Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2023 – 08:38 pm GMT

PDB ID	:	2BHT
Title	:	Crystal structure of O-acetylserine sulfhydrylase B
Authors	:	Claus, M.T.; Zocher, G.E.; Maier, T.H.P.; Schulz, G.E.
Deposited on	:	2005-01-18
Resolution	:	2.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

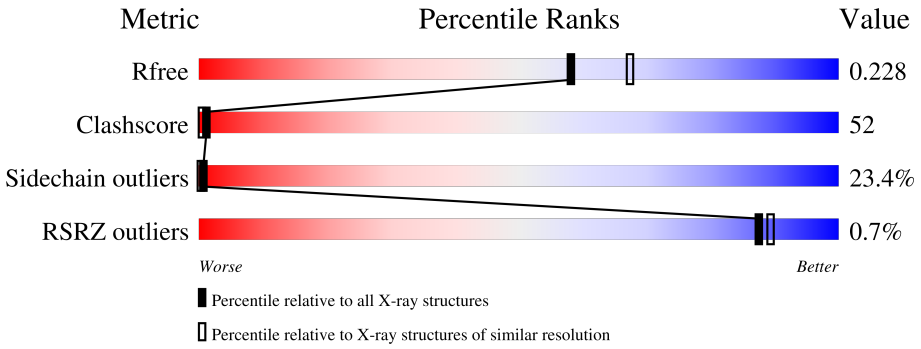
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	303	31% 51% 15% ·
1	B	303	% 25% 52% 14% · 7%
1	C	303	30% 55% 11% ·
1	D	303	% 37% 42% 15% · 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8978 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.

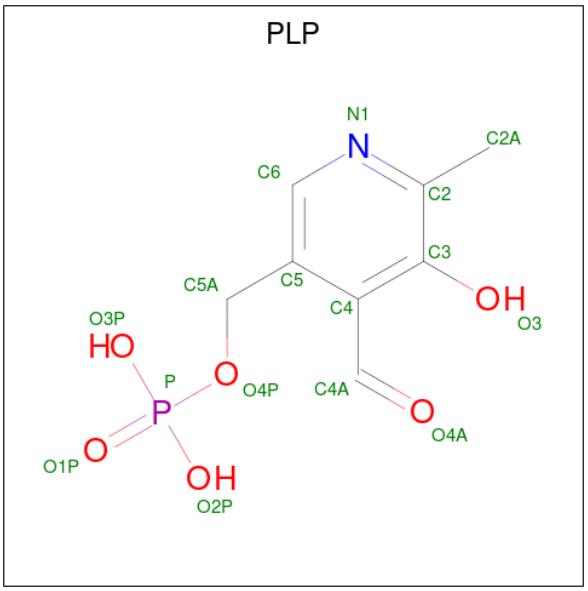
- Molecule 1 is a protein called CYSTEINE SYNTHASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2217	1375	398	429	15			
1	B	281	Total	C	N	O	S	0	0	0
			2122	1315	384	410	13			
1	C	292	Total	C	N	O	S	0	0	0
			2204	1368	396	425	15			
1	D	285	Total	C	N	O	S	0	0	0
			2152	1336	387	415	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ARG	GLU	engineered mutation	UNP P16703
A	148	LYS	TYR	engineered mutation	UNP P16703
A	184	GLU	ARG	engineered mutation	UNP P16703
B	57	ARG	GLU	engineered mutation	UNP P16703
B	148	LYS	TYR	engineered mutation	UNP P16703
B	184	GLU	ARG	engineered mutation	UNP P16703
C	57	ARG	GLU	engineered mutation	UNP P16703
C	148	LYS	TYR	engineered mutation	UNP P16703
C	184	GLU	ARG	engineered mutation	UNP P16703
D	57	ARG	GLU	engineered mutation	UNP P16703
D	148	LYS	TYR	engineered mutation	UNP P16703
D	184	GLU	ARG	engineered mutation	UNP P16703

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O P 15 8 1 5 1	0	0
2	B	1	Total C N O P 15 8 1 5 1	0	0
2	C	1	Total C N O P 15 8 1 5 1	0	0
2	D	1	Total C N O P 15 8 1 5 1	0	0

- Molecule 3 is water.

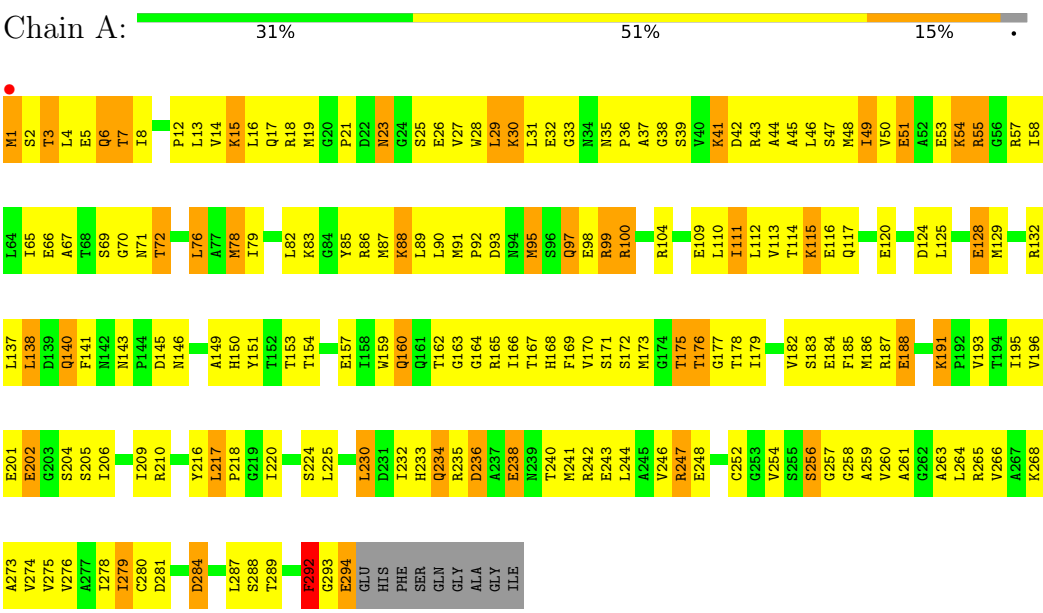
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	56	Total O 56 56	0	0
3	B	49	Total O 49 49	0	0
3	C	56	Total O 56 56	0	0
3	D	62	Total O 62 62	0	0

3 Residue-property plots (i)

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

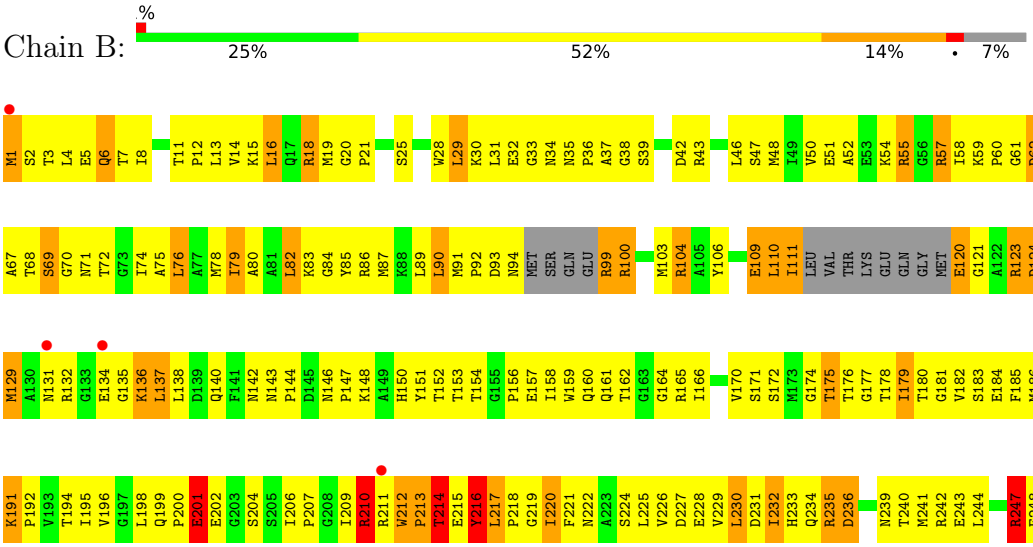
• Molecule 1: CYSTEINE SYNTHASE B

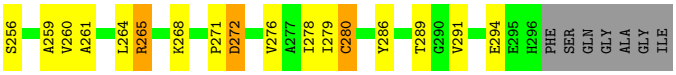
Chain A:



• Molecule 1: CYSTEINE SYNTHASE B

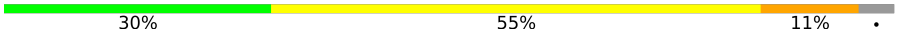
Chain B:

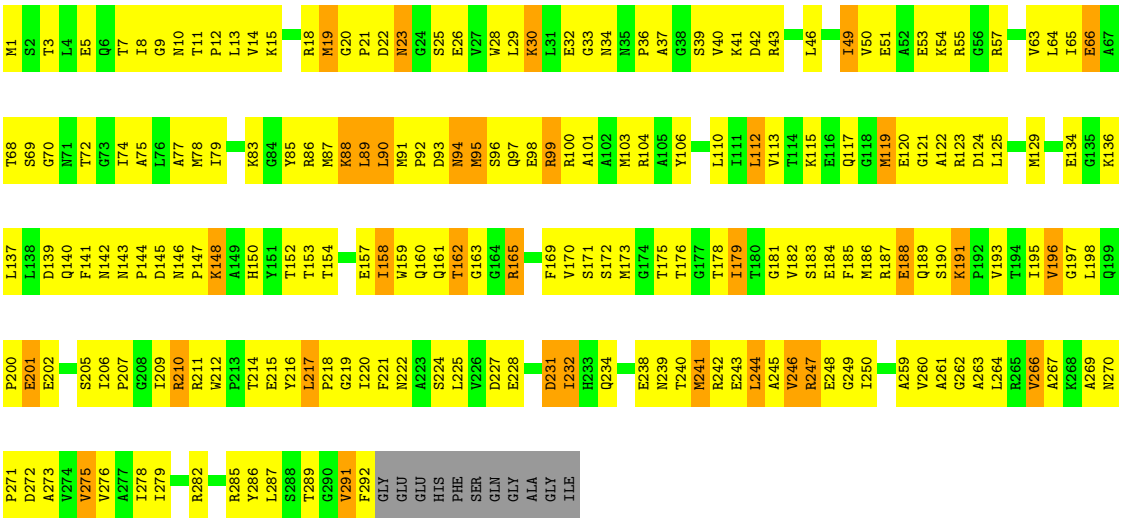




• Molecule 1: CYSTEINE SYNTHASE B

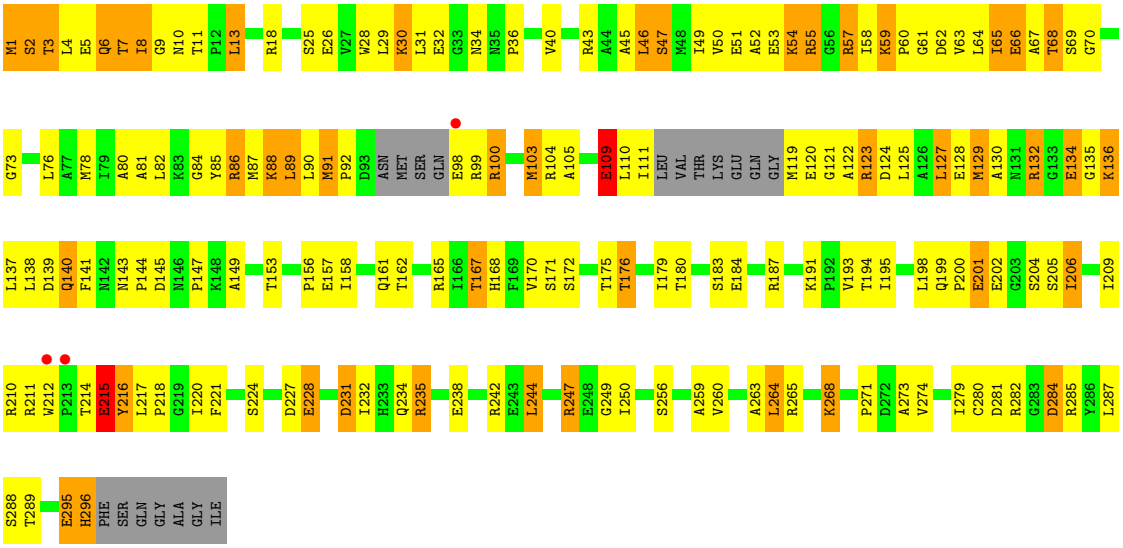
Chain C:





