Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:37 AM GMT

PDB ID	:	3FA3
Title	:	Crystal structure of 2,3-dimethylmalate lyase, a PEP mutase/isocitrate lyase superfamily member, trigonal crystal form
Authors	:	Narayanan, B.C.; Herzberg, O.
Deposited on	:	2008-11-14
Resolution	:	2.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

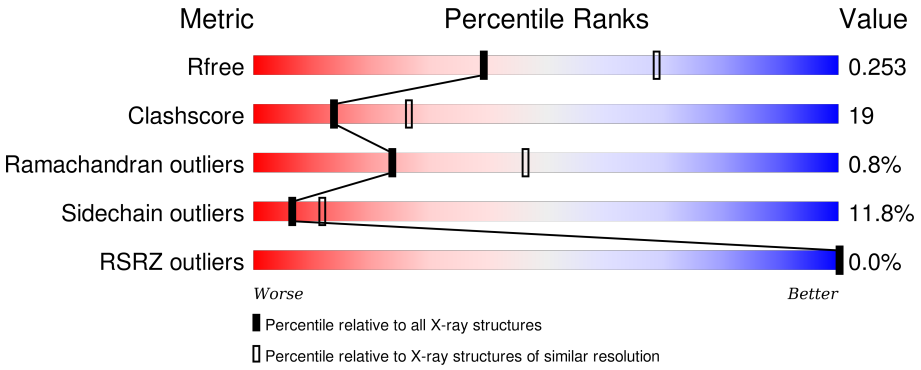
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	302	69% 26% 5%
1	B	302	65% 30% 5%
1	C	302	64% 30% 5%
1	D	302	67% 28%
1	E	302	70% 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	302	65% 31%
1	G	302	69% 26%
1	H	302	65% 30%
1	I	302	60% 35%
1	J	302	62% 28% 5%
1	K	302	64% 30% 5%
1	L	302	55% 39% 5%
1	M	302	59% 36%
1	N	302	56% 34% 5%
1	O	302	64% 31% 5%
1	P	302	% 55% 38% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	602	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36360 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.

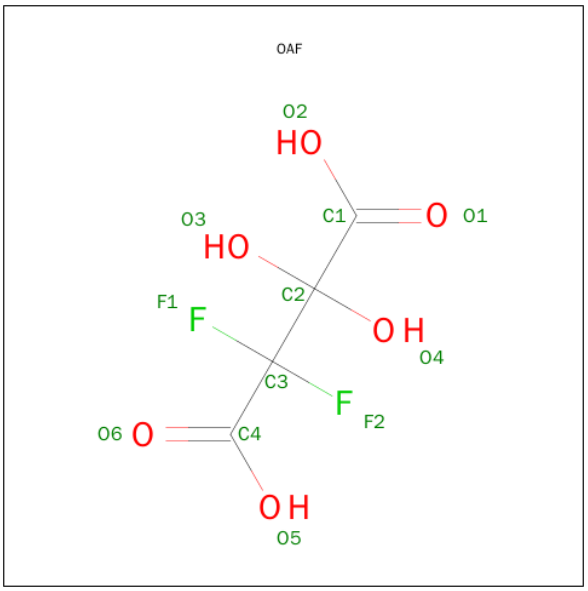
- Molecule 1 is a protein called 2,3-dimethylmalate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2222	1379	397	430	16			
1	B	302	Total	C	N	O	S	0	0	0
			2230	1384	399	431	16			
1	C	301	Total	C	N	O	S	0	0	0
			2228	1384	398	430	16			
1	D	301	Total	C	N	O	S	0	0	0
			2226	1384	398	428	16			
1	E	301	Total	C	N	O	S	0	0	0
			2228	1384	398	430	16			
1	F	301	Total	C	N	O	S	0	0	0
			2224	1381	397	430	16			
1	G	301	Total	C	N	O	S	0	0	0
			2228	1384	398	430	16			
1	H	301	Total	C	N	O	S	0	0	0
			2228	1384	398	430	16			
1	I	300	Total	C	N	O	S	0	0	0
			2216	1376	397	427	16			
1	J	292	Total	C	N	O	S	0	0	0
			2162	1344	383	420	15			
1	K	300	Total	C	N	O	S	0	0	0
			2218	1376	397	429	16			
1	L	300	Total	C	N	O	S	0	0	0
			2215	1375	396	428	16			
1	M	300	Total	C	N	O	S	0	0	0
			2220	1378	397	429	16			
1	N	292	Total	C	N	O	S	0	0	0
			2161	1342	383	421	15			
1	O	301	Total	C	N	O	S	0	0	0
			2211	1374	397	424	16			
1	P	301	Total	C	N	O	S	0	0	0
			2225	1381	398	430	16			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

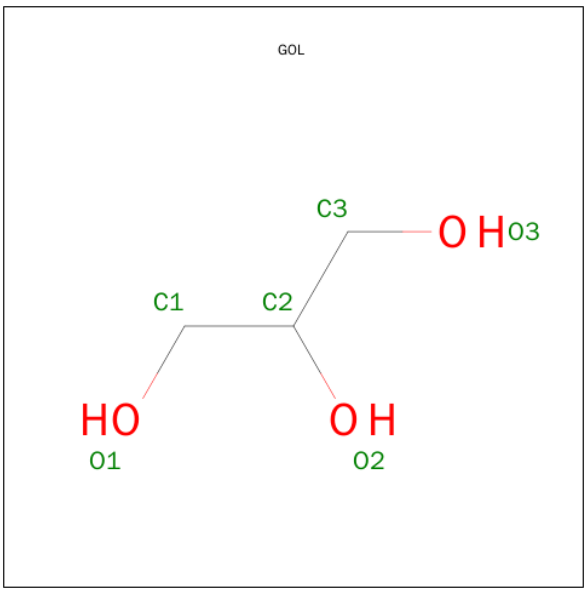
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	1	Total Mn 1 1	0	0
2	G	1	Total Mn 1 1	0	0
2	J	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	K	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	H	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	I	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0
2	N	1	Total Mn 1 1	0	0
2	O	1	Total Mn 1 1	0	0
2	L	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0
2	M	1	Total Mn 1 1	0	0

- Molecule 3 is 2,2-DIFLUORO-3,3-DIHYDROXYBUTANEDIOIC ACID (three-letter code: OAF) (formula: $C_4H_4F_2O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F O 12 4 2 6	0	0
3	B	1	Total C F O 12 4 2 6	0	0
3	C	1	Total C F O 12 4 2 6	0	0
3	D	1	Total C F O 12 4 2 6	0	0
3	E	1	Total C F O 12 4 2 6	0	0
3	F	1	Total C F O 12 4 2 6	0	0
3	G	1	Total C F O 12 4 2 6	0	0
3	H	1	Total C F O 12 4 2 6	0	0
3	I	1	Total C F O 12 4 2 6	0	0
3	K	1	Total C F O 12 4 2 6	0	0
3	L	1	Total C F O 12 4 2 6	0	0
3	M	1	Total C F O 12 4 2 6	0	0
3	O	1	Total C F O 12 4 2 6	0	0
3	P	1	Total C F O 12 4 2 6	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	M	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	59	Total O 59 59	0	0
5	B	59	Total O 59 59	0	0
5	C	52	Total O 52 52	0	0
5	D	57	Total O 57 57	0	0
5	E	65	Total O 65 65	0	0
5	F	55	Total O 55 55	0	0

Continued on next page...

Continued from previous page...

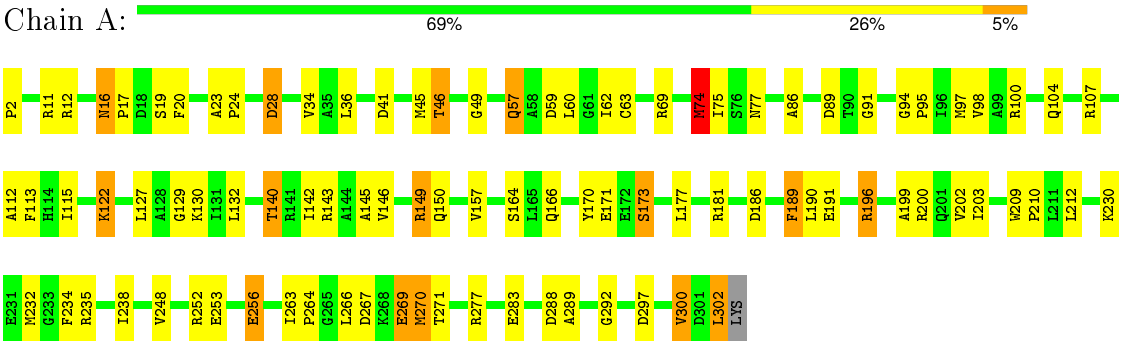
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	66	Total O 66 66	0	0
5	H	68	Total O 68 68	0	0
5	I	29	Total O 29 29	0	0
5	J	29	Total O 29 29	0	0
5	K	27	Total O 27 27	0	0
5	L	24	Total O 24 24	0	0
5	M	38	Total O 38 38	0	0
5	N	28	Total O 28 28	0	0
5	O	24	Total O 24 24	0	0
5	P	24	Total O 24 24	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

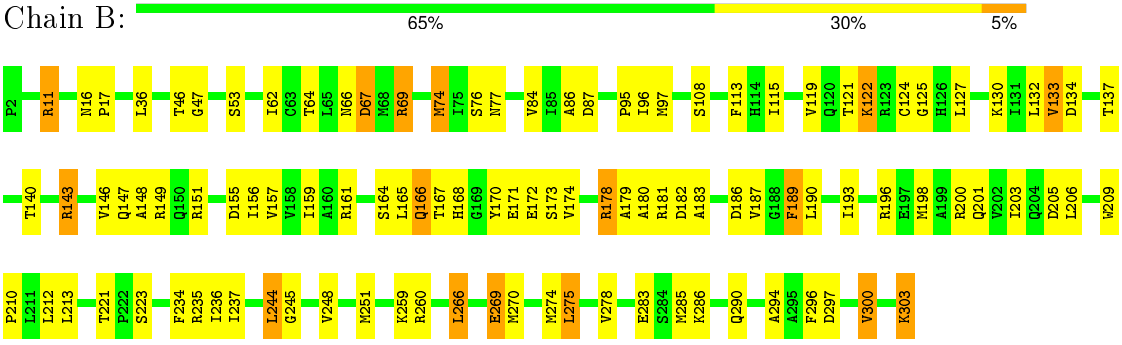
- Molecule 1: 2,3-dimethylmalate lyase

Chain A:



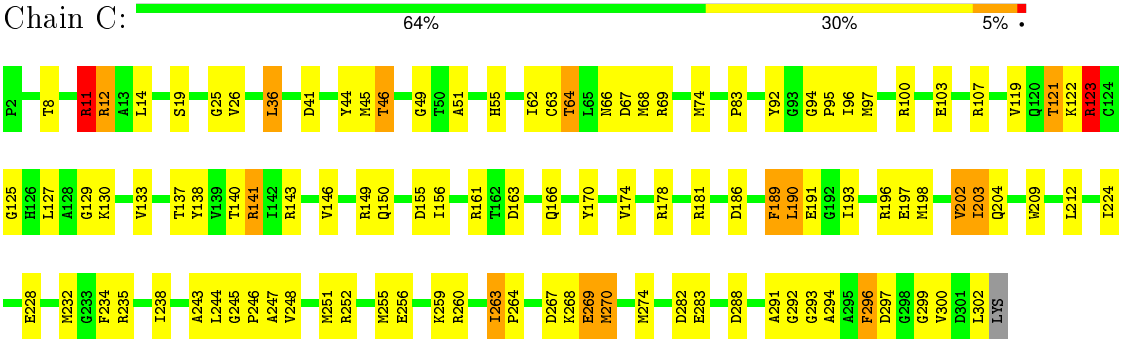
- Molecule 1: 2,3-dimethylmalate lyase

Chain B:



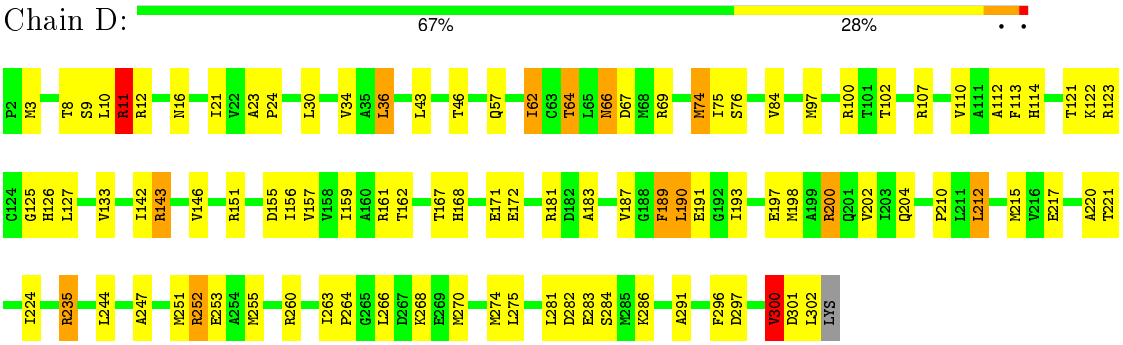
- Molecule 1: 2,3-dimethylmalate lyase

Chain C:



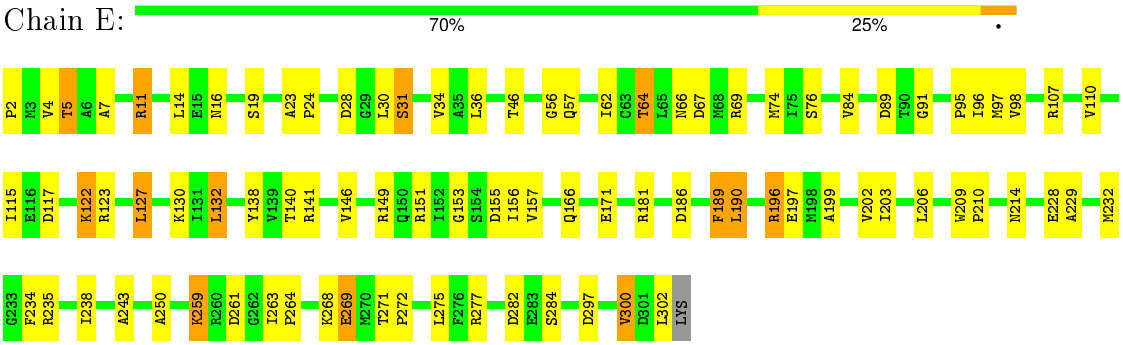
- Molecule 1: 2,3-dimethylmalate lyase

Chain D:



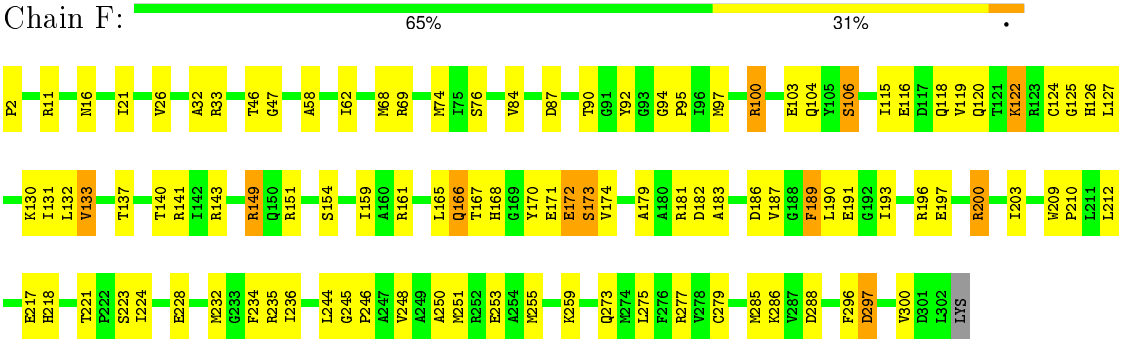
- Molecule 1: 2,3-dimethylmalate lyase

Chain E:



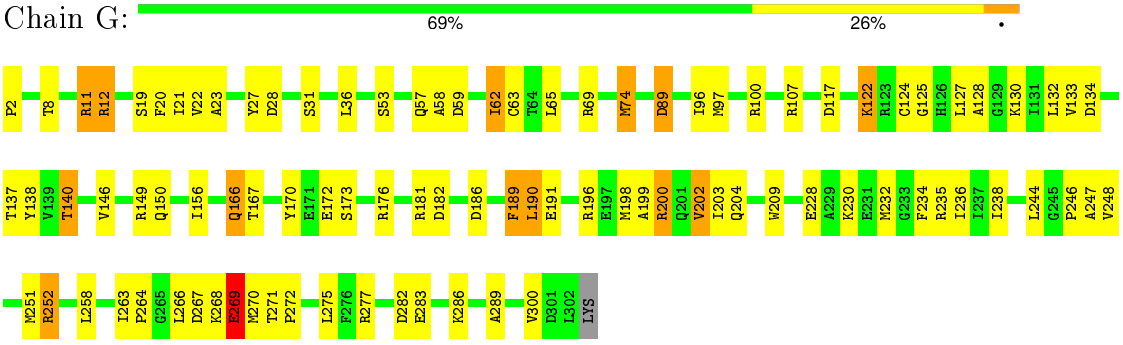
- Molecule 1: 2,3-dimethylmalate lyase

Chain F:



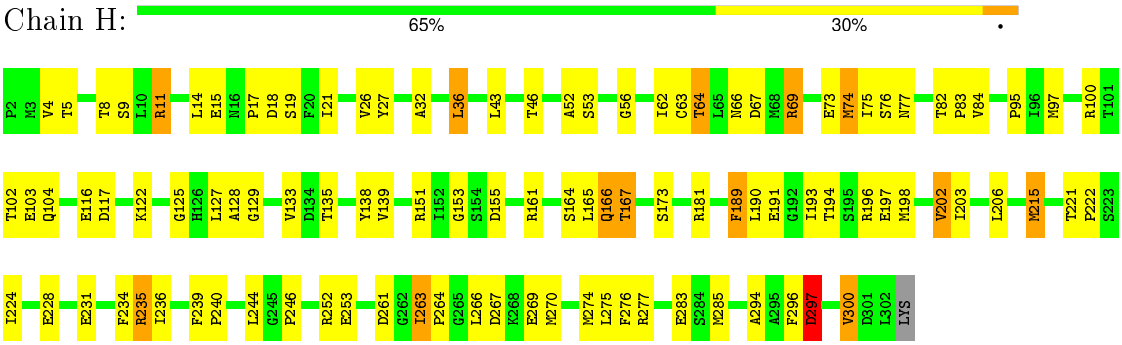
- Molecule 1: 2,3-dimethylmalate lyase

Chain G:



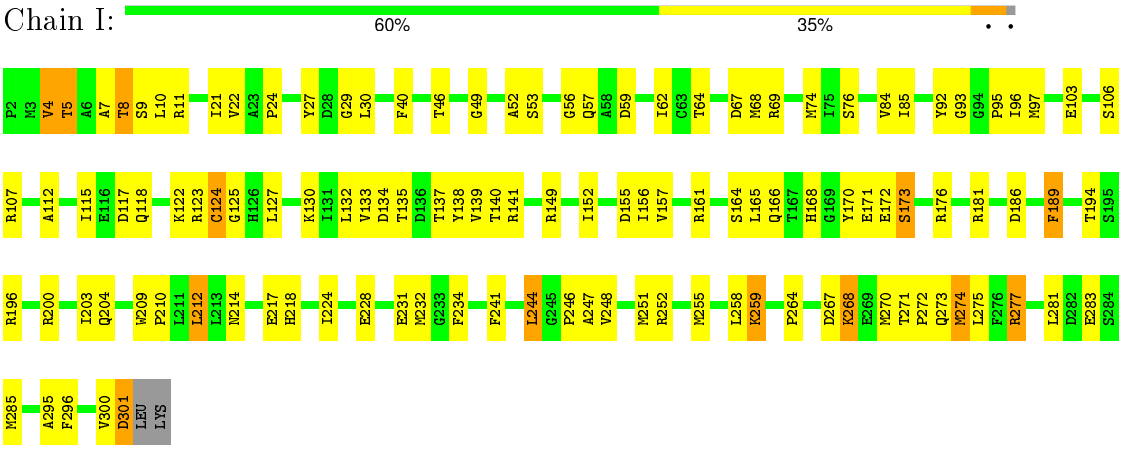
- Molecule 1: 2,3-dimethylmalate lyase

Chain H:



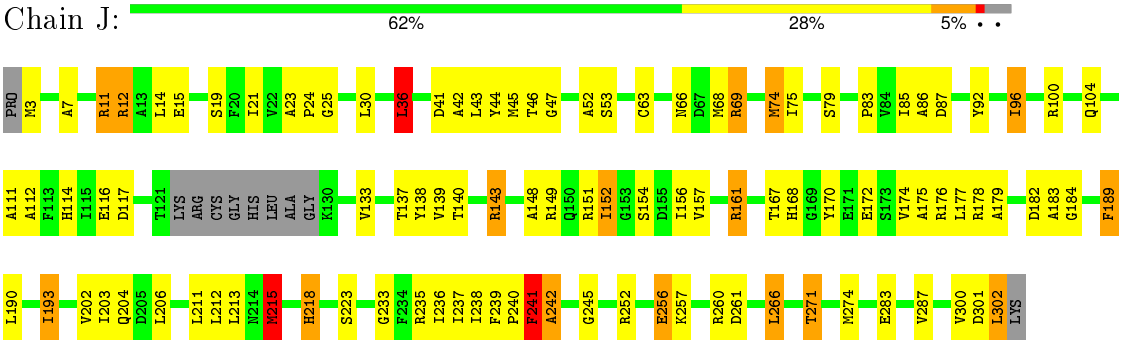
- Molecule 1: 2,3-dimethylmalate lyase

Chain I:



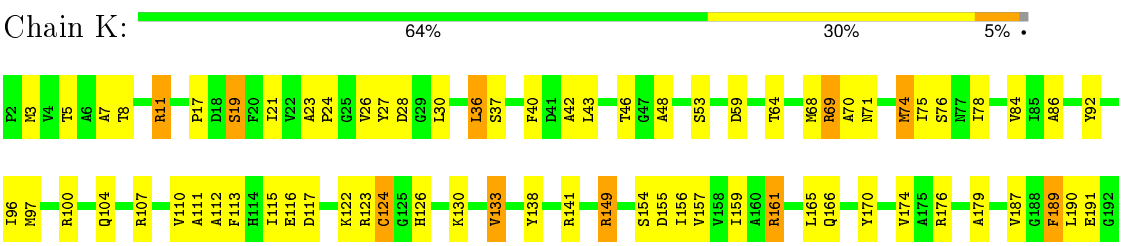
- Molecule 1: 2,3-dimethylmalate lyase

Chain J:



- Molecule 1: 2,3-dimethylmalate lyase

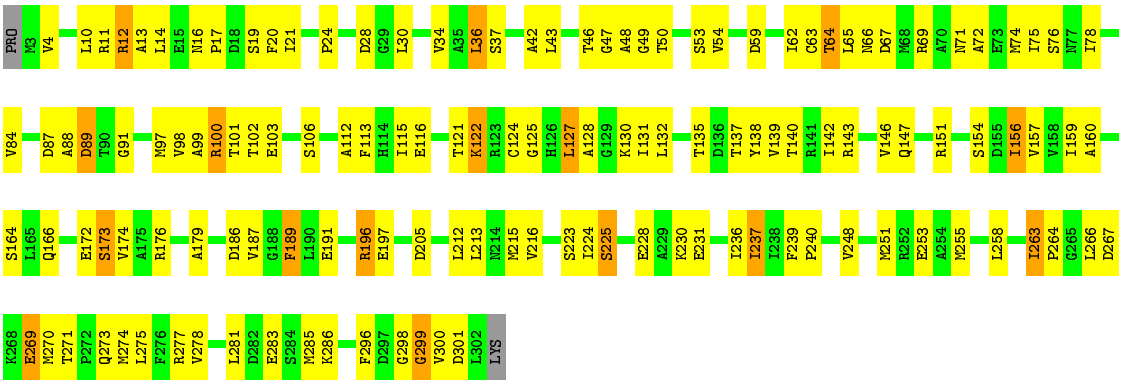
Chain K:



- Molecule 1: 2,3-dimethylmalate lyase

- Molecule 1: 2,3-dimethylmalate lyase

Chain L:

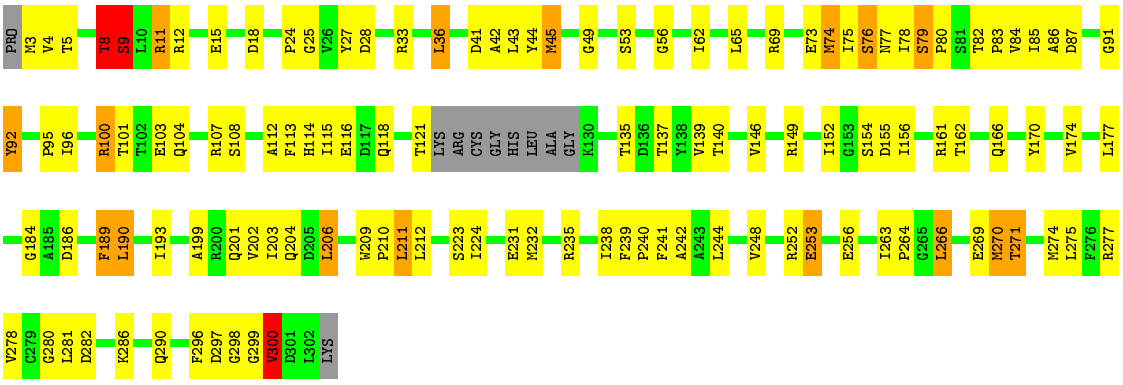


- Molecule 1: 2,3-dimethylmalate lyase

Chain M:

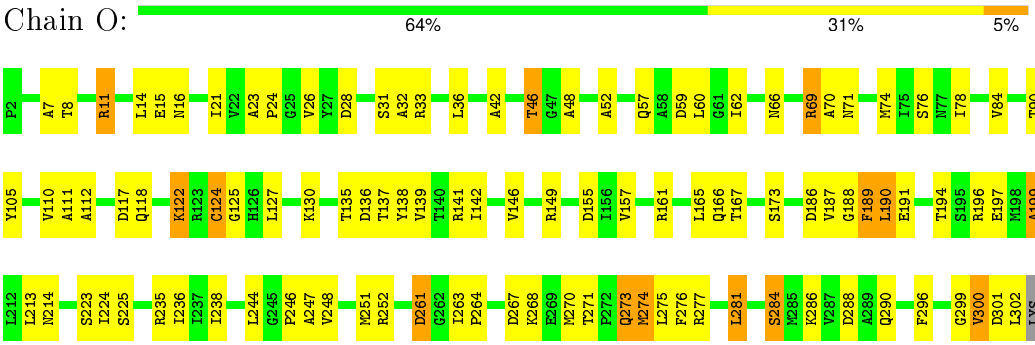
- Molecule 1: 2,3-dimethylmalate lyase

Chain N:



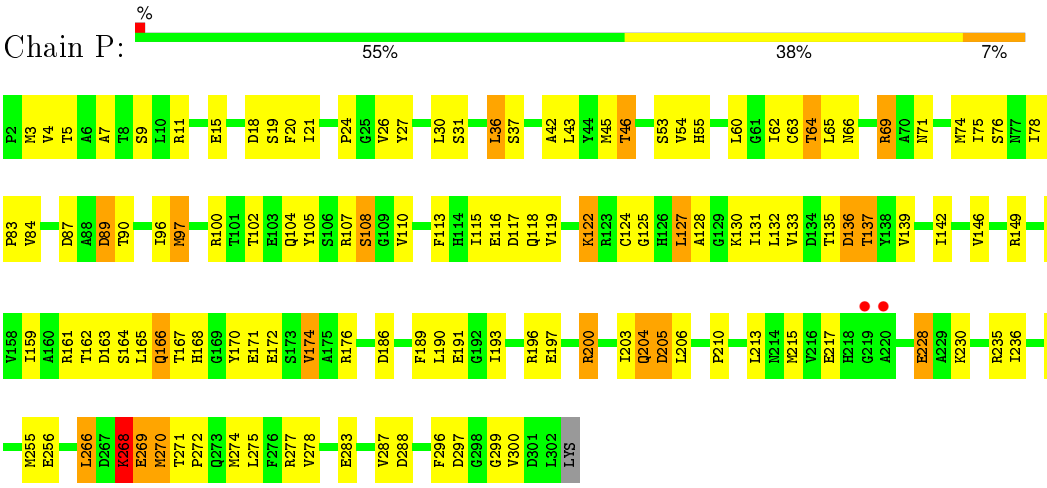
- Molecule 1: 2,3-dimethylmalate lyase

Chain O:



• Molecule 1: 2,3-dimethylmalate lyase

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	160.57Å 160.57Å 161.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.60 49.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-2.60) 94.3 (49.98-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.255 0.190 , 0.253	Depositor DCC
R_{free} test set	6752 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.9	EDS
Estimated twinning fraction	0.447 for -h,-k,l 0.084 for h,-h-k,-l 0.083 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 135026 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	36360	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.63 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.5454e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: OAF, MN, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.10	4/2255 (0.2%)	1.07	5/3053 (0.2%)
1	B	1.07	3/2263 (0.1%)	0.98	4/3063 (0.1%)
1	C	1.13	5/2261 (0.2%)	1.05	8/3060 (0.3%)
1	D	1.13	5/2259 (0.2%)	1.11	7/3057 (0.2%)
1	E	1.11	4/2261 (0.2%)	1.04	1/3060 (0.0%)
1	F	1.00	3/2257 (0.1%)	1.03	1/3056 (0.0%)
1	G	1.09	3/2261 (0.1%)	1.03	2/3060 (0.1%)
1	H	1.15	3/2261 (0.1%)	1.09	3/3060 (0.1%)
1	I	0.99	3/2249 (0.1%)	0.98	1/3044 (0.0%)
1	J	0.94	1/2192 (0.0%)	1.01	3/2967 (0.1%)
1	K	0.94	2/2251 (0.1%)	1.00	3/3046 (0.1%)
1	L	0.91	1/2247 (0.0%)	0.87	0/3041
1	M	0.94	0/2253	0.99	2/3049 (0.1%)
1	N	0.99	5/2191 (0.2%)	0.95	0/2966
1	O	0.98	1/2244 (0.0%)	0.94	0/3039
1	P	0.93	2/2258 (0.1%)	0.92	1/3056 (0.0%)
All	All	1.03	45/35963 (0.1%)	1.01	41/48677 (0.1%)

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	283	GLU	CG-CD	-15.69	1.28	1.51
1	P	63	CYS	CB-SG	-8.32	1.68	1.82
1	D	253	GLU	CG-CD	7.75	1.63	1.51
1	N	253	GLU	CG-CD	7.50	1.63	1.51
1	C	197	GLU	CG-CD	7.11	1.62	1.51
1	I	283	GLU	CG-CD	6.97	1.62	1.51
1	H	63	CYS	CB-SG	-6.93	1.70	1.82
1	L	63	CYS	CB-SG	-6.92	1.70	1.82
1	K	124	CYS	CB-SG	-6.83	1.70	1.82
1	D	253	GLU	CD-OE1	6.82	1.33	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	197	GLU	CD-OE2	6.64	1.32	1.25
1	G	283	GLU	CG-CD	6.58	1.61	1.51
1	F	171	GLU	CG-CD	6.56	1.61	1.51
1	H	197	GLU	CG-CD	6.45	1.61	1.51
1	H	253	GLU	CG-CD	6.45	1.61	1.51
1	B	171	GLU	CG-CD	6.37	1.61	1.51
1	C	63	CYS	CB-SG	-6.36	1.71	1.82
1	A	63	CYS	CB-SG	-6.33	1.71	1.82
1	F	200	ARG	CG-CD	6.23	1.67	1.51
1	G	269	GLU	CG-CD	6.20	1.61	1.51
1	A	171	GLU	CD-OE2	6.17	1.32	1.25
1	N	27	TYR	CD2-CE2	-6.10	1.30	1.39
1	G	63	CYS	CB-SG	-6.09	1.71	1.82
1	C	296	PHE	CD2-CE2	-6.02	1.27	1.39
1	E	4	VAL	CB-CG2	5.98	1.65	1.52
1	D	197	GLU	CG-CD	5.88	1.60	1.51
1	E	4	VAL	CB-CG1	5.80	1.65	1.52
1	N	253	GLU	CD-OE2	5.74	1.31	1.25
1	B	260	ARG	CG-CD	5.70	1.66	1.51
1	B	200	ARG	CG-CD	5.66	1.66	1.51
1	E	4	VAL	CA-CB	5.66	1.66	1.54
1	N	27	TYR	CD1-CE1	-5.63	1.30	1.39
1	C	283	GLU	CG-CD	5.53	1.60	1.51
1	A	283	GLU	CB-CG	5.50	1.62	1.52
1	P	269	GLU	CG-CD	5.42	1.60	1.51
1	J	241	PHE	CD2-CE2	5.35	1.50	1.39
1	O	124	CYS	CB-SG	-5.27	1.73	1.81
1	A	283	GLU	CG-CD	5.24	1.59	1.51
1	K	191	GLU	CB-CG	5.19	1.62	1.52
1	N	300	VAL	CA-CB	-5.16	1.44	1.54
1	I	4	VAL	CB-CG2	5.12	1.63	1.52
1	D	171	GLU	CD-OE2	5.11	1.31	1.25
1	F	197	GLU	CG-CD	5.08	1.59	1.51
1	E	269	GLU	CG-CD	5.07	1.59	1.51
1	I	171	GLU	CG-CD	5.05	1.59	1.51

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	235	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	C	141	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	J	161	ARG	NE-CZ-NH1	6.67	123.63	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	12	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	P	252	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	D	107	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	C	11	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	149	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	C	143	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	D	260	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	H	202	VAL	CB-CA-C	-5.92	100.15	111.40
1	M	261	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	28	ASP	CB-CG-OD1	5.64	123.38	118.30
1	K	123	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	C	11	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	D	200	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	D	235	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	C	141	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	107	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	G	200	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	F	149	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	B	74	MET	CG-SD-CE	-5.52	91.36	100.20
1	G	74	MET	CG-SD-CE	-5.52	91.37	100.20
1	B	69	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	67	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	J	215	MET	CG-SD-CE	5.50	109.00	100.20
1	A	74	MET	CG-SD-CE	-5.49	91.42	100.20
1	B	178	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	E	261	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	H	261	ASP	CB-CG-OD1	5.44	123.20	118.30
1	C	260	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	D	11	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	282	ASP	CB-CG-OD1	5.30	123.07	118.30
1	M	69	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	C	36	LEU	CB-CG-CD1	5.22	119.87	111.00
1	J	36	LEU	CA-CB-CG	5.22	127.30	115.30
1	I	117	ASP	CB-CG-OD1	5.20	122.98	118.30
1	D	296	PHE	CA-C-N	-5.17	105.83	117.20
1	C	123	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	K	275	LEU	CA-CB-CG	5.09	127.01	115.30
1	K	252	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	2222	0	2206	83	0
1	B	2230	0	2217	91	0
1	C	2228	0	2224	97	0
1	D	2226	0	2224	76	0
1	E	2228	0	2224	76	0
1	F	2224	0	2213	92	0
1	G	2228	0	2224	80	0
1	H	2228	0	2224	68	0
1	I	2216	0	2209	94	0
1	J	2162	0	2150	88	0
1	K	2218	0	2206	79	0
1	L	2215	0	2203	116	0
1	M	2220	0	2213	109	0
1	N	2161	0	2146	105	0
1	O	2211	0	2196	97	0
1	P	2225	0	2215	133	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	12	0	1	0	0
3	B	12	0	1	0	0
3	C	12	0	1	0	0
3	D	12	0	1	2	0
3	E	12	0	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	12	0	1	1	0
3	G	12	0	1	0	0
3	H	12	0	1	1	0
3	I	12	0	1	2	0
3	K	12	0	1	0	0
3	L	12	0	1	1	0
3	M	12	0	1	1	0
3	O	12	0	1	1	0
3	P	12	0	1	1	0
4	A	12	0	16	6	0
4	E	6	0	8	0	0
4	G	6	0	8	2	0
4	M	6	0	8	1	0
5	A	59	0	0	4	0
5	B	59	0	0	3	0
5	C	52	0	0	7	0
5	D	57	0	0	4	0
5	E	65	0	0	6	0
5	F	55	0	0	3	0
5	G	66	0	0	5	0
5	H	68	0	0	2	0
5	I	29	0	0	1	0
5	J	29	0	0	1	0
5	K	27	0	0	0	0
5	L	24	0	0	1	0
5	M	38	0	0	6	0
5	N	28	0	0	4	0
5	O	24	0	0	3	0
5	P	24	0	0	4	0
All	All	36360	0	35348	1315	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 19.

