17	0.44
1:I:321:GLU:CG	2:J:304:PHE:HB3	2.39	0.44
1:M:510:PHE:O	1:M:511:THR:HG23	2.18	0.44
1:A:410:LYS:HZ2	1:A:410:LYS:HB2	1.83	0.44
1:A:959:TRP:HZ3	1:A:963:ALA:HB2	1.79	0.44
1:A:1076:ILE:HD13	2:C:332:VAL:HG22	1.99	0.44
2:C:111:GLU:OE1	2:C:111:GLU:N	2.38	0.44
1:E:218:LEU:HD12	1:E:235:VAL:O	2.18	0.44
1:E:283:ALA:HB3	1:E:399:GLU:CG	2.48	0.44
1:E:521:ARG:HD2	1:E:531:GLU:N	2.32	0.44
1:E:732:LYS:NZ	1:E:739:LYS:HE2	1.98	0.44
1:E:988:LYS:HE3	2:F:206:TRP:HE3	1.83	0.44
1:E:1069:ALA:O	1:E:1073:LEU:HD23	2.18	0.44
2:F:107:ASN:CG	5:F:405:NAG:C1	2.91	0.44
2:F:130:ASN:HB3	2:F:265:ALA:HA	1.99	0.44
1:I:1071:ILE:HA	1:I:1074:ILE:HG12	1.99	0.44
1:M:716:HIS:NE2	1:M:774:ILE:O	2.51	0.44
2:N:91:CYS:HB2	2:N:106:ILE:HD11	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:ALA:O	1:A:661:GLU:HG2	2.18	0.44
1:A:686:TYR:HA	1:A:691:PHE:HB2	1.99	0.44
1:E:323:TRP:CH2	2:F:300:PRO:O	2.71	0.44
1:E:462:PHE:HE2	1:E:511:THR:HA	1.82	0.44
2:F:79:GLU:HB2	2:F:311:ILE:HG12	1.99	0.44
1:I:489:LEU:HD21	1:I:509:GLY:O	2.10	0.44
1:M:67:ILE:HG13	1:M:292:LEU:HD23	2.00	0.44
1:M:128:ILE:HG21	1:M:132:LYS:HB2	1.99	0.44
1:M:161:LEU:HA	1:M:161:LEU:HD23	1.76	0.44
1:M:821:VAL:HG13	1:M:822:SER:H	1.83	0.44
1:A:127:ILE:HD11	1:A:145:ASP:HB3	1.99	0.44
1:A:217:ASP:O	1:A:218:LEU:CB	2.66	0.44
2:C:143:LEU:HB3	2:C:214:PHE:CD1	2.53	0.44
1:E:46:VAL:O	1:E:117:ASP:OD2	2.36	0.44
2:F:63:PRO:O	2:F:66:ILE:HG22	2.18	0.44
1:I:143:VAL:HG13	1:I:263:TYR:CG	2.52	0.44
1:I:413:THR:HG21	1:I:815:GLY:HA2	2.00	0.44
1:I:599:ALA:HB1	1:I:640:MET:HE3	1.99	0.44
2:J:99:VAL:HG12	2:J:101:PRO:HD2	1.99	0.44
1:A:316:THR:OG1	1:A:317:PRO:CD	2.48	0.44
1:A:321:GLU:N	1:A:322:PRO:CD	2.80	0.44
1:A:379:ASP:OD2	2:C:35:GLN:NE2	2.50	0.44
1:A:754:SER:O	1:A:758:LEU:HD13	2.18	0.44
1:E:884:PHE:HZ	1:E:908:LEU:HD21	1.82	0.44
1:I:162:LEU:HB2	1:I:258:TYR:O	2.18	0.44
1:M:171:CYS:O	1:M:187:HIS:NE2	2.51	0.44
1:A:275:GLN:NE2	1:A:822:SER:C	2.75	0.43
1:A:489:LEU:HD12	1:A:491:TYR:CZ	2.53	0.43
2:F:157:CYS:HB3	2:F:172:GLY:HA2	1.99	0.43
2:F:186:PHE:HB3	2:F:194:PRO:HB2	1.99	0.43
1:I:1027:TRP:CE3	1:I:1030:LEU:HD21	2.53	0.43
1:M:475:LYS:H	1:M:475:LYS:CD	2.31	0.43
1:A:480:VAL:HG23	1:I:486:SER:CB	2.49	0.43
1:A:816:ASP:O	1:A:838:GLY:O	2.35	0.43
1:A:909:THR:O	1:A:913:ILE:HG23	2.18	0.43
2:C:241:TYR:C	2:C:250:ASN:HD21	2.26	0.43
1:E:346:SER:O	1:E:349:VAL:HG12	2.18	0.43
1:E:599:ALA:HB3	1:E:641:ASN:CB	2.48	0.43
1:I:192:ASP:OD1	1:I:193:THR:N	2.51	0.43
1:I:994:THR:HG22	1:I:1056:VAL:HG22	1.99	0.43
1:M:654:ASP:HB3	1:M:853:LYS:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1052:ARG:HE	1:M:1052:ARG:N	2.16	0.43
1:A:354:ILE:HG13	1:A:885:ILE:HD13	2.01	0.43
1:A:519:TYR:HD1	1:A:534:LEU:CB	2.31	0.43
1:A:792:PRO:C	1:A:823:MET:HE3	2.36	0.43
1:A:898:SER:C	2:C:132:ARG:HH22	2.25	0.43
1:A:910:MET:SD	1:A:911:TYR:N	2.91	0.43
2:C:51:LEU:HD11	2:C:344:LEU:HD12	1.99	0.43
1:E:348:MET:O	1:E:352:ASN:N	2.51	0.43
1:E:717:GLU:OE2	1:E:774:ILE:CB	2.67	0.43
1:I:73:LEU:O	1:I:77:LEU:HD13	2.18	0.43
1:I:260:VAL:HG12	1:I:260:VAL:O	2.18	0.43
1:I:335:LEU:CD1	1:I:338:LEU:HB2	2.44	0.43
2:J:100:THR:HB	2:J:101:PRO:HD3	2.00	0.43
1:M:147:VAL:HB	1:M:258:TYR:CG	2.54	0.43
1:M:272:LEU:HD12	1:M:272:LEU:H	1.83	0.43
1:M:295:TYR:C	1:M:355:ILE:HD11	2.43	0.43
1:M:526:ARG:NE	1:M:526:ARG:HA	2.33	0.43
1:A:173:VAL:HG22	1:A:251:LEU:HD12	2.01	0.43
1:A:673:LEU:HD12	1:A:795:LYS:HG3	1.99	0.43
1:A:816:ASP:OD2	1:A:837:GLU:HB3	2.16	0.43
2:C:143:LEU:HB3	2:C:214:PHE:CE1	2.53	0.43
2:C:258:ILE:HD13	2:C:258:ILE:HA	1.84	0.43
1:E:113:ARG:HD3	1:E:392:ASN:HB3	2.00	0.43
1:E:423:GLU:HB3	1:E:647:ALA:HB3	2.00	0.43
2:F:128:TYR:CD1	2:F:267:PRO:HB3	2.53	0.43
1:I:929:HIS:HB2	1:I:1016:ARG:HE	1.84	0.43
1:M:322:PRO:HB2	1:M:324:TYR:CE2	2.53	0.43
1:M:371:SER:HB2	1:M:391:VAL:HG22	1.99	0.43
1:M:999:VAL:O	1:M:1003:LEU:HB2	2.17	0.43
2:N:206:TRP:CG	2:N:207:TRP:H	2.36	0.43
1:A:233:GLU:OE2	1:A:243:ASN:N	2.51	0.43
1:A:311:TYR:CA	1:A:315:SER:HB2	2.45	0.43
1:A:353:PHE:CZ	1:A:909:THR:HG22	2.54	0.43
1:A:932:ILE:HD12	1:A:933:ASP:N	2.33	0.43
2:C:281:ASP:N	2:C:281:ASP:OD1	2.51	0.43
1:E:984:GLU:OE2	1:E:1062:SER:OG	2.36	0.43
1:I:233:GLU:HB2	1:I:243:ASN:HB3	1.99	0.43
1:M:493:SER:HB3	1:M:498:GLU:OE2	2.19	0.43
1:M:581:THR:O	1:M:585:VAL:HG23	2.18	0.43
1:M:752:ASP:OD2	1:M:754:SER:OG	2.34	0.43
1:A:218:LEU:HD22	1:A:267:GLU:CG	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LEU:CD2	1:A:520:MET:HB2	2.48	0.43
1:A:572:ARG:HG3	1:A:574:GLN:HE22	1.83	0.43
1:A:1009:LEU:O	1:A:1013:LEU:HG	2.18	0.43
2:C:141:SER:HB2	2:C:149:ALA:HB2	2.00	0.43
1:E:233:GLU:OE1	1:E:243:ASN:CA	2.66	0.43
1:E:421:PHE:HB3	1:E:648:VAL:HA	2.01	0.43
1:I:173:VAL:HG21	1:I:249:ALA:HB1	2.00	0.43
1:I:311:TYR:CD1	1:I:339:LYS:HG2	2.53	0.43
1:I:791:ALA:HB3	1:I:794:GLN:HE22	1.83	0.43
1:I:865:LEU:HD22	1:I:869:ARG:HH12	1.82	0.43
1:M:284:VAL:HG21	1:M:398:GLU:HB2	2.01	0.43
1:M:462:PHE:HZ	1:M:521:ARG:HE	1.65	0.43
1:A:56:LEU:HB2	1:A:57:PRO:HD3	2.01	0.43
1:A:359:MET:HA	1:A:877:PHE:CE2	2.54	0.43
1:A:719:LEU:HD22	1:A:778:ILE:HB	2.01	0.43
1:E:94:PRO:HB3	3:E:1202:P5S:HB	2.00	0.43
1:E:560:LEU:HG	1:E:561:PHE:N	2.34	0.43
1:E:695:THR:OG1	1:E:747:TYR:CD2	2.66	0.43
2:F:54:PHE:HB3	2:F:336:SER:O	2.18	0.43
2:F:129:GLN:HG3	2:F:134:TYR:CE1	2.54	0.43
1:I:678:MET:CE	1:I:700:LEU:CG	2.91	0.43
1:I:748:GLY:HA2	1:I:784:ALA:O	2.18	0.43
2:J:66:ILE:HB	2:J:330:ILE:HD11	2.01	0.43
1:M:750:ILE:HA	1:M:786:LEU:O	2.19	0.43
1:A:1072:LEU:HB2	2:C:329:TYR:CE1	2.53	0.43
2:C:341:VAL:O	2:C:345:VAL:HG23	2.19	0.43
1:E:183:ASN:ND2	1:E:183:ASN:H	2.15	0.43
1:E:474:ILE:HG12	1:E:475:LYS:H	1.84	0.43
1:E:500:ALA:HB2	1:E:594:ARG:NH2	2.34	0.43
1:E:721:GLU:O	1:E:725:LYS:N	2.50	0.43
1:M:47:SER:OG	1:M:843:ARG:NH1	2.47	0.43
1:M:158:ASP:O	1:M:159:LEU:HD13	2.18	0.43
1:M:272:LEU:HD11	1:M:818:ALA:O	2.19	0.43
1:A:528:GLU:HA	1:A:528:GLU:OE2	2.19	0.43
1:A:1042:GLY:HA2	1:A:1045:TRP:CZ2	2.54	0.43
1:E:356:PRO:O	1:E:359:MET:HG2	2.19	0.43
1:E:694:ASN:HB2	1:E:745:GLN:CB	2.49	0.43
1:E:831:ILE:HD13	1:E:847:TYR:HB2	2.00	0.43
1:I:888:GLN:HE22	1:I:901:PRO:CB	2.31	0.43
2:J:80:ILE:HD12	2:J:80:ILE:O	2.19	0.43
2:J:135:VAL:HG22	2:J:263:THR:HG21	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:143:VAL:HA	1:M:262:VAL:HB	2.01	0.43
1:M:750:ILE:HD12	1:M:786:LEU:HD22	2.01	0.43
2:N:290:ARG:CZ	2:N:292:TRP:NE1	2.82	0.43
1:A:218:LEU:CD2	1:A:246:LEU:HD23	2.49	0.43
1:A:723:ARG:NH2	1:A:781:LYS:O	2.52	0.43
2:C:121:TYR:CE1	2:C:272:LEU:HD12	2.54	0.43
1:E:127:ILE:HG12	1:E:146:VAL:O	2.19	0.43
1:I:93:LEU:HB3	1:I:94:PRO:HD3	2.01	0.43
1:I:590:MET:O	1:I:689:ARG:NH2	2.52	0.43
1:I:756:LEU:O	1:I:759:ILE:HG22	2.19	0.43
1:M:237:ARG:HD2	1:M:675:GLY:O	2.18	0.43
1:A:77:LEU:O	1:A:80:VAL:HG22	2.18	0.42
1:A:128:ILE:HG12	1:A:199:ALA:HB2	2.00	0.42
1:A:146:VAL:HA	1:A:259:GLY:O	2.18	0.42
1:A:360:TYR:O	1:A:363:VAL:HG12	2.19	0.42
1:A:519:TYR:CD2	1:A:519:TYR:O	2.72	0.42
1:A:633:PHE:HA	1:A:636:ILE:HD12	2.00	0.42
1:A:656:ALA:CB	1:A:688:CYS:SG	3.07	0.42
1:E:735:ARG:HG3	1:E:735:ARG:O	2.19	0.42
1:E:1009:LEU:HD13	1:E:1013:LEU:HD23	2.01	0.42
2:F:262:ARG:O	2:F:271:LYS:NZ	2.51	0.42
1:I:318:TYR:O	1:I:319:ASN:C	2.59	0.42
2:J:157:CYS:HB3	2:J:172:GLY:HA2	2.00	0.42
1:M:167:THR:HG21	1:M:474:ILE:HD13	2.01	0.42
1:M:1081:GLU:O	1:M:1085:ILE:HG12	2.19	0.42
1:A:98:VAL:HG22	1:A:361:VAL:HG13	2.01	0.42
1:A:417:ASN:HD22	1:A:417:ASN:C	2.27	0.42
1:E:829:VAL:HG13	1:E:830:GLY:N	2.34	0.42
1:I:195:ALA:O	1:I:196:LEU:HB2	2.19	0.42
1:I:880:LYS:NZ	1:I:1003:LEU:HD21	2.33	0.42
2:J:258:ILE:HD13	2:J:258:ILE:HA	1.91	0.42
1:M:149:VAL:HB	1:M:258:TYR:CE2	2.54	0.42
1:A:177:SER:CA	1:A:837:GLU:HG2	2.48	0.42
1:A:474:ILE:HG22	1:A:491:TYR:HB3	2.00	0.42
2:C:301:VAL:HG21	2:C:308:LYS:HD3	2.01	0.42
1:M:205:LEU:HD23	1:M:205:LEU:HA	1.87	0.42
1:M:284:VAL:O	1:M:288:ILE:HG12	2.19	0.42
1:M:860:LEU:HD11	1:M:942:TYR:CE2	2.54	0.42
1:E:958:TYR:OH	1:E:1084:LEU:HD22	2.18	0.42
1:I:273:ASN:HA	1:I:822:SER:CB	2.50	0.42
1:I:492:ILE:O	1:I:492:ILE:HG13	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:572:ARG:HG2	1:I:640:MET:HG3	2.01	0.42
1:M:700:LEU:HD22	1:M:751:ILE:HG12	2.02	0.42
1:A:29:VAL:CG2	1:A:31:GLU:HG2	2.49	0.42
1:A:321:GLU:HG2	1:A:322:PRO:HD3	2.01	0.42
1:E:374:ILE:HD11	1:E:391:VAL:CG1	2.49	0.42
1:E:621:ALA:HB3	1:E:623:GLN:HE21	1.85	0.42
1:E:921:LEU:HD23	1:E:921:LEU:HA	1.94	0.42
1:I:170:THR:HG1	1:I:473:GLU:CD	2.23	0.42
1:I:885:ILE:O	1:I:886:LEU:C	2.61	0.42
1:M:921:LEU:HD22	1:M:925:LEU:HD11	2.01	0.42
1:M:950:MET:HA	1:M:950:MET:HE3	2.02	0.42
2:N:46:THR:OG1	2:N:47:ALA:N	2.52	0.42
1:E:159:LEU:HD21	1:E:261:ALA:O	2.20	0.42
1:E:1015:THR:HG21	1:E:1018:TRP:CE2	2.54	0.42
2:F:310:MET:HG2	2:F:311:ILE:N	2.34	0.42
1:M:592:GLY:CA	1:M:686:TYR:HB2	2.50	0.42
1:A:194:ILE:O	1:A:198:THR:HG23	2.19	0.42
1:A:512:PHE:CE1	1:A:520:MET:CB	3.02	0.42
1:E:127:ILE:CD1	1:E:128:ILE:H	2.24	0.42
1:E:291:PHE:CE2	1:E:959:TRP:HZ3	2.38	0.42
1:E:988:LYS:HE3	2:F:206:TRP:CE3	2.55	0.42
1:I:659:THR:O	1:I:663:LEU:HD13	2.20	0.42
1:I:843:ARG:H	1:I:843:ARG:HG3	1.68	0.42
1:M:812:LEU:HD23	1:M:813:SER:N	2.34	0.42
1:M:907:TYR:O	1:M:911:TYR:HB3	2.19	0.42
1:M:1052:ARG:O	1:M:1053:MET:C	2.61	0.42
1:A:790:MET:SD	1:A:794:GLN:CA	3.07	0.42
1:A:792:PRO:C	1:A:823:MET:CE	2.80	0.42
1:A:1068:LEU:O	2:C:329:TYR:OH	2.34	0.42
2:C:81:ASP:HA	2:C:309:ARG:HB3	2.02	0.42
1:I:273:ASN:HA	1:I:822:SER:HB3	2.02	0.42
1:I:880:LYS:HE3	1:I:911:TYR:CE2	2.54	0.42
1:I:1005:PHE:HE1	1:I:1030:LEU:HD13	1.84	0.42
1:M:194:ILE:O	1:M:196:LEU:N	2.51	0.42
1:M:818:ALA:HB2	1:M:840:GLN:HE21	1.84	0.42
1:A:514:GLY:O	1:A:515:ASN:CB	2.68	0.42
1:A:964:ALA:O	1:A:965:PHE:C	2.62	0.42