• Molecule 1: CYSTEINE SYNTHASE B

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	149.94Å 149.94Å 194.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 74.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.10) 99.6 (74.97-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.10Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.225 , 0.244 0.235 , 0.228	Depositor DCC
R_{free} test set	4937 reflections (1.03%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 74.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.419 for -h,k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8978	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.92	1/2250 (0.0%)	0.68	2/3039 (0.1%)
1	B	0.47	2/2153 (0.1%)	0.67	4/2905 (0.1%)
1	C	0.23	0/2237	0.55	0/3022
1	D	0.24	0/2184	0.58	0/2948
All	All	0.54	3/8824 (0.0%)	0.62	6/11914 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
1	C	0	2
1	D	0	4
All	All	0	13

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	PHE	C-O	41.94	2.03	1.23
1	B	210	ARG	CZ-NH1	13.48	1.50	1.33
1	B	210	ARG	NE-CZ	12.76	1.49	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	292	PHE	O-C-N	-18.34	92.02	123.20
1	B	210	ARG	NE-CZ-NH1	13.94	127.27	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	292	PHE	CA-C-O	-9.78	99.56	120.10
1	B	247	ARG	CD-NE-CZ	7.70	134.38	123.60
1	B	210	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	B	247	ARG	NE-CZ-NH1	6.22	123.41	120.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Peptide
1	A	292	PHE	Mainchain
1	A	41	LYS	Mainchain
1	B	201	GLU	Peptide
1	B	213	PRO	Peptide
1	B	214	THR	Peptide
1	B	216	TYR	Peptide
1	C	201	GLU	Peptide
1	C	30	LYS	Peptide
1	D	109	GLU	Peptide
1	D	215	GLU	Peptide
1	D	216	TYR	Peptide
1	D	68	THR	Peptide

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	2217	0	2228	262	0
1	B	2122	0	2116	256	0
1	C	2204	0	2220	191	0
1	D	2152	0	2154	220	0
2	A	15	0	6	2	0
2	B	15	0	6	4	0
2	C	15	0	6	2	0
2	D	15	0	6	1	0
3	A	56	0	0	1	0
3	B	49	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	56	0	0	10	0
3	D	62	0	0	6	0
All	All	8978	0	8742	909	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 52.