All (1315) 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:N:210:PRO:C	1:N:211:LEU:HD12	1.49	1.29
1:N:210:PRO:O	1:N:211:LEU:HD12	1.23	1.27
1:C:8:THR:HG22	1:C:155:ASP:OD2	1.38	1.19
1:L:10:LEU:O	1:L:14:LEU:HD12	1.41	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:62:ILE:HG23	1:L:97:MET:HE3	1.14	1.13
1:N:210:PRO:C	1:N:211:LEU:CD1	2.17	1.12
1:B:303:LYS:HD2	1:B:303:LYS:H	1.05	1.11
1:L:12:ARG:HH11	1:L:12:ARG:HG3	0.95	1.10
1:L:12:ARG:HH11	1:L:12:ARG:CG	1.65	1.10
1:K:5:THR:HG23	1:K:8:THR:HG23	1.35	1.09
1:L:97:MET:HE1	1:L:100:ARG:HE	1.01	1.09
1:G:53:SER:OG	4:G:601:GOL:H32	1.47	1.09
1:O:271:THR:O	1:O:275:LEU:HD12	1.50	1.08
1:F:212:LEU:HD23	1:F:236:ILE:HB	1.36	1.08
1:L:124:CYS:HB3	1:L:127:LEU:HD13	1.21	1.08
1:M:127:LEU:HD13	1:N:300:VAL:CG1	1.87	1.05
1:J:3:MET:CE	1:L:106:SER:HB3	1.87	1.04
1:M:193:ILE:HG23	1:M:198:MET:HG2	1.36	1.04
1:M:127:LEU:HD13	1:N:300:VAL:HG11	1.37	1.03
4:A:605:GOL:H12	5:A:814:HOH:O	1.59	1.02
1:M:127:LEU:N	1:M:127:LEU:HD23	1.74	1.01
1:N:210:PRO:O	1:N:211:LEU:CD1	2.10	0.99
1:L:11:ARG:HH22	1:L:186:ASP:CG	1.66	0.98
1:B:196:ARG:HD2	1:O:196:ARG:HE	1.26	0.98
1:J:3:MET:HE1	1:L:106:SER:HB3	1.41	0.97
1:B:303:LYS:HD2	1:B:303:LYS:N	1.78	0.97
1:C:121:THR:O	1:C:121:THR:HG23	1.66	0.96
1:C:181:ARG:HD2	5:C:533:HOH:O	1.64	0.95
1:N:211:LEU:N	1:N:211:LEU:CD1	2.30	0.95
1:M:264:PRO:HB2	1:M:266:LEU:CD1	1.96	0.95
1:L:132:LEU:HD11	1:L:164:SER:HA	1.46	0.95
1:M:127:LEU:HB3	1:N:300:VAL:HG13	1.47	0.94
1:J:85:ILE:HG23	1:J:112:ALA:HB3	1.50	0.93
1:B:303:LYS:CD	1:B:303:LYS:H	1.81	0.93
1:L:12:ARG:NH1	1:L:12:ARG:HG3	1.68	0.93
1:C:291:ALA:N	1:C:292:GLY:HA2	1.81	0.93
1:D:266:LEU:HD22	1:D:270:MET:HE3	1.50	0.93
4:M:606:GOL:H31	5:M:815:HOH:O	1.67	0.92
1:O:8:THR:HG22	1:O:155:ASP:OD2	1.70	0.91
1:P:124:CYS:HB3	1:P:127:LEU:HD23	1.52	0.91
1:I:64:THR:HG21	1:L:66:ASN:OD1	1.70	0.90
1:F:203:ILE:HD11	1:F:234:PHE:CD1	2.07	0.90
1:L:97:MET:HE1	1:L:100:ARG:NE	1.86	0.90
1:O:300:VAL:CG2	1:P:127:LEU:HD12	2.02	0.89
1:F:212:LEU:CD2	1:F:236:ILE:HB	2.02	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:196:ARG:HH12	1:P:228:GLU:HG2	1.36	0.88
1:I:62:ILE:CG2	1:L:97:MET:HE3	2.03	0.87
1:M:127:LEU:CD1	1:N:300:VAL:HG11	2.05	0.87
1:L:11:ARG:NH2	1:L:186:ASP:CG	2.28	0.87
1:L:97:MET:CE	1:L:100:ARG:HE	1.88	0.86
1:G:53:SER:OG	4:G:601:GOL:C3	2.24	0.86
1:L:125:GLY:HA3	1:L:191:GLU:OE2	1.76	0.86
1:B:66:ASN:OD1	1:C:64:THR:HG21	1.76	0.86
1:F:97:MET:HE3	1:G:62:ILE:HA	1.58	0.86
1:L:263:ILE:HG13	1:L:264:PRO:CD	2.06	0.85
1:P:124:CYS:HB3	1:P:127:LEU:CD2	2.07	0.85
1:M:133:VAL:CG1	1:M:137:THR:HB	2.07	0.84
1:H:263:ILE:HG13	1:H:264:PRO:HD2	1.60	0.84
1:P:213:LEU:HD11	1:P:215:MET:CE	2.07	0.83
1:N:211:LEU:N	1:N:211:LEU:HD12	1.85	0.83
1:O:127:LEU:HB3	1:P:300:VAL:HG13	1.58	0.83
1:N:116:GLU:HG2	5:N:702:HOH:O	1.77	0.83
1:P:213:LEU:HD11	1:P:215:MET:HE2	1.62	0.82
1:J:271:THR:HG22	1:J:274:MET:H	1.43	0.82
1:F:210:PRO:HA	1:F:235:ARG:HG3	1.62	0.81
1:M:193:ILE:CG2	1:M:198:MET:HG2	2.09	0.81
1:B:182:ASP:HB3	5:B:679:HOH:O	1.79	0.81
1:A:143:ARG:HB3	1:C:291:ALA:O	1.81	0.81
1:L:124:CYS:CB	1:L:127:LEU:HD13	2.09	0.80
1:D:266:LEU:HD22	1:D:270:MET:CE	2.11	0.80
1:P:124:CYS:CB	1:P:127:LEU:HD23	2.12	0.80
1:P:97:MET:CE	1:P:97:MET:HA	2.12	0.80
1:M:132:LEU:HD11	1:M:164:SER:HA	1.62	0.80
1:P:135:THR:O	1:P:139:VAL:HG23	1.81	0.80
1:K:5:THR:CG2	1:K:8:THR:HG23	2.11	0.80
1:M:126:HIS:C	1:M:127:LEU:HD23	2.02	0.80
1:A:127:LEU:HB3	1:B:300:VAL:HG22	1.62	0.80
1:H:300:VAL:O	1:H:300:VAL:CG1	2.30	0.80
1:L:10:LEU:O	1:L:14:LEU:CD1	2.29	0.80
1:J:137:THR:O	1:J:140:THR:HB	1.82	0.79
1:I:62:ILE:HG23	1:L:97:MET:CE	2.05	0.79
1:D:270:MET:HE2	5:D:698:HOH:O	1.81	0.79
4:A:605:GOL:H31	5:A:814:HOH:O	1.81	0.79
1:G:12:ARG:HG3	5:G:466:HOH:O	1.81	0.79
1:F:125:GLY:HA2	1:F:130:LYS:HE2	1.64	0.78
1:J:143:ARG:HB3	1:J:183:ALA:HB1	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:ILE:HD11	1:G:96:ILE:HG21	1.64	0.78
1:L:223:SER:O	1:L:224:ILE:HG13	1.83	0.78
1:C:8:THR:CG2	1:C:155:ASP:OD2	2.28	0.78
1:F:196:ARG:HD3	1:F:224:ILE:HG12	1.63	0.78
1:P:300:VAL:O	1:P:300:VAL:CG1	2.31	0.78
1:M:63:CYS:HB2	5:M:572:HOH:O	1.83	0.78
1:M:300:VAL:HG12	1:M:301:ASP:N	1.99	0.77
1:L:112:ALA:HB2	1:L:157:VAL:HB	1.66	0.77
1:I:217:GLU:OE2	1:J:266:LEU:HB2	1.85	0.77
1:I:203:ILE:HD13	1:I:232:MET:O	1.85	0.77
1:N:100:ARG:O	1:N:104:GLN:HG3	1.85	0.77
1:G:127:LEU:HG	1:H:300:VAL:HG13	1.67	0.77
1:O:300:VAL:HA	1:P:128:ALA:HB3	1.67	0.76
1:B:203:ILE:HD11	1:B:234:PHE:CE1	2.20	0.76
1:M:217:GLU:OE2	1:N:266:LEU:HB2	1.86	0.76
1:E:30:LEU:HD11	1:F:244:LEU:HD11	1.66	0.76
1:F:143:ARG:HG3	1:F:183:ALA:HB1	1.67	0.76
1:B:132:LEU:HD11	1:B:164:SER:HA	1.67	0.76
1:N:87:ASP:OD1	1:N:114:HIS:CE1	2.39	0.76
1:B:97:MET:CE	1:C:62:ILE:HG23	2.16	0.76
1:K:300:VAL:CB	1:L:127:LEU:HD23	2.16	0.75
1:J:283:GLU:O	1:J:287:VAL:HG23	1.85	0.75
1:D:64:THR:HG22	1:D:67:ASP:H	1.52	0.75
1:L:11:ARG:NH2	1:L:186:ASP:OD1	2.20	0.75
1:B:125:GLY:HA2	1:B:130:LYS:HE2	1.67	0.75
1:C:270:MET:HG3	1:C:274:MET:HE3	1.68	0.74
1:C:149:ARG:HD2	1:C:156:ILE:O	1.86	0.74
1:B:11:ARG:NH2	1:B:149:ARG:HH12	1.84	0.74
1:B:97:MET:HE1	1:C:62:ILE:HG23	1.69	0.74
1:I:196:ARG:NH1	1:I:228:GLU:OE1	2.20	0.74
1:D:198:MET:O	1:D:202:VAL:HG23	1.88	0.74
1:F:200:ARG:HG3	1:F:232:MET:HE3	1.67	0.74
1:B:196:ARG:HD2	1:O:196:ARG:NE	2.01	0.74
1:O:127:LEU:HD22	1:P:300:VAL:HG11	1.68	0.74
1:F:33:ARG:HD3	1:F:279:CYS:HA	1.70	0.73
1:O:263:ILE:HG13	1:O:264:PRO:HD2	1.70	0.73
1:N:252:ARG:O	1:N:256:GLU:HG3	1.88	0.73
1:F:62:ILE:HA	1:G:97:MET:HE3	1.68	0.73
1:P:124:CYS:SG	1:P:127:LEU:HD23	2.28	0.73
1:E:97:MET:HE3	1:H:62:ILE:HA	1.69	0.73
1:M:300:VAL:CG1	1:M:301:ASP:N	2.52	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:GLU:O	1:C:274:MET:HG3	1.88	0.72
1:N:62:ILE:HG23	1:O:97:MET:HE3	1.70	0.72
1:E:302:LEU:HD11	1:F:126:HIS:O	1.87	0.72
1:C:121:THR:CG2	1:C:121:THR:O	2.35	0.72
1:P:300:VAL:O	1:P:300:VAL:HG12	1.88	0.72
1:N:91:GLY:O	1:N:92:TYR:HB2	1.89	0.72
1:E:30:LEU:CD1	1:F:244:LEU:CD1	2.67	0.72
1:L:267:ASP:OD1	1:L:269:GLU:HB3	1.90	0.72
1:I:30:LEU:HD21	1:I:275:LEU:HD21	1.70	0.72
1:M:97:MET:CE	1:M:100:ARG:HG3	2.20	0.72
1:L:135:THR:O	1:L:139:VAL:HG23	1.89	0.72
1:M:252:ARG:HD3	5:M:645:HOH:O	1.90	0.72
1:J:256:GLU:HB2	1:J:260:ARG:HH12	1.52	0.72
1:P:102:THR:HG23	1:P:113:PHE:HZ	1.54	0.72
1:M:127:LEU:CD2	1:M:127:LEU:N	2.49	0.71
1:M:264:PRO:HB2	1:M:266:LEU:HD13	1.72	0.71
1:O:246:PRO:HD3	1:P:266:LEU:HD21	1.72	0.71
1:A:41:ASP:HB2	1:I:296:PHE:HA	1.71	0.71
1:K:276:PHE:HE1	1:L:127:LEU:HD11	1.55	0.71
1:K:301:ASP:OD2	1:K:301:ASP:N	2.23	0.71
1:D:270:MET:HB3	1:D:275:LEU:HD21	1.71	0.71
1:G:62:ILE:HD13	1:G:62:ILE:N	2.05	0.71
1:P:97:MET:HE2	1:P:97:MET:HA	1.73	0.71
1:M:123:ARG:NH1	1:M:128:ALA:O	2.23	0.71
1:A:263:ILE:HG13	1:A:264:PRO:HD2	1.72	0.71
1:H:161:ARG:HA	1:H:189:PHE:O	1.89	0.71
1:C:12:ARG:HG3	5:C:771:HOH:O	1.91	0.71
1:A:302:LEU:C	1:A:302:LEU:HD23	2.12	0.71
1:P:210:PRO:HA	1:P:235:ARG:HG3	1.73	0.70
1:K:11:ARG:NH1	1:K:155:ASP:O	2.23	0.70
1:I:64:THR:HG22	1:I:67:ASP:OD2	1.91	0.70
1:K:8:THR:HG22	1:K:155:ASP:OD2	1.92	0.70
1:O:299:GLY:C	1:O:300:VAL:HG12	2.11	0.70
1:B:213:LEU:HD23	1:B:237:ILE:HD12	1.73	0.70
1:E:300:VAL:HG22	1:F:127:LEU:HB3	1.73	0.70
1:M:95:PRO:HD2	1:O:288:ASP:OD1	1.92	0.70
1:P:64:THR:HG23	1:P:66:ASN:H	1.56	0.70
1:F:297:ASP:OD1	1:F:297:ASP:N	2.20	0.70
1:P:196:ARG:HH12	1:P:228:GLU:CG	2.05	0.70
1:L:263:ILE:HG13	1:L:264:PRO:HD2	1.72	0.70
1:E:30:LEU:CD1	1:F:244:LEU:HD11	2.21	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:300:VAL:CG1	1:N:300:VAL:O	2.41	0.69
1:C:288:ASP:O	1:C:293:GLY:N	2.20	0.69
1:B:11:ARG:CZ	1:B:149:ARG:HH12	2.06	0.69
1:A:129:GLY:O	1:A:130:LYS:C	2.30	0.69
1:I:7:ALA:HB1	1:I:156:ILE:HA	1.73	0.69
1:H:52:ALA:O	1:H:56:GLY:HA2	1.93	0.69
1:E:97:MET:HE1	1:H:62:ILE:HG23	1.72	0.69
1:L:16:ASN:OD1	1:L:16:ASN:C	2.30	0.69
1:A:97:MET:CE	1:D:62:ILE:HA	2.21	0.69
1:A:97:MET:HE3	1:D:62:ILE:HA	1.74	0.69
1:L:13:ALA:O	1:L:19:SER:HB2	1.93	0.69
1:I:125:GLY:HA2	1:I:130:LYS:HD3	1.74	0.69
1:B:294:ALA:HB1	1:B:297:ASP:OD2	1.92	0.69
1:C:119:VAL:HG23	1:C:121:THR:HG22	1.76	0.68
1:M:267:ASP:HB2	5:M:560:HOH:O	1.92	0.68
1:A:232:MET:HE3	1:A:234:PHE:HE1	1.58	0.68
1:H:64:THR:HG22	1:H:67:ASP:H	1.58	0.68
1:M:214:ASN:ND2	3:M:501:OAF:O6	2.26	0.68
1:O:300:VAL:HG23	1:P:127:LEU:HD12	1.76	0.68
1:G:149:ARG:HD2	1:G:156:ILE:O	1.93	0.68
1:N:149:ARG:HG3	1:N:156:ILE:HG22	1.75	0.68
1:E:62:ILE:HG23	1:H:97:MET:HE3	1.75	0.68
1:D:97:MET:CE	1:D:100:ARG:HG3	2.24	0.68
1:A:196:ARG:O	1:A:199:ALA:HB3	1.94	0.68
1:E:30:LEU:HD11	1:F:244:LEU:CD1	2.24	0.68
1:A:112:ALA:HB2	1:A:157:VAL:HB	1.74	0.68
1:A:289:ALA:O	1:A:292:GLY:HA3	1.94	0.68
1:L:213:LEU:HD23	1:L:237:ILE:HG13	1.77	0.68
1:D:270:MET:CE	5:D:698:HOH:O	2.39	0.67
1:P:19:SER:O	1:P:235:ARG:NH2	2.24	0.67
1:I:52:ALA:O	1:I:56:GLY:HA2	1.94	0.67
1:P:102:THR:HG23	1:P:113:PHE:CZ	2.29	0.67
1:E:66:ASN:OD1	1:H:64:THR:HG21	1.95	0.67
1:I:95:PRO:HG3	1:I:140:THR:HG22	1.75	0.67
1:B:62:ILE:HG23	1:C:97:MET:HE1	1.75	0.67
1:F:97:MET:CE	1:G:62:ILE:HG23	2.25	0.67
1:B:62:ILE:HG23	1:C:97:MET:CE	2.24	0.67
1:P:76:SER:HA	1:P:84:VAL:HG21	1.77	0.67
1:I:271:THR:HB	1:I:272:PRO:HD2	1.75	0.67
1:M:161:ARG:HA	1:M:189:PHE:HB3	1.75	0.67
1:F:116:GLU:OE2	1:F:122:LYS:NZ	2.26	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:ARG:NH1	1:E:228:GLU:OE2	2.27	0.67
1:N:87:ASP:OD1	1:N:114:HIS:HE1	1.76	0.67
1:H:294:ALA:O	1:H:297:ASP:HB2	1.95	0.67
1:M:127:LEU:CD1	1:N:300:VAL:CG1	2.65	0.66
1:I:224:ILE:HG21	1:I:232:MET:HE3	1.77	0.66
1:C:137:THR:O	1:C:140:THR:HB	1.94	0.66
1:M:66:ASN:N	1:M:66:ASN:OD1	2.28	0.66
1:L:124:CYS:HB3	1:L:127:LEU:CD1	2.13	0.66
1:O:300:VAL:HG21	1:P:127:LEU:HD12	1.77	0.66
1:L:125:GLY:N	3:L:501:OAF:O5	2.24	0.66
1:J:256:GLU:HB2	1:J:260:ARG:NH1	2.10	0.66
1:B:47:GLY:HA3	1:B:87:ASP:OD2	1.95	0.66
1:C:224:ILE:HG21	1:C:232:MET:HE2	1.77	0.66
1:O:274:MET:HE3	1:O:275:LEU:HA	1.77	0.66
1:N:211:LEU:HD13	1:N:211:LEU:N	2.09	0.66
1:L:12:ARG:NH1	1:L:12:ARG:CG	2.38	0.66
1:D:64:THR:HG22	1:D:67:ASP:CG	2.16	0.66
1:F:133:VAL:HG21	1:F:137:THR:HG21	1.76	0.66
1:B:133:VAL:HG21	1:B:137:THR:HG21	1.77	0.66
1:P:275:LEU:O	1:P:278:VAL:HB	1.96	0.66
1:P:196:ARG:NH1	1:P:228:GLU:HG2	2.10	0.66
1:O:11:ARG:NH2	1:O:186:ASP:OD1	2.28	0.66
1:P:116:GLU:OE1	1:P:122:LYS:HD2	1.97	0.65
1:A:181:ARG:HG3	1:A:209:TRP:CE2	2.31	0.65
1:B:149:ARG:HD2	1:B:156:ILE:O	1.95	0.65
1:A:130:LYS:H	1:A:166:GLN:NE2	1.93	0.65
1:I:133:VAL:CG1	1:I:137:THR:HB	2.26	0.65
1:I:244:LEU:HD11	1:J:30:LEU:HD11	1.79	0.65
1:N:210:PRO:C	1:N:211:LEU:HD13	2.12	0.65
1:D:11:ARG:NH1	1:D:155:ASP:O	2.27	0.65
1:M:130:LYS:HD2	1:M:163:ASP:HB3	1.76	0.65
1:L:216:VAL:CG2	1:L:240:PRO:HG2	2.27	0.65
1:D:64:THR:CG2	1:D:67:ASP:H	2.09	0.65
1:N:170:TYR:O	1:N:174:VAL:HG23	1.96	0.65
1:O:275:LEU:HD23	1:P:244:LEU:CD2	2.26	0.65
1:A:252:ARG:O	1:A:256:GLU:HG2	1.96	0.65
1:F:97:MET:HE1	1:G:62:ILE:HG23	1.78	0.65
1:M:149:ARG:HG3	1:M:156:ILE:HG22	1.79	0.65
1:E:95:PRO:HG3	1:E:140:THR:HG22	1.79	0.65
1:B:62:ILE:HA	1:C:97:MET:HE3	1.79	0.65
1:E:11:ARG:HH12	1:E:157:VAL:HA	1.62	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:10:LEU:HG	1:L:14:LEU:HD11	1.79	0.64
1:C:247:ALA:O	1:C:251:MET:HG3	1.97	0.64
1:E:229:ALA:HA	1:E:232:MET:HE2	1.78	0.64
1:N:266:LEU:HD22	1:N:270:MET:HG2	1.79	0.64
1:I:212:LEU:C	1:I:212:LEU:HD23	2.17	0.64
1:J:3:MET:HE1	1:L:106:SER:CB	2.22	0.64
1:O:273:GLN:NE2	1:O:300:VAL:O	2.29	0.64
1:H:263:ILE:HG13	1:H:264:PRO:CD	2.26	0.64
1:P:97:MET:HE1	1:P:100:ARG:HE	1.62	0.64
1:O:277:ARG:HD3	5:O:595:HOH:O	1.96	0.64
1:E:30:LEU:HD13	1:F:244:LEU:CD1	2.28	0.64
1:L:46:THR:HG23	1:L:49:GLY:HA3	1.79	0.64
1:B:303:LYS:CD	1:B:303:LYS:N	2.42	0.64
1:H:300:VAL:O	1:H:300:VAL:HG13	1.97	0.64
1:E:199:ALA:O	1:E:202:VAL:HG12	1.98	0.64
1:O:274:MET:CE	1:O:275:LEU:HG	2.29	0.63
1:K:276:PHE:CE1	1:L:127:LEU:HD11	2.32	0.63
1:B:11:ARG:HH22	1:B:186:ASP:CG	2.00	0.63
1:I:300:VAL:O	1:I:301:ASP:HB2	1.96	0.63
1:L:225:SER:HB2	1:L:228:GLU:H	1.64	0.63
1:O:48:ALA:HA	1:O:59:ASP:HB2	1.81	0.63
1:K:97:MET:HE1	1:K:100:ARG:HD3	1.79	0.63
1:A:130:LYS:H	1:A:166:GLN:HE22	1.46	0.63
1:I:132:LEU:HD11	1:I:164:SER:HA	1.80	0.63
1:I:8:THR:HG23	1:I:155:ASP:OD2	1.98	0.63
1:N:286:LYS:O	1:N:290:GLN:HB2	1.98	0.63
1:J:112:ALA:HB2	1:J:157:VAL:HB	1.81	0.63
1:L:64:THR:HG23	1:L:66:ASN:H	1.64	0.63
1:M:228:GLU:O	1:M:232:MET:HG3	1.99	0.63
1:N:135:THR:O	1:N:139:VAL:HG23	1.98	0.63
1:A:57:GLN:HG3	1:A:62:ILE:HD13	1.81	0.63
1:O:301:ASP:O	1:O:302:LEU:CB	2.46	0.63
1:N:212:LEU:HD23	1:N:212:LEU:C	2.19	0.63
1:A:199:ALA:O	1:A:202:VAL:HG12	1.99	0.63
1:C:125:GLY:HA2	1:C:130:LYS:HE3	1.81	0.63
1:F:203:ILE:HD11	1:F:234:PHE:CE1	2.33	0.62
1:D:161:ARG:HA	1:D:189:PHE:O	1.99	0.62
1:M:23:ALA:HB3	1:M:238:ILE:HG22	1.80	0.62
1:K:116:GLU:HB3	1:K:161:ARG:HG2	1.81	0.62
1:B:210:PRO:HB3	1:B:235:ARG:HG3	1.81	0.62
1:J:45:MET:HE2	1:J:86:ALA:HB1	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:198:MET:O	1:H:202:VAL:HG23	2.00	0.62
1:A:46:THR:HG23	1:A:49:GLY:HA3	1.81	0.62
1:H:18:ASP:HB3	5:H:310:HOH:O	1.98	0.62
1:O:26:VAL:O	1:O:46:THR:HG22	1.99	0.62
1:K:24:PRO:HD2	1:K:42:ALA:O	1.99	0.62
1:C:270:MET:CE	1:C:274:MET:HE1	2.29	0.62
1:P:125:GLY:N	3:P:501:OAF:O5	2.27	0.62
1:F:62:ILE:HG23	1:G:97:MET:CE	2.30	0.62
1:G:117:ASP:HB3	1:G:138:TYR:CD1	2.35	0.62
1:H:14:LEU:HD21	1:H:236:ILE:HD11	1.80	0.62
1:N:62:ILE:HA	1:O:97:MET:HE3	1.81	0.61
1:P:299:GLY:HA2	5:P:397:HOH:O	2.00	0.61
1:O:135:THR:O	1:O:139:VAL:HG23	2.00	0.61
1:F:210:PRO:CA	1:F:235:ARG:HG3	2.28	0.61
1:P:125:GLY:HA3	1:P:191:GLU:OE2	2.00	0.61
1:G:20:PHE:CG	1:G:230:LYS:HG3	2.35	0.61
1:J:212:LEU:HD23	1:J:212:LEU:C	2.20	0.61
1:H:21:ILE:HB	1:H:236:ILE:HG12	1.82	0.61
1:D:97:MET:HE2	1:D:100:ARG:HG3	1.80	0.61
1:F:212:LEU:HD23	1:F:236:ILE:CB	2.22	0.61
1:P:119:VAL:HG13	1:P:131:ILE:HG22	1.83	0.61
1:H:11:ARG:NH1	1:H:155:ASP:O	2.33	0.61
1:C:282:ASP:HB2	5:C:320:HOH:O	2.00	0.61
1:O:299:GLY:O	1:O:300:VAL:HB	1.99	0.61
1:E:95:PRO:HG3	1:E:140:THR:CG2	2.31	0.61
1:I:107:ARG:O	1:K:107:ARG:HB3	2.00	0.61
1:J:206:LEU:HD12	1:J:211:LEU:HD21	1.83	0.61
1:E:64:THR:O	1:E:67:ASP:HB2	2.01	0.61
1:H:193:ILE:O	1:H:221:THR:HA	2.00	0.61
1:J:21:ILE:HB	1:J:236:ILE:HG13	1.83	0.61
1:M:95:PRO:HG3	1:M:140:THR:CG2	2.31	0.60
1:E:123:ARG:CG	1:E:127:LEU:HD12	2.31	0.60
1:I:161:ARG:NH2	3:I:501:OAF:O3	2.32	0.60
1:I:127:LEU:HD22	1:J:300:VAL:HB	1.81	0.60
1:M:96:ILE:O	1:M:100:ARG:HG2	2.01	0.60
1:J:170:TYR:O	1:J:174:VAL:HG23	2.01	0.60
1:H:161:ARG:HA	1:H:189:PHE:HB3	1.82	0.60
1:P:157:VAL:HG13	1:P:186:ASP:HB2	1.84	0.60
1:O:127:LEU:HD22	1:P:300:VAL:CG1	2.31	0.60
1:P:37:SER:HB2	5:P:749:HOH:O	2.00	0.60
1:O:300:VAL:CG2	1:P:127:LEU:CD1	2.78	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:97:MET:HE1	1:M:100:ARG:HG3	1.84	0.60
1:O:296:PHE:CZ	1:P:60:LEU:HD22	2.37	0.60
1:C:161:ARG:HA	1:C:189:PHE:HB3	1.83	0.60
1:E:76:SER:HA	1:E:84:VAL:HG21	1.84	0.60
1:P:213:LEU:HD11	1:P:215:MET:HE3	1.84	0.59
1:C:270:MET:HG3	1:C:274:MET:CE	2.32	0.59
1:N:146:VAL:HG11	1:N:184:GLY:O	2.02	0.59
1:A:57:GLN:HG3	1:A:62:ILE:CD1	2.33	0.59
1:M:274:MET:O	1:M:278:VAL:HG23	2.01	0.59
1:I:271:THR:HB	1:I:272:PRO:CD	2.32	0.59
1:C:270:MET:HA	1:C:274:MET:HE2	1.84	0.59
1:J:212:LEU:HD21	1:J:238:ILE:HG12	1.83	0.59
1:B:244:LEU:HD12	1:B:244:LEU:C	2.23	0.59
1:B:148:ALA:HA	1:B:151:ARG:NH1	2.18	0.59
1:O:161:ARG:HA	1:O:189:PHE:HB3	1.85	0.59
1:K:19:SER:O	1:K:235:ARG:NH1	2.36	0.59
1:F:125:GLY:CA	1:F:130:LYS:HE2	2.32	0.59
1:N:44:TYR:OH	1:N:114:HIS:NE2	2.30	0.59
1:F:179:ALA:O	1:F:182:ASP:HB3	2.03	0.59
1:I:258:LEU:HD13	1:I:264:PRO:HG3	1.84	0.59
1:N:235:ARG:HB3	1:N:235:ARG:NH1	2.17	0.59
1:A:11:ARG:NH2	1:A:186:ASP:OD1	2.36	0.59
1:L:281:LEU:O	1:L:285:MET:HB2	2.02	0.59
1:P:270:MET:HG2	1:P:275:LEU:HD21	1.85	0.59
1:K:161:ARG:HA	1:K:189:PHE:O	2.02	0.59
1:K:76:SER:HA	1:K:84:VAL:HG21	1.85	0.59
1:E:117:ASP:O	1:E:132:LEU:HD22	2.03	0.58
1:P:133:VAL:HG21	1:P:137:THR:HB	1.83	0.58
1:C:245:GLY:HA2	1:D:275:LEU:HD11	1.84	0.58
1:M:97:MET:HE2	1:M:100:ARG:HG3	1.86	0.58
1:J:149:ARG:HG2	1:J:154:SER:O	2.03	0.58
1:L:76:SER:HA	1:L:84:VAL:HG21	1.85	0.58
1:J:12:ARG:O	1:J:15:GLU:HB2	2.02	0.58
1:G:11:ARG:NH2	1:G:186:ASP:OD1	2.36	0.58
1:N:277:ARG:HD3	1:N:282:ASP:OD2	2.03	0.58
1:L:130:LYS:HE3	1:L:166:GLN:HG2	1.86	0.58
1:C:248:VAL:HG22	1:D:30:LEU:HD22	1.86	0.58
1:M:125:GLY:O	1:M:130:LYS:HE2	2.04	0.58
1:E:16:ASN:O	1:E:235:ARG:NH2	2.37	0.58
1:G:190:LEU:HD12	1:G:202:VAL:HG11	1.85	0.58
1:A:86:ALA:O	1:A:113:PHE:HA	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:133:VAL:HG11	1:M:137:THR:HB	1.85	0.58
1:M:7:ALA:HB1	1:M:156:ILE:HA	1.86	0.58
1:I:161:ARG:HA	1:I:189:PHE:HB3	1.85	0.58
1:N:206:LEU:CD2	1:N:209:TRP:HE3	2.16	0.58
1:K:113:PHE:HE2	1:K:156:ILE:HG12	1.69	0.58
1:O:296:PHE:CZ	1:P:60:LEU:CD2	2.87	0.58
1:E:282:ASP:HB2	5:E:375:HOH:O	2.03	0.58
1:H:267:ASP:OD1	1:H:269:GLU:HB3	2.04	0.58
1:I:268:LYS:HA	1:J:218:HIS:CD2	2.39	0.58
1:M:300:VAL:CG1	1:M:301:ASP:H	2.17	0.58
1:C:193:ILE:HG23	1:C:198:MET:HG2	1.86	0.58
1:A:266:LEU:HD21	1:B:245:GLY:HA3	1.84	0.58
1:I:181:ARG:HB2	1:I:209:TRP:CZ2	2.39	0.58
1:C:291:ALA:N	1:C:292:GLY:CA	2.63	0.58
1:O:23:ALA:HB3	1:O:238:ILE:HG22	1.86	0.58
1:E:149:ARG:NH1	5:E:596:HOH:O	2.35	0.58
1:C:291:ALA:H	1:C:292:GLY:HA2	1.69	0.57
1:I:214:ASN:ND2	3:I:501:OAF:O6	2.37	0.57
1:E:181:ARG:HG3	1:E:209:TRP:CE2	2.39	0.57
1:P:75:ILE:HA	1:P:78:ILE:HD12	1.86	0.57
1:F:212:LEU:CD2	1:F:236:ILE:CB	2.79	0.57
1:L:223:SER:C	1:L:224:ILE:HG13	2.25	0.57
1:E:97:MET:CE	1:H:62:ILE:HG23	2.34	0.57
1:H:285:MET:HG2	1:H:296:PHE:CG	2.39	0.57
1:L:196:ARG:HH11	1:L:196:ARG:HG2	1.69	0.57
1:P:197:GLU:HB3	5:P:774:HOH:O	2.05	0.57
1:M:273:GLN:HG3	1:M:277:ARG:HH12	1.69	0.57
1:B:285:MET:HG2	1:B:296:PHE:CG	2.38	0.57
1:N:91:GLY:O	1:N:92:TYR:CB	2.52	0.57
1:P:104:GLN:O	1:P:108:SER:HB2	2.04	0.57
1:D:102:THR:HG23	1:D:113:PHE:CZ	2.40	0.57
1:O:8:THR:CG2	1:O:155:ASP:OD2	2.51	0.57
1:B:259:LYS:HA	1:I:300:VAL:HG22	1.87	0.57
1:P:117:ASP:OD2	1:P:162:THR:HA	2.04	0.57
1:H:300:VAL:HG12	1:H:300:VAL:O	2.03	0.57
1:B:96:ILE:HG21	1:C:62:ILE:CD1	2.34	0.57
1:C:270:MET:HE2	1:C:274:MET:HE1	1.86	0.57
1:O:90:THR:HG21	1:O:118:GLN:O	2.04	0.57
1:N:11:ARG:NH2	1:N:186:ASP:OD1	2.37	0.57
1:O:21:ILE:HB	1:O:236:ILE:HG12	1.87	0.57
1:G:203:ILE:HD11	1:G:234:PHE:CE1	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:200:ARG:O	1:I:204:GLN:HG2	2.04	0.57
1:I:30:LEU:HD21	1:I:275:LEU:CD2	2.35	0.57
1:P:271:THR:O	1:P:275:LEU:HD23	2.05	0.57
1:J:174:VAL:O	1:J:177:LEU:N	2.38	0.57
1:L:189:PHE:CD2	1:L:189:PHE:C	2.78	0.57
1:P:124:CYS:SG	1:P:127:LEU:CD2	2.93	0.57
1:E:64:THR:HG22	1:E:67:ASP:H	1.69	0.57
1:D:142:ILE:O	1:D:146:VAL:HG23	2.04	0.57
1:J:152:ILE:HD12	1:J:154:SER:HB2	1.87	0.56
1:J:68:MET:HG3	1:J:92:TYR:OH	2.05	0.56
1:G:128:ALA:HA	1:G:166:GLN:HE22	1.70	0.56
1:A:132:LEU:HD11	1:A:164:SER:HA	1.87	0.56
1:G:96:ILE:HG12	5:G:516:HOH:O	2.04	0.56
1:I:29:GLY:HA3	1:J:52:ALA:O	2.04	0.56
1:A:62:ILE:HG23	1:D:97:MET:HE1	1.87	0.56
1:P:130:LYS:CE	1:P:166:GLN:HG2	2.34	0.56
1:B:149:ARG:HG3	1:B:156:ILE:HG22	1.87	0.56
1:C:163:ASP:OD1	1:C:191:GLU:HG2	2.05	0.56
1:P:132:LEU:HD11	1:P:164:SER:HA	1.87	0.56
1:O:76:SER:HA	1:O:84:VAL:HG21	1.85	0.56
1:G:270:MET:HB3	1:G:275:LEU:HD21	1.88	0.56
1:M:45:MET:HG3	1:M:75:ILE:HD12	1.87	0.56
1:D:281:LEU:HD21	1:D:300:VAL:HG11	1.88	0.56
1:L:189:PHE:HD2	1:L:189:PHE:C	2.09	0.56
1:M:57:GLN:HG2	1:M:62:ILE:HD12	1.87	0.56
1:C:263:ILE:HG13	1:C:264:PRO:CD	2.35	0.56
1:M:211:LEU:HB2	5:M:582:HOH:O	2.06	0.56