1:E:663:LEU:HD11	1:E:668:LEU:HD11	2.02	0.42
1:I:485:GLU:CG	1:I:488:GLU:HB2	2.49	0.42
1:I:703:LYS:CD	1:I:714:ARG:HD3	2.50	0.42
1:M:406:VAL:HG23	1:M:812:LEU:HD22	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:992:ASN:HB2	2:N:265:ALA:CB	2.49	0.42
1:A:66:ARG:NE	1:A:285:GLU:OE1	2.39	0.42
1:A:218:LEU:HB2	1:A:267:GLU:CD	2.45	0.42
1:A:237:ARG:NH1	1:A:676:ASP:O	2.53	0.42
1:A:350:LEU:HD11	1:A:888:GLN:HE22	1.84	0.42
1:A:485:GLU:OE1	1:A:485:GLU:N	2.53	0.42
1:A:959:TRP:CD2	1:A:959:TRP:C	2.98	0.42
2:C:100:THR:HB	2:C:101:PRO:HD3	2.01	0.42
1:E:272:LEU:HA	1:E:822:SER:HB3	2.02	0.42
1:I:321:GLU:HG2	2:J:304:PHE:HB3	2.02	0.42
1:I:588:ASN:HB2	1:I:593:TYR:CD1	2.55	0.42
1:M:310:LYS:HE2	3:M:1201:P5S:HN	1.85	0.42
1:M:748:GLY:CA	1:M:782:CYS:HB2	2.50	0.42
1:A:29:VAL:H	1:A:211:CYS:N	2.00	0.41
1:A:585:VAL:HG13	1:A:595:THR:HG21	2.02	0.41
2:C:185:LEU:HD11	2:C:312:LEU:CD2	2.49	0.41
1:E:66:ARG:NH2	1:E:285:GLU:OE1	2.51	0.41
1:E:87:SER:HB3	1:E:90:THR:HB	2.02	0.41
1:E:149:VAL:HG22	1:E:251:LEU:HD13	2.02	0.41
1:E:160:ILE:HD13	1:E:160:ILE:HA	1.97	0.41
1:E:187:HIS:HA	1:E:242:GLU:O	2.20	0.41
1:E:1019:THR:HG23	1:E:1022:ASN:H	1.84	0.41
1:I:295:TYR:O	1:I:298:ILE:HB	2.19	0.41
1:I:399:GLU:O	1:I:399:GLU:HG2	2.19	0.41
1:M:178:LEU:HD22	1:M:246:LEU:HD23	2.02	0.41
1:A:168:ASP:HB2	1:A:170:THR:HG22	2.02	0.41
1:A:724:LYS:O	1:A:728:HIS:ND1	2.53	0.41
1:A:974:THR:O	1:A:977:LEU:HG	2.20	0.41
1:E:413:THR:CG2	1:E:833:ILE:HG21	2.49	0.41
1:E:856:LYS:O	1:E:860:LEU:CB	2.68	0.41
1:E:902:LEU:O	1:E:996:GLY:HA3	2.21	0.41
2:F:299:TYR:O	2:F:301:VAL:HG22	2.21	0.41
1:I:468:LEU:HD12	1:I:469:CYS:SG	2.60	0.41
2:J:120:MET:HB2	2:J:312:LEU:HD12	2.02	0.41
2:J:233:PRO:HB2	2:J:236:TRP:HB2	2.02	0.41
1:M:29:VAL:HB	1:M:40:PHE:HZ	1.85	0.41
1:M:966:GLU:HB3	1:M:970:PHE:CE2	2.56	0.41
1:A:673:LEU:CD2	1:A:787:CYS:HB2	2.43	0.41
1:A:960:THR:O	1:A:963:ALA:N	2.53	0.41
1:E:771:TYR:HA	1:E:774:ILE:HD11	2.02	0.41
1:E:883:CYS:SG	1:E:966:GLU:HB2	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:209:ASP:O	2:F:214:PHE:HD2	2.03	0.41
1:I:149:VAL:HG11	1:I:155:PHE:CZ	2.55	0.41
1:I:159:LEU:HA	1:I:262:VAL:HG22	1.95	0.41
1:I:873:LEU:CD1	1:I:920:ILE:HG21	2.50	0.41
1:M:912:ASN:O	1:M:916:THR:OG1	2.37	0.41
1:A:516:ARG:NE	1:A:516:ARG:CA	2.83	0.41
1:E:339:LYS:HZ1	1:E:343:ASP:CB	2.31	0.41
1:E:346:SER:HB3	1:E:899:GLN:HG2	2.01	0.41
1:E:1036:PHE:CD1	1:E:1036:PHE:C	2.99	0.41
1:E:1086:VAL:HG21	2:F:50:VAL:HG21	2.01	0.41
2:F:46:THR:OG1	2:F:47:ALA:N	2.54	0.41
1:I:820:ASP:O	1:I:824:ILE:HG12	2.20	0.41
1:I:939:PRO:HA	1:I:942:TYR:CD1	2.55	0.41
1:M:147:VAL:HG12	1:M:258:TYR:CE2	2.55	0.41
1:M:147:VAL:CG1	1:M:258:TYR:CE2	3.03	0.41
1:M:821:VAL:HG13	1:M:822:SER:N	2.36	0.41
1:M:950:MET:HG3	1:M:950:MET:O	2.21	0.41
2:N:51:LEU:HD13	2:N:344:LEU:HB2	2.02	0.41
1:A:466:LEU:HD21	1:A:501:LEU:HB3	2.01	0.41
1:A:895:CYS:C	1:A:897:PHE:H	2.28	0.41
2:C:273:TYR:CD2	2:C:274:ARG:HG2	2.55	0.41
1:E:185:LYS:HD2	1:E:241:PRO:CB	2.44	0.41
1:E:907:TYR:OH	1:E:1033:TYR:CE1	2.73	0.41
2:F:193:TYR:HD1	2:F:194:PRO:HD2	1.86	0.41
1:I:253:ASN:O	1:I:474:ILE:HD11	2.21	0.41
1:M:294:VAL:HG21	1:M:959:TRP:CH2	2.55	0.41
1:M:593:TYR:CE1	1:M:649:GLU:HG2	2.56	0.41
1:M:975:TYR:HA	1:M:978:PHE:HB2	2.03	0.41
1:A:339:LYS:O	1:A:342:THR:HG22	2.19	0.41
1:A:458:ARG:NH1	1:A:458:ARG:HB3	2.36	0.41
1:A:1071:ILE:HG13	1:A:1072:LEU:N	2.36	0.41
2:C:63:PRO:O	2:C:66:ILE:HG22	2.20	0.41
2:C:107:ASN:HD22	2:C:290:ARG:HH21	1.68	0.41
2:C:198:ALA:O	2:C:276:ILE:HG23	2.20	0.41
2:C:331:ALA:O	2:C:332:VAL:C	2.64	0.41
1:E:865:LEU:HD12	1:E:869:ARG:NH2	2.35	0.41
1:I:862:HIS:HA	1:I:865:LEU:HD12	2.02	0.41
1:M:116:ALA:O	1:M:120:VAL:HG23	2.21	0.41
1:M:756:LEU:HD13	1:M:790:MET:HE1	2.03	0.41
1:M:819:ASN:HB3	7:M:1302:HOH:O	2.20	0.41
1:M:1055:PHE:CE1	2:N:213:LYS:HE2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ARG:HH11	1:A:675:GLY:HA2	1.85	0.41
1:A:488:GLU:OE1	1:A:488:GLU:HA	2.21	0.41
1:A:983:LEU:HB2	1:A:990:TYR:HE2	1.85	0.41
1:E:327:LYS:CG	1:E:331:GLU:H	2.34	0.41
1:E:673:LEU:CD1	1:E:795:LYS:HE2	2.51	0.41
1:E:700:LEU:O	1:E:701:THR:HG22	2.20	0.41
1:I:332:ARG:O	1:I:335:LEU:HG	2.21	0.41
1:I:521:ARG:HD2	1:I:531:GLU:HG3	2.02	0.41
2:J:32:ALA:HB1	2:J:38:LEU:HA	2.03	0.41
2:J:79:GLU:HB3	2:J:311:ILE:HG12	2.03	0.41
1:M:179:ASP:O	1:M:180:GLY:C	2.64	0.41
1:A:173:VAL:HG11	1:A:249:ALA:HB1	2.03	0.41
2:C:45:LEU:HA	2:C:49:THR:HG21	2.02	0.41
2:C:84:GLY:C	2:C:86:GLU:H	2.29	0.41
1:E:818:ALA:O	1:E:821:VAL:HG12	2.21	0.41
2:F:90:PRO:HG2	2:F:105:THR:O	2.20	0.41
2:F:120:MET:SD	2:F:183:LEU:HD13	2.61	0.41
1:I:321:GLU:N	1:I:322:PRO:HD2	2.35	0.41
1:M:183:ASN:OD1	1:M:239:LEU:HB3	2.20	0.41
1:M:694:ASN:C	1:M:694:ASN:HD22	2.28	0.41
1:A:29:VAL:HG13	1:A:209:ILE:O	2.21	0.41
1:A:219:TYR:O	1:A:234:ALA:CA	2.64	0.41
1:A:409:BFD:OD2	1:A:409:BFD:F3	2.29	0.41
1:A:909:THR:OG1	1:A:910:MET:N	2.53	0.41
1:A:1000:PHE:O	1:A:1003:LEU:HB3	2.21	0.41
1:A:1004:VAL:HG13	1:A:1005:PHE:HD1	1.86	0.41
1:A:1067:TRP:O	1:A:1071:ILE:HG23	2.20	0.41
1:A:1075:PHE:CZ	2:C:57:ILE:HD12	2.56	0.41
2:C:233:PRO:HG2	2:C:236:TRP:CB	2.51	0.41
2:C:339:LEU:HD12	2:C:339:LEU:HA	1.97	0.41
1:E:67:ILE:CD1	1:E:293:ILE:HG12	2.51	0.41
1:E:67:ILE:HD11	1:E:289:ASN:O	2.20	0.41
1:E:151:ALA:HB2	1:E:255:GLU:HA	2.03	0.41
1:E:178:LEU:O	1:E:819:ASN:HB2	2.21	0.41
1:E:254:THR:CG2	1:E:255:GLU:H	2.32	0.41
1:E:254:THR:CG2	1:E:255:GLU:N	2.84	0.41
1:E:495:SER:HB2	1:E:496:PRO:HD2	2.03	0.41
1:E:775:PHE:O	1:E:778:ILE:HG22	2.20	0.41
1:E:865:LEU:C	1:E:867:TYR:N	2.78	0.41
1:E:887:PRO:O	1:E:888:GLN:C	2.64	0.41
1:E:952:GLN:O	1:E:956:PHE:CE2	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:51:LEU:N	2:F:52:PRO:HD2	2.36	0.41
1:I:173:VAL:CG2	1:I:249:ALA:HB1	2.50	0.41
1:I:233:GLU:CD	1:I:242:GLU:H	2.29	0.41
1:I:618:ALA:HB3	1:I:625:ARG:HH11	1.86	0.41
1:I:915:PHE:CG	1:I:916:THR:N	2.88	0.41
1:M:93:LEU:HB3	1:M:94:PRO:HD3	2.02	0.41
1:M:143:VAL:HG13	1:M:263:TYR:H	1.86	0.41
1:M:666:ALA:HB1	1:M:943:MET:CB	2.51	0.41
1:M:799:VAL:O	1:M:803:LYS:HG3	2.20	0.41
1:M:992:ASN:CB	2:N:265:ALA:CB	2.97	0.41
1:A:59:ASN:O	1:A:63:GLN:HB2	2.21	0.41
1:A:458:ARG:HB3	1:A:458:ARG:HH11	1.85	0.41
2:C:169:ALA:HB3	2:C:232:LYS:HZ2	1.85	0.41
1:E:150:GLN:HE21	1:E:150:GLN:HB3	1.68	0.41
1:E:218:LEU:O	1:E:235:VAL:HG13	2.21	0.41
1:E:232:LEU:HD12	1:E:242:GLU:OE1	2.21	0.41
1:E:397:ASN:HA	1:E:847:TYR:OH	2.21	0.41
1:E:1066:THR:O	1:E:1070:ILE:HG12	2.21	0.41
1:I:402:GLN:O	1:I:810:ILE:HD13	2.21	0.41
1:M:587:ARG:O	1:M:591:ASP:HB2	2.21	0.41
1:M:1070:ILE:HA	1:M:1073:LEU:HB2	2.03	0.41
2:N:315:ILE:HG22	2:N:320:GLY:HA2	2.03	0.41
1:A:712:GLU:HG3	1:A:771:TYR:CE2	2.56	0.40
2:C:120:MET:HE3	2:C:120:MET:HB2	1.88	0.40
1:E:93:LEU:N	1:E:94:PRO:HD2	2.36	0.40
1:E:1045:TRP:CZ2	1:E:1053:MET:O	2.74	0.40
2:F:46:THR:H	2:F:49:THR:CG2	2.33	0.40
2:F:292:TRP:HH2	5:F:405:NAG:HO6	1.58	0.40
1:I:79:GLN:HB2	1:I:84:THR:HG21	2.04	0.40
2:J:54:PHE:HA	2:J:57:ILE:HG12	2.04	0.40
2:J:178:MET:HG2	2:J:260:TRP:NE1	2.36	0.40
1:M:931:ASN:HB3	1:M:934:THR:HG22	2.03	0.40
2:N:105:THR:HG22	2:N:294:ASN:HB3	2.02	0.40
1:A:268:THR:O	1:A:272:LEU:HG	2.21	0.40
1:A:382:ASP:CB	1:A:386:ASN:CG	2.95	0.40
1:A:966:GLU:HA	1:A:969:VAL:HG12	2.02	0.40
2:C:142:GLN:OE1	2:C:149:ALA:C	2.64	0.40
1:E:185:LYS:HZ1	1:E:187:HIS:HB3	1.86	0.40
1:E:860:LEU:CD1	1:E:939:PRO:HB3	2.49	0.40
1:E:1034:VAL:HG12	1:E:1057:PHE:CZ	2.57	0.40
1:I:489:LEU:HD22	1:I:509:GLY:CA	2.50	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:966:GLU:O	1:I:969:VAL:HG12	2.20	0.40
1:I:991:GLY:O	1:I:994:THR:OG1	2.39	0.40
1:M:287:SER:HB2	1:M:951:LEU:HD22	2.03	0.40
1:A:379:ASP:OD2	1:A:857:LYS:NZ	2.54	0.40
1:A:870:ILE:HG13	1:A:871:ALA:N	2.37	0.40
1:A:1079:PHE:N	1:A:1080:PRO:HD2	2.35	0.40
2:C:113:SER:CB	2:C:287:PRO:HA	2.51	0.40
1:E:52:LEU:HD22	1:E:52:LEU:H	1.86	0.40
1:E:158:ASP:C	1:E:159:LEU:HD22	2.42	0.40
1:E:277:LYS:NZ	1:E:825:LEU:O	2.42	0.40
1:I:272:LEU:HD11	1:I:792:PRO:CG	2.52	0.40
1:I:476:THR:CG2	1:I:492:ILE:HD11	2.52	0.40
1:I:485:GLU:CG	1:I:488:GLU:OE2	2.69	0.40
1:I:980:THR:O	2:J:270:ARG:NH1	2.55	0.40
1:I:1005:PHE:CE1	1:I:1030:LEU:HB2	2.56	0.40
1:M:429:HIS:HB3	1:M:431:TYR:CE2	2.56	0.40
1:M:953:LEU:HA	1:M:956:PHE:HB3	2.03	0.40
1:A:86:THR:HG21	1:A:349:VAL:HG21	2.02	0.40
1:A:689:ARG:HA	1:A:689:ARG:HE	1.86	0.40
1:A:697:LEU:HD22	1:A:747:TYR:CE2	2.57	0.40
1:E:599:ALA:CB	1:E:641:ASN:HB3	2.51	0.40
1:I:1001:THR:HA	1:I:1004:VAL:HG12	2.03	0.40
1:M:186:THR:C	1:M:187:HIS:CG	3.00	0.40
1:M:873:LEU:HD11	1:M:920:ILE:HD12	2.04	0.40
2:N:276:ILE:HG21	2:N:285:THR:HG21	2.04	0.40
1:A:321:GLU:HG3	1:A:322:PRO:N	2.37	0.40
1:A:572:ARG:HD2	1:A:573:VAL:H	1.87	0.40
1:E:183:ASN:OD1	1:E:239:LEU:HD21	2.21	0.40
1:I:64:PHE:CE1	1:I:73:LEU:HD22	2.56	0.40
1:I:532:TYR:HD1	1:I:553:THR:HG21	1.85	0.40
1:I:906:ALA:O	1:I:910:MET:HB2	2.22	0.40
1:I:1078:LEU:HB3	1:I:1082:ILE:HD13	2.04	0.40
1:I:1090:VAL:O	1:I:1091:ARG:HB2	2.21	0.40
2:J:222:ASN:HD21	2:J:225:GLU:CB	2.32	0.40
1:M:87:SER:HA	1:M:88:PRO:HD3	1.93	0.40
1:M:451:PHE:HB3	1:M:526:ARG:NH2	2.37	0.40
1:M:1051:GLN:OE1	2:N:140:ASP:N	2.53	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	1061/1129 (94%)	917 (86%)	143 (14%)	1 (0%)	48 80
1	E	1061/1129 (94%)	875 (82%)	186 (18%)	0	100 100
1	I	1061/1129 (94%)	878 (83%)	182 (17%)	1 (0%)	48 80
1	M	1061/1129 (94%)	885 (83%)	176 (17%)	0	100 100
2	C	322/361 (89%)	266 (83%)	56 (17%)	0	100 100
2	F	322/361 (89%)	275 (85%)	47 (15%)	0	100 100
2	J	322/361 (89%)	281 (87%)	41 (13%)	0	100 100
2	N	322/361 (89%)	297 (92%)	25 (8%)	0	100 100
All	All	5532/5960 (93%)	4674 (84%)	856 (16%)	2 (0%)	100 100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	316	THR
1	A	570	PHE