All (909) 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:D:110:LEU:O	1:D:111:ILE:HD13	1.44	1.15
1:B:152:THR:HG23	1:B:153:THR:HG23	1.38	1.04
1:D:99:ARG:NH2	1:D:288:SER:OG	1.94	1.00
1:A:168:HIS:HB2	1:A:275:VAL:HG22	1.46	0.97
1:A:292:PHE:C	1:A:292:PHE:O	2.03	0.97
1:D:67:ALA:HB1	1:D:90:LEU:HD13	1.43	0.94
1:D:7:THR:HB	1:D:36:PRO:HG3	1.45	0.94
1:A:183:SER:HB2	1:A:195:ILE:HD13	1.47	0.94
1:A:234:GLN:HG2	1:A:235:ARG:HD2	1.50	0.94
1:A:175:THR:HG22	1:A:177:GLY:H	1.32	0.92
1:B:171:SER:HB3	1:B:179:ILE:HD12	1.49	0.92
1:B:12:PRO:HG2	1:B:31:LEU:HB2	1.52	0.92
1:D:4:LEU:HD11	1:D:36:PRO:HB3	1.53	0.91
1:A:25:SER:HB2	1:A:273:ALA:HB3	1.51	0.90
1:C:201:GLU:HG2	1:C:231:ASP:HB3	1.53	0.89
1:B:48:MET:HG2	1:B:138:LEU:HD22	1.53	0.89
1:C:158:ILE:HG21	1:C:276:VAL:HG11	1.54	0.88
1:A:37:ALA:HB2	1:A:78:MET:HE2	1.56	0.86
1:D:200:PRO:HD3	1:D:209:ILE:HD12	1.58	0.85
1:D:47:SER:HB2	1:D:149:ALA:HB2	1.60	0.84
1:D:4:LEU:HD23	1:D:82:LEU:HD21	1.56	0.84
1:B:201:GLU:HA	1:B:211:ARG:HH11	1.43	0.84
1:A:252:CYS:HB2	1:A:279:ILE:HD13	1.59	0.84
1:B:147:PRO:HA	1:B:150:HIS:HD2	1.42	0.84
1:A:79:ILE:HA	1:A:82:LEU:HD12	1.58	0.83
1:A:217:LEU:HD13	1:A:217:LEU:O	1.77	0.83
1:D:90:LEU:HB2	1:D:122:ALA:HB3	1.61	0.83
1:B:2:SER:HA	1:B:6:GLN:HE21	1.41	0.82
1:D:63:VAL:HG22	1:D:86:ARG:HB2	1.59	0.82
1:B:104:ARG:HH12	1:B:110:LEU:HG	1.43	0.82
1:B:71:ASN:HA	1:B:74:ILE:HD12	1.59	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ALA:HB3	1:A:42:ASP:OD1	1.79	0.82
1:D:204:SER:HB3	1:D:234:GLN:HB2	1.61	0.81
1:D:215:GLU:HA	1:D:217:LEU:H	1.44	0.80
1:D:68:THR:H	1:D:90:LEU:HD22	1.45	0.80
1:C:50:VAL:O	1:C:54:LYS:HG3	1.83	0.79
1:B:68:THR:HG21	1:B:72:THR:HB	1.65	0.78
1:B:16:LEU:HD23	1:B:19:MET:O	1.84	0.77
1:D:59:LYS:HB3	1:D:62:ASP:OD1	1.83	0.77
1:A:41:LYS:HD2	1:A:72:THR:HG23	1.66	0.77
1:B:140:GLN:OE1	1:B:175:THR:HG21	1.84	0.77
1:C:90:LEU:HD21	1:C:125:LEU:HD23	1.65	0.77
1:B:146:ASN:OD1	1:B:177:GLY:HA3	1.86	0.76
1:A:45:ALA:O	1:A:49:ILE:HG23	1.85	0.76
1:A:153:THR:O	1:A:157:GLU:HG3	1.86	0.76
1:B:67:ALA:HB2	1:B:90:LEU:HD23	1.68	0.76
1:A:48:MET:HB3	1:A:138:LEU:HD12	1.66	0.75
1:A:246:VAL:HG12	1:A:247:ARG:HG2	1.68	0.75
1:A:30:LYS:O	1:A:279:ILE:HG23	1.86	0.75
1:C:144:PRO:O	1:C:147:PRO:HD2	1.86	0.75
1:A:54:LYS:HZ1	1:A:55:ARG:HH11	1.31	0.75
1:D:244:LEU:HD11	1:D:260:VAL:HG21	1.68	0.75
1:C:34:ASN:HA	1:C:282:ARG:HH21	1.49	0.75
1:C:162:THR:O	1:C:165:ARG:HG3	1.87	0.74
1:A:46:LEU:O	1:A:50:VAL:HG22	1.86	0.74
1:A:230:LEU:HG	1:A:265:ARG:NH1	2.03	0.74
1:D:100:ARG:H	1:D:100:ARG:HD2	1.53	0.74
1:C:176:THR:HG21	1:C:221:PHE:HD1	1.53	0.74
1:A:13:LEU:HA	1:A:29:LEU:O	1.88	0.73
1:A:151:TYR:CD2	1:A:184:GLU:HB2	2.22	0.73
1:C:148:LYS:O	1:C:152:THR:HG23	1.89	0.73
1:A:233:HIS:HD2	1:A:235:ARG:H	1.37	0.73
1:C:125:LEU:O	1:C:129:MET:HG3	1.89	0.73
1:D:180:THR:O	1:D:184:GLU:HG3	1.88	0.72
1:A:37:ALA:HB2	1:A:78:MET:CE	2.19	0.72
1:A:95:MET:HG3	1:A:99:ARG:HD3	1.70	0.72
1:D:167:THR:HG21	1:D:273:ALA:HA	1.71	0.72
1:A:16:LEU:HD13	1:A:19:MET:HB2	1.69	0.72
1:A:91:MET:HE2	1:A:95:MET:HB3	1.71	0.72
1:D:206:ILE:HG12	1:D:209:ILE:HG12	1.72	0.72
1:C:91:MET:O	1:C:112:LEU:HD12	1.88	0.72
1:A:49:ILE:O	1:A:53:GLU:HG3	1.88	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:SER:OG	1:B:92:PRO:HB3	1.88	0.72
1:B:65:ILE:HD11	1:B:134:GLU:O	1.90	0.72
1:B:33:GLY:O	1:B:38:GLY:HA2	1.90	0.71
1:B:52:ALA:O	1:B:58:ILE:HG12	1.90	0.71
1:B:90:LEU:O	1:B:111:ILE:HD13	1.90	0.71
1:B:144:PRO:O	1:B:147:PRO:HD2	1.91	0.71
1:A:5:GLU:HA	1:A:8:ILE:HD12	1.73	0.71
1:C:243:GLU:HG3	1:C:247:ARG:HG3	1.71	0.71
1:A:91:MET:CE	1:A:95:MET:HB3	2.20	0.71
1:A:146:ASN:ND2	1:A:175:THR:HG21	2.05	0.71
1:C:19:MET:SD	1:C:243:GLU:HG2	2.31	0.71
1:D:99:ARG:CZ	1:D:288:SER:OG	2.39	0.71
1:C:234:GLN:HG2	1:C:238:GLU:OE2	1.91	0.71
1:B:201:GLU:HA	1:B:211:ARG:NH1	2.05	0.70
1:A:49:ILE:HD11	1:A:83:LYS:HD2	1.74	0.70
1:B:185:PHE:O	1:B:188:GLU:HG3	1.90	0.70
1:D:11:THR:OG1	1:D:30:LYS:HD2	1.92	0.70
1:A:91:MET:HG3	1:A:92:PRO:HD2	1.72	0.70
1:C:172:SER:HB3	1:C:209:ILE:HG21	1.74	0.70
1:A:175:THR:HG22	1:A:177:GLY:N	2.07	0.70
1:D:64:LEU:HD21	1:D:85:TYR:CD1	2.27	0.70
1:C:240:THR:O	1:C:244:LEU:HD12	1.92	0.70
1:D:183:SER:O	1:D:187:ARG:HG2	1.91	0.70
1:D:91:MET:HA	1:D:121:GLY:HA3	1.73	0.70
1:C:14:VAL:HG22	1:D:3:THR:N	2.06	0.69
1:A:3:THR:HG22	1:A:6:GLN:H	1.56	0.69
1:B:28:TRP:HB2	1:B:276:VAL:HG22	1.73	0.69
1:A:91:MET:O	1:A:112:LEU:HA	1.93	0.69
1:D:3:THR:O	1:D:6:GLN:HB2	1.92	0.69
1:A:12:PRO:HG2	1:A:31:LEU:HB2	1.75	0.69
1:A:175:THR:HB	2:A:320:PLP:O3P	1.93	0.69
1:C:144:PRO:O	1:C:148:LYS:HB3	1.92	0.69
1:D:98:GLU:HB3	1:D:99:ARG:HH21	1.58	0.69
1:A:3:THR:HG22	1:A:6:GLN:HG2	1.75	0.69
1:B:2:SER:HA	1:B:6:GLN:NE2	2.08	0.69
1:B:30:LYS:HB3	1:B:278:ILE:HD13	1.75	0.69
1:B:212:TRP:HA	1:B:214:THR:N	2.08	0.69
1:D:205:SER:HB3	1:D:234:GLN:NE2	2.08	0.69
1:A:21:PRO:HD3	1:A:268:LYS:NZ	2.09	0.68
1:A:54:LYS:HZ1	1:A:55:ARG:HD3	1.56	0.68
1:D:5:GLU:OE2	1:D:82:LEU:HB3	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:MET:HE2	1:C:198:LEU:N	2.09	0.68
1:B:7:THR:OG1	1:B:36:PRO:HG3	1.93	0.68
1:D:5:GLU:O	1:D:8:ILE:HG13	1.94	0.68
1:D:66:GLU:OE1	1:D:66:GLU:HA	1.93	0.68
1:B:176:THR:HG23	1:B:218:PRO:HG2	1.76	0.68
1:C:12:PRO:HA	1:D:1:MET:HG3	1.75	0.67
1:C:26:GLU:O	1:C:275:VAL:HG23	1.93	0.67
1:A:201:GLU:HG2	1:A:202:GLU:H	1.59	0.67
1:C:158:ILE:HA	1:C:161:GLN:HB2	1.76	0.67
1:B:194:THR:HA	1:B:227:ASP:OD2	1.94	0.67
1:C:21:PRO:HB3	1:C:267:ALA:HB1	1.74	0.67
1:B:91:MET:HB2	1:B:111:ILE:HD13	1.76	0.67
1:A:28:TRP:HH2	1:B:1:MET:HB2	1.60	0.67
1:A:50:VAL:HG12	1:A:53:GLU:OE1	1.95	0.67
1:B:28:TRP:O	1:B:276:VAL:HA	1.95	0.67
1:A:21:PRO:HD3	1:A:268:LYS:HZ2	1.60	0.66
1:A:104:ARG:NH1	1:A:110:LEU:HB3	2.09	0.66
1:B:175:THR:O	1:B:220:ILE:HD11	1.95	0.66
1:D:91:MET:O	1:D:111:ILE:HB	1.96	0.66
1:B:48:MET:HG3	1:B:143:ASN:ND2	2.09	0.66
1:B:68:THR:HG22	1:B:69:SER:H	1.59	0.66
1:B:148:LYS:O	1:B:152:THR:HG22	1.96	0.66
1:C:260:VAL:O	1:C:264:LEU:HD22	1.95	0.66
1:C:94:ASN:ND2	1:C:115:LYS:HG3	2.11	0.66
1:D:127:LEU:HD13	1:D:128:GLU:N	2.10	0.66
1:A:146:ASN:HD21	1:A:175:THR:HG21	1.61	0.66
1:C:89:LEU:HD23	1:C:103:MET:SD	2.36	0.66
1:D:143:ASN:OD1	1:D:145:ASP:HB2	1.96	0.66
1:B:217:LEU:HG	1:B:221:PHE:CD2	2.30	0.65
1:D:129:MET:HA	1:D:132:ARG:HB3	1.77	0.65
1:A:124:ASP:O	1:A:128:GLU:HG2	1.97	0.65
1:A:51:GLU:OE1	1:A:51:GLU:HA	1.95	0.65
1:B:74:ILE:O	1:B:78:MET:HB2	1.96	0.65
1:B:35:ASN:HB3	1:B:42:ASP:OD2	1.97	0.65
1:B:200:PRO:HA	1:B:232:ILE:O	1.96	0.65
1:A:173:MET:O	1:A:209:ILE:HB	1.97	0.65
1:B:18:ARG:HD2	1:B:247:ARG:O	1.96	0.65
1:B:212:TRP:HB3	1:B:214:THR:OG1	1.97	0.65
2:C:320:PLP:O1P	3:C:2010:HOH:O	2.14	0.65
1:B:67:ALA:HA	1:B:90:LEU:HB2	1.79	0.65
1:A:19:MET:SD	1:A:244:LEU:HD23	2.37	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:THR:HG23	1:B:225:LEU:HD12	1.77	0.64
1:C:246:VAL:HG23	1:C:247:ARG:H	1.62	0.64
1:A:172:SER:HB3	1:A:209:ILE:HG21	1.78	0.64
1:B:20:GLY:HA2	1:B:264:LEU:HD22	1.78	0.64
1:A:25:SER:HA	1:A:273:ALA:H	1.61	0.64
1:A:114:THR:HG22	1:A:116:GLU:H	1.63	0.64
1:A:233:HIS:NE2	1:A:235:ARG:HD3	2.12	0.64
1:B:93:ASP:O	1:B:94:ASN:O	2.15	0.64
1:C:289:THR:OG1	1:C:291:VAL:HG22	1.98	0.64
1:C:241:MET:HE1	1:C:291:VAL:HB	1.80	0.64
1:D:139:ASP:O	1:D:143:ASN:HB2	1.98	0.64
1:A:233:HIS:CD2	1:A:235:ARG:H	2.16	0.64
1:B:59:LYS:O	1:B:62:ASP:HB2	1.97	0.64
1:A:14:VAL:HG22	1:A:29:LEU:HB2	1.78	0.63
1:A:114:THR:HB	1:A:117:GLN:HG3	1.79	0.63
1:A:266:VAL:O	1:A:269:ALA:HB3	1.99	0.63
1:B:211:ARG:O	1:B:214:THR:HG23	1.98	0.63
1:B:65:ILE:O	1:B:137:LEU:HA	1.97	0.63
1:C:176:THR:HG21	1:C:221:PHE:CD1	2.33	0.63
1:B:19:MET:HE1	1:B:243:GLU:HB2	1.81	0.63
1:B:15:LYS:HD3	1:B:28:TRP:CZ2	2.33	0.63
1:A:244:LEU:HD11	1:A:260:VAL:HG21	1.81	0.63
1:A:293:GLY:O	1:A:294:GLU:OE1	2.16	0.63
1:D:73:GLY:HA3	1:D:103:MET:SD	2.39	0.63
1:D:67:ALA:CB	1:D:90:LEU:HD13	2.25	0.62
1:D:110:LEU:HD23	1:D:110:LEU:H	1.63	0.62
1:C:51:GLU:O	1:C:55:ARG:HG3	2.00	0.62
1:C:244:LEU:HD22	1:C:250:ILE:HG21	1.82	0.62
1:B:260:VAL:O	1:B:264:LEU:HG	2.00	0.62
1:A:14:VAL:HG22	1:A:31:LEU:HD11	1.81	0.62
1:D:193:VAL:O	1:D:195:ILE:HD12	1.98	0.62
1:A:54:LYS:NZ	1:A:55:ARG:HH11	1.98	0.62
1:C:13:LEU:H	1:D:1:MET:HG2	1.64	0.62
1:A:195:ILE:O	1:A:195:ILE:HG13	1.98	0.62
1:B:195:ILE:HG22	1:B:226:VAL:HA	1.82	0.62
1:C:175:THR:O	1:C:220:ILE:HD11	1.99	0.62
1:A:13:LEU:HD12	1:A:30:LYS:HD3	1.81	0.62
1:A:162:THR:O	1:A:165:ARG:HB3	2.00	0.62
1:B:175:THR:HG23	2:B:320:PLP:O3P	2.00	0.62
1:A:167:THR:HG22	1:A:274:VAL:O	2.00	0.61
1:B:11:THR:OG1	1:B:30:LYS:HE3	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ILE:O	1:B:162:THR:HG23	1.99	0.61
1:D:256:SER:HB3	1:D:279:ILE:HG23	1.82	0.61
1:B:37:ALA:HB3	1:B:42:ASP:OD1	2.00	0.61
1:D:125:LEU:HD23	1:D:125:LEU:O	2.00	0.61
1:B:83:LYS:HB2	1:B:85:TYR:CD2	2.34	0.61
1:B:183:SER:O	1:B:187:ARG:HG2	2.00	0.61
1:C:11:THR:OG1	1:C:30:LYS:HE3	2.00	0.61
1:C:210:ARG:NH1	1:C:210:ARG:HB2	2.16	0.61
1:A:233:HIS:CD2	1:A:235:ARG:HD3	2.35	0.61
1:B:239:ASN:O	1:B:242:ARG:HB2	2.00	0.61
1:B:244:LEU:HD11	1:B:260:VAL:HG21	1.82	0.61
1:A:279:ILE:HD11	1:A:281:ASP:O	2.01	0.61
1:D:110:LEU:C	1:D:111:ILE:HD13	2.20	0.61
1:D:127:LEU:HD13	1:D:128:GLU:HG3	1.82	0.61
1:B:3:THR:O	1:B:7:THR:HG23	2.01	0.60
1:A:170:VAL:HG21	1:A:263:ALA:HA	1.82	0.60
1:B:151:TYR:HB2	1:B:184:GLU:OE1	2.01	0.60
1:B:192:PRO:HG2	3:B:2027:HOH:O	2.00	0.60
1:B:212:TRP:HA	1:B:214:THR:HG23	1.84	0.60
1:A:169:PHE:CE2	1:A:171:SER:HB2	2.37	0.60
1:B:128:GLU:HG2	1:B:129:MET:CG	2.32	0.60
1:D:88:LYS:NZ	1:D:88:LYS:HB3	2.16	0.60
1:A:63:VAL:HG11	1:A:88:LYS:HE2	1.83	0.60
1:B:59:LYS:H	1:B:62:ASP:HB2	1.67	0.60
1:B:183:SER:HB3	1:B:225:LEU:HD13	1.83	0.60
1:C:197:GLY:O	1:C:198:LEU:HD23	2.02	0.60
1:A:185:PHE:O	1:A:188:GLU:HG3	2.02	0.60
1:B:147:PRO:HA	1:B:150:HIS:CD2	2.33	0.60
1:A:167:THR:HG23	1:A:168:HIS:ND1	2.16	0.60
1:B:18:ARG:HD3	1:B:247:ARG:NH1	2.17	0.60