1:P:132:LEU:HD12	1:P:168:HIS:CE1	2.41	0.56
1:E:263:ILE:HG13	1:E:264:PRO:CD	2.35	0.56
1:G:146:VAL:O	1:G:150:GLN:HG2	2.06	0.56
1:F:62:ILE:HG23	1:G:97:MET:HE1	1.86	0.56
1:I:149:ARG:HG2	1:I:156:ILE:HG22	1.87	0.56
1:N:238:ILE:HD12	1:N:240:PRO:HG3	1.87	0.56
1:J:3:MET:HE3	1:L:106:SER:HB3	1.83	0.56
1:L:273:GLN:O	1:L:277:ARG:HB2	2.06	0.56
1:O:130:LYS:H	1:O:166:GLN:NE2	2.03	0.56
1:D:114:HIS:HB3	1:D:159:ILE:HB	1.88	0.56
1:L:12:ARG:N	1:L:12:ARG:CD	2.68	0.56
1:F:200:ARG:HG3	1:F:232:MET:CE	2.33	0.56
1:B:244:LEU:O	1:B:248:VAL:HG23	2.06	0.56
1:F:181:ARG:CZ	1:F:209:TRP:HB2	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:GLN:HE22	1:D:291:ALA:HA	1.71	0.56
1:C:198:MET:O	1:C:202:VAL:HG22	2.06	0.56
1:B:170:TYR:O	1:B:174:VAL:HG23	2.06	0.56
1:M:203:ILE:HD11	1:M:234:PHE:CD1	2.41	0.56
1:O:299:GLY:O	1:O:300:VAL:CB	2.53	0.55
1:A:203:ILE:HD11	1:A:234:PHE:CE1	2.40	0.55
1:L:91:GLY:HA3	1:L:98:VAL:HG22	1.87	0.55
1:O:122:LYS:HD3	1:O:122:LYS:C	2.26	0.55
1:N:86:ALA:O	1:N:113:PHE:HA	2.06	0.55
1:L:112:ALA:CB	1:L:157:VAL:HB	2.36	0.55
1:F:170:TYR:O	1:F:174:VAL:HG23	2.06	0.55
1:I:135:THR:O	1:I:139:VAL:HG23	2.06	0.55
1:B:97:MET:HE1	1:C:62:ILE:CG2	2.35	0.55
1:A:170:TYR:O	1:A:173:SER:HB2	2.06	0.55
1:C:11:ARG:NH2	1:C:186:ASP:OD1	2.39	0.55
1:O:274:MET:HE3	1:O:275:LEU:CA	2.37	0.55
1:C:267:ASP:OD1	1:C:269:GLU:HB3	2.07	0.55
1:D:57:GLN:HG2	1:D:62:ILE:HD12	1.89	0.55
1:I:46:THR:HG23	1:I:49:GLY:HA3	1.86	0.55
1:M:271:THR:HB	1:M:272:PRO:CD	2.36	0.55
1:M:127:LEU:HD13	1:N:300:VAL:HG13	1.83	0.55
1:A:232:MET:CE	1:A:234:PHE:HE1	2.18	0.55
1:B:244:LEU:CD1	1:B:244:LEU:C	2.75	0.55
1:O:124:CYS:HB3	1:O:127:LEU:HG	1.89	0.55
1:F:16:ASN:O	1:F:235:ARG:NH2	2.39	0.55
1:M:142:ILE:O	1:M:146:VAL:HG22	2.07	0.55
1:J:74:MET:CE	1:J:75:ILE:HG13	2.36	0.55
1:I:172:GLU:O	1:I:173:SER:C	2.45	0.55
1:J:14:LEU:HD21	1:J:236:ILE:HD11	1.88	0.55
1:N:235:ARG:HH11	1:N:235:ARG:HB3	1.72	0.55
1:N:45:MET:HG3	1:N:75:ILE:HD12	1.87	0.55
1:A:300:VAL:O	1:A:300:VAL:HG13	2.07	0.55
1:J:117:ASP:HB3	1:J:138:TYR:CD1	2.41	0.55
1:J:143:ARG:CB	1:J:183:ALA:HB1	2.34	0.55
1:O:130:LYS:HD2	1:O:166:GLN:NE2	2.22	0.55
1:C:14:LEU:O	1:C:235:ARG:NH2	2.40	0.55
1:N:206:LEU:CD2	1:N:209:TRP:CE3	2.90	0.55
1:G:133:VAL:HG21	1:G:137:THR:HG21	1.88	0.55
1:M:275:LEU:HD22	1:N:244:LEU:HD23	1.89	0.54
1:N:199:ALA:O	1:N:203:ILE:HG13	2.07	0.54
1:J:85:ILE:HG23	1:J:112:ALA:CB	2.32	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:190:LEU:HB3	1:K:193:ILE:HD11	1.87	0.54
1:L:12:ARG:HD3	1:L:12:ARG:N	2.22	0.54
1:A:266:LEU:HD23	1:A:270:MET:HG3	1.89	0.54
1:P:132:LEU:HD12	1:P:168:HIS:ND1	2.22	0.54
1:F:168:HIS:CB	1:F:172:GLU:HG2	2.38	0.54
1:O:125:GLY:HA3	1:O:191:GLU:OE2	2.07	0.54
1:I:152:ILE:HD12	1:K:3:MET:CE	2.38	0.54
1:B:178:ARG:NH2	1:B:205:ASP:O	2.41	0.54
1:A:89:ASP:OD2	1:A:122:LYS:NZ	2.34	0.54
1:M:244:LEU:HD23	1:M:244:LEU:C	2.28	0.54
1:K:276:PHE:HE1	1:L:127:LEU:CD1	2.19	0.54
1:P:113:PHE:HE1	1:P:115:ILE:HD11	1.72	0.54
1:P:130:LYS:HE2	1:P:166:GLN:HG2	1.89	0.54
1:C:300:VAL:HB	1:D:127:LEU:HD22	1.90	0.54
1:G:22:VAL:O	1:G:22:VAL:HG23	2.07	0.54
1:G:125:GLY:HA3	1:G:191:GLU:OE2	2.08	0.54
1:N:62:ILE:HG23	1:O:97:MET:CE	2.38	0.54
1:P:4:VAL:HG22	1:P:5:THR:H	1.72	0.54
1:E:57:GLN:HG2	1:E:62:ILE:HD13	1.89	0.54
1:J:47:GLY:HA3	1:J:87:ASP:OD2	2.08	0.54
1:G:300:VAL:HB	1:H:127:LEU:HD22	1.89	0.54
1:F:285:MET:HG2	1:F:296:PHE:CG	2.43	0.54
1:I:224:ILE:HG21	1:I:232:MET:CE	2.37	0.54
1:B:266:LEU:HD13	1:B:270:MET:SD	2.48	0.54
1:N:76:SER:HA	1:N:84:VAL:HG21	1.89	0.54
1:N:300:VAL:O	1:N:300:VAL:HG13	2.08	0.54
1:K:30:LEU:HD22	1:L:248:VAL:HG22	1.90	0.54
1:B:286:LYS:O	1:B:290:GLN:HG3	2.08	0.54
1:K:113:PHE:CE2	1:K:156:ILE:HG12	2.43	0.53
1:C:64:THR:HG22	1:C:67:ASP:H	1.72	0.53
1:P:116:GLU:HA	1:P:161:ARG:O	2.08	0.53
1:E:268:LYS:HD2	1:F:218:HIS:CE1	2.43	0.53
1:L:20:PHE:CG	1:L:230:LYS:HG3	2.43	0.53
1:N:103:GLU:HB3	1:N:107:ARG:HH12	1.72	0.53
1:J:215:MET:HE3	1:J:215:MET:HA	1.89	0.53
1:I:281:LEU:O	1:I:285:MET:HG2	2.08	0.53
1:E:11:ARG:HH22	1:E:186:ASP:CG	2.12	0.53
1:P:163:ASP:OD1	1:P:191:GLU:HG2	2.09	0.53
1:B:178:ARG:HH21	1:B:206:LEU:HD23	1.73	0.53
1:B:76:SER:HA	1:B:84:VAL:HG21	1.90	0.53
1:F:26:VAL:HG11	1:F:32:ALA:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:ARG:NH2	5:E:685:HOH:O	2.33	0.53
1:L:100:ARG:O	1:L:101:THR:C	2.45	0.53
1:G:8:THR:HG22	1:G:12:ARG:HE	1.72	0.53
1:E:11:ARG:NH2	1:E:186:ASP:OD1	2.41	0.53
1:K:116:GLU:CB	1:K:161:ARG:HG2	2.38	0.53
1:C:146:VAL:O	1:C:150:GLN:HG2	2.09	0.53
1:A:263:ILE:CG1	1:A:264:PRO:HD2	2.39	0.53
1:P:283:GLU:O	1:P:287:VAL:HG23	2.09	0.53
1:M:133:VAL:HG12	1:M:137:THR:HB	1.90	0.53
1:K:53:SER:O	1:L:28:ASP:HB2	2.08	0.53
1:F:133:VAL:CG2	1:F:137:THR:HG21	2.38	0.53
1:F:168:HIS:HB3	1:F:172:GLU:HG2	1.90	0.53
1:H:19:SER:O	1:H:235:ARG:NH1	2.41	0.53
1:G:181:ARG:HG3	1:G:209:TRP:CD2	2.43	0.53
1:L:138:TYR:OH	1:L:160:ALA:HB1	2.08	0.53
1:E:277:ARG:HD2	5:E:594:HOH:O	2.08	0.53
1:A:300:VAL:HG22	1:B:127:LEU:HB3	1.91	0.53
1:I:76:SER:HA	1:I:84:VAL:HG21	1.90	0.53
1:H:117:ASP:HB3	1:H:138:TYR:CD1	2.44	0.53
1:E:190:LEU:HD12	1:E:202:VAL:HG21	1.91	0.52
1:M:224:ILE:HG21	1:M:232:MET:HE2	1.91	0.52
1:K:28:ASP:OD2	1:L:53:SER:OG	2.23	0.52
1:M:10:LEU:HD23	1:M:157:VAL:HG21	1.90	0.52
1:K:23:ALA:HB3	1:K:238:ILE:HG22	1.91	0.52
1:B:278:VAL:O	1:B:278:VAL:HG12	2.08	0.52
1:J:239:PHE:O	1:J:241:PHE:N	2.42	0.52
1:F:193:ILE:O	1:F:221:THR:HA	2.09	0.52
1:O:28:ASP:OD2	1:O:28:ASP:C	2.47	0.52
1:D:36:LEU:HD13	1:D:43:LEU:HD21	1.90	0.52
1:I:21:ILE:H	1:I:21:ILE:HD12	1.75	0.52
1:G:228:GLU:O	1:G:232:MET:HG3	2.08	0.52
1:K:170:TYR:O	1:K:174:VAL:HG23	2.09	0.52
1:L:130:LYS:HB2	1:L:166:GLN:NE2	2.25	0.52
1:J:7:ALA:HB2	1:J:111:ALA:HA	1.90	0.52
1:K:117:ASP:HB3	1:K:138:TYR:CD1	2.44	0.52
1:A:288:ASP:O	1:A:292:GLY:HA2	2.08	0.52
1:E:11:ARG:NH1	1:E:155:ASP:O	2.43	0.52
1:A:113:PHE:HE1	1:A:115:ILE:HD11	1.74	0.52
1:L:113:PHE:HE1	1:L:115:ILE:HD11	1.75	0.52
1:N:33:ARG:HD3	1:N:78:ILE:HG21	1.90	0.52
1:M:29:GLY:N	1:N:53:SER:O	2.38	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:CYS:HB3	1:B:127:LEU:HG	1.92	0.52
1:F:68:MET:HG3	1:F:92:TYR:OH	2.09	0.52
1:L:46:THR:CG2	1:L:49:GLY:HA3	2.40	0.52
1:A:248:VAL:HG21	1:B:275:LEU:HD12	1.92	0.52
1:K:59:ASP:OD1	1:K:124:CYS:HB2	2.08	0.52
1:N:36:LEU:HD23	1:N:78:ILE:HG22	1.91	0.52
1:E:91:GLY:HA3	1:E:98:VAL:HG22	1.91	0.52
1:N:77:ASN:HB2	5:N:748:HOH:O	2.08	0.52
1:P:124:CYS:CB	1:P:127:LEU:CD2	2.81	0.52
1:A:181:ARG:HG3	1:A:209:TRP:CD2	2.45	0.52
1:H:166:GLN:HG3	1:H:167:THR:N	2.24	0.52
1:C:123:ARG:HG3	1:C:127:LEU:HD12	1.91	0.52
1:G:275:LEU:HD12	1:H:244:LEU:HD23	1.92	0.52
1:A:16:ASN:O	1:A:235:ARG:NH2	2.42	0.52
1:I:96:ILE:HG21	1:L:62:ILE:HD11	1.92	0.52
1:E:11:ARG:NH2	1:E:186:ASP:CG	2.63	0.52
4:A:602:GOL:H31	1:C:107:ARG:HH12	1.75	0.52
1:A:97:MET:HE1	1:D:62:ILE:HG23	1.92	0.51
1:G:133:VAL:HG22	1:G:134:ASP:H	1.74	0.51
1:I:92:TYR:HB3	5:I:548:HOH:O	2.10	0.51
1:F:103:GLU:O	1:F:106:SER:HB2	2.10	0.51
1:P:136:ASP:N	1:P:136:ASP:OD1	2.43	0.51
1:C:181:ARG:CD	5:C:533:HOH:O	2.36	0.51
1:P:97:MET:CE	1:P:100:ARG:HE	2.21	0.51
1:A:266:LEU:HD23	1:A:270:MET:CG	2.40	0.51
1:E:181:ARG:CZ	1:E:209:TRP:HB2	2.40	0.51
1:B:77:ASN:ND2	1:B:108:SER:O	2.42	0.51
1:J:271:THR:CG2	1:J:274:MET:H	2.21	0.51
1:K:8:THR:CG2	1:K:155:ASP:OD2	2.56	0.51
5:C:531:HOH:O	1:D:266:LEU:HD12	2.11	0.51
1:E:229:ALA:HA	1:E:232:MET:CE	2.40	0.51
1:D:212:LEU:C	1:D:212:LEU:HD23	2.29	0.51
1:F:212:LEU:CD2	1:F:236:ILE:CG2	2.89	0.51
1:N:95:PRO:HD2	1:P:288:ASP:OD2	2.10	0.51
1:O:117:ASP:HB3	1:O:138:TYR:CD1	2.46	0.51
1:H:74:MET:HG3	1:H:75:ILE:N	2.25	0.51
1:E:210:PRO:HB3	1:E:235:ARG:HG3	1.93	0.51
1:I:165:LEU:HD21	1:I:194:THR:HG23	1.92	0.51
1:P:161:ARG:HA	1:P:189:PHE:O	2.10	0.51
1:H:97:MET:CE	1:H:100:ARG:HG3	2.41	0.51
1:K:48:ALA:HA	1:K:59:ASP:HB2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:165:LEU:CD2	1:I:194:THR:HG23	2.41	0.51
1:L:142:ILE:O	1:L:146:VAL:HG23	2.11	0.51
1:L:10:LEU:O	1:L:10:LEU:HG	2.11	0.51
1:J:44:TYR:OH	1:J:114:HIS:NE2	2.27	0.51
1:G:21:ILE:HB	1:G:236:ILE:HG12	1.93	0.51
1:K:7:ALA:HB2	1:K:111:ALA:HA	1.93	0.51
1:B:11:ARG:NH2	1:B:186:ASP:OD1	2.42	0.51
1:P:45:MET:HG3	1:P:75:ILE:HD12	1.93	0.51
1:K:86:ALA:O	1:K:113:PHE:HA	2.11	0.50
1:O:97:MET:CE	1:O:97:MET:HA	2.41	0.50
1:D:102:THR:HG23	1:D:113:PHE:HZ	1.76	0.50
1:L:189:PHE:CD1	1:L:212:LEU:HD22	2.45	0.50
1:O:191:GLU:OE2	3:O:501:OAF:O6	2.29	0.50
1:J:239:PHE:O	1:J:240:PRO:C	2.48	0.50
1:M:4:VAL:HG12	1:M:5:THR:N	2.26	0.50
1:L:64:THR:HG23	1:L:66:ASN:N	2.25	0.50
1:K:40:PHE:CZ	1:L:258:LEU:HD23	2.46	0.50
1:M:117:ASP:HB3	1:M:138:TYR:CD1	2.46	0.50
1:P:24:PRO:HD2	1:P:42:ALA:O	2.11	0.50
1:O:196:ARG:O	1:O:199:ALA:HB3	2.11	0.50
1:L:130:LYS:HB2	1:L:166:GLN:HE21	1.76	0.50
1:G:19:SER:O	1:G:235:ARG:NH1	2.44	0.50
1:M:128:ALA:HB3	1:N:300:VAL:HA	1.92	0.50
1:M:149:ARG:HG3	1:M:156:ILE:CG2	2.41	0.50
1:E:123:ARG:HG3	1:E:127:LEU:HD12	1.94	0.50
1:N:25:GLY:HA3	1:N:240:PRO:HA	1.94	0.50
1:K:27:TYR:CD2	1:K:53:SER:HB2	2.46	0.50
1:I:10:LEU:HD23	1:I:157:VAL:HG21	1.93	0.50
1:M:284:SER:O	1:M:287:VAL:HB	2.11	0.50
1:C:119:VAL:CG2	1:C:121:THR:HG22	2.40	0.50
1:N:206:LEU:HD22	1:N:209:TRP:CE3	2.47	0.50
1:E:300:VAL:HG13	1:E:300:VAL:O	2.12	0.50
1:A:129:GLY:O	1:A:130:LYS:O	2.30	0.50
1:N:263:ILE:HG13	1:N:264:PRO:CD	2.42	0.50
1:C:270:MET:CE	1:C:274:MET:CE	2.89	0.50
1:P:89:ASP:HB3	1:P:122:LYS:HD3	1.94	0.50
1:C:228:GLU:O	1:C:232:MET:HG3	2.11	0.50
1:M:245:GLY:HA3	1:N:266:LEU:HD21	1.92	0.50
1:D:64:THR:HG22	1:D:67:ASP:N	2.23	0.50
1:F:228:GLU:O	1:F:232:MET:HG3	2.11	0.50
1:G:244:LEU:O	1:G:248:VAL:HG23	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:16:ASN:O	1:O:235:ARG:NH2	2.44	0.50
1:P:26:VAL:O	1:P:46:THR:HG22	2.11	0.50
1:M:264:PRO:HB2	1:M:266:LEU:HD11	1.88	0.49
1:B:210:PRO:CB	1:B:235:ARG:HG3	2.42	0.49
1:N:11:ARG:HH22	1:N:186:ASP:CG	2.15	0.49
1:K:252:ARG:HA	1:L:34:VAL:HG13	1.94	0.49
1:J:19:SER:O	1:J:235:ARG:NH1	2.45	0.49
1:I:273:GLN:O	1:I:277:ARG:HG2	2.12	0.49
1:I:273:GLN:O	1:I:277:ARG:CG	2.60	0.49
1:K:97:MET:CE	1:K:100:ARG:HD3	2.42	0.49
1:G:252:ARG:HH11	1:G:252:ARG:HB3	1.76	0.49
1:O:261:ASP:O	1:O:263:ILE:HG22	2.11	0.49
1:B:181:ARG:HG3	1:B:209:TRP:CE2	2.48	0.49
1:P:130:LYS:HE2	1:P:166:GLN:OE1	2.13	0.49
1:I:172:GLU:HG3	1:I:176:ARG:HD2	1.94	0.49
1:A:77:ASN:HB2	4:A:602:GOL:H12	1.93	0.49
1:K:281:LEU:HG	1:K:285:MET:CE	2.42	0.49
1:C:64:THR:CG2	1:C:66:ASN:HB2	2.43	0.49
1:G:62:ILE:N	1:G:62:ILE:CD1	2.75	0.49
1:P:97:MET:HE3	1:P:97:MET:HA	1.91	0.49
1:C:123:ARG:HD2	1:C:130:LYS:HG3	1.94	0.49
1:E:5:THR:HG23	5:E:520:HOH:O	2.13	0.49
1:A:267:ASP:OD2	1:A:269:GLU:HG2	2.12	0.49
1:E:96:ILE:HG21	1:H:62:ILE:CD1	2.43	0.49
1:N:36:LEU:HD13	1:N:43:LEU:HD11	1.94	0.49
1:F:90:THR:HB	1:F:141:ARG:NH1	2.28	0.49
1:K:68:MET:HG3	1:K:92:TYR:OH	2.12	0.49
1:N:298:GLY:O	1:N:299:GLY:O	2.30	0.49
1:I:103:GLU:O	1:I:106:SER:HB2	2.13	0.49
1:G:203:ILE:HD11	1:G:234:PHE:CD1	2.47	0.49
1:O:275:LEU:CD2	1:P:244:LEU:CD2	2.91	0.49
1:M:97:MET:HE3	1:P:62:ILE:HA	1.95	0.49
1:I:277:ARG:HG3	1:I:277:ARG:HH11	1.77	0.49
1:N:85:ILE:HG23	1:N:112:ALA:HB3	1.95	0.49
1:L:24:PRO:HD2	1:L:42:ALA:O	2.12	0.49
1:F:191:GLU:OE2	3:F:501:OAF:O6	2.31	0.49
1:D:274:MET:SD	1:D:275:LEU:HD22	2.52	0.49
1:O:276:PHE:HE1	1:P:127:LEU:HD21	1.77	0.49
1:O:263:ILE:HG13	1:O:264:PRO:CD	2.41	0.49
1:N:149:ARG:HD2	1:N:156:ILE:O	2.13	0.49
1:G:20:PHE:HB2	1:G:230:LYS:HE3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:273:GLN:O	1:M:277:ARG:HG2	2.13	0.49
1:K:214:ASN:HA	1:K:238:ILE:HG12	1.95	0.49
1:O:213:LEU:HA	5:O:564:HOH:O	2.13	0.49
1:A:23:ALA:HB3	1:A:238:ILE:HG22	1.93	0.49
1:G:124:CYS:HB3	1:G:127:LEU:HD22	1.94	0.49
1:I:112:ALA:HB2	1:I:157:VAL:HB	1.95	0.49
1:D:126:HIS:CE1	1:D:220:ALA:H	2.31	0.49
1:B:97:MET:CE	1:C:62:ILE:HA	2.43	0.48
1:K:195:SER:HB2	1:K:198:MET:H	1.77	0.48
1:F:2:PRO:HB2	1:H:153:GLY:O	2.12	0.48
1:O:247:ALA:O	1:O:251:MET:HG3	2.13	0.48
1:P:27:TYR:HD2	1:P:53:SER:HB2	1.78	0.48
1:P:268:LYS:H	1:P:268:LYS:NZ	2.11	0.48
1:A:266:LEU:HD23	1:A:270:MET:CB	2.43	0.48
1:B:269:GLU:HG3	1:B:270:MET:N	2.28	0.48
1:O:194:THR:HB	5:O:484:HOH:O	2.14	0.48
1:D:215:MET:CE	1:D:224:ILE:H	2.26	0.48
1:O:188:GLY:HA3	1:O:211:LEU:HD23	1.95	0.48
1:I:133:VAL:HG12	1:I:137:THR:HB	1.93	0.48
1:M:57:GLN:CG	1:M:62:ILE:HD12	2.43	0.48
1:M:203:ILE:HD11	1:M:234:PHE:CE1	2.48	0.48
1:K:193:ILE:O	1:K:221:THR:HA	2.13	0.48
1:M:112:ALA:CB	1:M:157:VAL:HB	2.43	0.48
1:A:146:VAL:O	1:A:150:GLN:HG3	2.12	0.48
1:F:288:ASP:OD2	1:H:95:PRO:HG2	2.13	0.48
1:I:118:GLN:NE2	1:I:123:ARG:O	2.43	0.48
1:M:128:ALA:HB3	1:N:300:VAL:CA	2.43	0.48
1:I:189:PHE:C	1:I:189:PHE:CD2	2.87	0.48
1:M:159:ILE:HG12	1:M:187:VAL:HB	1.95	0.48
1:L:298:GLY:O	1:L:299:GLY:O	2.30	0.48
1:E:89:ASP:OD2	1:E:122:LYS:NZ	2.30	0.48
1:F:21:ILE:HG22	1:F:236:ILE:HG23	1.96	0.48
1:J:3:MET:HE2	1:L:154:SER:HB2	1.96	0.48
1:K:286:LYS:NZ	1:P:18:ASP:OD2	2.35	0.48
1:G:189:PHE:C	1:G:189:PHE:CD2	2.87	0.48
1:N:96:ILE:HG21	1:O:62:ILE:HD11	1.95	0.48
1:L:298:GLY:O	1:L:299:GLY:C	2.51	0.48
1:K:112:ALA:HB2	1:K:157:VAL:HB	1.95	0.48
1:K:74:MET:O	1:K:78:ILE:HD12	2.13	0.48
1:C:270:MET:HE3	1:C:274:MET:HE1	1.95	0.48
1:G:271:THR:O	1:G:275:LEU:HD23	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:41:ASP:O	1:N:83:PRO:HD2	2.14	0.48
1:G:247:ALA:O	1:G:251:MET:HG3	2.14	0.48
1:B:165:LEU:HB3	5:B:658:HOH:O	2.13	0.48
1:H:76:SER:HA	1:H:84:VAL:HG21	1.95	0.48
1:G:23:ALA:HB3	1:G:238:ILE:HG22	1.95	0.48
1:L:36:LEU:HD23	1:L:43:LEU:HD11	1.95	0.48
1:J:182:ASP:C	1:J:184:GLY:H	2.16	0.48
1:A:69:ARG:HG3	1:A:104:GLN:HB3	1.96	0.48
1:I:271:THR:O	1:I:274:MET:HB3	2.13	0.48
1:D:161:ARG:NH2	3:D:501:OAF:O3	2.42	0.48
1:E:34:VAL:HG11	1:F:251:MET:HB3	1.95	0.48
1:N:280:GLY:O	1:N:281:LEU:C	2.52	0.48
1:H:274:MET:SD	1:H:274:MET:C	2.92	0.48
1:L:64:THR:HG23	1:L:65:LEU:N	2.28	0.47
1:O:7:ALA:HB2	1:O:111:ALA:HA	1.96	0.47
1:D:210:PRO:HA	1:D:235:ARG:HG3	1.95	0.47
1:C:255:MET:HG3	1:D:34:VAL:HG12	1.96	0.47
1:K:97:MET:CE	1:K:97:MET:HA	2.44	0.47
1:I:164:SER:O	1:I:168:HIS:N	2.46	0.47
1:D:125:GLY:HA3	1:D:191:GLU:OE2	2.13	0.47
1:P:117:ASP:OD1	1:P:132:LEU:HD22	2.14	0.47
1:H:129:GLY:H	1:H:166:GLN:HE22	1.62	0.47
1:N:96:ILE:HD11	1:P:288:ASP:HB2	1.96	0.47
1:E:271:THR:O	1:E:272:PRO:C	2.52	0.47
1:M:179:ALA:O	1:M:182:ASP:HB2	2.14	0.47
1:B:159:ILE:HG12	1:B:187:VAL:HB	1.96	0.47
1:I:271:THR:CB	1:I:272:PRO:CD	2.91	0.47
1:A:269:GLU:O	1:A:271:THR:N	2.46	0.47
1:E:250:ALA:HB2	1:F:250:ALA:HB2	1.95	0.47
1:D:112:ALA:HB2	1:D:157:VAL:HB	1.95	0.47
1:C:25:GLY:HA2	1:C:44:TYR:O	2.15	0.47
1:P:300:VAL:O	1:P:300:VAL:HG13	2.13	0.47
1:F:165:LEU:HB3	5:F:512:HOH:O	2.13	0.47
1:O:196:ARG:NH1	1:O:224:ILE:HG12	2.29	0.47
1:C:181:ARG:HG3	1:C:209:TRP:CE2	2.49	0.47
1:O:11:ARG:O	1:O:15:GLU:HG3	2.13	0.47
1:H:269:GLU:HB2	5:H:719:HOH:O	2.14	0.47
1:I:281:LEU:HD11	1:I:285:MET:CE	2.43	0.47
1:E:98:VAL:HG11	1:E:141:ARG:O	2.14	0.47
1:C:203:ILE:HD11	1:C:234:PHE:CE1	2.49	0.47
1:G:196:ARG:HD3	1:G:228:GLU:OE2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:263:ILE:HG13	1:N:264:PRO:HD2	1.97	0.47
1:E:23:ALA:HB3	1:E:238:ILE:HG22	1.97	0.47
1:G:170:TYR:O	1:G:173:SER:HB2	2.14	0.47
1:N:116:GLU:OE1	1:N:118:GLN:HG3	2.15	0.47
1:E:284:SER:HB2	1:G:96:ILE:HD12	1.95	0.47
1:C:269:GLU:O	1:C:269:GLU:HG2	2.15	0.47
1:P:76:SER:HA	1:P:84:VAL:CG2	2.43	0.47
1:I:181:ARG:CZ	1:I:209:TRP:HB2	2.45	0.47
1:P:118:GLN:HA	1:P:132:LEU:HA	1.96	0.47
1:M:271:THR:HB	1:M:272:PRO:HD2	1.96	0.47
1:P:26:VAL:HB	1:P:31:SER:OG	2.15	0.47
1:A:277:ARG:HD2	5:A:664:HOH:O	2.15	0.47
1:E:153:GLY:O	1:G:2:PRO:HB2	2.15	0.47
1:G:89:ASP:OD1	1:G:122:LYS:HD3	2.15	0.47
1:H:135:THR:O	1:H:139:VAL:HG23	2.14	0.47
5:N:388:HOH:O	1:P:107:ARG:HG2	2.13	0.47
1:P:20:PHE:CE1	1:P:230:LYS:HA	2.49	0.47
1:F:245:GLY:N	1:F:246:PRO:CD	2.78	0.47
1:F:62:ILE:CD1	1:G:96:ILE:HG21	2.40	0.47
1:A:181:ARG:HD3	5:A:423:HOH:O	2.15	0.47
1:B:16:ASN:O	1:B:235:ARG:NH2	2.47	0.47
1:M:27:TYR:CD2	1:M:53:SER:HB2	2.50	0.47
1:J:161:ARG:HA	1:J:189:PHE:O	2.15	0.47
1:D:97:MET:HA	1:D:97:MET:CE	2.45	0.47
1:O:214:ASN:HA	1:O:238:ILE:HG13	1.96	0.47
1:I:152:ILE:HD12	1:K:3:MET:HE1	1.96	0.47
1:K:36:LEU:CD2	1:K:43:LEU:HD11	2.45	0.47
1:N:271:THR:HG23	1:N:274:MET:H	1.80	0.47
1:N:116:GLU:HB3	1:N:161:ARG:HG2	1.97	0.47
1:C:263:ILE:HG13	1:C:264:PRO:HD2	1.96	0.47
1:J:215:MET:CE	1:J:215:MET:HA	2.45	0.47
1:N:274:MET:O	1:N:278:VAL:HG23	2.15	0.47
1:O:244:LEU:HD23	1:O:248:VAL:HG23	1.97	0.47
1:K:133:VAL:HG21	1:K:141:ARG:NH2	2.30	0.47
1:N:206:LEU:HD22	1:N:209:TRP:HE3	1.78	0.46
1:C:64:THR:HG22	1:C:67:ASP:CG	2.35	0.46
1:E:56:GLY:O	1:F:33:ARG:NH1	2.40	0.46
1:H:97:MET:HE2	1:H:100:ARG:HG3	1.97	0.46
1:J:235:ARG:HB3	1:J:235:ARG:NH1	2.30	0.46
1:A:23:ALA:O	1:A:238:ILE:HA	2.15	0.46
1:G:58:ALA:HA	5:G:670:HOH:O	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:THR:O	1:D:12:ARG:HG2	2.15	0.46
1:F:62:ILE:HD12	1:G:97:MET:HE3	1.98	0.46
1:D:57:GLN:CG	1:D:62:ILE:HD12	2.46	0.46
1:I:95:PRO:HB2	1:K:288:ASP:HA	1.97	0.46
1:I:300:VAL:HG12	1:I:301:ASP:N	2.31	0.46
1:J:212:LEU:C	1:J:212:LEU:CD2	2.84	0.46
1:L:21:ILE:HD13	1:L:236:ILE:HG12	1.97	0.46
1:L:159:ILE:HG12	1:L:187:VAL:HB	1.97	0.46
1:G:277:ARG:HD2	5:G:575:HOH:O	2.16	0.46
1:K:130:LYS:H	1:K:166:GLN:NE2	2.13	0.46
1:O:274:MET:HE3	1:O:275:LEU:N	2.31	0.46
1:O:246:PRO:CD	1:P:266:LEU:HD21	2.42	0.46
1:M:130:LYS:CD	1:M:163:ASP:HB3	2.44	0.46
1:J:11:ARG:O	1:J:15:GLU:HG3	2.16	0.46
1:N:244:LEU:HD12	1:N:244:LEU:N	2.30	0.46
1:E:28:ASP:OD1	1:E:31:SER:OG	2.32	0.46
1:L:275:LEU:O	1:L:278:VAL:HB	2.15	0.46
1:K:256:GLU:O	1:K:260:ARG:HG3	2.15	0.46
1:H:26:VAL:HG11	1:H:32:ALA:HA	1.97	0.46
1:J:149:ARG:CG	1:J:154:SER:O	2.63	0.46
1:C:190:LEU:HD12	1:C:202:VAL:HG11	1.97	0.46
1:I:85:ILE:HG12	1:I:112:ALA:HB3	1.96	0.46
1:G:263:ILE:HG13	1:G:264:PRO:HD2	1.95	0.46
1:D:168:HIS:HB3	1:D:172:GLU:HG2	1.97	0.46
1:A:41:ASP:OD1	4:A:605:GOL:H11	2.16	0.46
1:C:270:MET:HE3	1:C:274:MET:CE	2.46	0.46
1:I:181:ARG:HB2	1:I:209:TRP:CH2	2.51	0.46
1:J:63:CYS:HB2	5:J:656:HOH:O	2.16	0.46
1:G:258:LEU:HD11	1:H:239:PHE:CE1	2.51	0.46
1:O:52:ALA:HB1	1:P:30:LEU:HG	1.97	0.46
1:D:247:ALA:O	1:D:251:MET:HG3	2.15	0.46
1:N:209:TRP:O	1:N:211:LEU:HD13	2.15	0.46
1:O:127:LEU:CB	1:P:300:VAL:HG13	2.36	0.46
1:I:275:LEU:HD11	1:J:52:ALA:HB2	1.98	0.46
1:D:97:MET:HA	1:D:97:MET:HE3	1.98	0.46
1:N:49:GLY:HA2	1:N:244:LEU:HD21	1.97	0.46
1:N:271:THR:CG2	1:N:274:MET:H	2.28	0.46
1:G:172:GLU:O	1:G:176:ARG:HG3	2.15	0.46
1:L:10:LEU:HG	1:L:14:LEU:CD1	2.46	0.46
1:O:300:VAL:HG23	1:P:127:LEU:CD1	2.42	0.46
1:G:130:LYS:HE3	1:G:166:GLN:HG2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ARG:C	1:B:180:ALA:N	2.69	0.46
1:G:189:PHE:HD2	1:G:189:PHE:C	2.19	0.46
1:M:128:ALA:HB3	1:N:300:VAL:C	2.35	0.46
1:I:203:ILE:HD11	1:I:234:PHE:CD1	2.51	0.46
1:J:283:GLU:H	1:J:283:GLU:CD	2.18	0.46
1:D:161:ARG:HA	1:D:189:PHE:HB3	1.97	0.46
1:J:25:GLY:HA3	1:J:240:PRO:HA	1.97	0.46
1:J:161:ARG:HA	1:J:189:PHE:HB3	1.97	0.46
1:E:243:ALA:HB3	5:E:434:HOH:O	2.15	0.46
1:J:112:ALA:CB	1:J:157:VAL:HB	2.45	0.46
1:B:300:VAL:HG13	1:B:300:VAL:O	2.15	0.46
1:P:299:GLY:CA	5:P:397:HOH:O	2.63	0.46
1:K:190:LEU:HD12	1:K:202:VAL:HG11	1.98	0.46
1:A:189:PHE:HD2	1:A:189:PHE:C	2.20	0.46
1:P:36:LEU:CD1	1:P:43:LEU:HD21	2.46	0.46
1:F:122:LYS:HE3	1:F:122:LYS:HB2	1.69	0.46
1:P:133:VAL:CG2	1:P:137:THR:HB	2.45	0.46
1:N:239:PHE:O	1:N:240:PRO:C	2.55	0.46
1:C:19:SER:O	1:C:235:ARG:NH1	2.49	0.46
1:M:112:ALA:HB2	1:M:157:VAL:HB	1.97	0.46
1:L:113:PHE:HD2	1:L:156:ILE:HD11	1.80	0.46
1:K:218:HIS:HB3	1:L:271:THR:HG22	1.97	0.46