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	946/1004 (94%)	939 (99%)	7 (1%)	76 78
1	E	946/1004 (94%)	939 (99%)	7 (1%)	76 78
1	I	946/1004 (94%)	943 (100%)	3 (0%)	86 85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	M	946/1004 (94%)	942 (100%)	4 (0%)	84 83
2	C	288/316 (91%)	287 (100%)	1 (0%)	86 85
2	F	288/316 (91%)	288 (100%)	0	100 100
2	J	288/316 (91%)	288 (100%)	0	100 100
2	N	288/316 (91%)	288 (100%)	0	100 100
All	All	4936/5280 (94%)	4914 (100%)	22 (0%)	84 83

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	TYR
1	A	220	LYS
1	A	226	ASN
1	A	227	ILE
1	A	489	LEU
1	A	515	ASN
1	A	574	GLN
2	C	199	LEU
1	E	316	THR
1	E	324	TYR
1	E	622	LEU
1	E	718	LEU
1	E	942	TYR
1	E	1009	LEU
1	E	1013	LEU
1	I	309	LEU
1	I	469	CYS
1	I	485	GLU
1	M	35	TYR
1	M	36	ILE
1	M	39	ARG
1	M	117	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	59	ASN
1	A	114	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	187	HIS
1	A	275	GLN
1	A	397	ASN
1	A	536	HIS
1	A	574	GLN
1	A	655	GLN
1	A	864	HIS
1	A	928	GLN
2	C	254	ASN
2	C	298	ASN
1	E	243	ASN
1	E	314	GLN
1	E	623	GLN
1	E	744	HIS
1	E	761	ASN
1	E	892	GLN
1	E	948	ASN
1	E	952	GLN
2	F	35	GLN
2	F	92	ASN
2	F	144	ASN
2	F	176	ASN
2	F	180	ASN
2	F	211	ASN
2	F	249	ASN
2	F	254	ASN
1	I	38	GLN
1	I	273	ASN
1	I	289	ASN
1	I	314	GLN
1	I	329	GLN
1	I	392	ASN
1	I	429	HIS
1	I	574	GLN
1	I	797	GLN
1	I	881	ASN
1	I	900	GLN
1	I	912	ASN
2	J	36	GLN
2	J	347	ASN
1	M	392	ASN
1	M	402	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	429	HIS
1	M	470	HIS
1	M	623	GLN
1	M	653	GLN
1	M	694	ASN
1	M	992	ASN
2	N	107	ASN
2	N	117	ASN
2	N	142	GLN
2	N	216	ASN
2	N	235	ASN
2	N	249	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	BFD	E	409	1	8,11,12	6.05	3 (37%)	2,15,17	1.27	0
1	BFD	M	409	1	8,11,12	6.10	3 (37%)	2,15,17	2.07	1 (50%)
1	BFD	I	409	1	8,11,12	6.08	3 (37%)	2,15,17	2.47	1 (50%)
1	BFD	A	409	4,1	8,11,12	6.06	3 (37%)	2,15,17	1.91	1 (50%)