1:C:94:ASN:ND2	1:C:94:ASN:H	2.00	0.59
1:A:66:GLU:HG3	1:A:76:LEU:HD13	1.83	0.59
1:D:128:GLU:O	1:D:132:ARG:HB2	2.03	0.59
1:B:195:ILE:H	1:B:227:ASP:HB2	1.66	0.59
1:C:25:SER:CB	1:C:273:ALA:H	2.15	0.59
1:D:98:GLU:O	1:D:99:ARG:HB2	2.02	0.59
1:B:99:ARG:NH1	1:C:115:LYS:HB2	2.17	0.59
1:D:1:MET:O	1:D:2:SER:HB2	2.01	0.59
1:B:153:THR:O	1:B:156:PRO:HD2	2.02	0.59
1:B:29:LEU:HD22	1:B:260:VAL:HG22	1.85	0.59
1:A:143:ASN:OD1	1:A:145:ASP:HB2	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ILE:HD12	1:A:276:VAL:CG2	2.33	0.59
1:A:88:LYS:HA	1:A:109:GLU:O	2.03	0.58
1:A:138:LEU:HD13	1:A:143:ASN:ND2	2.17	0.58
1:C:117:GLN:HB3	1:C:121:GLY:HA3	1.85	0.58
1:A:58:ILE:HD12	1:A:85:TYR:CE1	2.37	0.58
1:D:26:GLU:HB3	1:D:274:VAL:HA	1.83	0.58
1:B:90:LEU:HD12	1:B:111:ILE:CG2	2.33	0.58
1:C:46:LEU:HA	1:C:79:ILE:HD12	1.85	0.58
1:C:242:ARG:HD3	1:C:291:VAL:O	2.04	0.58
1:D:141:PHE:O	1:D:220:ILE:HG23	2.03	0.58
1:D:176:THR:HG22	1:D:220:ILE:HD11	1.86	0.58
1:B:198:LEU:HD13	1:B:259:ALA:HA	1.85	0.58
1:D:52:ALA:HB1	1:D:57:ARG:HB3	1.85	0.58
1:B:78:MET:HG2	1:B:106:TYR:CE1	2.39	0.58
1:D:88:LYS:CE	1:D:109:GLU:HB2	2.34	0.58
1:D:199:GLN:HG3	1:D:200:PRO:O	2.04	0.58
1:A:201:GLU:HG2	1:A:202:GLU:HG3	1.86	0.58
1:C:246:VAL:O	1:D:81:ALA:HB1	2.04	0.58
1:B:198:LEU:HD23	1:B:230:LEU:HD13	1.86	0.57
1:B:213:PRO:HG3	1:B:216:TYR:O	2.04	0.57
1:B:233:HIS:ND1	1:B:235:ARG:HG2	2.18	0.57
1:C:3:THR:HG22	1:C:5:GLU:N	2.19	0.57
1:C:94:ASN:H	1:C:94:ASN:HD22	1.52	0.57
1:B:240:THR:HA	1:B:243:GLU:HG3	1.86	0.57
1:C:19:MET:HG2	1:C:247:ARG:CZ	2.34	0.57
1:D:111:ILE:HG22	1:D:111:ILE:O	2.04	0.57
1:D:129:MET:HA	1:D:132:ARG:CB	2.34	0.57
1:C:25:SER:HB2	1:C:273:ALA:O	2.05	0.57
1:D:36:PRO:HB2	1:D:78:MET:HE2	1.85	0.57
1:C:287:LEU:HD13	1:D:98:GLU:N	2.19	0.57
1:A:179:ILE:HG12	1:A:195:ILE:HD12	1.86	0.57
1:B:247:ARG:HH11	1:B:247:ARG:HG2	1.68	0.57
1:C:29:LEU:HB3	1:C:279:ILE:HG12	1.86	0.57
1:C:201:GLU:HA	1:C:231:ASP:OD1	2.04	0.57
1:B:30:LYS:NZ	1:B:161:GLN:HE22	2.03	0.57
1:C:20:GLY:HA2	1:C:264:LEU:HD12	1.87	0.57
1:C:51:GLU:HB2	1:C:145:ASP:OD2	2.05	0.57
1:D:63:VAL:HG13	1:D:86:ARG:O	2.04	0.57
1:B:100:ARG:HB3	1:B:103:MET:HE1	1.87	0.57
1:B:195:ILE:O	1:B:227:ASP:HB2	2.03	0.57
1:C:183:SER:O	1:C:187:ARG:HG3	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ARG:HD2	1:C:225:LEU:HD23	1.86	0.57
1:D:68:THR:H	1:D:90:LEU:CD2	2.17	0.57
1:B:215:GLU:O	1:B:216:TYR:HD2	1.88	0.57
1:A:160:GLN:HA	1:A:160:GLN:NE2	2.20	0.57
1:C:77:ALA:HB1	1:C:106:TYR:HB2	1.87	0.57
1:D:122:ALA:HB1	1:D:125:LEU:HB3	1.86	0.57
1:D:176:THR:HG23	1:D:180:THR:OG1	2.05	0.57
1:D:198:LEU:CD1	1:D:259:ALA:HA	2.34	0.57
1:D:215:GLU:O	1:D:215:GLU:HG3	2.03	0.57
1:B:198:LEU:CD1	1:B:259:ALA:HA	2.34	0.56
1:A:234:GLN:O	1:A:238:GLU:HG2	2.05	0.56
1:B:16:LEU:CD1	1:B:29:LEU:HD11	2.35	0.56
1:B:233:HIS:HB3	1:B:236:ASP:OD1	2.05	0.56
1:C:29:LEU:HB3	1:C:279:ILE:CG1	2.35	0.56
1:C:207:PRO:HG2	1:C:286:TYR:HE2	1.69	0.56
1:D:47:SER:CB	1:D:149:ALA:HB2	2.34	0.56
1:D:88:LYS:HE3	1:D:109:GLU:HB2	1.86	0.56
1:D:158:ILE:O	1:D:162:THR:HG23	2.06	0.56
1:A:13:LEU:CD1	1:A:30:LYS:HD3	2.35	0.56
1:B:154:THR:O	1:B:158:ILE:HD12	2.06	0.56
1:B:196:VAL:HG13	1:B:228:GLU:HB3	1.87	0.56
1:D:206:ILE:HG12	1:D:209:ILE:CG1	2.35	0.56
1:B:91:MET:HG2	1:B:92:PRO:O	2.05	0.56
1:B:8:ILE:HG13	1:B:36:PRO:HG2	1.87	0.56
1:B:210:ARG:HD3	1:B:214:THR:HG21	1.87	0.56
1:C:248:GLU:O	1:D:82:LEU:HD13	2.04	0.56
1:D:49:ILE:HG22	1:D:49:ILE:O	2.05	0.56
1:B:201:GLU:OE2	1:B:233:HIS:HB2	2.05	0.56
1:C:91:MET:HG3	1:C:95:MET:HG2	1.88	0.56
1:B:239:ASN:O	1:B:243:GLU:HG3	2.06	0.56
1:C:13:LEU:H	1:D:1:MET:CG	2.18	0.56
1:A:4:LEU:HD23	1:A:82:LEU:HD11	1.86	0.56
1:C:171:SER:HB3	1:C:179:ILE:CD1	2.36	0.56
1:D:135:GLY:O	1:D:136:LYS:HB2	2.06	0.56
1:D:201:GLU:HA	1:D:231:ASP:OD2	2.05	0.56
1:D:50:VAL:O	1:D:54:LYS:HB2	2.07	0.55
1:B:178:THR:O	1:B:182:VAL:HG23	2.06	0.55
1:A:49:ILE:HG13	1:A:50:VAL:N	2.21	0.55
1:C:101:ALA:CB	1:D:287:LEU:HD22	2.36	0.55
1:C:154:THR:O	1:C:158:ILE:HG13	2.06	0.55
1:B:90:LEU:HD11	1:B:128:GLU:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:THR:O	1:B:165:ARG:HB2	2.06	0.55
1:D:53:GLU:HG3	1:D:85:TYR:OH	2.07	0.55
1:D:98:GLU:OE2	1:D:285:ARG:O	2.25	0.55
1:D:217:LEU:HG	1:D:218:PRO:HD2	1.88	0.55
1:C:92:PRO:HA	1:C:113:VAL:HG22	1.88	0.55
1:B:123:ARG:N	1:B:124:ASP:HA	2.22	0.55
1:D:4:LEU:HD12	1:D:7:THR:OG1	2.07	0.55
1:B:3:THR:H	1:B:6:GLN:HG3	1.72	0.55
1:B:83:LYS:HB2	1:B:85:TYR:HD2	1.72	0.55
1:B:289:THR:OG1	1:B:291:VAL:HG12	2.06	0.55
1:D:179:ILE:O	1:D:183:SER:HB2	2.07	0.55
1:D:215:GLU:HA	1:D:217:LEU:N	2.17	0.55
1:B:212:TRP:HB2	1:B:216:TYR:HB2	1.89	0.55
1:B:286:TYR:O	1:B:289:THR:HG23	2.06	0.55
1:A:186:MET:CE	1:A:193:VAL:HG11	2.37	0.55
1:B:25:SER:HB3	1:B:271:PRO:O	2.07	0.55
1:D:217:LEU:HD21	1:D:221:PHE:CD2	2.42	0.55
1:B:174:GLY:O	1:B:212:TRP:HZ2	1.89	0.55
1:B:230:LEU:H	1:B:230:LEU:HD12	1.72	0.55
1:D:11:THR:HB	1:D:31:LEU:O	2.07	0.55
1:A:18:ARG:HB3	1:A:247:ARG:HH22	1.73	0.54
1:A:271:PRO:O	1:A:272:ASP:HB2	2.07	0.54
1:C:88:LYS:HE2	1:C:134:GLU:OE2	2.06	0.54
1:D:98:GLU:N	1:D:285:ARG:HB3	2.22	0.54
1:A:95:MET:HE3	1:A:95:MET:HA	1.90	0.54
1:A:198:LEU:CD1	1:A:259:ALA:HA	2.37	0.54
1:C:243:GLU:O	1:C:246:VAL:HG23	2.06	0.54
1:B:21:PRO:HD3	1:B:268:LYS:HE3	1.89	0.54
1:A:175:THR:HG23	1:A:220:ILE:HD11	1.89	0.54
1:C:7:THR:HG22	3:D:2009:HOH:O	2.07	0.54
1:C:206:ILE:HD11	1:C:234:GLN:CA	2.38	0.54
1:D:9:GLY:O	1:D:10:ASN:HB2	2.08	0.54
1:A:244:LEU:O	1:A:248:GLU:HB2	2.08	0.54
1:A:246:VAL:HG12	1:A:247:ARG:CG	2.36	0.54
1:C:25:SER:HB3	1:C:273:ALA:H	1.72	0.53
1:D:172:SER:HA	1:D:198:LEU:HB2	1.90	0.53
1:B:150:HIS:CD2	1:B:178:THR:HA	2.43	0.53
1:A:21:PRO:HG3	1:A:268:LYS:HG2	1.91	0.53
1:C:179:ILE:HG22	3:C:2036:HOH:O	2.07	0.53
1:D:176:THR:HG23	1:D:180:THR:HG1	1.74	0.53
1:A:37:ALA:HB3	1:A:42:ASP:CG	2.29	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:SER:HA	1:B:280:CYS:O	2.08	0.53
1:C:8:ILE:HD12	1:C:46:LEU:HD22	1.91	0.53
1:C:120:GLU:O	1:C:124:ASP:OD2	2.26	0.53
1:D:129:MET:HE2	1:D:132:ARG:HE	1.74	0.53
1:C:12:PRO:HA	1:D:1:MET:CG	2.38	0.53
1:B:75:ALA:O	1:B:78:MET:HB3	2.09	0.53
1:C:262:GLY:O	1:C:266:VAL:HG23	2.08	0.53
1:A:201:GLU:HB3	1:A:204:SER:OG	2.09	0.53
1:B:46:LEU:N	1:B:79:ILE:HD13	2.24	0.53
1:D:3:THR:HA	3:D:2001:HOH:O	2.08	0.53
1:A:49:ILE:HD11	1:A:83:LYS:CD	2.39	0.53
1:B:191:LYS:HG3	1:B:192:PRO:N	2.22	0.53
1:C:78:MET:HE2	1:C:79:ILE:HG12	1.89	0.53
1:C:271:PRO:O	1:C:272:ASP:HB2	2.09	0.53
1:A:7:THR:HG22	1:A:36:PRO:HG3	1.91	0.52
1:A:48:MET:HB3	1:A:138:LEU:CD1	2.37	0.52
1:C:36:PRO:HD2	1:C:42:ASP:OD2	2.09	0.52
1:D:25:SER:HB3	1:D:271:PRO:HA	1.91	0.52
1:A:141:PHE:O	1:A:220:ILE:HG12	2.09	0.52
1:B:150:HIS:CE1	1:B:178:THR:HG23	2.44	0.52
1:D:264:LEU:O	1:D:268:LYS:HE3	2.10	0.52
1:A:90:LEU:HD11	1:A:129:MET:HE1	1.91	0.52
1:A:175:THR:O	1:A:176:THR:HG22	2.10	0.52
1:C:200:PRO:HA	1:C:232:ILE:O	2.10	0.52
1:D:175:THR:O	1:D:176:THR:HG22	2.10	0.52
1:A:18:ARG:HB3	1:A:247:ARG:NH2	2.24	0.52
1:B:180:THR:O	1:B:225:LEU:HD13	2.10	0.52
1:B:182:VAL:O	1:B:186:MET:HG2	2.10	0.52
1:C:37:ALA:HB1	1:C:74:ILE:HG22	1.92	0.52
1:D:7:THR:O	1:D:36:PRO:HD3	2.09	0.52
1:A:44:ALA:O	1:A:48:MET:HG3	2.09	0.52
1:C:33:GLY:HA3	1:C:282:ARG:HG3	1.91	0.52
1:D:60:PRO:HA	1:D:85:TYR:CZ	2.44	0.52
1:A:14:VAL:HG13	1:A:31:LEU:HD11	1.92	0.52
1:A:60:PRO:HD3	1:A:85:TYR:OH	2.09	0.52
1:A:179:ILE:CG1	1:A:195:ILE:HD12	2.39	0.52
1:A:196:VAL:HG11	1:A:230:LEU:HD22	1.92	0.52
1:A:238:GLU:HB2	1:A:242:ARG:NH1	2.24	0.52
1:B:195:ILE:H	1:B:227:ASP:CB	2.23	0.52
1:C:119:MET:HA	1:C:122:ALA:HB3	1.92	0.52
1:D:98:GLU:HG3	1:D:99:ARG:N	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:PHE:HA	1:A:188:GLU:OE2	2.10	0.52
1:A:166:ILE:HD11	1:A:168:HIS:O	2.10	0.52
1:D:98:GLU:HB2	1:D:285:ARG:O	2.09	0.52
1:A:198:LEU:HD13	1:A:232:ILE:HD11	1.92	0.52
1:A:284:ASP:HA	1:A:287:LEU:CD1	2.40	0.52
1:C:292:PHE:HB3	1:D:105:ALA:HB2	1.91	0.52
1:D:88:LYS:HE3	1:D:109:GLU:OE1	2.10	0.52
1:B:213:PRO:HA	1:B:216:TYR:H	1.75	0.51
1:C:242:ARG:O	1:C:246:VAL:HG22	2.09	0.51
1:D:238:GLU:HG2	1:D:242:ARG:NH2	2.25	0.51
1:D:99:ARG:NH1	1:D:288:SER:OG	2.42	0.51
1:A:196:VAL:CG1	1:A:230:LEU:HD22	2.40	0.51
1:C:186:MET:O	1:C:189:GLN:HG2	2.11	0.51
1:D:119:MET:O	1:D:120:GLU:HB2	2.09	0.51
1:A:97:GLN:HA	1:A:100:ARG:HB2	1.91	0.51
1:A:12:PRO:HG2	1:A:31:LEU:CB	2.40	0.51
1:B:99:ARG:NH1	3:B:2016:HOH:O	2.43	0.51
1:B:128:GLU:HG2	1:B:129:MET:HG3	1.93	0.51
1:A:14:VAL:CG2	1:A:29:LEU:HB2	2.41	0.51
1:A:15:LYS:HB2	1:A:28:TRP:CE3	2.46	0.51
1:B:104:ARG:NH1	1:B:110:LEU:H	2.08	0.51
1:C:201:GLU:HG2	1:C:231:ASP:CB	2.34	0.51
1:B:159:TRP:HB2	1:B:185:PHE:HE2	1.76	0.51
1:B:170:VAL:CG1	1:B:198:LEU:HD11	2.41	0.51
1:C:15:LYS:HD2	1:C:28:TRP:CH2	2.46	0.51
1:C:187:ARG:HD2	1:C:225:LEU:CD2	2.41	0.51
1:A:33:GLY:O	1:A:38:GLY:HA2	2.11	0.51
1:B:214:THR:OG1	1:B:214:THR:O	2.29	0.51
1:C:113:VAL:HB	1:C:117:GLN:OE1	2.11	0.51
1:C:159:TRP:HB2	1:C:185:PHE:HE2	1.76	0.51
1:B:199:GLN:O	1:B:231:ASP:HA	2.11	0.50
1:C:21:PRO:HB3	1:C:267:ALA:CB	2.40	0.50
1:A:90:LEU:HD11	1:A:129:MET:CE	2.42	0.50
1:A:21:PRO:HD3	1:A:268:LYS:HG2	1.93	0.50
1:A:91:MET:HE2	1:A:95:MET:CB	2.41	0.50
1:C:241:MET:HE1	1:C:291:VAL:CG1	2.41	0.50
1:A:91:MET:HE3	1:A:99:ARG:HB3	1.92	0.50
1:A:183:SER:OG	1:A:225:LEU:HB3	2.12	0.50
1:B:70:GLY:O	1:B:74:ILE:HG13	2.12	0.50
1:B:194:THR:HG23	1:B:227:ASP:HB3	1.93	0.50
1:D:28:TRP:O	1:D:29:LEU:HD23	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:LYS:HZ2	1:D:110:LEU:HD23	1.76	0.50
1:A:5:GLU:HA	1:A:8:ILE:CD1	2.40	0.50
1:A:39:SER:HA	1:A:280:CYS:O	2.12	0.50
1:A:191:LYS:HD2	1:A:191:LYS:N	2.26	0.50
1:A:293:GLY:O	1:A:294:GLU:HB2	2.11	0.50
1:B:61:GLY:O	1:B:86:ARG:HD3	2.11	0.50
1:B:90:LEU:HD12	1:B:111:ILE:HG23	1.94	0.50
1:D:3:THR:HG22	3:D:2001:HOH:O	2.11	0.50
1:A:3:THR:HG23	1:A:5:GLU:OE1	2.11	0.50
1:B:14:VAL:HG21	1:B:31:LEU:HD11	1.93	0.50
1:D:51:GLU:HB3	1:D:55:ARG:NH1	2.27	0.50