1:I:246:PRO:O	1:I:247:ALA:C	2.54	0.46
1:I:189:PHE:C	1:I:189:PHE:HD2	2.20	0.45
1:L:36:LEU:CD2	1:L:43:LEU:HD11	2.45	0.45
1:L:176:ARG:O	1:L:179:ALA:HB3	2.16	0.45
1:F:100:ARG:O	1:F:104:GLN:HG3	2.16	0.45
1:O:300:VAL:HA	1:P:128:ALA:CB	2.42	0.45
1:F:244:LEU:O	1:F:248:VAL:HG23	2.16	0.45
1:P:133:VAL:HG21	1:P:137:THR:CB	2.46	0.45
1:C:212:LEU:HD21	1:C:238:ILE:HG12	1.97	0.45
1:M:87:ASP:OD1	1:M:114:HIS:CE1	2.69	0.45
1:C:170:TYR:CZ	1:C:174:VAL:HG21	2.52	0.45
1:C:246:PRO:HD3	1:D:266:LEU:HD21	1.98	0.45
1:L:143:ARG:O	1:L:147:GLN:HG3	2.16	0.45
1:C:51:ALA:O	1:C:55:HIS:HB2	2.17	0.45
1:C:181:ARG:HG3	1:C:209:TRP:CD2	2.51	0.45
1:O:97:MET:HA	1:O:97:MET:HE2	1.99	0.45
1:B:269:GLU:HA	5:B:429:HOH:O	2.17	0.45
1:A:189:PHE:CD2	1:A:189:PHE:C	2.89	0.45
1:A:34:VAL:HG11	1:B:251:MET:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:21:ILE:HB	1:P:236:ILE:HG12	1.99	0.45
1:C:294:ALA:O	1:C:297:ASP:HB2	2.17	0.45
1:E:123:ARG:HG2	1:E:127:LEU:HD12	1.98	0.45
1:N:239:PHE:O	1:N:241:PHE:N	2.50	0.45
1:N:36:LEU:HD23	1:N:78:ILE:CG2	2.47	0.45
1:E:122:LYS:C	1:E:122:LYS:HD3	2.36	0.45
1:L:172:GLU:O	1:L:176:ARG:HG3	2.17	0.45
1:G:28:ASP:OD1	1:G:31:SER:OG	2.29	0.45
1:L:48:ALA:HA	1:L:59:ASP:HB2	1.97	0.45
1:C:296:PHE:HB2	5:C:738:HOH:O	2.16	0.45
1:F:159:ILE:HG12	1:F:187:VAL:HB	1.98	0.45
1:F:212:LEU:HD21	1:F:236:ILE:CG2	2.47	0.45
1:C:264:PRO:HD2	1:D:217:GLU:OE1	2.17	0.45
1:E:89:ASP:O	1:E:115:ILE:HA	2.16	0.45
1:P:71:ASN:O	1:P:75:ILE:HG13	2.16	0.45
1:J:36:LEU:HD13	1:J:43:LEU:HD11	1.98	0.45
1:N:8:THR:O	1:N:9:SER:C	2.55	0.45
1:A:191:GLU:HA	1:A:191:GLU:OE1	2.16	0.45
1:G:191:GLU:HA	1:G:191:GLU:OE1	2.17	0.45
1:E:62:ILE:O	1:E:62:ILE:CG2	2.64	0.45
1:M:189:PHE:C	1:M:189:PHE:CD2	2.89	0.45
1:I:248:VAL:HG22	1:J:30:LEU:HD22	1.98	0.45
1:M:198:MET:HB2	1:M:198:MET:HE3	1.83	0.45
1:L:132:LEU:HD11	1:L:164:SER:CA	2.32	0.45
1:P:165:LEU:HD22	1:P:190:LEU:HD21	1.98	0.45
1:I:95:PRO:HG3	1:I:140:THR:CG2	2.45	0.45
1:J:149:ARG:CD	1:J:156:ILE:HG22	2.47	0.45
1:J:100:ARG:O	1:J:104:GLN:HG3	2.17	0.45
1:J:202:VAL:CG1	1:J:203:ILE:N	2.79	0.45
1:C:243:ALA:HB2	1:D:255:MET:CE	2.47	0.45
1:L:137:THR:O	1:L:140:THR:HB	2.16	0.45
1:F:97:MET:HE3	1:G:62:ILE:CA	2.39	0.45
1:I:209:TRP:O	1:I:210:PRO:C	2.55	0.45
1:P:30:LEU:HA	1:P:30:LEU:HD23	1.80	0.45
1:P:251:MET:O	1:P:255:MET:HG2	2.17	0.45
1:I:29:GLY:N	1:J:53:SER:O	2.50	0.44
1:A:203:ILE:HD11	1:A:234:PHE:CD1	2.52	0.44
1:P:271:THR:O	1:P:272:PRO:C	2.54	0.44
1:G:133:VAL:HG22	1:G:134:ASP:N	2.32	0.44
1:O:69:ARG:O	1:O:70:ALA:C	2.53	0.44
1:C:97:MET:HE2	1:C:100:ARG:HG3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:176:ARG:O	1:K:179:ALA:HB3	2.17	0.44
1:M:138:TYR:O	1:M:141:ARG:HB2	2.18	0.44
1:A:94:GLY:H	1:D:121:THR:HG21	1.82	0.44
1:O:142:ILE:O	1:O:146:VAL:HG23	2.17	0.44
1:J:203:ILE:HG21	1:J:233:GLY:HA3	1.99	0.44
1:B:64:THR:O	1:B:67:ASP:HB2	2.16	0.44
1:H:36:LEU:HD13	1:H:43:LEU:HD11	1.99	0.44
1:B:95:PRO:O	1:B:96:ILE:C	2.54	0.44
1:J:149:ARG:HG3	1:J:154:SER:HB3	1.98	0.44
1:P:69:ARG:HG3	1:P:104:GLN:HB3	1.99	0.44
1:O:187:VAL:HG12	1:O:188:GLY:N	2.33	0.44
1:P:79:SER:HA	1:P:80:PRO:HD3	1.85	0.44
1:P:172:GLU:O	1:P:176:ARG:HG3	2.17	0.44
1:N:209:TRP:O	1:N:211:LEU:CD1	2.65	0.44
1:E:57:GLN:CG	1:E:62:ILE:HD13	2.47	0.44
1:D:16:ASN:O	1:D:235:ARG:NH2	2.50	0.44
1:B:146:VAL:HG21	1:B:183:ALA:O	2.17	0.44
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.76	0.44
1:N:300:VAL:HG12	1:N:300:VAL:O	2.12	0.44
1:A:200:ARG:HG2	1:A:232:MET:HG2	1.99	0.44
1:A:142:ILE:O	1:A:146:VAL:HG23	2.18	0.44
1:E:250:ALA:CB	1:F:250:ALA:HB2	2.48	0.44
1:N:224:ILE:HD13	1:N:232:MET:CE	2.47	0.44
1:C:138:TYR:O	1:C:141:ARG:HB2	2.18	0.44
1:M:91:GLY:HA3	1:M:98:VAL:HG22	1.99	0.44
1:O:273:GLN:H	1:O:273:GLN:HG2	1.40	0.44
1:L:64:THR:HG22	1:L:67:ASP:H	1.83	0.44
1:P:193:ILE:HD12	1:P:213:LEU:HD23	1.99	0.44
1:I:93:GLY:HA3	1:I:97:MET:HG3	1.99	0.44
1:A:95:PRO:HG3	1:A:140:THR:HG23	2.00	0.44
1:K:272:PRO:HA	1:K:275:LEU:HD23	1.99	0.44
1:K:8:THR:HG22	1:K:155:ASP:HB2	1.99	0.44
1:M:189:PHE:HD2	1:M:189:PHE:C	2.21	0.44
1:P:45:MET:HG3	1:P:75:ILE:CD1	2.48	0.44
1:A:145:ALA:O	1:A:149:ARG:HB2	2.18	0.44
1:M:48:ALA:HA	1:M:59:ASP:HB2	2.00	0.44
1:I:27:TYR:CD2	1:I:53:SER:HB2	2.53	0.44
1:H:27:TYR:HD2	1:H:53:SER:HB2	1.82	0.44
1:F:151:ARG:NH2	5:F:596:HOH:O	2.43	0.44
1:O:300:VAL:O	1:O:300:VAL:HG22	2.17	0.44
1:N:161:ARG:HA	1:N:189:PHE:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:THR:HG23	1:D:66:ASN:N	2.33	0.44
1:A:112:ALA:CB	1:A:157:VAL:HB	2.45	0.44
1:E:268:LYS:HD2	1:F:218:HIS:HE1	1.83	0.44
1:K:224:ILE:HG21	1:K:232:MET:HE2	2.00	0.44
1:A:59:ASP:O	1:A:60:LEU:HD23	2.17	0.44
1:O:105:TYR:O	1:O:110:VAL:HB	2.17	0.44
1:N:137:THR:O	1:N:140:THR:HB	2.18	0.43
1:J:24:PRO:HD2	1:J:42:ALA:O	2.18	0.43
1:F:210:PRO:CB	1:F:235:ARG:HG3	2.47	0.43
1:I:241:PHE:HD1	1:I:244:LEU:HD22	1.84	0.43
1:C:129:GLY:H	1:C:166:GLN:HE22	1.66	0.43
1:J:45:MET:CE	1:J:86:ALA:HB1	2.47	0.43
1:P:11:ARG:HH22	1:P:149:ARG:NH1	2.16	0.43
1:K:159:ILE:HG12	1:K:187:VAL:HB	2.01	0.43
1:L:266:LEU:HD13	1:L:270:MET:HE3	2.00	0.43
1:B:122:LYS:HE3	1:B:122:LYS:HB2	1.69	0.43
1:I:62:ILE:HG22	1:I:62:ILE:O	2.17	0.43
1:F:209:TRP:CD1	1:F:210:PRO:HD2	2.53	0.43
1:J:252:ARG:O	1:J:256:GLU:HG2	2.17	0.43
1:P:66:ASN:N	1:P:66:ASN:OD1	2.52	0.43
1:N:149:ARG:HG2	1:N:154:SER:O	2.18	0.43
1:M:45:MET:HG3	1:M:75:ILE:CD1	2.47	0.43
1:J:69:ARG:HG3	1:J:104:GLN:HB3	2.00	0.43
1:C:41:ASP:O	1:C:83:PRO:HD2	2.18	0.43
1:F:47:GLY:HA3	1:F:87:ASP:OD2	2.18	0.43
1:F:97:MET:HE3	1:G:62:ILE:HG23	1.98	0.43
1:A:232:MET:HE3	1:A:234:PHE:CE1	2.46	0.43
1:I:244:LEU:O	1:I:248:VAL:HG23	2.17	0.43
1:N:49:GLY:CA	1:N:244:LEU:HD21	2.48	0.43
1:D:123:ARG:HB2	1:D:123:ARG:HE	1.56	0.43
1:N:79:SER:HA	1:N:80:PRO:HD3	1.76	0.43
1:K:155:ASP:O	1:K:156:ILE:C	2.57	0.43
1:P:190:LEU:HD22	1:P:193:ILE:HG12	2.01	0.43
1:J:236:ILE:HG22	1:J:237:ILE:N	2.32	0.43
1:M:30:LEU:HD21	1:M:275:LEU:CD1	2.47	0.43
1:C:68:MET:HG3	1:C:92:TYR:OH	2.17	0.43
1:P:54:VAL:HG12	1:P:55:HIS:CD2	2.54	0.43
1:K:69:ARG:HG3	1:K:104:GLN:HB3	2.01	0.43
1:H:15:GLU:O	1:H:17:PRO:HD3	2.18	0.43
1:H:191:GLU:OE2	3:H:501:OAF:O6	2.36	0.43
1:M:78:ILE:HD11	1:N:56:GLY:HA3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:ALA:HB1	1:E:156:ILE:HA	2.00	0.43
1:H:8:THR:HG23	1:H:155:ASP:OD2	2.18	0.43
1:M:62:ILE:O	1:M:62:ILE:HG22	2.18	0.43
1:H:125:GLY:HA3	1:H:191:GLU:OE2	2.18	0.43
1:K:26:VAL:O	1:K:46:THR:HG22	2.18	0.43
1:B:161:ARG:HA	1:B:189:PHE:HB3	1.99	0.43
1:L:75:ILE:HA	1:L:78:ILE:HD12	2.00	0.43
1:K:301:ASP:C	1:L:128:ALA:HB2	2.39	0.43
1:N:74:MET:HA	5:N:748:HOH:O	2.18	0.43
1:O:112:ALA:HB2	1:O:157:VAL:HB	2.00	0.43
1:O:33:ARG:HD3	1:O:78:ILE:HG21	2.01	0.43
1:M:181:ARG:NH1	1:M:209:TRP:HB2	2.34	0.43
1:L:122:LYS:H	1:L:122:LYS:HG3	1.62	0.43
1:G:97:MET:HA	1:G:100:ARG:HG3	2.01	0.43
1:E:228:GLU:O	1:E:232:MET:HE2	2.18	0.43
1:G:190:LEU:HD12	1:G:202:VAL:CG1	2.49	0.43
1:I:68:MET:HG3	1:I:92:TYR:OH	2.18	0.43
1:K:69:ARG:O	1:K:70:ALA:C	2.54	0.43
1:F:94:GLY:O	1:F:95:PRO:C	2.57	0.43
1:P:200:ARG:HA	1:P:203:ILE:HD12	2.00	0.43
1:M:127:LEU:CB	1:N:300:VAL:HG13	2.34	0.43
1:B:96:ILE:HG21	1:C:62:ILE:HD11	2.01	0.43
1:B:97:MET:HE3	1:C:62:ILE:HA	2.01	0.43
1:P:161:ARG:HD2	1:P:189:PHE:CE1	2.53	0.43
1:C:123:ARG:NH1	1:C:129:GLY:HA3	2.34	0.43
1:I:170:TYR:O	1:I:173:SER:HB2	2.18	0.43
1:G:252:ARG:HB3	1:G:252:ARG:NH1	2.33	0.43
1:H:102:THR:O	1:H:103:GLU:C	2.57	0.43
1:M:274:MET:HB2	5:M:807:HOH:O	2.18	0.43
1:B:96:ILE:HG21	1:C:62:ILE:HD12	2.01	0.43
1:C:96:ILE:O	1:C:100:ARG:HG2	2.19	0.43
1:M:146:VAL:HG12	1:M:158:VAL:HG21	2.01	0.43
1:P:27:TYR:CD2	1:P:53:SER:HB2	2.53	0.43
1:D:263:ILE:HG12	1:D:264:PRO:HD2	2.01	0.43
1:A:20:PHE:CG	1:A:230:LYS:HG3	2.53	0.43
1:F:161:ARG:HA	1:F:189:PHE:HB3	2.01	0.43
1:K:126:HIS:ND1	1:K:219:GLY:HA3	2.34	0.43
1:M:76:SER:HA	1:M:84:VAL:HG21	2.00	0.43
1:D:191:GLU:OE2	3:D:501:OAF:O6	2.37	0.42
1:E:117:ASP:HB3	1:E:138:TYR:CD1	2.54	0.42
1:D:215:MET:CE	1:D:224:ILE:HB	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:266:LEU:HD21	1:H:246:PRO:HD3	2.00	0.42
1:B:157:VAL:HG13	1:B:186:ASP:HB2	2.00	0.42
1:I:300:VAL:CG1	1:I:301:ASP:N	2.83	0.42
1:J:174:VAL:O	1:J:178:ARG:N	2.49	0.42
1:D:123:ARG:HG2	1:D:127:LEU:HB2	2.01	0.42
1:L:113:PHE:HE1	1:L:115:ILE:CD1	2.31	0.42
1:D:210:PRO:HB3	1:D:235:ARG:HG3	2.01	0.42
1:P:21:ILE:CD1	1:P:236:ILE:HG12	2.48	0.42
1:H:266:LEU:HD22	1:H:270:MET:CE	2.49	0.42
1:J:168:HIS:HB3	1:J:172:GLU:HG2	2.01	0.42
1:O:275:LEU:HD23	1:P:244:LEU:HD23	2.01	0.42
1:P:113:PHE:O	1:P:159:ILE:HB	2.19	0.42
1:H:215:MET:HE3	1:H:224:ILE:HB	2.00	0.42
1:P:296:PHE:O	1:P:297:ASP:C	2.57	0.42
1:H:203:ILE:HD11	1:H:234:PHE:CE1	2.54	0.42
1:C:26:VAL:O	1:C:45:MET:HA	2.20	0.42
1:A:41:ASP:CB	1:I:296:PHE:HA	2.45	0.42
1:H:52:ALA:O	1:H:56:GLY:CA	2.66	0.42
1:P:157:VAL:HG13	1:P:186:ASP:CB	2.48	0.42
1:B:244:LEU:CD1	1:B:244:LEU:O	2.66	0.42
1:B:244:LEU:HD12	1:B:244:LEU:O	2.19	0.42
1:G:271:THR:HB	1:G:272:PRO:HD2	2.01	0.42
1:M:146:VAL:HG11	1:M:184:GLY:O	2.19	0.42
1:I:59:ASP:OD1	1:I:124:CYS:HB2	2.20	0.42
1:H:196:ARG:NH1	1:H:228:GLU:OE1	2.53	0.42
1:O:14:LEU:HD23	1:O:14:LEU:HA	1.65	0.42
1:M:270:MET:HG2	1:M:274:MET:HE1	2.02	0.42
1:B:16:ASN:OD1	1:B:17:PRO:HD2	2.19	0.42
1:G:199:ALA:O	1:G:202:VAL:HG23	2.19	0.42
1:F:217:GLU:O	1:F:218:HIS:HB2	2.19	0.42
1:K:130:LYS:HG3	1:K:166:GLN:NE2	2.34	0.42
1:J:23:ALA:HA	1:J:24:PRO:HD2	1.92	0.42
1:F:186:ASP:O	1:F:210:PRO:HG2	2.20	0.42
1:D:64:THR:HG23	1:D:66:ASN:H	1.84	0.42
1:L:16:ASN:OD1	1:L:17:PRO:N	2.51	0.42
1:P:149:ARG:NH1	1:P:186:ASP:OD2	2.52	0.42
1:J:74:MET:HE3	1:J:75:ILE:HG13	2.02	0.42
1:M:59:ASP:OD1	1:M:124:CYS:HB2	2.19	0.42
1:L:116:GLU:OE2	1:L:122:LYS:HE3	2.20	0.42
1:L:122:LYS:HE2	1:L:122:LYS:HB2	1.94	0.42
1:D:193:ILE:O	1:D:221:THR:HA	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:65:LEU:HD13	1:N:101:THR:OG1	2.19	0.42
1:C:46:THR:HG23	1:C:49:GLY:HA3	2.00	0.42
1:N:73:GLU:HB2	1:N:108:SER:HB3	2.02	0.42
1:F:131:ILE:HD13	1:F:131:ILE:HA	1.91	0.42
1:G:27:TYR:CD2	1:G:53:SER:HB2	2.55	0.42
1:L:263:ILE:HG13	1:L:264:PRO:HD3	1.95	0.42
1:O:90:THR:O	1:O:141:ARG:HD3	2.19	0.42
1:F:251:MET:O	1:F:255:MET:HG2	2.19	0.42
1:L:47:GLY:O	1:L:48:ALA:C	2.57	0.42
1:B:143:ARG:HA	1:B:146:VAL:HG22	2.01	0.42
1:L:251:MET:O	1:L:255:MET:HG2	2.20	0.42
1:B:86:ALA:O	1:B:113:PHE:HA	2.19	0.42
1:L:50:THR:O	1:L:54:VAL:HB	2.20	0.42
1:P:7:ALA:HB1	1:P:156:ILE:N	2.34	0.42
1:J:96:ILE:H	1:J:96:ILE:HG12	1.25	0.42
1:O:270:MET:HG2	1:O:274:MET:HE1	2.02	0.42
1:C:95:PRO:HG3	1:C:140:THR:CG2	2.50	0.42
1:B:137:THR:O	1:B:140:THR:HB	2.19	0.42
1:E:14:LEU:HA	1:E:235:ARG:NH2	2.35	0.42
1:F:132:LEU:HD12	1:F:168:HIS:CE1	2.55	0.42
1:G:300:VAL:HA	1:H:128:ALA:HB3	2.01	0.42
1:A:17:PRO:HA	1:A:235:ARG:HE	1.85	0.42
1:K:74:MET:CE	1:K:75:ILE:HG13	2.50	0.42
1:C:122:LYS:NZ	5:C:309:HOH:O	2.38	0.42
1:P:105:TYR:CD2	1:P:110:VAL:HG21	2.55	0.42
1:G:267:ASP:OD1	1:G:269:GLU:HB3	2.19	0.42
1:L:121:THR:HG22	5:L:763:HOH:O	2.20	0.42
1:F:119:VAL:CG1	1:F:120:GLN:N	2.83	0.42
1:K:5:THR:CG2	1:K:8:THR:CG2	2.93	0.42
1:N:45:MET:HE2	1:N:86:ALA:HB1	2.01	0.42
1:M:30:LEU:HA	1:M:30:LEU:HD23	1.81	0.42
1:M:4:VAL:CG1	1:M:5:THR:N	2.83	0.42
1:G:246:PRO:HD3	1:H:266:LEU:HD21	2.01	0.42
1:H:82:THR:HA	1:H:83:PRO:HD2	1.90	0.42
1:G:282:ASP:HB2	5:G:405:HOH:O	2.20	0.42
1:O:24:PRO:HD2	1:O:42:ALA:O	2.20	0.42
1:M:116:GLU:OE2	1:M:122:LYS:NZ	2.42	0.42
1:F:130:LYS:H	1:F:166:GLN:NE2	2.17	0.42
1:I:49:GLY:O	1:I:52:ALA:HB3	2.20	0.42
4:A:602:GOL:H32	1:C:103:GLU:OE1	2.20	0.42
1:K:281:LEU:HG	1:K:285:MET:HE2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:MET:HG3	1:D:75:ILE:N	2.35	0.42
1:D:10:LEU:N	5:D:752:HOH:O	2.53	0.42
1:H:4:VAL:HG12	1:H:5:THR:N	2.35	0.42
1:C:130:LYS:HE2	1:C:163:ASP:HB3	2.01	0.41
1:O:296:PHE:HZ	1:P:60:LEU:HD22	1.82	0.41
1:K:17:PRO:HA	1:K:235:ARG:NH2	2.35	0.41
1:M:273:GLN:CA	1:M:273:GLN:OE1	2.67	0.41
1:P:166:GLN:HG3	1:P:167:THR:N	2.35	0.41
1:K:165:LEU:HB2	1:K:190:LEU:HD21	2.02	0.41
1:P:200:ARG:HG3	1:P:200:ARG:H	1.61	0.41
1:B:121:THR:HG21	1:C:94:GLY:H	1.85	0.41
1:M:162:THR:HG22	1:M:177:LEU:HD21	2.02	0.41
1:F:58:ALA:HA	5:F:529:HOH:O	2.18	0.41
1:D:143:ARG:HG3	1:D:183:ALA:HB1	2.01	0.41
1:I:24:PRO:HG3	1:I:40:PHE:CD1	2.55	0.41
1:D:252:ARG:HH11	1:D:252:ARG:HB3	1.83	0.41
1:N:11:ARG:O	1:N:15:GLU:HG3	2.20	0.41
1:E:23:ALA:HA	1:E:24:PRO:HD2	1.97	0.41
1:F:189:PHE:CD2	1:F:189:PHE:C	2.93	0.41
1:D:143:ARG:NH1	5:D:690:HOH:O	2.53	0.41
1:M:152:ILE:HG13	1:M:154:SER:HB3	2.02	0.41
1:B:168:HIS:HB3	1:B:172:GLU:HG2	2.02	0.41
1:P:142:ILE:O	1:P:146:VAL:HG23	2.19	0.41
1:P:170:TYR:O	1:P:174:VAL:HG23	2.21	0.41
1:J:193:ILE:HG12	1:J:193:ILE:H	1.66	0.41
1:M:266:LEU:HB3	1:M:270:MET:SD	2.60	0.41
1:F:125:GLY:C	1:F:130:LYS:HE2	2.40	0.41
1:P:89:ASP:O	1:P:115:ILE:HA	2.19	0.41
1:B:209:TRP:HA	1:B:210:PRO:HD3	1.94	0.41
1:O:296:PHE:HZ	1:P:60:LEU:CD2	2.33	0.41
1:D:159:ILE:HG12	1:D:187:VAL:HB	2.02	0.41
1:A:45:MET:HG3	1:A:75:ILE:CD1	2.51	0.41
1:M:263:ILE:CG2	1:M:263:ILE:O	2.69	0.41
1:A:297:ASP:OD1	1:A:297:ASP:C	2.57	0.41
1:B:203:ILE:HD11	1:B:234:PHE:CD1	2.54	0.41
1:L:213:LEU:HD21	1:L:215:MET:HE3	2.02	0.41
1:O:26:VAL:HG11	1:O:32:ALA:HB2	2.01	0.41
1:I:181:ARG:NH2	1:I:209:TRP:HB2	2.35	0.41
1:M:45:MET:SD	1:M:71:ASN:HB3	2.60	0.41
1:D:263:ILE:HA	1:D:264:PRO:HD3	1.93	0.41
1:D:190:LEU:HD13	1:D:193:ILE:HG12	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LEU:HA	1:B:236:ILE:O	2.19	0.41
1:O:136:ASP:O	1:O:137:THR:C	2.59	0.41
1:M:88:ALA:O	1:M:89:ASP:HB2	2.20	0.41
1:E:203:ILE:HD11	1:E:234:PHE:CE1	2.56	0.41
1:L:88:ALA:O	1:L:89:ASP:C	2.59	0.41
1:M:28:ASP:C	1:M:28:ASP:OD1	2.59	0.41
1:D:274:MET:SD	1:D:274:MET:C	2.99	0.41
1:H:116:GLU:HB3	1:H:161:ARG:HD3	2.01	0.41
1:E:123:ARG:HD2	1:E:130:LYS:HG2	2.00	0.41
1:G:275:LEU:HD12	1:H:244:LEU:CD2	2.51	0.41
1:E:263:ILE:HG13	1:E:264:PRO:HD3	2.00	0.41
1:F:170:TYR:O	1:F:173:SER:HB2	2.20	0.41
1:J:117:ASP:OD2	1:J:176:ARG:HD3	2.21	0.41
1:M:30:LEU:HD22	1:N:248:VAL:CG2	2.51	0.41
1:K:117:ASP:OD2	1:K:176:ARG:NH1	2.54	0.41
1:A:95:PRO:HG3	1:A:140:THR:CG2	2.49	0.41
1:J:41:ASP:O	1:J:83:PRO:HD2	2.21	0.41
1:K:194:THR:HA	1:K:220:ALA:O	2.21	0.41
1:N:177:LEU:HD21	1:N:189:PHE:H	1.85	0.41
1:B:278:VAL:CG1	1:B:278:VAL:O	2.68	0.41
1:K:110:VAL:HG12	1:K:112:ALA:H	1.85	0.41
1:A:28:ASP:OD2	1:B:53:SER:OG	2.25	0.41
1:J:148:ALA:HA	1:J:151:ARG:NH1	2.35	0.41
1:J:257:LYS:O	1:J:261:ASP:N	2.48	0.41
1:A:212:LEU:C	1:A:212:LEU:HD23	2.40	0.41
1:C:302:LEU:HD12	1:C:302:LEU:HA	1.97	0.41
1:C:244:LEU:HD23	1:D:275:LEU:HD12	2.02	0.41
1:O:300:VAL:CA	1:P:128:ALA:HB3	2.44	0.41
1:J:133:VAL:HG22	1:J:137:THR:HB	2.02	0.41
1:D:97:MET:HE3	1:D:100:ARG:HG3	2.00	0.41
1:H:221:THR:HA	1:H:222:PRO:HD3	1.91	0.41
1:O:57:GLN:HG2	1:O:62:ILE:HD13	2.02	0.41
1:P:82:THR:HA	1:P:83:PRO:HD3	1.79	0.41
1:N:162:THR:HG23	1:N:190:LEU:HD23	2.02	0.41
1:P:65:LEU:HD12	1:P:65:LEU:O	2.20	0.41
1:H:73:GLU:O	1:H:77:ASN:ND2	2.48	0.41
1:M:300:VAL:HG13	1:M:301:ASP:H	1.83	0.41
1:O:130:LYS:H	1:O:166:GLN:HE21	1.68	0.41
1:F:189:PHE:C	1:F:189:PHE:HD2	2.24	0.41
1:H:203:ILE:HD11	1:H:234:PHE:CD1	2.56	0.41
1:N:24:PRO:HD2	1:N:42:ALA:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:165:LEU:HA	1:O:165:LEU:HD12	1.88	0.41
1:A:74:MET:SD	1:A:74:MET:C	2.99	0.41
1:L:30:LEU:HA	1:L:30:LEU:HD23	1.94	0.41
1:H:69:ARG:HG3	1:H:104:GLN:HB3	2.01	0.41
1:K:113:PHE:N	1:K:113:PHE:CD2	2.89	0.41
1:B:130:LYS:H	1:B:166:GLN:NE2	2.18	0.41
1:A:232:MET:CE	1:A:234:PHE:CE1	2.99	0.41
1:F:122:LYS:H	1:F:122:LYS:HG3	1.70	0.41
1:A:256:GLU:HG2	1:A:256:GLU:H	1.74	0.41
1:A:252:ARG:HH21	1:B:274:MET:CE	2.33	0.41
1:C:129:GLY:O	1:C:130:LYS:C	2.60	0.41
1:C:189:PHE:CD2	1:C:189:PHE:C	2.94	0.41
1:J:149:ARG:HD2	1:J:156:ILE:HG22	2.03	0.41
1:L:196:ARG:CG	1:L:196:ARG:HH11	2.32	0.41
1:J:241:PHE:O	1:J:242:ALA:C	2.59	0.41
1:K:214:ASN:HA	1:K:238:ILE:CG1	2.51	0.41
1:A:235:ARG:HA	1:A:235:ARG:HD2	1.73	0.41
1:E:271:THR:O	1:E:275:LEU:HD23	2.21	0.41
1:D:162:THR:HG23	1:D:190:LEU:HD23	2.02	0.41
1:A:91:GLY:HA3	1:A:98:VAL:HG22	2.03	0.41
1:D:23:ALA:HA	1:D:24:PRO:HD3	1.83	0.41
1:I:138:TYR:O	1:I:141:ARG:N	2.50	0.41
1:D:110:VAL:O	1:D:156:ILE:HD12	2.21	0.41
1:E:107:ARG:HG2	1:G:107:ARG:O	2.20	0.41
1:B:193:ILE:O	1:B:221:THR:HA	2.20	0.41
1:B:198:MET:HA	1:B:201:GLN:HB2	2.02	0.41
1:E:259:LYS:HA	1:E:259:LYS:HD2	1.66	0.41
1:H:164:SER:O	1:H:165:LEU:C	2.57	0.41
1:I:270:MET:HG2	1:J:245:GLY:CA	2.51	0.41
1:A:143:ARG:CB	1:C:291:ALA:O	2.62	0.41
1:B:181:ARG:CZ	1:B:209:TRP:HB2	2.51	0.41
1:M:85:ILE:HG12	1:M:112:ALA:HB3	2.02	0.41
1:A:23:ALA:HA	1:A:24:PRO:HD2	1.88	0.41
1:J:179:ALA:O	1:J:182:ASP:HB2	2.21	0.41
1:H:239:PHE:O	1:H:240:PRO:C	2.60	0.41
1:L:99:ALA:O	1:L:103:GLU:HG3	2.21	0.41
1:K:21:ILE:HB	1:K:236:ILE:HG12	2.03	0.41
1:F:76:SER:HA	1:F:84:VAL:HG21	2.03	0.41
1:G:124:CYS:SG	1:G:125:GLY:N	2.94	0.40
1:B:140:THR:HA	1:D:291:ALA:O	2.21	0.40
1:P:90:THR:HG21	1:P:118:GLN:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:137:THR:O	1:G:140:THR:HB	2.21	0.40
1:N:8:THR:HG23	1:N:155:ASP:OD2	2.21	0.40
1:J:202:VAL:HG13	1:J:203:ILE:N	2.36	0.40
1:E:110:VAL:HG12	1:E:156:ILE:HD11	2.03	0.40
1:P:204:GLN:C	1:P:206:LEU:H	2.25	0.40
1:F:253:GLU:OE1	1:F:253:GLU:HA	2.21	0.40
1:I:4:VAL:CG1	1:I:5:THR:N	2.84	0.40
1:L:12:ARG:HD3	1:L:12:ARG:H	1.84	0.40
1:B:210:PRO:HA	1:B:235:ARG:HG3	2.03	0.40
1:G:181:ARG:HG3	1:G:209:TRP:CG	2.56	0.40
1:E:189:PHE:CE2	1:E:214:ASN:HB2	2.56	0.40
1:J:302:LEU:HA	1:J:302:LEU:HD12	1.51	0.40
1:L:164:SER:OG	1:L:173:SER:HA	2.21	0.40
1:N:62:ILE:CG2	1:O:97:MET:HE3	2.44	0.40
1:L:285:MET:HG2	1:L:296:PHE:CG	2.56	0.40
1:C:202:VAL:O	1:C:203:ILE:C	2.60	0.40
1:F:118:GLN:HA	1:F:132:LEU:HA	2.03	0.40
1:O:165:LEU:HB2	1:O:190:LEU:HD21	2.03	0.40
1:I:251:MET:O	1:I:255:MET:HB2	2.21	0.40
1:G:59:ASP:HB2	1:H:276:PHE:CE2	2.57	0.40
1:K:149:ARG:HG3	1:K:154:SER:O	2.21	0.40
1:F:11:ARG:NH2	1:F:186:ASP:OD1	2.51	0.40
1:M:100:ARG:H	1:M:100:ARG:HG2	1.76	0.40
1:G:198:MET:O	1:G:202:VAL:HG22	2.21	0.40
1:J:138:TYR:O	1:J:139:VAL:C	2.60	0.40
1:B:275:LEU:O	1:B:278:VAL:HB	2.22	0.40
1:L:102:THR:HG23	1:L:113:PHE:CZ	2.56	0.40
1:I:97:MET:HE3	1:L:62:ILE:HD13	2.03	0.40
1:K:130:LYS:HE2	1:K:166:GLN:CD	2.42	0.40
1:O:69:ARG:HG3	1:O:104:GLN:HB3	2.03	0.40
1:J:66:ASN:OD1	1:K:64:THR:HG21	2.21	0.40
1:D:76:SER:HA	1:D:84:VAL:HG21	2.03	0.40
1:O:281:LEU:O	1:O:284:SER:HB2	2.22	0.40
1:A:209:TRP:HA	1:A:210:PRO:HD3	2.00	0.40
1:B:210:PRO:CA	1:B:235:ARG:HG3	2.50	0.40
1:J:174:VAL:O	1:J:175:ALA:C	2.60	0.40
1:M:57:GLN:HG2	1:M:62:ILE:CD1	2.49	0.40
1:M:47:GLY:HA3	1:M:87:ASP:OD2	2.21	0.40
1:N:152:ILE:HD12	1:P:3:MET:CE	2.51	0.40
1:F:273:GLN:O	1:F:277:ARG:HG3	2.21	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	299/302 (99%)	278 (93%)	20 (7%)	1 (0%)	46	72
1	B	300/302 (99%)	284 (95%)	15 (5%)	1 (0%)	46	72
1	C	299/302 (99%)	286 (96%)	11 (4%)	2 (1%)	26	51
1	D	299/302 (99%)	289 (97%)	8 (3%)	2 (1%)	26	51
1	E	299/302 (99%)	279 (93%)	20 (7%)	0	100	100
1	F	299/302 (99%)	279 (93%)	19 (6%)	1 (0%)	46	72
1	G	299/302 (99%)	282 (94%)	15 (5%)	2 (1%)	26	51
1	H	299/302 (99%)	284 (95%)	14 (5%)	1 (0%)	46	72
1	I	298/302 (99%)	271 (91%)	24 (8%)	3 (1%)	19	39
1	J	288/302 (95%)	260 (90%)	27 (9%)	1 (0%)	46	72
1	K	298/302 (99%)	275 (92%)	20 (7%)	3 (1%)	19	39
1	L	298/302 (99%)	268 (90%)	22 (7%)	8 (3%)	6	10
1	M	298/302 (99%)	270 (91%)	26 (9%)	2 (1%)	26	51
1	N	288/302 (95%)	266 (92%)	18 (6%)	4 (1%)	14	28
1	O	299/302 (99%)	268 (90%)	28 (9%)	3 (1%)	19	39
1	P	299/302 (99%)	262 (88%)	32 (11%)	5 (2%)	11	22
All	All	4759/4832 (98%)	4401 (92%)	319 (7%)	39 (1%)	24	46