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
1	BFD	E	409	1	-	1/5/11/13	-
1	BFD	M	409	1	-	3/5/11/13	-
1	BFD	I	409	1	-	2/5/11/13	-
1	BFD	A	409	4,1	-	2/5/11/13	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	409	BFD	F3-BE	10.20	1.77	1.54
1	I	409	BFD	F3-BE	10.19	1.77	1.54
1	A	409	BFD	F3-BE	10.14	1.76	1.54
1	E	409	BFD	F3-BE	10.13	1.76	1.54
1	M	409	BFD	F2-BE	9.79	1.76	1.54
1	M	409	BFD	F1-BE	9.70	1.75	1.54
1	E	409	BFD	F2-BE	9.70	1.75	1.54
1	I	409	BFD	F2-BE	9.70	1.75	1.54
1	I	409	BFD	F1-BE	9.69	1.75	1.54
1	A	409	BFD	F2-BE	9.66	1.75	1.54
1	A	409	BFD	F1-BE	9.65	1.75	1.54
1	E	409	BFD	F1-BE	9.64	1.75	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	409	BFD	CA-CB-CG	-3.15	106.02	112.78
1	M	409	BFD	CA-CB-CG	-2.55	107.30	112.78
1	A	409	BFD	OD2-CG-CB	-2.46	118.94	124.65

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	409	BFD	N-CA-CB-CG
1	I	409	BFD	C-CA-CB-CG
1	M	409	BFD	C-CA-CB-CG
1	M	409	BFD	N-CA-CB-CG
1	A	409	BFD	CA-CB-CG-OD1
1	A	409	BFD	CA-CB-CG-OD2
1	E	409	BFD	CA-CB-CG-OD2
1	M	409	BFD	CA-CB-CG-OD2

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	409	BFD	5	0
1	M	409	BFD	2	0
1	A	409	BFD	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 4 are monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	C	406	-	13,13,15	0.50	0	12,17,21	0.45	0
3	P5S	I	1201	-	9,10,53	0.94	0	9,14,60	1.46	2 (22%)
3	P5S	C	401	-	52,53,53	0.98	2 (3%)	54,60,60	1.08	2 (3%)
5	NAG	F	402	-	14,14,15	0.48	0	17,19,21	0.47	0
5	NAG	N	405	-	13,13,15	0.35	0	12,17,21	0.52	0
3	P5S	E	1201	-	9,10,53	0.94	0	9,14,60	1.05	1 (11%)
5	NAG	F	405	-	13,13,15	0.34	0	12,17,21	0.58	0
5	NAG	C	403	-	14,14,15	0.56	0	17,19,21	0.98	2 (11%)
5	NAG	J	405	-	13,13,15	0.55	0	12,17,21	0.58	0
3	P5S	I	1202	-	9,10,53	0.95	0	9,14,60	1.11	0
5	NAG	N	401	-	14,14,15	0.42	0	17,19,21	0.39	0
5	NAG	J	401	-	14,14,15	0.19	0	17,19,21	0.51	0
3	P5S	E	1202	-	9,10,53	0.95	0	9,14,60	1.39	2 (22%)
5	NAG	N	404	-	14,14,15	0.29	0	17,19,21	0.67	1 (5%)
5	NAG	J	402	-	14,14,15	0.22	0	17,19,21	0.38	0
5	NAG	N	402	-	14,14,15	0.22	0	17,19,21	0.44	0
5	NAG	J	404	-	14,14,15	0.37	0	17,19,21	0.74	1 (5%)
5	NAG	C	405	-	14,14,15	0.62	0	17,19,21	0.84	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	P5S	A	1201	-	9,10,53	0.96	0	9,14,60	1.19	1 (11%)
6	AH2	F	403	-	11,11,11	0.97	0	15,15,15	1.08	1 (6%)
6	AH2	N	403	-	11,11,11	0.79	0	15,15,15	1.30	2 (13%)
5	NAG	C	402	-	14,14,15	1.19	1 (7%)	17,19,21	0.64	0
3	P5S	M	1201	-	9,10,53	0.94	0	9,14,60	1.28	2 (22%)
6	AH2	J	403	-	11,11,11	0.81	0	15,15,15	1.24	1 (6%)
5	NAG	F	404	-	14,14,15	0.26	0	17,19,21	0.62	1 (5%)
5	NAG	F	401	-	14,14,15	1.09	1 (7%)	17,19,21	1.02	2 (11%)
6	AH2	C	404	-	11,11,11	0.71	0	15,15,15	1.12	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	406	-	-	2/6/19/26	0/1/1/1
3	P5S	I	1201	-	-	5/10/10/59	-
3	P5S	C	401	-	-	19/59/59/59	-
5	NAG	F	402	-	-	1/6/23/26	0/1/1/1
5	NAG	N	405	-	-	1/6/19/26	0/1/1/1
3	P5S	E	1201	-	-	9/10/10/59	-
5	NAG	F	405	-	-	3/6/19/26	1/1/1/1
5	NAG	C	403	-	-	2/6/23/26	0/1/1/1
5	NAG	J	405	-	-	4/6/19/26	1/1/1/1
3	P5S	I	1202	-	-	0/10/10/59	-
5	NAG	N	401	-	-	2/6/23/26	0/1/1/1
5	NAG	J	401	-	-	3/6/23/26	0/1/1/1
3	P5S	E	1202	-	-	4/10/10/59	-
5	NAG	N	404	-	-	3/6/23/26	0/1/1/1
5	NAG	J	402	-	-	1/6/23/26	0/1/1/1
5	NAG	N	402	-	-	0/6/23/26	0/1/1/1
5	NAG	J	404	-	-	2/6/23/26	0/1/1/1
5	NAG	C	405	-	-	1/6/23/26	0/1/1/1
3	P5S	A	1201	-	-	3/10/10/59	-
6	AH2	F	403	-	-	1/2/19/19	0/1/1/1
6	AH2	N	403	-	-	1/2/19/19	1/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	402	-	-	4/6/23/26	0/1/1/1
3	P5S	M	1201	-	-	2/10/10/59	-
6	AH2	J	403	-	-	2/2/19/19	1/1/1/1
5	NAG	F	404	-	-	0/6/23/26	0/1/1/1
5	NAG	F	401	-	-	4/6/23/26	0/1/1/1
6	AH2	C	404	-	-	1/2/19/19	1/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	P5S	O37-C38	4.53	1.47	1.34
3	C	401	P5S	O19-C17	4.44	1.46	1.33
5	C	402	NAG	O5-C1	-4.20	1.36	1.43
5	F	401	NAG	O5-C1	-3.53	1.37	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	P5S	O37-C38-C39	4.41	121.02	111.48
6	J	403	AH2	C1-O5-C5	3.92	117.44	112.19
6	N	403	AH2	C1-O5-C5	3.79	117.27	112.19
6	C	404	AH2	C1-O5-C5	3.42	116.78	112.19
3	I	1201	P5S	OG-CB-CA	3.25	110.89	108.06
5	C	405	NAG	C1-O5-C5	3.14	116.39	112.19
3	C	401	P5S	O19-C17-C20	2.89	120.66	111.83
6	F	403	AH2	C1-O5-C5	2.73	115.85	112.19
5	J	404	NAG	C1-O5-C5	2.70	115.81	112.19
5	C	403	NAG	C1-O5-C5	2.68	115.78	112.19
3	E	1202	P5S	OG-CB-CA	2.59	110.31	108.06
3	M	1201	P5S	OG-CB-CA	2.53	110.26	108.06
3	A	1201	P5S	OXT-C-O	-2.47	118.48	124.08
5	N	404	NAG	C1-O5-C5	2.34	115.32	112.19
5	C	403	NAG	C3-C4-C5	2.33	114.46	110.23
5	F	401	NAG	C1-O5-C5	-2.32	109.07	112.19
5	F	401	NAG	C2-N2-C7	2.28	125.96	122.90
3	E	1202	P5S	OXT-C-O	-2.22	119.05	124.08
6	N	403	AH2	O2-C2-C3	-2.16	105.67	110.15
3	I	1201	P5S	OXT-C-O	-2.15	119.19	124.08
5	F	404	NAG	C1-O5-C5	2.14	115.05	112.19
3	M	1201	P5S	OXT-C-O	-2.09	119.35	124.08
3	E	1201	P5S	OXT-C-O	-2.01	119.51	124.08

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1201	P5S	C-CA-CB-OG
3	A	1201	P5S	N-CA-CB-OG
3	C	401	P5S	O-C-CA-N
3	C	401	P5S	O-C-CA-CB
3	C	401	P5S	OXT-C-CA-CB
3	C	401	P5S	N-CA-CB-OG
3	C	401	P5S	C39-C38-O37-C2
3	E	1201	P5S	O-C-CA-N
3	E	1201	P5S	O-C-CA-CB
3	E	1201	P5S	OXT-C-CA-CB
3	E	1201	P5S	C-CA-CB-OG
3	E	1201	P5S	N-CA-CB-OG
3	E	1201	P5S	CB-OG-P12-O13
3	E	1202	P5S	C-CA-CB-OG
3	E	1202	P5S	N-CA-CB-OG
3	I	1201	P5S	C-CA-CB-OG
3	I	1201	P5S	N-CA-CB-OG
3	I	1201	P5S	CB-OG-P12-O13
5	C	406	NAG	C4-C5-C6-O6
5	C	406	NAG	O5-C5-C6-O6
5	F	405	NAG	C1-C2-N2-C7
5	F	405	NAG	C8-C7-N2-C2
5	F	405	NAG	O7-C7-N2-C2
5	N	405	NAG	C1-C2-N2-C7
3	C	401	P5S	O47-C38-O37-C2
5	F	401	NAG	O5-C5-C6-O6
5	C	403	NAG	O5-C5-C6-O6
5	C	402	NAG	O5-C5-C6-O6
6	J	403	AH2	O5-C5-C6-O6
5	J	404	NAG	O5-C5-C6-O6
5	F	401	NAG	C4-C5-C6-O6
5	C	403	NAG	C4-C5-C6-O6
3	E	1201	P5S	OXT-C-CA-N
3	M	1201	P5S	OXT-C-CA-N
5	C	402	NAG	C4-C5-C6-O6
5	C	402	NAG	C8-C7-N2-C2
5	C	402	NAG	O7-C7-N2-C2
5	F	401	NAG	C8-C7-N2-C2
5	F	401	NAG	O7-C7-N2-C2
5	J	401	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	J	401	NAG	O7-C7-N2-C2
5	N	401	NAG	C8-C7-N2-C2
5	N	401	NAG	O7-C7-N2-C2
5	N	404	NAG	O5-C5-C6-O6
6	J	403	AH2	C4-C5-C6-O6
3	C	401	P5S	OXT-C-CA-N
5	C	405	NAG	O5-C5-C6-O6
3	C	401	P5S	C20-C21-C22-C23
5	J	404	NAG	C4-C5-C6-O6
6	N	403	AH2	O5-C5-C6-O6
3	C	401	P5S	C-CA-CB-OG
6	C	404	AH2	O5-C5-C6-O6
6	F	403	AH2	O5-C5-C6-O6
3	C	401	P5S	C25-C26-C27-C28
5	J	402	NAG	O5-C5-C6-O6
5	J	401	NAG	O5-C5-C6-O6
3	C	401	P5S	C45-C46-C48-C49
5	J	405	NAG	O5-C5-C6-O6
3	C	401	P5S	O19-C1-C2-C3
3	M	1201	P5S	O-C-CA-N
5	J	405	NAG	C1-C2-N2-C7
3	C	401	P5S	C22-C23-C24-C25
3	I	1201	P5S	CB-OG-P12-O16
3	C	401	P5S	C20-C17-O19-C1
3	I	1201	P5S	CA-CB-OG-P12
3	C	401	P5S	O18-C17-O19-C1
3	C	401	P5S	O19-C1-C2-O37
3	C	401	P5S	C39-C40-C41-C42
5	N	404	NAG	C4-C5-C6-O6
5	F	402	NAG	C1-C2-N2-C7
5	N	404	NAG	C1-C2-N2-C7
5	J	405	NAG	C3-C2-N2-C7
3	E	1201	P5S	CB-OG-P12-O16
3	E	1202	P5S	CB-OG-P12-O15
3	C	401	P5S	C44-C45-C46-C48
3	C	401	P5S	C29-C30-C31-C32
3	A	1201	P5S	CA-CB-OG-P12
3	E	1201	P5S	CA-CB-OG-P12
5	J	405	NAG	C4-C5-C6-O6
3	E	1202	P5S	OXT-C-CA-N