1:D:63:VAL:HG22	1:D:86:ARG:CB	2.37	0.50
1:D:92:PRO:HA	1:D:111:ILE:O	2.12	0.50
1:A:104:ARG:HH12	1:A:110:LEU:HB3	1.76	0.50
1:A:198:LEU:HD12	1:A:259:ALA:HA	1.93	0.50
1:B:51:GLU:O	1:B:55:ARG:HG2	2.11	0.50
1:B:226:VAL:HG12	1:B:227:ASP:H	1.76	0.50
1:C:139:ASP:O	1:C:143:ASN:HB2	2.12	0.50
1:D:4:LEU:HD23	1:D:82:LEU:HD11	1.94	0.50
1:B:235:ARG:HG3	1:B:236:ASP:N	2.27	0.50
1:C:20:GLY:HA2	1:C:264:LEU:CD1	2.41	0.50
1:C:245:ALA:O	1:C:249:GLY:HA2	2.11	0.50
1:A:70:GLY:HA3	1:A:99:ARG:HG2	1.93	0.50
1:C:210:ARG:HB2	1:C:210:ARG:HH11	1.75	0.50
1:C:263:ALA:HA	1:C:266:VAL:HG23	1.94	0.50
1:A:185:PHE:O	1:A:188:GLU:OE2	2.29	0.49
1:C:285:ARG:HB2	3:C:2054:HOH:O	2.11	0.49
1:D:4:LEU:CD2	1:D:82:LEU:HD21	2.36	0.49
1:D:295:GLU:O	1:D:296:HIS:O	2.30	0.49
1:A:65:ILE:O	1:A:137:LEU:HD12	2.12	0.49
1:C:243:GLU:O	1:C:247:ARG:HG3	2.12	0.49
1:A:256:SER:HB3	1:A:279:ILE:HB	1.93	0.49
1:C:106:TYR:HE1	1:D:249:GLY:O	1.95	0.49
1:C:178:THR:N	3:C:2010:HOH:O	2.44	0.49
1:C:244:LEU:HD22	1:C:250:ILE:CG2	2.41	0.49
1:D:124:ASP:OD1	1:D:124:ASP:O	2.30	0.49
1:A:95:MET:HA	1:A:95:MET:CE	2.41	0.49
1:B:5:GLU:OE1	1:B:82:LEU:HG	2.13	0.49
1:B:32:GLU:HB2	1:B:279:ILE:O	2.13	0.49
1:B:58:ILE:HG21	1:B:64:LEU:HD21	1.95	0.49
1:B:69:SER:HB2	1:B:92:PRO:CD	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLU:O	1:B:110:LEU:O	2.30	0.49
1:D:26:GLU:HG2	1:D:28:TRP:NE1	2.27	0.49
1:D:53:GLU:OE2	1:D:85:TYR:OH	2.29	0.49
1:D:90:LEU:O	1:D:91:MET:O	2.30	0.49
1:A:26:GLU:OE1	1:A:165:ARG:NH2	2.46	0.49
1:A:88:LYS:O	1:A:89:LEU:HD13	2.11	0.49
1:B:222:ASN:OD1	1:B:224:SER:OG	2.30	0.49
1:D:36:PRO:HB2	1:D:78:MET:CE	2.43	0.49
1:D:66:GLU:O	1:D:89:LEU:HA	2.12	0.49
1:A:95:MET:CG	1:A:99:ARG:HD3	2.42	0.49
1:B:212:TRP:HB2	1:B:213:PRO:HA	1.95	0.49
1:A:47:SER:O	1:A:51:GLU:HB2	2.12	0.49
1:A:54:LYS:HZ3	1:A:55:ARG:HG2	1.78	0.49
1:A:124:ASP:OD2	1:A:216:TYR:OH	2.30	0.49
1:C:46:LEU:HB2	1:C:79:ILE:HD11	1.95	0.49
1:D:98:GLU:N	1:D:285:ARG:HD2	2.28	0.49
1:D:215:GLU:OE2	1:D:217:LEU:O	2.30	0.49
1:B:123:ARG:HA	1:B:124:ASP:OD1	2.12	0.49
1:B:256:SER:HB3	1:B:279:ILE:HD12	1.94	0.49
1:C:63:VAL:HG22	1:C:86:ARG:HB3	1.94	0.49
1:C:78:MET:CE	1:C:79:ILE:HG12	2.43	0.49
1:B:64:LEU:HD12	1:B:85:TYR:HB3	1.94	0.49
1:B:89:LEU:O	1:B:110:LEU:O	2.31	0.49
1:B:111:ILE:HG22	1:B:111:ILE:O	2.13	0.49
1:B:210:ARG:NE	1:B:214:THR:OG1	2.46	0.49
1:B:232:ILE:O	1:B:232:ILE:HG12	2.13	0.49
1:C:143:ASN:O	1:C:146:ASN:HB3	2.13	0.49
1:C:184:GLU:O	1:C:188:GLU:OE1	2.30	0.49
1:D:4:LEU:O	1:D:7:THR:OG1	2.30	0.49
1:B:194:THR:O	1:B:195:ILE:HD12	2.12	0.48
1:B:206:ILE:HG23	1:B:254:VAL:HG12	1.94	0.48
1:D:64:LEU:HB2	1:D:87:MET:CE	2.44	0.48
1:A:66:GLU:HG3	1:A:76:LEU:CD1	2.43	0.48
1:B:170:VAL:HG12	1:B:198:LEU:HD11	1.95	0.48
1:B:181:GLY:O	1:B:184:GLU:HB3	2.13	0.48
1:C:68:THR:O	1:C:91:MET:HB2	2.13	0.48
1:D:144:PRO:C	1:D:147:PRO:HD2	2.33	0.48
1:D:45:ALA:HB1	1:D:76:LEU:HD23	1.95	0.48
1:B:135:GLY:HA2	1:B:136:LYS:HE2	1.95	0.48
1:C:243:GLU:HG3	1:C:247:ARG:CG	2.40	0.48
1:A:258:GLY:O	1:A:261:ALA:HB3	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:PHE:O	1:A:293:GLY:N	2.46	0.48
1:D:274:VAL:HG12	1:D:274:VAL:O	2.13	0.48
1:A:25:SER:HB3	1:A:271:PRO:HA	1.96	0.48
1:B:43:ARG:HH22	1:B:157:GLU:CD	2.17	0.48
1:B:151:TYR:CD1	1:B:184:GLU:HB3	2.48	0.48
1:C:19:MET:CE	1:C:243:GLU:HG2	2.43	0.48
1:D:67:ALA:HA	1:D:90:LEU:HD22	1.95	0.48
1:A:35:ASN:HB3	1:A:42:ASP:OD2	2.14	0.48
1:A:150:HIS:CD2	1:A:178:THR:HA	2.49	0.48
1:A:206:ILE:HG23	1:A:254:VAL:CG2	2.43	0.48
1:C:187:ARG:NH1	1:C:224:SER:O	2.46	0.48
1:D:68:THR:N	1:D:90:LEU:HD22	2.23	0.48
1:B:99:ARG:NH1	1:C:93:ASP:OD2	2.47	0.48
1:C:143:ASN:HA	1:C:144:PRO:HD3	1.76	0.48
1:C:159:TRP:HB2	1:C:185:PHE:CE2	2.48	0.48
1:A:32:GLU:OE1	1:A:43:ARG:HD2	2.14	0.48
1:A:37:ALA:CB	1:A:78:MET:HE2	2.37	0.48
1:A:186:MET:HE2	1:A:193:VAL:HG11	1.96	0.48
1:A:240:THR:HB	1:A:257:GLY:O	2.14	0.48
1:D:176:THR:HG22	1:D:220:ILE:CD1	2.43	0.48
1:A:69:SER:O	1:A:95:MET:HG2	2.13	0.47
1:C:157:GLU:O	1:C:161:GLN:HG3	2.14	0.47
1:A:15:LYS:NZ	1:A:16:LEU:O	2.47	0.47
1:B:212:TRP:CB	1:B:216:TYR:HB2	2.44	0.47
1:A:165:ARG:NH2	1:A:274:VAL:HG13	2.30	0.47
1:B:80:ALA:HB2	1:B:87:MET:CE	2.44	0.47
1:B:91:MET:HB2	1:B:111:ILE:CD1	2.44	0.47
1:C:23:ASN:HB2	1:C:271:PRO:HB3	1.96	0.47
1:A:16:LEU:HD13	1:A:19:MET:CB	2.43	0.47
1:A:54:LYS:NZ	1:A:55:ARG:HG2	2.29	0.47
1:A:90:LEU:HD21	1:A:125:LEU:HG	1.96	0.47
1:D:32:GLU:OE1	1:D:43:ARG:NH1	2.47	0.47
1:C:240:THR:HG21	1:C:261:ALA:N	2.29	0.47
1:D:8:ILE:HG12	1:D:36:PRO:HG2	1.97	0.47
1:D:168:HIS:CD2	1:D:194:THR:HB	2.50	0.47
1:B:58:ILE:HB	1:B:85:TYR:HE1	1.78	0.47
1:B:69:SER:HB2	1:B:92:PRO:HD3	1.97	0.47
1:B:180:THR:O	1:B:225:LEU:CD1	2.62	0.47
1:D:49:ILE:HD11	1:D:76:LEU:HD22	1.96	0.47
1:D:256:SER:CB	1:D:279:ILE:HG23	2.44	0.47
1:A:12:PRO:HG2	1:A:31:LEU:HD22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LYS:HB2	1:A:28:TRP:CZ3	2.49	0.47
1:A:54:LYS:HZ1	1:A:55:ARG:CD	2.25	0.47
1:A:65:ILE:HG21	1:A:129:MET:HE2	1.95	0.47
1:A:93:ASP:O	1:A:93:ASP:OD2	2.32	0.47
1:A:198:LEU:HB3	1:A:232:ILE:CG1	2.45	0.47
1:A:200:PRO:HB3	1:A:204:SER:O	2.14	0.47
1:A:216:TYR:O	1:A:218:PRO:HD3	2.14	0.47
1:C:41:LYS:HE2	1:C:72:THR:OG1	2.15	0.47
1:C:196:VAL:HB	1:C:228:GLU:CG	2.44	0.47
1:B:183:SER:HA	1:B:186:MET:HB2	1.97	0.47
1:B:142:ASN:HD22	1:B:219:GLY:HA3	1.79	0.47
1:C:9:GLY:O	1:C:10:ASN:HB2	2.15	0.47
1:C:212:TRP:CD1	1:C:218:PRO:HD3	2.50	0.47
1:D:280:CYS:O	1:D:281:ASP:HB3	2.15	0.47
1:B:90:LEU:HD12	1:B:111:ILE:HG22	1.97	0.47
1:B:153:THR:C	1:B:156:PRO:HD2	2.36	0.47
1:C:101:ALA:HB1	1:D:287:LEU:HD22	1.95	0.47
1:D:46:LEU:HD23	1:D:46:LEU:HA	1.74	0.47
1:D:140:GLN:H	1:D:140:GLN:HG3	1.42	0.47
1:C:144:PRO:C	1:C:147:PRO:HD2	2.36	0.46
1:D:149:ALA:O	1:D:153:THR:OG1	2.30	0.46
1:A:91:MET:CE	1:A:99:ARG:HB3	2.45	0.46
1:A:129:MET:HG2	1:A:134:GLU:OE1	2.15	0.46
1:A:16:LEU:HD22	1:A:248:GLU:CD	2.36	0.46
1:A:170:VAL:CG1	1:A:198:LEU:HD11	2.45	0.46
1:B:4:LEU:HB3	1:B:82:LEU:HD21	1.96	0.46
1:A:166:ILE:HD12	1:A:276:VAL:HB	1.97	0.46
1:C:32:GLU:CD	1:C:43:ARG:HE	2.18	0.46
1:C:246:VAL:HG23	1:C:247:ARG:HG2	1.97	0.46
1:B:233:HIS:O	1:B:236:ASP:OD1	2.33	0.46
1:C:241:MET:HE1	1:C:291:VAL:CB	2.46	0.46
1:D:13:LEU:HG	1:D:161:GLN:HB3	1.97	0.46
1:D:64:LEU:HB2	1:D:87:MET:HE2	1.98	0.46
1:B:99:ARG:O	1:B:100:ARG:HB2	2.14	0.46
1:D:65:ILE:CD1	1:D:130:ALA:HB2	2.45	0.46
1:D:90:LEU:CB	1:D:122:ALA:HB3	2.39	0.46
1:A:217:LEU:C	1:A:217:LEU:HD22	2.36	0.46
1:B:200:PRO:O	1:B:211:ARG:HD2	2.15	0.46
1:B:244:LEU:HD11	1:B:260:VAL:CG2	2.44	0.46
1:D:98:GLU:HB3	1:D:99:ARG:HE	1.80	0.46
1:C:171:SER:HB3	1:C:179:ILE:HD12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ILE:HD11	1:C:234:GLN:HA	1.98	0.46
1:D:162:THR:O	1:D:165:ARG:HG3	2.16	0.46
1:D:170:VAL:HG21	1:D:263:ALA:HA	1.98	0.46
1:A:17:GLN:N	1:A:248:GLU:OE1	2.49	0.46
1:A:120:GLU:HG2	1:A:216:TYR:CD1	2.50	0.46
1:A:234:GLN:HG2	1:A:235:ARG:CD	2.35	0.46
1:B:76:LEU:HD12	1:B:76:LEU:HA	1.82	0.45
1:B:180:THR:O	1:B:184:GLU:HB2	2.17	0.45
1:A:98:GLU:OE2	1:A:288:SER:OG	2.30	0.45
1:D:66:GLU:HG2	1:D:138:LEU:HB2	1.98	0.45
1:A:63:VAL:HG11	1:A:88:LYS:CE	2.45	0.45
1:A:91:MET:HE3	1:A:95:MET:HB3	1.95	0.45
1:B:211:ARG:NH1	1:B:231:ASP:OD2	2.50	0.45
1:C:14:VAL:HG22	1:D:2:SER:C	2.36	0.45
1:D:59:LYS:O	1:D:61:GLY:N	2.50	0.45
1:A:15:LYS:HB2	1:A:28:TRP:CD2	2.51	0.45
1:A:30:LYS:HD2	1:A:30:LYS:HA	1.84	0.45
1:A:266:VAL:O	1:A:270:ASN:N	2.50	0.45
1:B:25:SER:N	1:B:271:PRO:O	2.50	0.45
1:B:80:ALA:O	1:B:84:GLY:N	2.50	0.45
1:C:3:THR:HG22	1:C:5:GLU:H	1.81	0.45
1:D:52:ALA:O	1:D:57:ARG:N	2.47	0.45
1:D:99:ARG:NH2	3:D:2056:HOH:O	2.49	0.45
1:A:8:ILE:HG13	1:A:36:PRO:CG	2.47	0.45
1:A:41:LYS:HG3	1:A:71:ASN:HB3	1.98	0.45
1:A:114:THR:HG22	1:A:116:GLU:N	2.30	0.45
1:A:284:ASP:N	1:A:284:ASP:OD1	2.50	0.45
1:B:59:LYS:O	1:B:61:GLY:N	2.49	0.45
1:B:79:ILE:O	1:B:83:LYS:HG3	2.17	0.45
1:D:30:LYS:HA	1:D:30:LYS:HD3	1.86	0.45
1:D:40:VAL:HG22	1:D:40:VAL:O	2.16	0.45
1:D:194:THR:HG21	1:D:228:GLU:OE1	2.16	0.45
1:D:204:SER:CB	1:D:234:GLN:HB2	2.40	0.45
1:A:198:LEU:HB3	1:A:232:ILE:HG13	1.98	0.45
1:A:200:PRO:HD3	1:A:209:ILE:HD12	1.99	0.45
1:B:83:LYS:NZ	3:B:2014:HOH:O	2.50	0.45
1:B:153:THR:OG1	1:B:154:THR:N	2.50	0.45
1:B:164:GLY:O	1:B:191:LYS:NZ	2.50	0.45
1:B:234:GLN:OE1	1:C:117:GLN:NE2	2.50	0.45
1:C:75:ALA:O	1:C:78:MET:HE2	2.16	0.45
1:D:65:ILE:HD11	1:D:130:ALA:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:THR:OG1	1:D:73:GLY:N	2.50	0.45
1:D:128:GLU:O	1:D:132:ARG:N	2.50	0.45
1:D:235:ARG:CZ	1:D:295:GLU:HB3	2.47	0.45
1:A:128:GLU:HG2	1:A:128:GLU:H	1.59	0.45
1:A:241:MET:O	1:A:244:LEU:HB2	2.17	0.45
1:A:260:VAL:O	1:A:264:LEU:HD13	2.17	0.45
1:C:18:ARG:NH1	1:C:247:ARG:O	2.50	0.45
1:D:232:ILE:HD13	1:D:265:ARG:NH2	2.31	0.45
1:A:188:GLU:HG3	1:A:188:GLU:H	1.50	0.45
1:C:173:MET:HE3	1:C:173:MET:HB2	1.82	0.45
1:D:3:THR:OG1	1:D:6:GLN:NE2	2.50	0.45
1:D:260:VAL:O	1:D:264:LEU:HB2	2.16	0.45
1:B:60:PRO:HB3	1:B:83:LYS:O	2.17	0.45
1:B:150:HIS:CE1	1:B:178:THR:HA	2.52	0.45
1:B:211:ARG:NH2	1:B:231:ASP:OD2	2.50	0.45
1:C:170:VAL:HG22	1:C:196:VAL:HG13	1.99	0.45
1:A:41:LYS:CG	1:A:71:ASN:HB3	2.46	0.45
1:A:236:ASP:N	1:A:236:ASP:OD1	2.50	0.45
1:B:199:GLN:HG3	1:B:231:ASP:OD1	2.16	0.45
1:D:26:GLU:OE2	1:D:28:TRP:NE1	2.50	0.45
1:D:98:GLU:HB3	1:D:99:ARG:NH2	2.29	0.45
1:A:7:THR:HG23	1:A:7:THR:O	2.16	0.44
1:A:235:ARG:HA	1:A:238:GLU:CG	2.47	0.44
1:C:120:GLU:HB3	1:C:216:TYR:CZ	2.52	0.44
1:D:67:ALA:O	1:D:140:GLN:NE2	2.50	0.44
1:D:127:LEU:CD1	1:D:128:GLU:HG3	2.46	0.44
1:A:58:ILE:HD12	1:A:85:TYR:CZ	2.52	0.44
1:A:67:ALA:O	1:A:140:GLN:NE2	2.50	0.44
1:A:182:VAL:O	1:A:186:MET:HG2	2.17	0.44
1:A:186:MET:HE3	1:A:193:VAL:HG11	1.99	0.44
1:B:272:ASP:OD1	1:B:272:ASP:N	2.50	0.44
1:C:150:HIS:HB2	1:C:181:GLY:HA3	1.99	0.44
1:D:34:ASN:OD1	1:D:282:ARG:NH2	2.50	0.44
1:D:43:ARG:NH2	1:D:157:GLU:OE1	2.50	0.44
1:A:16:LEU:HD23	1:A:16:LEU:HA	1.82	0.44