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	MET
1	C	299	GLY
1	I	295	ALA
1	J	242	ALA
1	L	151	ARG
1	L	299	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	300	VAL
1	D	297	ASP
1	K	268	LYS
1	L	72	ALA
1	M	242	ALA
1	M	295	ALA
1	N	9	SER
1	N	92	TYR
1	N	242	ALA
1	O	268	LYS
1	P	87	ASP
1	P	89	ASP
1	B	179	ALA
1	L	87	ASP
1	L	205	ASP
1	P	205	ASP
1	P	268	LYS
1	D	300	VAL
1	G	289	ALA
1	H	297	ASP
1	I	259	LYS
1	L	71	ASN
1	L	89	ASP
1	G	89	ASP
1	I	173	SER
1	N	8	THR
1	P	266	LEU
1	C	203	ILE
1	F	106	SER
1	K	264	PRO
1	O	199	ALA
1	K	298	GLY
1	L	156	ILE

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	225/228 (99%)	206 (92%)	19 (8%)	14 26
1	B	226/228 (99%)	201 (89%)	25 (11%)	8 13
1	C	227/228 (100%)	204 (90%)	23 (10%)	9 17
1	D	226/228 (99%)	196 (87%)	30 (13%)	5 8
1	E	227/228 (100%)	202 (89%)	25 (11%)	8 14
1	F	226/228 (99%)	203 (90%)	23 (10%)	9 17
1	G	227/228 (100%)	204 (90%)	23 (10%)	9 17
1	H	227/228 (100%)	199 (88%)	28 (12%)	6 11
1	I	225/228 (99%)	199 (88%)	26 (12%)	7 12
1	J	220/228 (96%)	194 (88%)	26 (12%)	6 12
1	K	225/228 (99%)	202 (90%)	23 (10%)	9 17
1	L	224/228 (98%)	196 (88%)	28 (12%)	6 10
1	M	226/228 (99%)	197 (87%)	29 (13%)	5 10
1	N	220/228 (96%)	181 (82%)	39 (18%)	2 3
1	O	222/228 (97%)	194 (87%)	28 (13%)	5 10
1	P	226/228 (99%)	197 (87%)	29 (13%)	5 10
All	All	3599/3648 (99%)	3175 (88%)	424 (12%)	6 12