All (5) ring outliers are listed below:

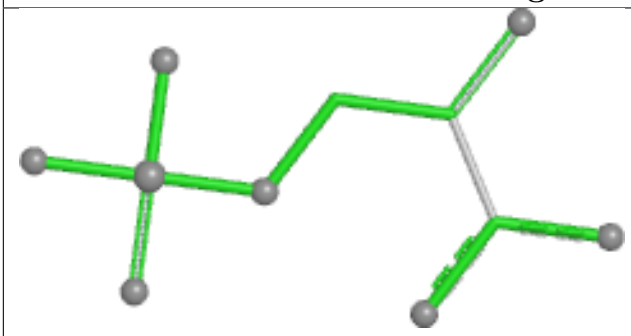
Mol	Chain	Res	Type	Atoms
5	F	405	NAG	C1-C2-C3-C4-C5-O5
6	N	403	AH2	C1-C2-C3-C4-C5-O5
6	J	403	AH2	C1-C2-C3-C4-C5-O5
6	C	404	AH2	C1-C2-C3-C4-C5-O5
5	J	405	NAG	C1-C2-C3-C4-C5-O5

12 monomers are involved in 75 short contacts:

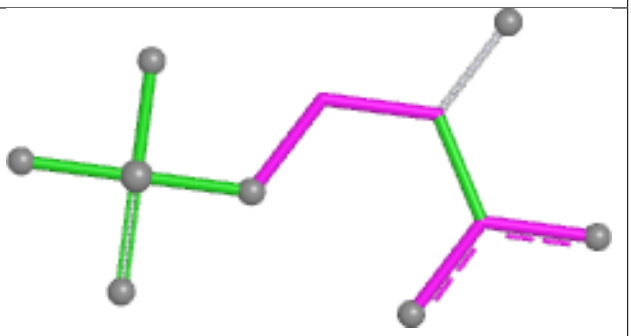
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	406	NAG	1	0
3	I	1201	P5S	9	0
3	C	401	P5S	2	0
5	N	405	NAG	15	0
5	F	405	NAG	19	0
5	J	405	NAG	7	0
3	E	1202	P5S	1	0
5	J	404	NAG	13	0
5	C	402	NAG	2	0
3	M	1201	P5S	1	0
5	F	404	NAG	4	0
5	F	401	NAG	1	0