1:B:15:LYS:HD3	1:B:28:TRP:CE2	2.53	0.44
1:C:3:THR:CG2	1:C:5:GLU:HB2	2.48	0.44
1:C:170:VAL:HA	1:C:196:VAL:O	2.18	0.44
1:C:217:LEU:HD22	1:C:217:LEU:N	2.32	0.44
1:C:269:ALA:O	1:C:270:ASN:ND2	2.50	0.44
1:D:65:ILE:HG13	1:D:137:LEU:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ALA:O	1:D:84:GLY:N	2.50	0.44
1:A:159:TRP:CE2	1:A:164:GLY:HA2	2.52	0.44
1:B:66:GLU:OE1	1:B:66:GLU:HA	2.17	0.44
1:B:195:ILE:O	1:B:227:ASP:N	2.50	0.44
1:B:247:ARG:NH1	1:B:247:ARG:HG2	2.31	0.44
1:C:182:VAL:HG12	1:C:186:MET:HG2	2.00	0.44
1:C:239:ASN:HA	1:C:242:ARG:HH21	1.82	0.44
1:D:132:ARG:O	1:D:134:GLU:N	2.50	0.44
1:D:206:ILE:HA	3:D:2033:HOH:O	2.16	0.44
1:A:202:GLU:H	1:A:202:GLU:HG3	1.44	0.44
1:B:204:SER:OG	1:B:233:HIS:HA	2.18	0.44
1:C:187:ARG:NH2	1:C:227:ASP:OD1	2.50	0.44
1:C:222:ASN:ND2	1:C:224:SER:OG	2.49	0.44
1:B:2:SER:OG	1:B:3:THR:N	2.50	0.44
1:B:21:PRO:CD	1:B:268:LYS:HE3	2.48	0.44
1:B:131:ASN:N	1:B:131:ASN:OD1	2.50	0.44
1:B:174:GLY:N	2:B:320:PLP:O2P	2.50	0.44
1:C:239:ASN:OD1	1:C:242:ARG:NH2	2.50	0.44
1:A:187:ARG:HA	1:A:187:ARG:HD3	1.63	0.44
1:A:233:HIS:CD2	1:A:235:ARG:HB2	2.52	0.44
1:B:83:LYS:HB2	1:B:85:TYR:CE2	2.52	0.44
1:B:195:ILE:HG22	1:B:195:ILE:O	2.16	0.44
1:C:99:ARG:NH1	3:C:2023:HOH:O	2.50	0.44
1:D:129:MET:CE	1:D:132:ARG:HE	2.30	0.44
1:A:159:TRP:O	1:A:163:GLY:N	2.50	0.44
1:C:173:MET:HG2	1:C:179:ILE:HG21	2.00	0.44
1:D:4:LEU:HD11	1:D:36:PRO:CB	2.36	0.44
1:D:64:LEU:O	1:D:88:LYS:N	2.49	0.44
1:D:64:LEU:HD12	1:D:87:MET:CE	2.48	0.44
1:D:167:THR:HG23	1:D:168:HIS:ND1	2.33	0.44
1:A:14:VAL:HG13	1:A:31:LEU:CD1	2.48	0.44
1:A:91:MET:CE	1:A:95:MET:CB	2.93	0.44
1:B:199:GLN:NE2	1:B:231:ASP:OD1	2.50	0.44
1:C:125:LEU:HG	1:C:129:MET:HG3	2.00	0.44
1:D:18:ARG:HD2	1:D:247:ARG:O	2.18	0.44
1:A:104:ARG:NH1	3:A:2026:HOH:O	2.50	0.43
1:B:261:ALA:O	1:B:265:ARG:HG2	2.18	0.43
1:C:169:PHE:CE2	1:C:182:VAL:HB	2.53	0.43
1:D:68:THR:HG23	1:D:68:THR:O	2.17	0.43
1:A:26:GLU:OE1	1:A:165:ARG:NH1	2.50	0.43
1:A:241:MET:CA	1:A:257:GLY:HA3	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:SER:HA	1:B:198:LEU:HB2	1.99	0.43
1:A:3:THR:HG23	1:A:5:GLU:H	1.83	0.43
1:A:71:ASN:ND2	2:A:320:PLP:H2A1	2.33	0.43
1:B:19:MET:CE	1:B:243:GLU:HB2	2.47	0.43
1:B:35:ASN:O	1:B:38:GLY:N	2.50	0.43
1:B:209:ILE:HG23	2:B:320:PLP:H6	1.99	0.43
1:C:19:MET:HE1	1:C:244:LEU:HA	2.00	0.43
1:C:43:ARG:NH1	1:C:153:THR:OG1	2.49	0.43
1:C:79:ILE:O	1:C:83:LYS:HB2	2.18	0.43
1:C:95:MET:HB2	3:C:2021:HOH:O	2.17	0.43
1:C:240:THR:HG21	1:C:261:ALA:H	1.83	0.43
1:D:187:ARG:CZ	1:D:195:ILE:HD13	2.48	0.43
1:A:125:LEU:HA	1:A:128:GLU:HG3	2.01	0.43
1:A:230:LEU:HD12	1:A:230:LEU:HA	1.76	0.43
1:A:243:GLU:O	1:A:247:ARG:HB2	2.18	0.43
1:B:110:LEU:N	1:B:110:LEU:HD12	2.33	0.43
1:A:41:LYS:HA	1:A:41:LYS:HD3	1.72	0.43
1:A:150:HIS:HA	1:A:154:THR:OG1	2.18	0.43
1:A:270:ASN:N	1:A:270:ASN:OD1	2.51	0.43
1:B:3:THR:HG22	1:B:6:GLN:HG2	2.00	0.43
1:C:163:GLY:HA3	3:C:2033:HOH:O	2.17	0.43
1:C:217:LEU:HD22	1:C:217:LEU:H	1.83	0.43
1:C:68:THR:N	1:C:90:LEU:O	2.50	0.43
1:D:127:LEU:HD13	1:D:128:GLU:H	1.82	0.43
1:A:275:VAL:O	1:A:275:VAL:HG12	2.18	0.43
1:B:289:THR:HG23	3:B:2045:HOH:O	2.18	0.43
1:C:49:ILE:HD13	1:C:79:ILE:CG2	2.48	0.43
1:D:137:LEU:HG	1:D:138:LEU:N	2.34	0.43
1:A:6:GLN:HE21	1:A:6:GLN:HB3	1.56	0.43
1:A:23:ASN:N	1:A:23:ASN:HD22	2.16	0.43
1:B:8:ILE:CG1	1:B:36:PRO:HG2	2.49	0.43
1:B:206:ILE:HA	1:B:207:PRO:HD2	1.93	0.43
1:C:144:PRO:HD2	3:C:2032:HOH:O	2.19	0.43
1:C:198:LEU:HD12	1:C:259:ALA:HA	1.99	0.43
1:D:153:THR:C	1:D:156:PRO:HD2	2.39	0.43
1:D:247:ARG:HE	1:D:247:ARG:HB3	1.75	0.43
1:A:58:ILE:HA	1:A:136:LYS:HE2	2.00	0.43
1:A:93:ASP:HB2	1:D:289:THR:O	2.18	0.43
1:A:264:LEU:O	1:A:268:LYS:HG3	2.19	0.43
1:C:19:MET:HE1	1:C:243:GLU:C	2.39	0.43
1:D:57:ARG:NH2	3:D:2017:HOH:O	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:THR:CG2	1:A:6:GLN:HG2	2.46	0.43
1:A:128:GLU:O	1:A:132:ARG:HG3	2.19	0.43
1:A:258:GLY:O	1:A:261:ALA:N	2.50	0.43
1:A:292:PHE:O	1:A:293:GLY:HA2	2.18	0.43
1:D:70:GLY:O	1:D:73:GLY:N	2.52	0.43
1:D:198:LEU:HD12	1:D:259:ALA:HA	2.00	0.43
1:A:195:ILE:HD11	1:A:225:LEU:O	2.19	0.42
1:B:51:GLU:OE1	1:B:51:GLU:HA	2.18	0.42
1:B:69:SER:HB2	1:B:92:PRO:N	2.34	0.42
1:A:111:ILE:O	1:A:111:ILE:HG22	2.18	0.42
1:D:9:GLY:HA2	1:D:43:ARG:CZ	2.49	0.42
1:A:26:GLU:N	1:A:273:ALA:O	2.52	0.42
1:A:111:ILE:HG13	1:D:295:GLU:HG2	2.01	0.42
1:A:252:CYS:SG	1:A:256:SER:HB2	2.59	0.42
1:C:123:ARG:HD3	1:C:141:PHE:CD2	2.55	0.42
1:C:191:LYS:HA	1:C:191:LYS:HD3	1.79	0.42
1:D:78:MET:O	1:D:82:LEU:HD22	2.19	0.42
1:A:4:LEU:O	1:A:7:THR:HG22	2.20	0.42
1:B:120:GLU:HB2	1:B:121:GLY:H	1.68	0.42
1:B:217:LEU:HD13	1:B:217:LEU:HA	1.84	0.42
1:B:241:MET:HE3	1:B:291:VAL:HG22	2.02	0.42
1:C:285:ARG:HD3	1:D:284:ASP:OD2	2.19	0.42
1:B:89:LEU:O	1:B:90:LEU:HD13	2.20	0.42
1:B:213:PRO:HB3	1:B:216:TYR:O	2.18	0.42
1:C:91:MET:CE	1:C:100:ARG:HG2	2.50	0.42
1:D:232:ILE:HD13	1:D:265:ARG:HH22	1.85	0.42
1:A:23:ASN:ND2	1:A:25:SER:OG	2.53	0.42
1:A:150:HIS:CG	1:A:178:THR:HA	2.55	0.42
1:B:67:ALA:CB	1:B:90:LEU:HB2	2.50	0.42
1:B:210:ARG:HD3	1:B:214:THR:CG2	2.49	0.42
1:B:240:THR:O	1:B:243:GLU:N	2.53	0.42
1:B:241:MET:CE	1:B:291:VAL:HG22	2.48	0.42
1:C:19:MET:CE	1:C:244:LEU:HA	2.50	0.42
1:D:130:ALA:HA	1:D:136:LYS:H	1.84	0.42
1:D:167:THR:O	1:D:168:HIS:ND1	2.53	0.42
1:B:235:ARG:O	1:B:239:ASN:HB2	2.20	0.42
1:C:29:LEU:HD22	1:C:279:ILE:HD11	2.00	0.42
1:C:77:ALA:HB1	1:C:106:TYR:CB	2.49	0.42
1:C:157:GLU:O	1:C:161:GLN:N	2.51	0.42
1:A:57:ARG:NH2	1:A:137:LEU:O	2.50	0.42
1:A:113:VAL:HG23	1:A:114:THR:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ARG:HE	1:B:18:ARG:HB3	1.44	0.42
1:B:19:MET:HG3	1:B:248:GLU:OE2	2.20	0.42
1:B:201:GLU:HG2	1:B:231:ASP:HB3	2.02	0.42
1:C:183:SER:OG	1:C:195:ILE:HG13	2.19	0.42
1:C:215:GLU:HG2	1:C:216:TYR:CD2	2.54	0.42
1:A:198:LEU:CD2	1:A:230:LEU:HB2	2.49	0.42
1:B:150:HIS:HB2	1:B:181:GLY:HA3	2.02	0.42
1:B:226:VAL:HG12	1:B:227:ASP:N	2.34	0.42
1:B:243:GLU:O	1:B:247:ARG:HB2	2.20	0.42
1:C:49:ILE:HG22	1:C:50:VAL:N	2.34	0.42
1:C:53:GLU:HG3	1:C:85:TYR:OH	2.19	0.42
1:A:25:SER:HA	1:A:273:ALA:N	2.31	0.42
1:A:51:GLU:O	1:A:54:LYS:HB3	2.20	0.42
1:B:57:ARG:HH11	1:B:57:ARG:HG2	1.85	0.42
1:B:180:THR:CG2	1:B:225:LEU:HD12	2.48	0.42
1:B:235:ARG:HE	1:B:235:ARG:HB2	1.47	0.42
1:C:95:MET:N	3:C:2021:HOH:O	2.53	0.42
1:D:167:THR:HG23	1:D:167:THR:O	2.19	0.42
1:B:212:TRP:HB3	1:B:214:THR:O	2.19	0.41
1:B:236:ASP:OD1	1:B:236:ASP:N	2.50	0.41
1:C:66:GLU:OE2	1:C:140:GLN:N	2.52	0.41
1:C:142:ASN:OD1	1:C:219:GLY:N	2.50	0.41
1:D:59:LYS:HA	1:D:60:PRO:HD3	1.87	0.41
1:D:88:LYS:C	1:D:89:LEU:HD13	2.39	0.41
1:B:82:LEU:HB3	1:B:83:LYS:HG2	2.01	0.41
1:B:128:GLU:HA	1:B:129:MET:HA	1.65	0.41
1:C:146:ASN:HB3	1:C:147:PRO:HD3	2.02	0.41
1:D:90:LEU:HD23	1:D:90:LEU:H	1.84	0.41
1:A:58:ILE:HG22	1:A:136:LYS:HD3	2.02	0.41
1:B:202:GLU:HG3	1:B:211:ARG:HD3	2.02	0.41
1:C:207:PRO:HG2	1:C:286:TYR:CE2	2.54	0.41
1:D:4:LEU:HA	1:D:7:THR:OG1	2.20	0.41
1:A:8:ILE:HG12	1:A:42:ASP:HB3	2.02	0.41
1:A:30:LYS:HB3	1:A:278:ILE:HD13	2.03	0.41
1:B:137:LEU:HD12	1:B:138:LEU:N	2.34	0.41
1:D:55:ARG:HE	1:D:55:ARG:HB2	1.51	0.41
1:D:211:ARG:NH1	1:D:231:ASP:OD1	2.50	0.41
1:A:14:VAL:O	1:A:29:LEU:N	2.50	0.41
1:A:15:LYS:HA	1:A:27:VAL:O	2.20	0.41
1:B:11:THR:HB	1:B:12:PRO:HD2	2.02	0.41
1:B:43:ARG:HH21	1:B:153:THR:CB	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:LEU:HA	1:C:136:LYS:O	2.21	0.41
2:C:320:PLP:P	3:C:2010:HOH:O	2.78	0.41
1:D:63:VAL:C	1:D:64:LEU:HD23	2.40	0.41
1:D:88:LYS:HB3	1:D:88:LYS:HZ3	1.84	0.41
1:A:166:ILE:HD12	1:A:276:VAL:HG23	2.02	0.41
1:A:238:GLU:HG2	1:A:238:GLU:H	1.49	0.41
1:B:4:LEU:HA	1:B:7:THR:HG23	2.02	0.41
1:B:199:GLN:HG2	1:B:229:VAL:CG1	2.51	0.41
1:C:214:THR:O	1:C:217:LEU:HD13	2.21	0.41
1:A:149:ALA:O	1:A:153:THR:N	2.51	0.41
1:A:150:HIS:NE2	1:A:178:THR:OG1	2.50	0.41
1:A:178:THR:HG22	1:A:179:ILE:N	2.34	0.41
1:A:293:GLY:O	1:A:294:GLU:CB	2.68	0.41
1:B:172:SER:HB3	1:B:209:ILE:HG21	2.02	0.41
1:D:26:GLU:HG2	1:D:28:TRP:CD1	2.56	0.41
1:D:65:ILE:CG2	1:D:88:LYS:HB2	2.51	0.41
1:B:5:GLU:CD	1:B:82:LEU:HG	2.41	0.41
1:D:65:ILE:HG23	1:D:88:LYS:HB2	2.02	0.41
1:D:172:SER:OG	1:D:259:ALA:HB2	2.21	0.41
1:A:32:GLU:OE2	1:A:43:ARG:NH1	2.54	0.41
1:A:115:LYS:HG2	1:A:116:GLU:N	2.35	0.41
1:B:59:LYS:H	1:B:62:ASP:CB	2.34	0.41
1:B:171:SER:O	1:B:198:LEU:N	2.52	0.41
1:B:174:GLY:HA3	2:B:320:PLP:H5A1	2.03	0.41
1:B:196:VAL:HG13	1:B:228:GLU:CB	2.49	0.41
1:B:198:LEU:HD23	1:B:230:LEU:CD1	2.49	0.41
1:D:7:THR:HB	1:D:36:PRO:CG	2.33	0.41
1:D:57:ARG:NH1	1:D:57:ARG:HG2	2.36	0.41
1:D:99:ARG:HH22	1:D:288:SER:HG	1.60	0.41
1:D:123:ARG:O	1:D:123:ARG:HG3	2.21	0.41
1:D:268:LYS:HE3	1:D:268:LYS:HB2	1.69	0.41
1:A:150:HIS:HA	1:A:154:THR:CB	2.50	0.41
1:C:12:PRO:HG2	1:C:34:ASN:ND2	2.36	0.41
1:C:78:MET:HB2	1:C:106:TYR:CE1	2.55	0.41
1:C:150:HIS:CD2	1:C:178:THR:HA	2.56	0.41
1:D:52:ALA:CB	1:D:58:ILE:HG12	2.51	0.40
1:D:211:ARG:HH12	1:D:231:ASP:CG	2.22	0.40
1:A:54:LYS:HZ1	1:A:55:ARG:NH1	2.08	0.40
1:A:87:MET:HE2	1:A:87:MET:HB3	1.80	0.40
1:A:170:VAL:HG12	1:A:198:LEU:HD11	2.02	0.40
1:C:13:LEU:HG	1:C:28:TRP:HE3	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:GLU:HG3	1:C:232:ILE:C	2.41	0.40
1:C:206:ILE:HA	1:C:207:PRO:HD3	1.86	0.40
1:B:67:ALA:CA	1:B:90:LEU:HB2	2.48	0.40
1:C:171:SER:HB3	1:C:179:ILE:HD13	2.03	0.40
1:B:46:LEU:O	1:B:50:VAL:HG23	2.21	0.40
1:B:99:ARG:HH22	1:C:93:ASP:CG	2.25	0.40
1:B:99:ARG:HH12	1:C:115:LYS:HB2	1.83	0.40
1:B:150:HIS:CG	1:B:178:THR:HA	2.56	0.40
1:B:166:ILE:HG23	1:B:166:ILE:O	2.21	0.40
1:B:212:TRP:CG	1:B:216:TYR:HB2	2.57	0.40
1:A:220:ILE:HG12	1:A:220:ILE:H	1.70	0.40
1:B:104:ARG:NH1	1:B:110:LEU:N	2.70	0.40
1:B:253:GLY:HA3	1:B:286:TYR:CE2	2.57	0.40
1:C:70:GLY:CA	1:C:99:ARG:HG2	2.52	0.40
1:D:59:LYS:HB3	1:D:62:ASP:CG	2.42	0.40
1:D:175:THR:O	1:D:220:ILE:HD11	2.21	0.40
1:D:175:THR:OG1	2:D:320:PLP:O3P	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