All (424) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	16	ASN
1	A	19	SER
1	A	36	LEU
1	A	46	THR
1	A	57	GLN
1	A	74	MET
1	A	100	ARG
1	A	122	LYS
1	A	140	THR
1	A	173	SER
1	A	189	PHE
1	A	190	LEU
1	A	196	ARG
1	A	253	GLU
1	A	256	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	269	GLU
1	A	300	VAL
1	A	302	LEU
1	B	11	ARG
1	B	36	LEU
1	B	46	THR
1	B	69	ARG
1	B	74	MET
1	B	115	ILE
1	B	119	VAL
1	B	122	LYS
1	B	133	VAL
1	B	134	ASP
1	B	143	ARG
1	B	155	ASP
1	B	166	GLN
1	B	167	THR
1	B	173	SER
1	B	189	PHE
1	B	190	LEU
1	B	223	SER
1	B	244	LEU
1	B	266	LEU
1	B	269	GLU
1	B	275	LEU
1	B	283	GLU
1	B	300	VAL
1	B	303	LYS
1	C	11	ARG
1	C	12	ARG
1	C	36	LEU
1	C	46	THR
1	C	64	THR
1	C	69	ARG
1	C	74	MET
1	C	121	THR
1	C	123	ARG
1	C	133	VAL
1	C	178	ARG
1	C	189	PHE
1	C	190	LEU
1	C	196	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	202	VAL
1	C	204	GLN
1	C	252	ARG
1	C	256	GLU
1	C	259	LYS
1	C	263	ILE
1	C	268	LYS
1	C	269	GLU
1	C	270	MET
1	D	3	MET
1	D	9	SER
1	D	11	ARG
1	D	21	ILE
1	D	36	LEU
1	D	46	THR
1	D	62	ILE
1	D	64	THR
1	D	66	ASN
1	D	69	ARG
1	D	74	MET
1	D	122	LYS
1	D	133	VAL
1	D	143	ARG
1	D	151	ARG
1	D	167	THR
1	D	181	ARG
1	D	189	PHE
1	D	190	LEU
1	D	200	ARG
1	D	204	GLN
1	D	212	LEU
1	D	244	LEU
1	D	252	ARG
1	D	268	LYS
1	D	284	SER
1	D	286	LYS
1	D	300	VAL
1	D	301	ASP
1	D	302	LEU
1	E	2	PRO
1	E	5	THR
1	E	11	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	19	SER
1	E	31	SER
1	E	36	LEU
1	E	46	THR
1	E	64	THR
1	E	69	ARG
1	E	74	MET
1	E	122	LYS
1	E	127	LEU
1	E	132	LEU
1	E	146	VAL
1	E	166	GLN
1	E	171	GLU
1	E	189	PHE
1	E	190	LEU
1	E	196	ARG
1	E	197	GLU
1	E	206	LEU
1	E	259	LYS
1	E	269	GLU
1	E	297	ASP
1	E	300	VAL
1	F	46	THR
1	F	69	ARG
1	F	74	MET
1	F	100	ARG
1	F	115	ILE
1	F	122	LYS
1	F	124	CYS
1	F	133	VAL
1	F	140	THR
1	F	149	ARG
1	F	154	SER
1	F	166	GLN
1	F	167	THR
1	F	172	GLU
1	F	173	SER
1	F	189	PHE
1	F	190	LEU
1	F	223	SER
1	F	259	LYS
1	F	275	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	286	LYS
1	F	297	ASP
1	F	300	VAL
1	G	11	ARG
1	G	12	ARG
1	G	36	LEU
1	G	57	GLN
1	G	62	ILE
1	G	65	LEU
1	G	69	ARG
1	G	74	MET
1	G	122	LYS
1	G	132	LEU
1	G	140	THR
1	G	166	GLN
1	G	167	THR
1	G	182	ASP
1	G	189	PHE
1	G	190	LEU
1	G	200	ARG
1	G	202	VAL
1	G	204	GLN
1	G	252	ARG
1	G	268	LYS
1	G	269	GLU
1	G	286	LYS
1	H	9	SER
1	H	11	ARG
1	H	36	LEU
1	H	46	THR
1	H	64	THR
1	H	66	ASN
1	H	69	ARG
1	H	74	MET
1	H	122	LYS
1	H	133	VAL
1	H	151	ARG
1	H	166	GLN
1	H	167	THR
1	H	173	SER
1	H	181	ARG
1	H	189	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	190	LEU
1	H	194	THR
1	H	206	LEU
1	H	215	MET
1	H	231	GLU
1	H	252	ARG
1	H	263	ILE
1	H	275	LEU
1	H	277	ARG
1	H	283	GLU
1	H	297	ASP
1	H	300	VAL
1	I	5	THR
1	I	8	THR
1	I	9	SER
1	I	11	ARG
1	I	22	VAL
1	I	57	GLN
1	I	69	ARG
1	I	74	MET
1	I	115	ILE
1	I	122	LYS
1	I	124	CYS
1	I	134	ASP
1	I	166	GLN
1	I	186	ASP
1	I	189	PHE
1	I	212	LEU
1	I	218	HIS
1	I	231	GLU
1	I	244	LEU
1	I	252	ARG
1	I	259	LYS
1	I	267	ASP
1	I	268	LYS
1	I	274	MET
1	I	277	ARG
1	I	301	ASP
1	J	11	ARG
1	J	12	ARG
1	J	36	LEU
1	J	46	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	69	ARG
1	J	74	MET
1	J	79	SER
1	J	96	ILE
1	J	116	GLU
1	J	143	ARG
1	J	152	ILE
1	J	167	THR
1	J	189	PHE
1	J	190	LEU
1	J	193	ILE
1	J	204	GLN
1	J	213	LEU
1	J	215	MET
1	J	218	HIS
1	J	223	SER
1	J	241	PHE
1	J	256	GLU
1	J	266	LEU
1	J	271	THR
1	J	301	ASP
1	J	302	LEU
1	K	11	ARG
1	K	19	SER
1	K	36	LEU
1	K	37	SER
1	K	69	ARG
1	K	71	ASN
1	K	74	MET
1	K	96	ILE
1	K	115	ILE
1	K	122	LYS
1	K	133	VAL
1	K	149	ARG
1	K	161	ARG
1	K	189	PHE
1	K	195	SER
1	K	197	GLU
1	K	202	VAL
1	K	223	SER
1	K	225	SER
1	K	256	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	266	LEU
1	K	267	ASP
1	K	301	ASP
1	L	4	VAL
1	L	12	ARG
1	L	36	LEU
1	L	37	SER
1	L	64	THR
1	L	69	ARG
1	L	74	MET
1	L	100	ARG
1	L	122	LYS
1	L	127	LEU
1	L	131	ILE
1	L	173	SER
1	L	174	VAL
1	L	189	PHE
1	L	196	ARG
1	L	197	GLU
1	L	225	SER
1	L	231	GLU
1	L	237	ILE
1	L	239	PHE
1	L	253	GLU
1	L	263	ILE
1	L	269	GLU
1	L	274	MET
1	L	283	GLU
1	L	286	LYS
1	L	300	VAL
1	L	301	ASP
1	M	11	ARG
1	M	12	ARG
1	M	37	SER
1	M	66	ASN
1	M	69	ARG
1	M	74	MET
1	M	78	ILE
1	M	82	THR
1	M	122	LYS
1	M	127	LEU
1	M	134	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	143	ARG
1	M	151	ARG
1	M	155	ASP
1	M	167	THR
1	M	189	PHE
1	M	190	LEU
1	M	195	SER
1	M	198	MET
1	M	204	GLN
1	M	211	LEU
1	M	228	GLU
1	M	231	GLU
1	M	259	LYS
1	M	273	GLN
1	M	274	MET
1	M	277	ARG
1	M	285	MET
1	M	301	ASP
1	N	3	MET
1	N	4	VAL
1	N	5	THR
1	N	8	THR
1	N	9	SER
1	N	11	ARG
1	N	12	ARG
1	N	18	ASP
1	N	28	ASP
1	N	36	LEU
1	N	45	MET
1	N	69	ARG
1	N	74	MET
1	N	76	SER
1	N	79	SER
1	N	82	THR
1	N	100	ARG
1	N	115	ILE
1	N	121	THR
1	N	166	GLN
1	N	189	PHE
1	N	190	LEU
1	N	193	ILE
1	N	201	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	202	VAL
1	N	204	GLN
1	N	206	LEU
1	N	211	LEU
1	N	223	SER
1	N	231	GLU
1	N	253	GLU
1	N	266	LEU
1	N	269	GLU
1	N	270	MET
1	N	271	THR
1	N	275	LEU
1	N	296	PHE
1	N	297	ASP
1	N	300	VAL
1	O	11	ARG
1	O	31	SER
1	O	36	LEU
1	O	46	THR
1	O	60	LEU
1	O	66	ASN
1	O	69	ARG
1	O	71	ASN
1	O	74	MET
1	O	122	LYS
1	O	149	ARG
1	O	167	THR
1	O	173	SER
1	O	189	PHE
1	O	190	LEU
1	O	197	GLU
1	O	201	GLN
1	O	223	SER
1	O	225	SER
1	O	252	ARG
1	O	261	ASP
1	O	267	ASP
1	O	273	GLN
1	O	274	MET
1	O	281	LEU
1	O	284	SER
1	O	286	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	290	GLN
1	P	9	SER
1	P	15	GLU
1	P	36	LEU
1	P	46	THR
1	P	64	THR
1	P	69	ARG
1	P	74	MET
1	P	96	ILE
1	P	97	MET
1	P	108	SER
1	P	122	LYS
1	P	127	LEU
1	P	136	ASP
1	P	137	THR
1	P	154	SER
1	P	166	GLN
1	P	171	GLU
1	P	174	VAL
1	P	200	ARG
1	P	204	GLN
1	P	205	ASP
1	P	217	GLU
1	P	228	GLU
1	P	256	GLU
1	P	268	LYS
1	P	269	GLU
1	P	270	MET
1	P	274	MET
1	P	277	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	B	120	GLN
1	B	166	GLN
1	F	166	GLN
1	F	168	HIS
1	H	166	GLN
1	H	204	GLN
1	K	166	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	166	GLN
1	O	166	GLN
1	P	204	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 35 ligands modelled in this entry, 16 are monoatomic - leaving 19 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	$\#\|Z\| > 2$
3	OAF	A	501	2	2,11,11	1.25	0	1,18,18	1.14	0
4	GOL	A	602	-	5,5,5	0.87	0	5,5,5	1.64	1 (20%)
4	GOL	A	605	-	5,5,5	0.44	0	5,5,5	0.98	0
3	OAF	B	501	2	2,11,11	0.80	0	1,18,18	3.20	1 (100%)
3	OAF	C	501	2	2,11,11	1.51	0	1,18,18	0.11	0
3	OAF	D	501	2	2,11,11	0.86	0	1,18,18	3.11	1 (100%)
3	OAF	E	501	2	2,11,11	1.77	1 (50%)	1,18,18	2.73	1 (100%)
4	GOL	E	604	-	5,5,5	0.64	0	5,5,5	0.76	0
3	OAF	F	501	2	2,11,11	1.21	0	1,18,18	0.15	0
3	OAF	G	501	2	2,11,11	1.47	0	1,18,18	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	G	601	-	5,5,5	0.87	0	5,5,5	1.69	2 (40%)
3	OAF	H	501	2	2,11,11	0.61	0	1,18,18	2.17	1 (100%)
3	OAF	I	501	2	2,11,11	0.33	0	1,18,18	1.87	0
3	OAF	K	501	2	2,11,11	1.47	0	1,18,18	0.70	0
3	OAF	L	501	2	2,11,11	0.64	0	1,18,18	2.03	1 (100%)
3	OAF	M	501	2	2,11,11	0.36	0	1,18,18	2.21	1 (100%)
4	GOL	M	606	-	5,5,5	0.45	0	5,5,5	0.95	0
3	OAF	O	501	2	2,11,11	1.10	0	1,18,18	3.45	1 (100%)
3	OAF	P	501	2	2,11,11	1.04	0	1,18,18	4.28	1 (100%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OAF	A	501	2	-	0/0/21/21	0/0/0/0
4	GOL	A	602	-	-	0/4/4/4	0/0/0/0
4	GOL	A	605	-	-	0/4/4/4	0/0/0/0
3	OAF	B	501	2	-	0/0/21/21	0/0/0/0
3	OAF	C	501	2	-	0/0/21/21	0/0/0/0
3	OAF	D	501	2	-	0/0/21/21	0/0/0/0
3	OAF	E	501	2	-	0/0/21/21	0/0/0/0
4	GOL	E	604	-	-	0/4/4/4	0/0/0/0
3	OAF	F	501	2	-	0/0/21/21	0/0/0/0
3	OAF	G	501	2	-	0/0/21/21	0/0/0/0
4	GOL	G	601	-	-	0/4/4/4	0/0/0/0
3	OAF	H	501	2	-	0/0/21/21	0/0/0/0
3	OAF	I	501	2	-	0/0/21/21	0/0/0/0
3	OAF	K	501	2	-	0/0/21/21	0/0/0/0
3	OAF	L	501	2	-	0/0/21/21	0/0/0/0
3	OAF	M	501	2	-	0/0/21/21	0/0/0/0
4	GOL	M	606	-	-	0/4/4/4	0/0/0/0
3	OAF	O	501	2	-	0/0/21/21	0/0/0/0
3	OAF	P	501	2	-	0/0/21/21	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	501	OAF	F2-C3	-2.08	1.28	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	501	OAF	F1-C3-F2	-2.73	100.14	106.40
4	G	601	GOL	O3-C3-C2	-2.04	100.30	110.18
3	L	501	OAF	F1-C3-F2	2.03	111.06	106.40
3	H	501	OAF	F1-C3-F2	2.17	111.38	106.40
3	M	501	OAF	F1-C3-F2	2.21	111.48	106.40
4	G	601	GOL	O1-C1-C2	2.40	121.81	110.18
4	A	602	GOL	O2-C2-C3	2.51	120.15	108.65
3	D	501	OAF	F1-C3-F2	3.11	113.53	106.40
3	B	501	OAF	F1-C3-F2	3.20	113.76	106.40
3	O	501	OAF	F1-C3-F2	3.45	114.34	106.40
3	P	501	OAF	F1-C3-F2	4.28	116.22	106.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	GOL	3	0
4	A	605	GOL	3	0
3	D	501	OAF	2	0
3	F	501	OAF	1	0
4	G	601	GOL	2	0
3	H	501	OAF	1	0
3	I	501	OAF	2	0
3	L	501	OAF	1	0
3	M	501	OAF	1	0
4	M	606	GOL	1	0
3	O	501	OAF	1	0
3	P	501	OAF	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	301/302 (99%)	-0.72	0 100 100	33, 37, 40, 44	0
1	B	302/302 (100%)	-0.66	0 100 100	33, 37, 42, 44	0
1	C	301/302 (99%)	-0.71	0 100 100	31, 37, 41, 44	0
1	D	301/302 (99%)	-0.75	0 100 100	33, 37, 41, 45	0
1	E	301/302 (99%)	-0.71	0 100 100	33, 37, 41, 44	0
1	F	301/302 (99%)	-0.66	0 100 100	32, 37, 41, 45	0
1	G	301/302 (99%)	-0.73	0 100 100	33, 37, 40, 45	0
1	H	301/302 (99%)	-0.72	0 100 100	32, 37, 41, 44	0
1	I	300/302 (99%)	-0.56	0 100 100	32, 38, 41, 46	0
1	J	292/302 (96%)	-0.51	0 100 100	33, 38, 42, 46	0
1	K	300/302 (99%)	-0.55	0 100 100	33, 38, 42, 48	0
1	L	300/302 (99%)	-0.37	0 100 100	33, 38, 44, 48	0
1	M	300/302 (99%)	-0.52	0 100 100	32, 37, 42, 47	0
1	N	292/302 (96%)	-0.53	0 100 100	32, 38, 42, 48	0
1	O	301/302 (99%)	-0.62	0 100 100	33, 38, 42, 46	0
1	P	301/302 (99%)	-0.34	2 (0%) 89 87	34, 38, 43, 47	0
All	All	4795/4832 (99%)	-0.60	2 (0%) 100 100	31, 37, 42, 48	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	220	ALA	2.3
1	P	219	GLY	2.2