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

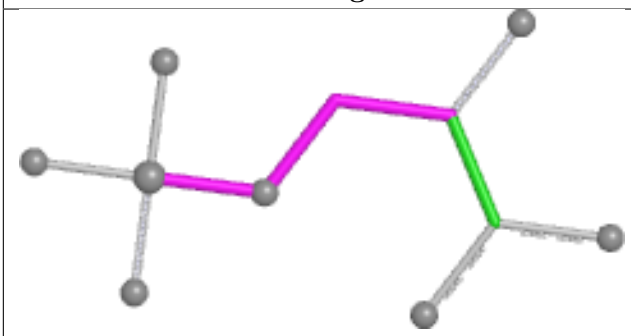
Ligand P5S I 1201



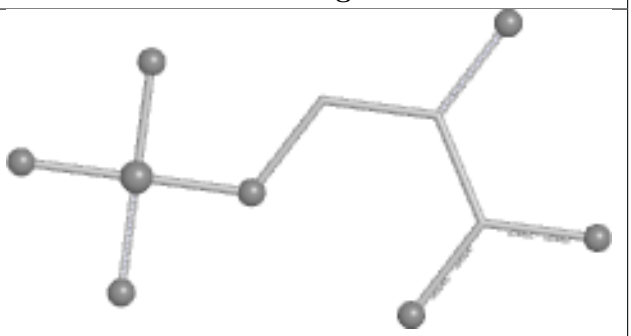
Bond lengths



Bond angles

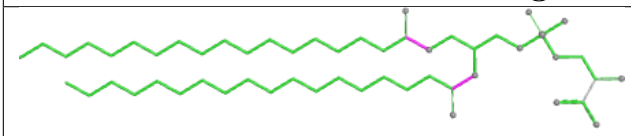


Torsions

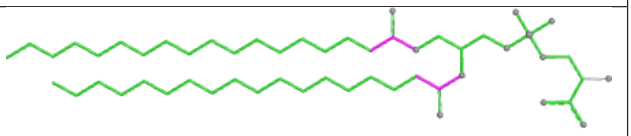


Rings

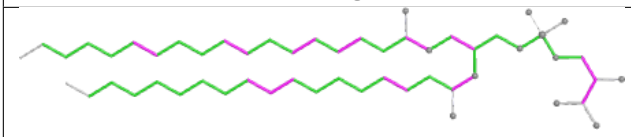
Ligand P5S C 401



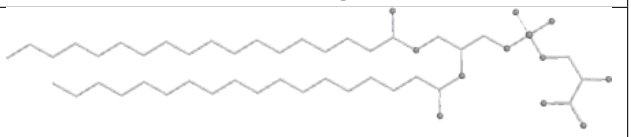
Bond lengths



Bond angles

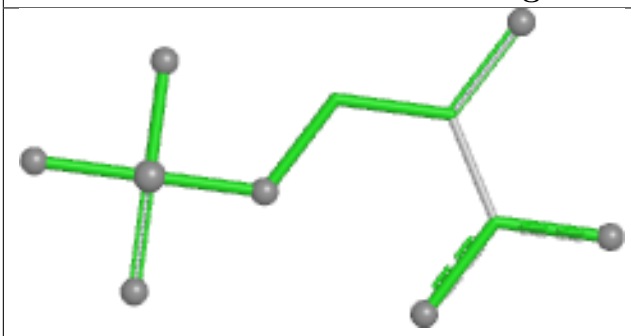


Torsions

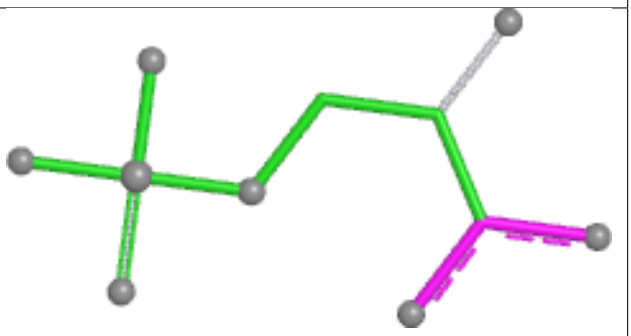


Rings

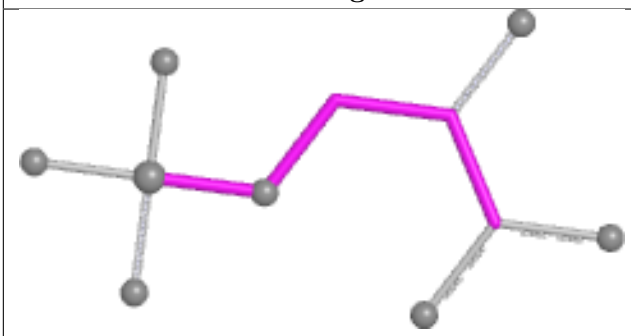
Ligand P5S E 1201



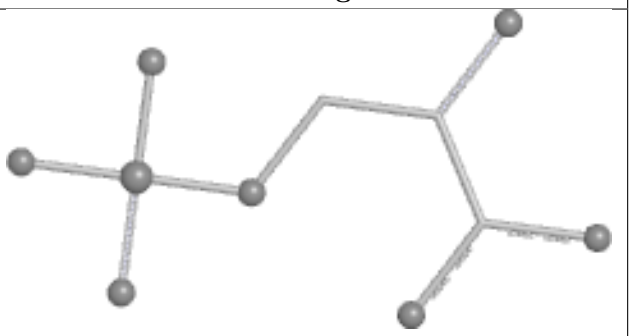
Bond lengths



Bond angles

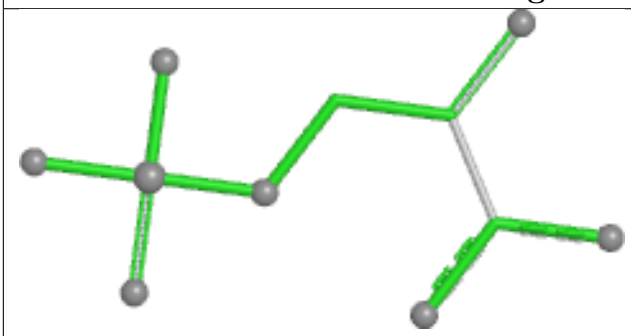


Torsions

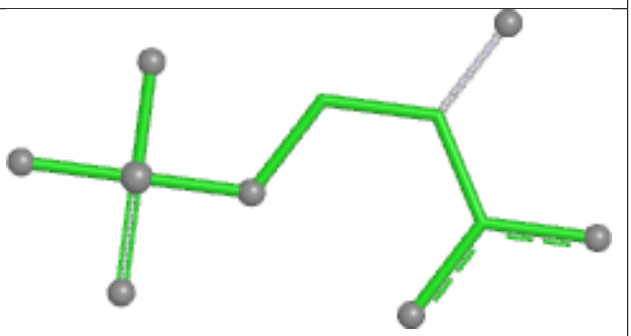


Rings

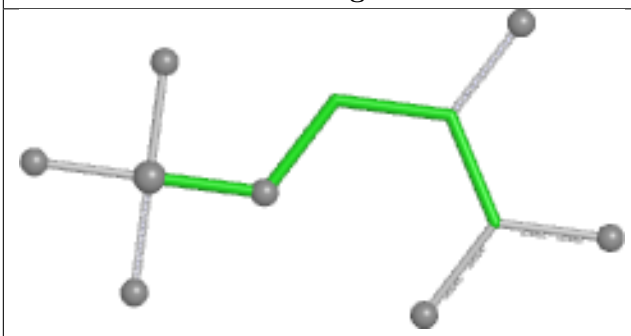
Ligand P5S I 1202



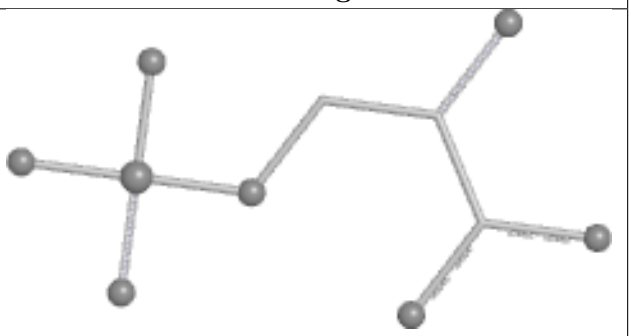
Bond lengths



Bond angles

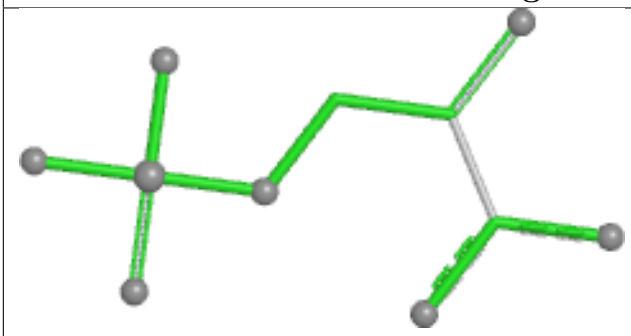


Torsions

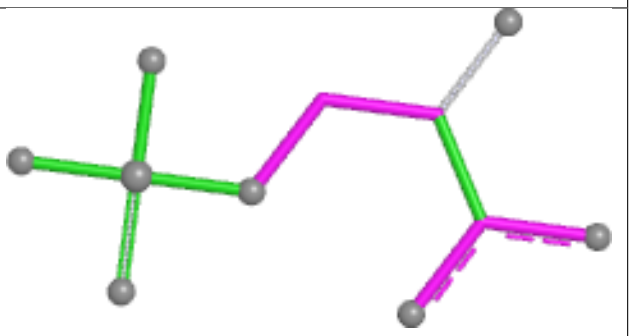


Rings

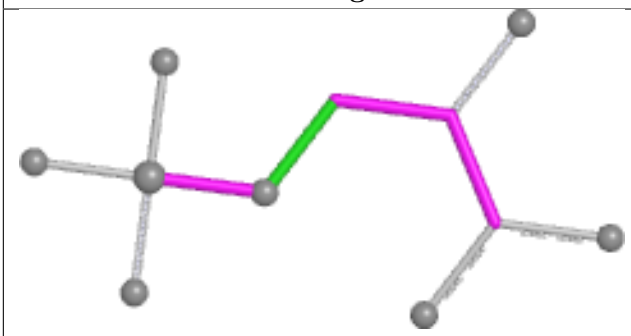
Ligand P5S E 1202



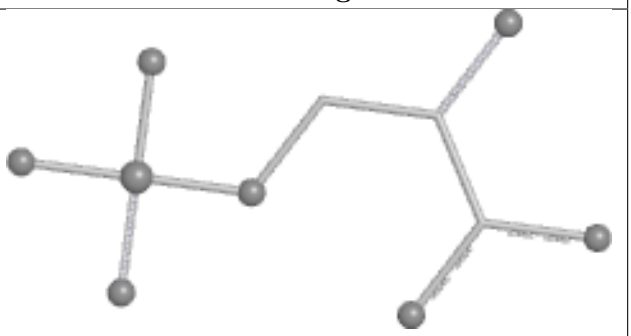
Bond lengths



Bond angles

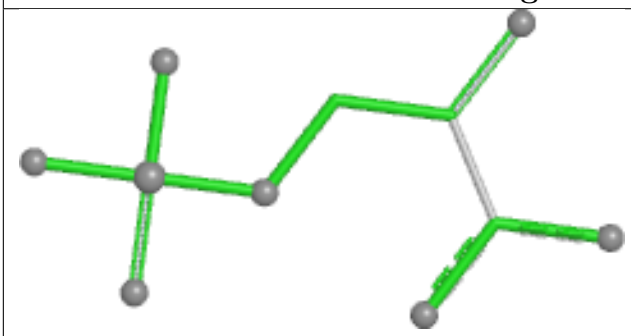


Torsions

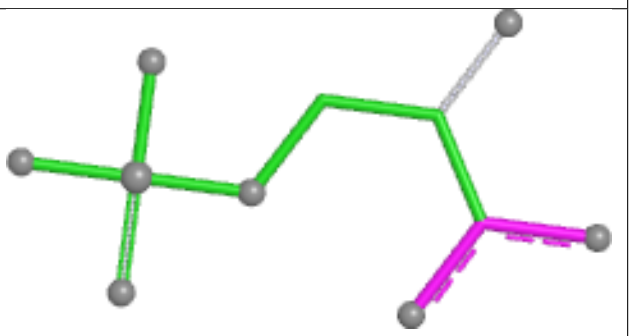


Rings

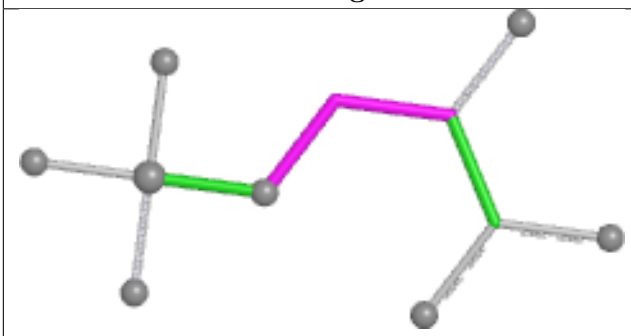
Ligand P5S A 1201



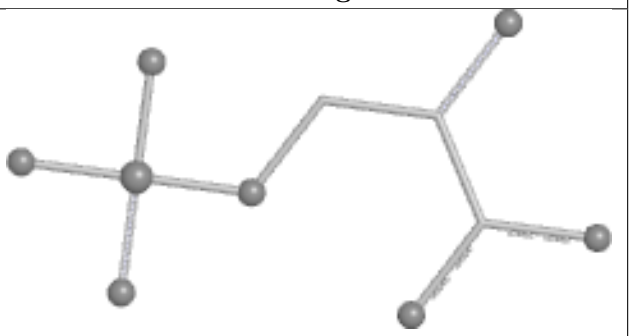
Bond lengths



Bond angles

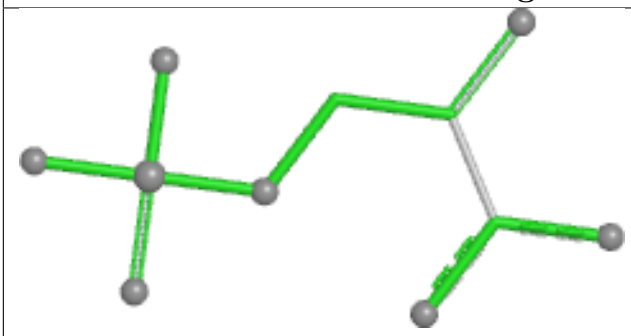


Torsions

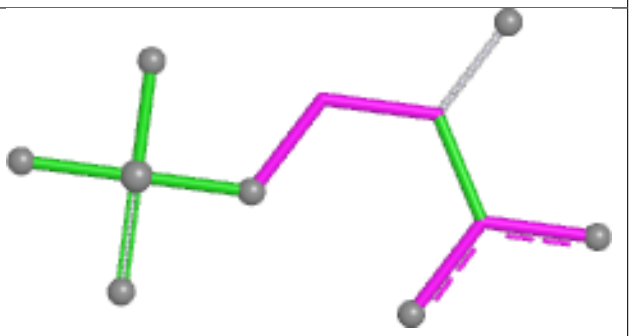


Rings

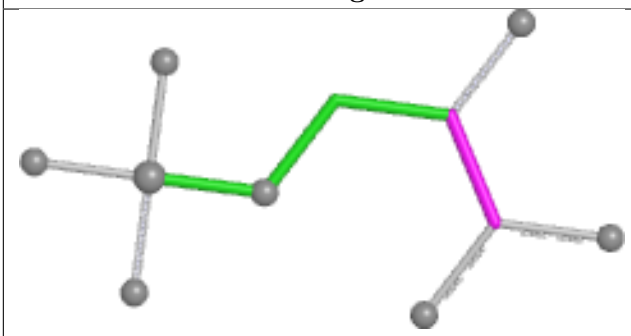
Ligand P5S M 1201



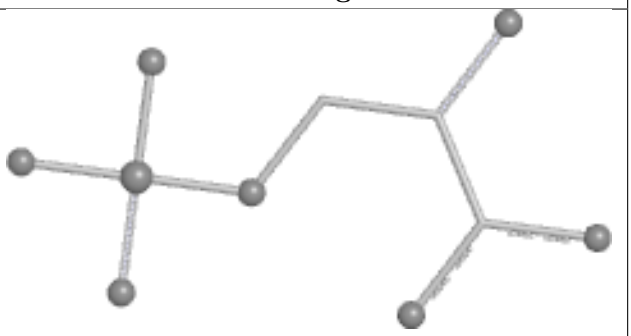
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	1063/1129 (94%)	0.49	68 (6%) 25 22	24, 120, 194, 235	0
1	E	1063/1129 (94%)	0.61	97 (9%) 15 16	31, 115, 211, 246	0
1	I	1063/1129 (94%)	0.63	77 (7%) 21 20	96, 173, 226, 261	0
1	M	1063/1129 (94%)	0.90	134 (12%) 8 11	124, 214, 315, 367	0
2	C	324/361 (89%)	0.27	19 (5%) 28 24	21, 79, 153, 183	0
2	F	324/361 (89%)	0.05	5 (1%) 72 50	25, 71, 136, 166	0
2	J	324/361 (89%)	0.67	25 (7%) 19 18	118, 189, 255, 281	0
2	N	324/361 (89%)	0.81	31 (9%) 13 16	204, 340, 392, 416	0
All	All	5548/5960 (93%)	0.61	456 (8%) 17 18	21, 164, 320, 416	0