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	234/240 (98%)	184 (79%)	50 (21%)	1 0
1	B	223/240 (93%)	168 (75%)	55 (25%)	0 0
1	C	233/240 (97%)	181 (78%)	52 (22%)	1 0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	226/240 (94%)	169 (75%)	57 (25%)	0 0
All	All	916/960 (95%)	702 (77%)	214 (23%)	1 0

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	SER
1	A	3	THR
1	A	6	GLN
1	A	7	THR
1	A	15	LYS
1	A	23	ASN
1	A	29	LEU
1	A	30	LYS
1	A	49	ILE
1	A	51	GLU
1	A	54	LYS
1	A	55	ARG
1	A	59	LYS
1	A	72	THR
1	A	76	LEU
1	A	78	MET
1	A	86	ARG
1	A	88	LYS
1	A	95	MET
1	A	97	GLN
1	A	99	ARG
1	A	100	ARG
1	A	111	ILE
1	A	115	LYS
1	A	128	GLU
1	A	138	LEU
1	A	140	GLN
1	A	160	GLN
1	A	175	THR
1	A	176	THR
1	A	188	GLU
1	A	191	LYS
1	A	202	GLU
1	A	205	SER
1	A	210	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	217	LEU
1	A	224	SER
1	A	230	LEU
1	A	234	GLN
1	A	236	ASP
1	A	238	GLU
1	A	247	ARG
1	A	256	SER
1	A	270	ASN
1	A	272	ASP
1	A	279	ILE
1	A	284	ASP
1	A	289	THR
1	A	294	GLU
1	B	1	MET
1	B	6	GLN
1	B	13	LEU
1	B	16	LEU
1	B	18	ARG
1	B	29	LEU
1	B	34	ASN
1	B	47	SER
1	B	54	LYS
1	B	55	ARG
1	B	57	ARG
1	B	62	ASP
1	B	63	VAL
1	B	66	GLU
1	B	69	SER
1	B	76	LEU
1	B	79	ILE
1	B	82	LEU
1	B	90	LEU
1	B	99	ARG
1	B	100	ARG
1	B	104	ARG
1	B	109	GLU
1	B	110	LEU
1	B	111	ILE
1	B	120	GLU
1	B	123	ARG
1	B	124	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	128	GLU
1	B	129	MET
1	B	132	ARG
1	B	136	LYS
1	B	137	LEU
1	B	160	GLN
1	B	175	THR
1	B	179	ILE
1	B	188	GLU
1	B	190	SER
1	B	191	LYS
1	B	201	GLU
1	B	210	ARG
1	B	212	TRP
1	B	214	THR
1	B	216	TYR
1	B	217	LEU
1	B	220	ILE
1	B	230	LEU
1	B	232	ILE
1	B	235	ARG
1	B	236	ASP
1	B	247	ARG
1	B	265	ARG
1	B	272	ASP
1	B	280	CYS
1	B	294	GLU
1	C	1	MET
1	C	19	MET
1	C	22	ASP
1	C	23	ASN
1	C	39	SER
1	C	40	VAL
1	C	49	ILE
1	C	57	ARG
1	C	65	ILE
1	C	66	GLU
1	C	69	SER
1	C	87	MET
1	C	88	LYS
1	C	89	LEU
1	C	90	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	94	ASN
1	C	95	MET
1	C	96	SER
1	C	97	GLN
1	C	98	GLU
1	C	99	ARG
1	C	104	ARG
1	C	110	LEU
1	C	112	LEU
1	C	119	MET
1	C	137	LEU
1	C	148	LYS
1	C	158	ILE
1	C	160	GLN
1	C	162	THR
1	C	165	ARG
1	C	179	ILE
1	C	188	GLU
1	C	190	SER
1	C	191	LYS
1	C	193	VAL
1	C	196	VAL
1	C	202	GLU
1	C	205	SER
1	C	210	ARG
1	C	211	ARG
1	C	217	LEU
1	C	231	ASP
1	C	232	ILE
1	C	241	MET
1	C	244	LEU
1	C	246	VAL
1	C	247	ARG
1	C	266	VAL
1	C	275	VAL
1	C	278	ILE
1	C	291	VAL
1	D	1	MET
1	D	2	SER
1	D	3	THR
1	D	6	GLN
1	D	7	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	8	ILE
1	D	13	LEU
1	D	30	LYS
1	D	46	LEU
1	D	47	SER
1	D	54	LYS
1	D	55	ARG
1	D	57	ARG
1	D	59	LYS
1	D	65	ILE
1	D	66	GLU
1	D	69	SER
1	D	86	ARG
1	D	88	LYS
1	D	89	LEU
1	D	91	MET
1	D	100	ARG
1	D	103	MET
1	D	104	ARG
1	D	109	GLU
1	D	123	ARG
1	D	127	LEU
1	D	129	MET
1	D	132	ARG
1	D	134	GLU
1	D	136	LYS
1	D	140	GLN
1	D	167	THR
1	D	171	SER
1	D	176	THR
1	D	191	LYS
1	D	201	GLU
1	D	202	GLU
1	D	206	ILE
1	D	210	ARG
1	D	212	TRP
1	D	214	THR
1	D	215	GLU
1	D	216	TYR
1	D	224	SER
1	D	227	ASP
1	D	228	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	231	ASP
1	D	235	ARG
1	D	244	LEU
1	D	247	ARG
1	D	250	ILE
1	D	264	LEU
1	D	268	LYS
1	D	284	ASP
1	D	295	GLU
1	D	296	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	97	GLN
1	A	160	GLN
1	A	233	HIS
1	A	234	GLN
1	B	6	GLN
1	B	94	ASN
1	B	142	ASN
1	B	150	HIS
1	B	160	GLN
1	B	233	HIS
1	B	270	ASN
1	C	6	GLN
1	C	94	ASN
1	C	97	GLN
1	C	160	GLN
1	C	233	HIS
1	C	270	ASN
1	D	6	GLN
1	D	296	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PLP	A	320	1	15,15,16	2.05	4 (26%)	20,22,23	1.86	4 (20%)
2	PLP	D	320	1	15,15,16	2.09	4 (26%)	20,22,23	1.85	4 (20%)
2	PLP	C	320	1	15,15,16	2.10	4 (26%)	20,22,23	1.72	3 (15%)
2	PLP	B	320	1	15,15,16	2.07	4 (26%)	20,22,23	1.75	3 (15%)