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	A	602	6/6	0.95	0.17	4.21	33,35,39,40	0
4	GOL	G	601	6/6	0.96	0.13	0.65	31,35,37,38	0
4	GOL	M	606	6/6	0.97	0.14	0.15	35,38,39,41	0
4	GOL	A	605	6/6	0.96	0.12	-0.36	36,39,41,42	0
3	OAF	L	501	12/12	0.98	0.12	-0.61	38,41,43,44	0
3	OAF	A	501	12/12	0.99	0.10	-0.72	33,35,36,37	0
4	GOL	E	604	6/6	0.95	0.11	-0.89	37,40,41,43	0
3	OAF	B	501	12/12	0.98	0.08	-1.20	28,32,36,36	0
3	OAF	O	501	12/12	0.98	0.09	-1.29	30,35,37,38	0
3	OAF	G	501	12/12	0.99	0.08	-1.43	31,34,37,38	0
3	OAF	F	501	12/12	0.99	0.08	-1.50	32,33,35,35	0
3	OAF	C	501	12/12	0.99	0.08	-1.52	32,34,35,36	0
3	OAF	P	501	12/12	0.97	0.10	-1.54	37,40,42,42	0
3	OAF	E	501	12/12	0.99	0.08	-1.59	28,32,34,34	0
3	OAF	I	501	12/12	0.99	0.07	-1.72	35,36,38,41	0
3	OAF	K	501	12/12	0.98	0.09	-1.74	33,36,38,39	0
3	OAF	D	501	12/12	0.99	0.07	-1.97	30,31,33,34	0
3	OAF	H	501	12/12	0.99	0.08	-2.16	33,36,36,39	0
3	OAF	M	501	12/12	0.99	0.07	-2.38	29,34,36,37	0
2	MN	N	401	1/1	0.97	0.04	-3.47	43,43,43,43	0
2	MN	D	401	1/1	1.00	0.04	-3.56	36,36,36,36	0
2	MN	P	401	1/1	0.97	0.03	-4.21	42,42,42,42	0
2	MN	A	401	1/1	1.00	0.04	-4.94	33,33,33,33	0
2	MN	B	401	1/1	1.00	0.03	-5.44	37,37,37,37	0
2	MN	C	401	1/1	1.00	0.03	-5.46	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MN	O	401	1/1	0.99	0.03	-5.84	39,39,39,39	0
2	MN	F	401	1/1	1.00	0.03	-5.90	36,36,36,36	0
2	MN	J	401	1/1	0.99	0.03	-5.91	43,43,43,43	0
2	MN	I	401	1/1	1.00	0.03	-6.20	39,39,39,39	0
2	MN	H	401	1/1	1.00	0.03	-6.22	35,35,35,35	0
2	MN	E	401	1/1	1.00	0.02	-6.48	36,36,36,36	0
2	MN	G	401	1/1	0.99	0.05	-6.78	34,34,34,34	0
2	MN	L	401	1/1	0.99	0.02	-7.04	41,41,41,41	0
2	MN	K	401	1/1	0.99	0.03	-7.36	38,38,38,38	0
2	MN	M	401	1/1	1.00	0.01	-10.59	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.