All (456) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	560	LEU	13.6
1	E	551	VAL	11.6
1	E	550	ILE	10.6
1	A	192	ASP	9.4
1	E	460	GLU	8.9
1	E	561	PHE	8.6
1	E	220	LYS	8.4
1	A	240	GLY	8.2
1	E	459	GLU	8.1
1	M	252	LYS	8.0
1	M	240	GLY	8.0
1	M	152	ASP	7.8
1	E	599	ALA	7.8
2	J	136	LYS	7.7
1	I	559	LEU	7.4
1	E	600	PHE	7.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	461	LEU	6.8
1	M	1044	ILE	6.7
1	E	193	THR	6.7
1	E	463	LEU	6.5
1	M	893	PHE	6.3
1	M	192	ASP	6.3
1	A	1054	TYR	6.3
1	E	559	LEU	6.2
1	M	194	ILE	6.0
1	M	549	VAL	6.0
1	I	953	LEU	5.9
1	I	461	LEU	5.9
1	E	240	GLY	5.8
1	I	560	LEU	5.7
1	E	549	VAL	5.6
1	A	654	ASP	5.5
1	M	945	ILE	5.4
2	F	126	ASN	5.4
1	A	37	ALA	5.2
1	I	192	ASP	5.2
2	N	242	MET	5.2
2	N	268	THR	5.2
1	M	1089	ASN	5.1
1	I	134	VAL	5.0
1	A	239	LEU	5.0
1	I	599	ALA	5.0
2	C	247	PRO	4.9
1	A	941	LEU	4.9
1	E	1043	ILE	4.9
1	M	236	ALA	4.8
1	M	695	THR	4.8
1	I	248	GLY	4.8
1	I	463	LEU	4.8
1	E	311	TYR	4.7
1	E	641	ASN	4.7
1	I	600	PHE	4.7
1	M	699	GLU	4.7
1	A	551	VAL	4.7
1	I	603	ILE	4.7
1	E	562	CYS	4.6
1	A	313	TRP	4.6
1	M	713	ASP	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	695	THR	4.5
1	M	241	PRO	4.5
1	M	1045	TRP	4.5
1	M	253	ASN	4.4
1	M	704	THR	4.4
1	E	245	LEU	4.4
1	M	855	LEU	4.4
1	M	234	ALA	4.4
1	E	222	VAL	4.3
2	C	128	TYR	4.3
2	J	271	LYS	4.3
1	A	658	GLU	4.3
1	M	1037	SER	4.3
1	I	550	ILE	4.2
1	E	602	GLU	4.2
2	N	241	TYR	4.2
2	N	349	LYS	4.2
1	A	234	ALA	4.2
1	E	784	ALA	4.2
2	N	137	SER	4.2
1	E	745	GLN	4.2
1	A	312	VAL	4.1
2	C	126	ASN	4.1
2	N	238	LYS	4.1
2	J	74	ASN	4.1
1	A	656	ALA	4.1
1	I	952	GLN	4.0
2	N	172	GLY	4.0
1	M	151	ALA	4.0
1	M	390	LEU	4.0
2	C	198	ALA	4.0
1	M	414	LEU	4.0
1	M	1091	ARG	4.0
1	I	954	GLY	4.0
1	M	972	PHE	4.0
1	I	460	GLU	3.9
1	M	737	PHE	3.9
1	M	193	THR	3.9
1	A	270	MET	3.8
1	M	120	VAL	3.8
2	N	346	ILE	3.8
1	M	1088	LYS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	327	ILE	3.8
1	M	602	GLU	3.8
1	M	792	PRO	3.8
1	A	1060	MET	3.7
1	I	696	GLU	3.7
2	C	277	GLU	3.7
1	A	1091	ARG	3.7
1	I	744	HIS	3.7
1	M	976	PHE	3.7
2	N	223	LEU	3.7
1	E	171	CYS	3.6
1	E	438	VAL	3.6
1	E	431	TYR	3.6
1	I	223	GLY	3.6
1	M	542	ALA	3.6
1	A	836	LYS	3.6
1	I	457	ASN	3.6
1	I	690	LEU	3.6
1	M	793	LEU	3.6
1	M	218	LEU	3.6
1	E	312	VAL	3.6
1	E	532	TYR	3.5
1	E	37	ALA	3.5
2	C	267	PRO	3.5
1	M	791	ALA	3.5
1	M	454	VAL	3.5
1	I	177	SER	3.5
1	M	641	ASN	3.5
1	M	858	LEU	3.5
1	A	235	VAL	3.5
1	I	270	MET	3.5
1	I	837	GLU	3.4
2	N	140	ASP	3.4
1	A	688	CYS	3.4
2	J	261	MET	3.4
1	I	176	ALA	3.4
2	C	203	GLY	3.3
2	C	199	LEU	3.3
1	E	959	TRP	3.3
1	E	1045	TRP	3.3
1	I	688	CYS	3.3
2	J	175	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	600	PHE	3.3
1	I	941	LEU	3.3
1	E	152	ASP	3.3
1	I	195	ALA	3.3
1	M	89	VAL	3.3
1	M	559	LEU	3.3
1	M	856	LYS	3.3
1	M	944	LYS	3.3
1	E	273	ASN	3.3
1	E	844	ASN	3.3
1	M	268	THR	3.3
1	A	569	VAL	3.2
2	J	317	TRP	3.2
2	J	348	HIS	3.2
1	A	517	ASN	3.2
1	A	655	GLN	3.2
1	M	358	SER	3.2
1	E	622	LEU	3.2
1	A	172	TYR	3.2
1	M	554	GLN	3.2
1	M	635	ASP	3.2
1	M	655	GLN	3.2
1	E	91	SER	3.2
1	M	543	VAL	3.1
1	M	239	LEU	3.1
1	I	128	ILE	3.1
1	M	251	LEU	3.1
2	N	245	SER	3.1
2	N	305	ASP	3.1
1	M	941	LEU	3.1
1	E	842	ALA	3.1
1	A	241	PRO	3.1
1	A	453	LYS	3.1
1	I	601	LYS	3.1
1	M	496	PRO	3.1
1	A	428	GLY	3.1
1	E	543	VAL	3.0
1	M	34	ALA	3.0
1	I	133	ARG	3.0
1	M	114	HIS	3.0
1	A	454	VAL	3.0
1	M	906	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	515	ASN	3.0
1	E	218	LEU	3.0
2	N	224	GLU	3.0
1	A	316	THR	3.0
1	E	437	GLU	3.0
1	E	271	ALA	3.0
1	M	487	ALA	3.0
1	A	519	TYR	3.0
1	I	834	LYS	3.0
1	I	697	LEU	3.0
1	M	391	VAL	3.0
1	M	447	THR	3.0
1	E	195	ALA	3.0
1	E	192	ASP	3.0
1	I	677	LYS	2.9
1	I	746	GLU	2.9
1	M	385	ILE	2.9
1	M	117	ASP	2.9
1	A	318	TYR	2.9
1	A	744	HIS	2.9
2	N	239	PRO	2.9
2	C	118	VAL	2.9
1	M	313	TRP	2.9
1	A	883	CYS	2.9
1	A	570	PHE	2.9
1	E	439	ASP	2.9
2	C	115	GLU	2.9
2	F	203	GLY	2.9
1	E	956	PHE	2.9
1	E	494	SER	2.8
1	M	562	CYS	2.8
1	I	641	ASN	2.8
1	E	818	ALA	2.8
1	A	559	LEU	2.8
2	N	222	ASN	2.8
1	A	170	THR	2.8
1	M	49	LYS	2.8
2	J	128	TYR	2.8
1	E	246	LEU	2.8
1	M	91	SER	2.8
1	I	698	LEU	2.8
1	M	890	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	350	TYR	2.8
1	I	561	PHE	2.7
1	I	854	HIS	2.7
1	I	654	ASP	2.7
1	A	787	CYS	2.7
1	E	570	PHE	2.7
1	M	50	TYR	2.7
1	E	170	THR	2.7
1	E	253	ASN	2.7
1	M	611	ILE	2.7
2	J	127	PHE	2.7
1	M	658	GLU	2.7
1	M	707	GLU	2.7
1	E	603	ILE	2.7
2	N	120	MET	2.7
1	A	737	PHE	2.7
1	I	239	LEU	2.7
1	M	113	ARG	2.7
1	M	895	CYS	2.7
1	E	252	LYS	2.7
2	J	237	LEU	2.7
1	I	385	ILE	2.7
1	M	794	GLN	2.7
2	J	132	ARG	2.7
1	I	818	ALA	2.7
2	J	134	TYR	2.7
1	E	212	GLU	2.7
1	E	276	GLY	2.6
2	F	172	GLY	2.6
1	M	1033	TYR	2.6
1	E	435	THR	2.6
1	M	488	GLU	2.6
1	I	737	PHE	2.6
1	M	345	LEU	2.6
2	N	237	LEU	2.6
1	I	328	THR	2.6
1	M	235	VAL	2.6
1	A	815	GLY	2.6
1	A	942	TYR	2.6
1	E	205	LEU	2.6
1	M	254	THR	2.6
1	A	727	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1056	VAL	2.6
2	N	208	THR	2.6
1	M	652	LEU	2.6
1	E	840	GLN	2.6
1	I	147	VAL	2.5
1	M	859	LEU	2.5
1	I	596	LEU	2.5
1	A	199	ALA	2.5
2	N	233	PRO	2.5
1	M	474	ILE	2.5
2	J	44	ILE	2.5
1	M	484	THR	2.5
1	M	702	THR	2.5
1	A	571	PRO	2.5
2	C	276	ILE	2.5
2	J	137	SER	2.5
1	M	305	VAL	2.5
2	J	259	VAL	2.5
2	J	324	PHE	2.5
1	E	36	ILE	2.5
1	I	474	ILE	2.5
1	M	550	ILE	2.5
1	A	254	THR	2.5
1	E	334	THR	2.5
1	A	315	SER	2.5
1	I	123	SER	2.5
1	E	672	VAL	2.5
1	I	598	VAL	2.5
2	C	194	PRO	2.5
1	A	237	ARG	2.5
1	E	211	CYS	2.5
1	E	458	ARG	2.5
1	M	1042	GLY	2.5
1	A	910	MET	2.5
1	E	262	VAL	2.5
1	M	854	HIS	2.4
1	M	894	PHE	2.4
1	A	834	LYS	2.4
1	M	631	LYS	2.4
2	N	136	LYS	2.4
2	J	43	PRO	2.4
1	A	203	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	557	ASP	2.4
1	E	134	VAL	2.4
1	E	1047	PHE	2.4
1	M	705	ILE	2.4
1	M	717	GLU	2.4
1	M	743	GLU	2.4
1	M	1046	PRO	2.4
1	M	556	GLY	2.4
1	A	262	VAL	2.4
1	E	209	ILE	2.4
1	A	1040	TRP	2.4
1	E	604	ALA	2.4
2	N	126	ASN	2.4
2	N	244	ASP	2.4
1	E	34	ALA	2.4
1	M	587	ARG	2.4
1	I	275	GLN	2.4
2	J	42	GLN	2.4
1	I	124	THR	2.4
1	A	219	TYR	2.4
1	M	653	GLN	2.4
1	M	663	LEU	2.4
1	M	1087	LEU	2.4
2	C	234	VAL	2.4
1	M	818	ALA	2.4
1	A	171	CYS	2.3
2	J	257	PHE	2.3
1	I	742	THR	2.3
1	A	140	LYS	2.3
1	E	215	GLN	2.3
1	I	691	PHE	2.3
1	A	202	ILE	2.3
1	A	536	HIS	2.3
1	I	440	GLY	2.3
1	E	263	TYR	2.3
2	C	350	TYR	2.3
1	M	176	ALA	2.3
1	M	400	LEU	2.3
1	E	792	PRO	2.3
1	E	434	VAL	2.3
1	M	1034	VAL	2.3
1	A	271	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1043	ILE	2.3
2	N	338	LEU	2.3
1	A	195	ALA	2.3
1	E	705	ILE	2.3
1	M	847	TYR	2.3
1	A	624	ASP	2.3
1	I	500	ALA	2.3
1	I	784	ALA	2.3
1	E	30	SER	2.3
1	E	190	VAL	2.3
1	E	504	GLY	2.3
1	M	92	GLY	2.3
1	M	677	LYS	2.3
2	F	163	ASN	2.2
1	I	715	LEU	2.2
1	M	978	PHE	2.2
1	E	479	ALA	2.2
1	E	485	GLU	2.2
1	M	153	GLU	2.2
1	M	649	GLU	2.2
1	I	466	LEU	2.2
1	M	112	LEU	2.2
2	C	235	ASN	2.2
2	N	216	ASN	2.2
2	N	198	ALA	2.2
2	J	349	LYS	2.2
1	E	642	LEU	2.2
1	M	354	ILE	2.2
1	M	497	ASP	2.2
1	M	979	GLN	2.2
1	I	583	VAL	2.2
1	I	977	LEU	2.2
1	E	815	GLY	2.2
2	C	49	THR	2.2
1	M	536	HIS	2.2
1	E	313	TRP	2.2
2	J	280	SER	2.2
2	N	128	TYR	2.2
1	E	241	PRO	2.2
1	M	255	GLU	2.2
1	I	225	ILE	2.2
1	I	916	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	152	ASP	2.2
1	M	953	LEU	2.2
1	I	458	ARG	2.2
1	A	376	TRP	2.1
1	E	269	LYS	2.1
2	C	200	LYS	2.1
2	J	156	GLU	2.1
1	I	193	THR	2.1
1	I	957	LEU	2.1
1	M	819	ASN	2.1
1	I	499	ILE	2.1
1	I	551	VAL	2.1
1	M	913	ILE	2.1
1	I	532	TYR	2.1
1	M	853	LYS	2.1
2	N	141	SER	2.1
1	M	150	GLN	2.1
2	J	135	VAL	2.1
1	I	514	GLY	2.1
1	M	513	LEU	2.1
1	E	507	ARG	2.1
1	M	37	ALA	2.1
1	I	229	SER	2.1
1	M	1070	ILE	2.1
1	A	456	LYS	2.1
2	F	201	LYS	2.1
1	A	133	ARG	2.1
1	I	290	ALA	2.1
2	N	276	ILE	2.1
1	E	238	SER	2.1
1	M	601	LYS	2.1
1	E	457	ASN	2.1
2	J	269	PHE	2.1
1	M	909	THR	2.1
1	I	740	ALA	2.1
2	C	280	SER	2.1
1	I	130	ASN	2.1
1	I	218	LEU	2.1
1	M	246	LEU	2.1
1	E	722	TYR	2.0
1	M	408	THR	2.0
1	M	820	ASP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	185	LYS	2.0
2	C	204	ILE	2.0
2	J	60	ILE	2.0
1	E	941	LEU	2.0
1	E	146	VAL	2.0
1	E	472	VAL	2.0
1	M	1086	VAL	2.0
1	A	130	ASN	2.0
1	E	228	TYR	2.0
1	A	545	ARG	2.0
1	A	659	THR	2.0
2	N	264	ALA	2.0
1	M	171	CYS	2.0
1	E	631	LYS	2.0
1	E	703	LYS	2.0
1	A	225	ILE	2.0
1	E	960	THR	2.0
1	M	584	HIS	2.0
1	M	272	LEU	2.0
1	E	234	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
1	BFD	M	409	12/13	0.76	0.15	184,209,238,250	0
1	BFD	I	409	12/13	0.83	0.11	148,153,162,162	0
1	BFD	A	409	12/13	0.93	0.11	70,84,106,109	0
1	BFD	E	409	12/13	0.94	0.09	59,78,88,89	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

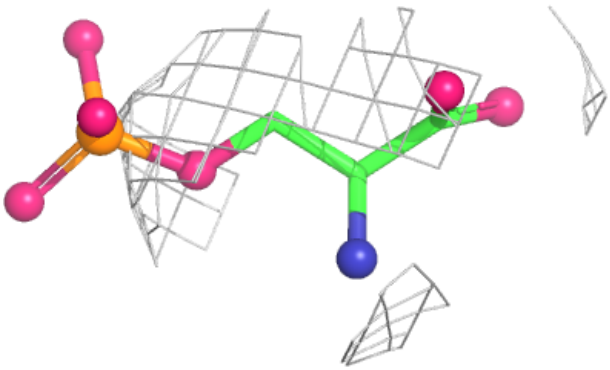
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

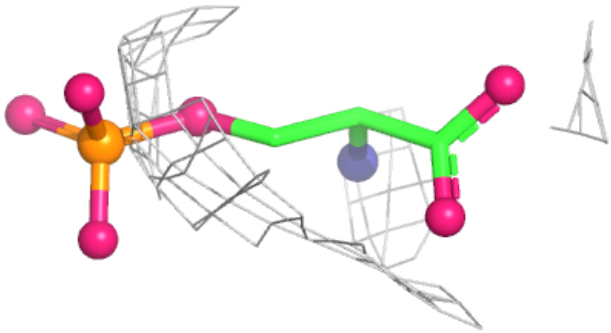
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	AH2	N	403	11/11	-0.10	0.21	347,350,356,359	0
6	AH2	J	403	11/11	0.38	0.10	155,161,168,172	0
3	P5S	M	1201	11/54	0.45	0.12	293,299,310,312	0
5	NAG	N	404	14/15	0.46	0.14	398,409,413,415	0
5	NAG	J	405	13/15	0.47	0.16	255,269,274,276	0
6	AH2	F	403	11/11	0.50	0.14	143,165,168,170	0
6	AH2	C	404	11/11	0.57	0.13	117,126,144,145	0
5	NAG	N	405	13/15	0.61	0.12	356,362,366,367	0
5	NAG	N	402	14/15	0.62	0.11	309,312,317,319	0
5	NAG	N	401	14/15	0.66	0.12	335,342,344,344	0
5	NAG	J	404	14/15	0.67	0.12	238,242,246,249	0
3	P5S	I	1202	11/54	0.75	0.18	151,162,189,189	0
3	P5S	I	1201	11/54	0.75	0.09	220,231,238,239	0
3	P5S	C	401	54/54	0.77	0.21	92,120,135,141	0
5	NAG	J	401	14/15	0.79	0.13	145,176,183,185	0
5	NAG	J	402	14/15	0.79	0.10	156,172,186,190	0
5	NAG	F	405	13/15	0.80	0.15	125,133,149,153	0
3	P5S	E	1202	11/54	0.81	0.18	78,97,159,160	0
4	MG	E	1203	1/1	0.82	0.17	91,91,91,91	0
5	NAG	C	405	14/15	0.89	0.11	99,111,127,137	0
3	P5S	A	1201	11/54	0.89	0.13	107,117,167,172	0
5	NAG	F	401	14/15	0.90	0.14	66,80,102,109	0
5	NAG	F	404	14/15	0.90	0.11	61,100,139,145	0
5	NAG	C	406	13/15	0.90	0.10	70,93,122,127	0
5	NAG	C	402	14/15	0.91	0.14	41,71,97,98	0
5	NAG	F	402	14/15	0.92	0.09	45,82,110,113	0
4	MG	A	1202	1/1	0.93	0.11	172,172,172,172	0
5	NAG	C	403	14/15	0.93	0.10	75,107,121,124	0
3	P5S	E	1201	11/54	0.97	0.07	70,85,102,110	0
4	MG	I	1203	1/1	0.97	0.06	139,139,139,139	0
4	MG	M	1202	1/1	0.98	0.17	185,185,185,185	0

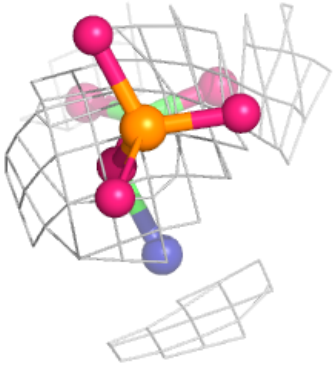
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P5S M 1201:

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

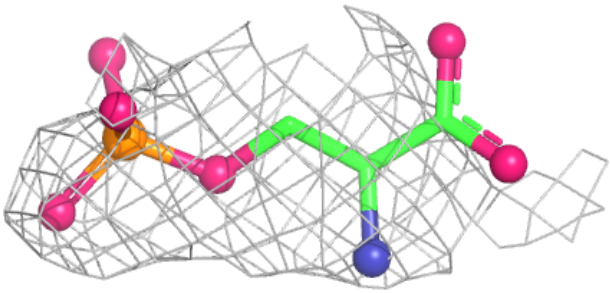


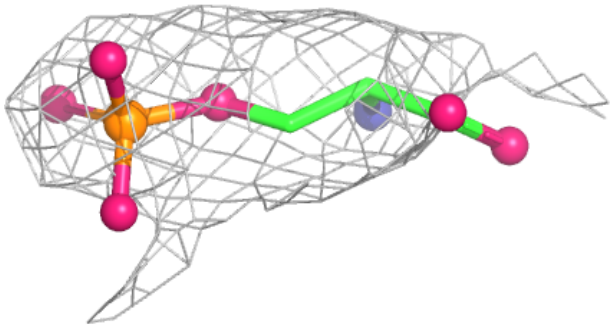


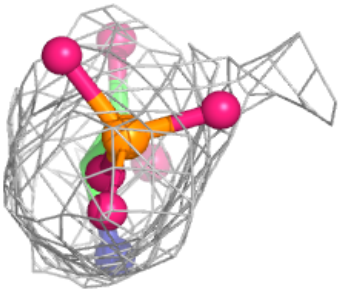


Electron density around P5S I 1202:

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

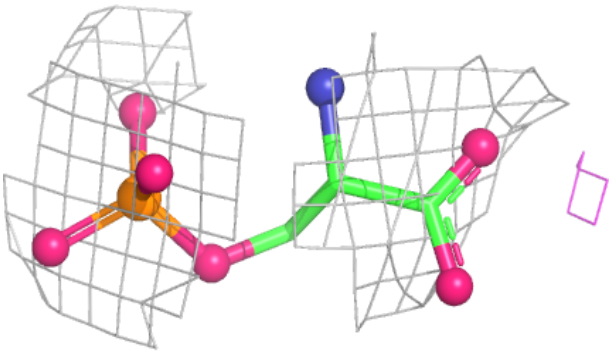


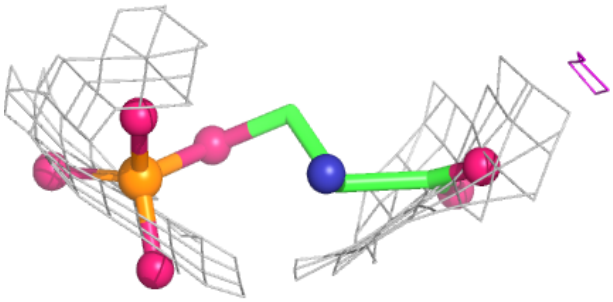


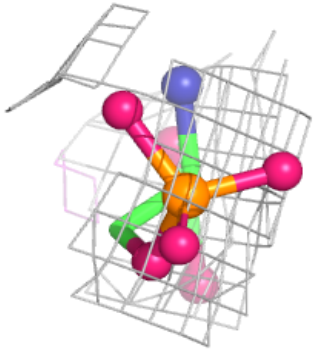


Electron density around P5S I 1201:

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

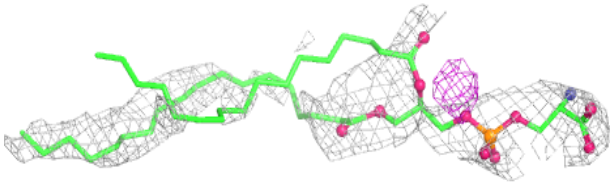


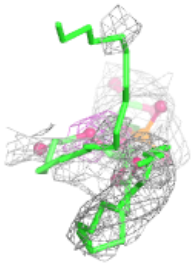




Electron density around P5S C 401:

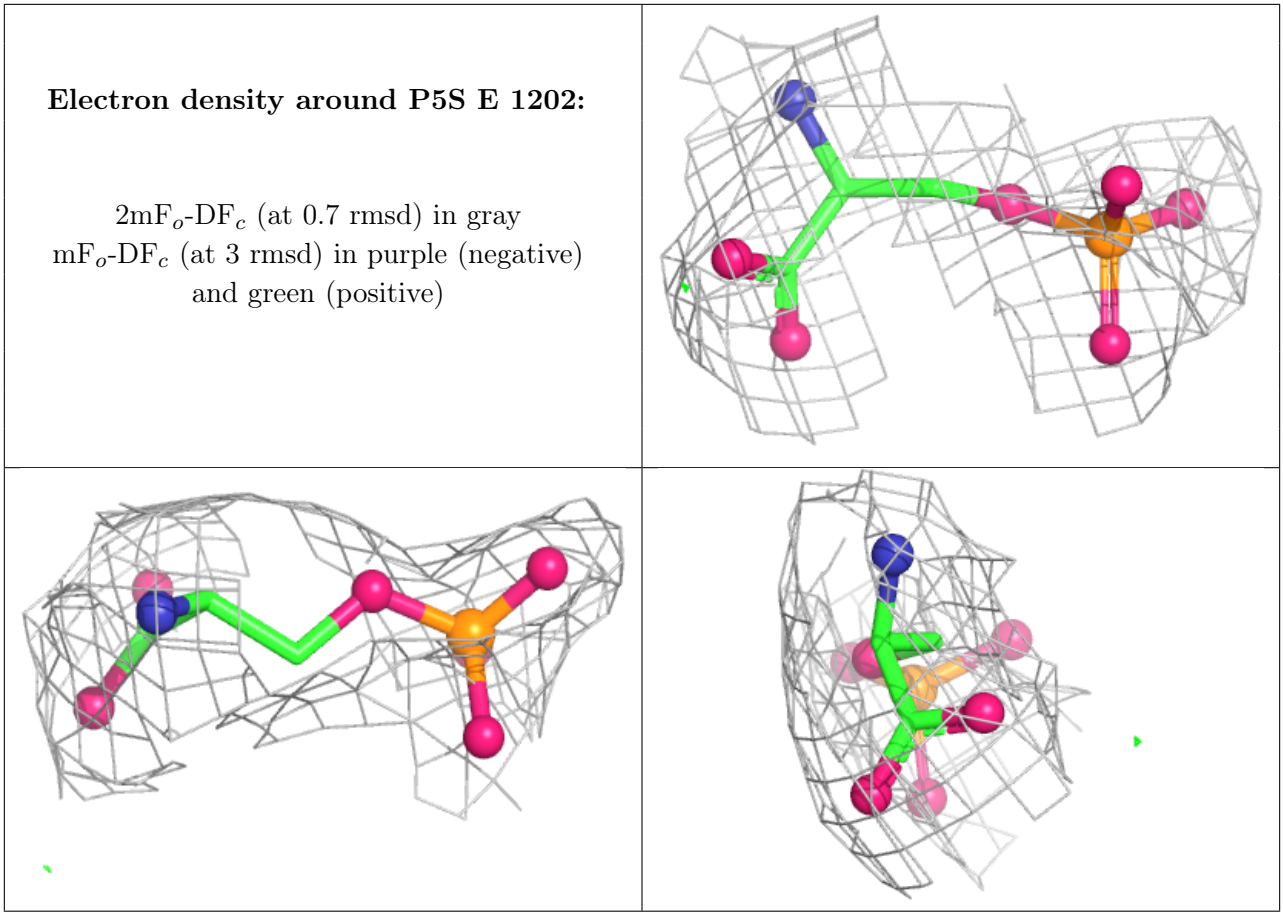
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





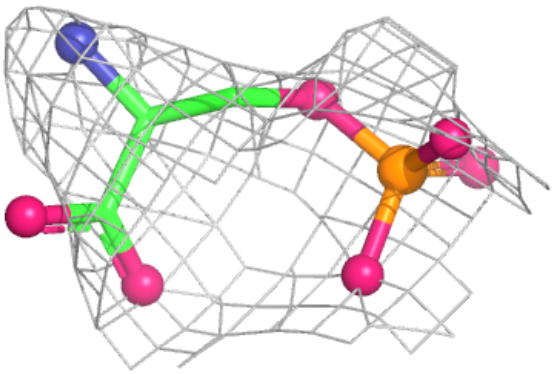
Electron density around P5S E 1202:

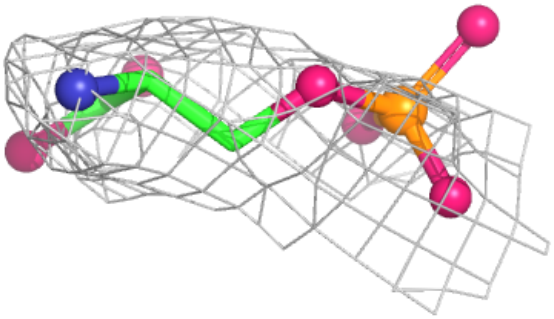
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

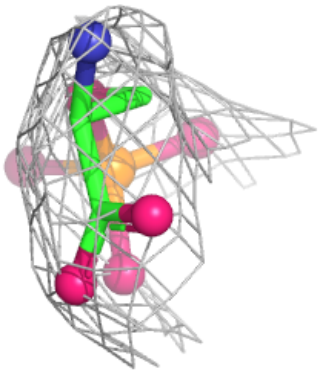


Electron density around P5S A 1201:

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

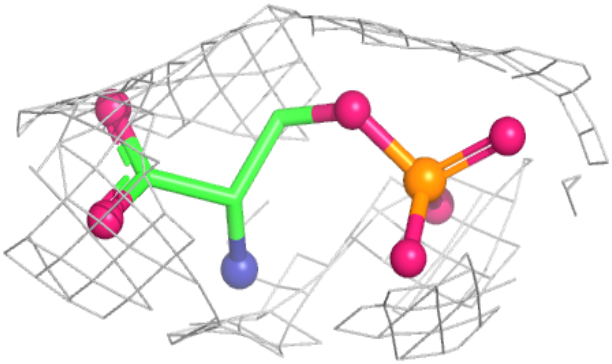


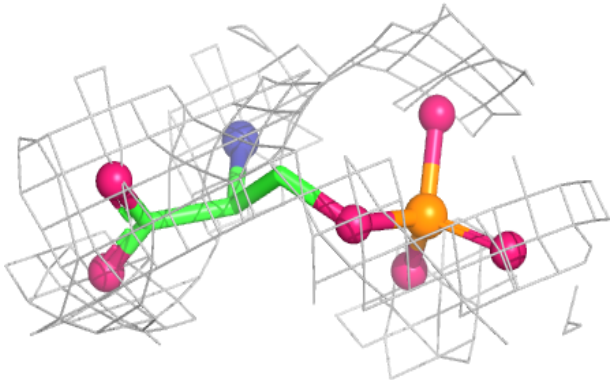


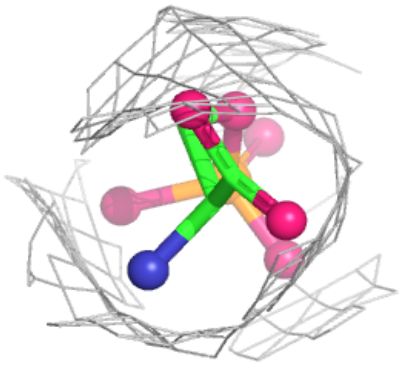


Electron density around P5S E 1201:

$2mF_o$-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.