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
2	PLP	A	320	1	-	0/6/6/8	0/1/1/1
2	PLP	D	320	1	-	0/6/6/8	0/1/1/1
2	PLP	C	320	1	-	2/6/6/8	0/1/1/1
2	PLP	B	320	1	-	0/6/6/8	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	320	PLP	O3-C3	-5.87	1.23	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	320	PLP	O3-C3	-5.87	1.23	1.37
2	B	320	PLP	O3-C3	-5.82	1.23	1.37
2	A	320	PLP	O3-C3	-5.79	1.23	1.37
2	C	320	PLP	P-O1P	2.98	1.60	1.50
2	B	320	PLP	P-O1P	2.88	1.59	1.50
2	D	320	PLP	P-O1P	2.87	1.59	1.50
2	A	320	PLP	P-O1P	2.73	1.59	1.50
2	C	320	PLP	O4P-C5A	-2.35	1.36	1.45
2	D	320	PLP	O4P-C5A	-2.31	1.36	1.45
2	A	320	PLP	O4P-C5A	-2.27	1.36	1.45
2	B	320	PLP	O4P-C5A	-2.21	1.36	1.45
2	A	320	PLP	P-O3P	-2.14	1.46	1.54
2	D	320	PLP	P-O3P	-2.10	1.46	1.54
2	B	320	PLP	P-O3P	-2.09	1.46	1.54
2	C	320	PLP	P-O3P	-2.06	1.46	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	320	PLP	O4P-C5A-C5	6.12	121.00	109.35
2	A	320	PLP	O4P-C5A-C5	5.81	120.43	109.35
2	C	320	PLP	O4P-C5A-C5	5.62	120.06	109.35
2	B	320	PLP	O4P-C5A-C5	5.56	119.95	109.35
2	A	320	PLP	C6-C5-C4	3.15	120.63	118.16
2	D	320	PLP	C6-C5-C4	2.60	120.20	118.16
2	B	320	PLP	C6-C5-C4	2.54	120.16	118.16
2	C	320	PLP	O3P-P-O4P	2.46	113.28	106.73
2	A	320	PLP	C3-C4-C5	-2.38	116.17	118.74
2	C	320	PLP	C6-C5-C4	2.32	119.99	118.16
2	B	320	PLP	O3P-P-O4P	2.30	112.84	106.73
2	D	320	PLP	O3P-P-O4P	2.25	112.72	106.73
2	D	320	PLP	C3-C4-C5	-2.11	116.47	118.74
2	A	320	PLP	O3P-P-O4P	2.08	112.27	106.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	320	PLP	C4-C5-C5A-O4P
2	C	320	PLP	C6-C5-C5A-O4P

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	320	PLP	2	0
2	D	320	PLP	1	0
2	C	320	PLP	2	0
2	B	320	PLP	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	294/303 (97%)	-0.47	1 (0%)	94	94	19, 38, 66, 97	0
1	B	281/303 (92%)	-0.27	4 (1%)	75	78	17, 42, 80, 144	0
1	C	292/303 (96%)	-0.50	0	100	100	18, 37, 58, 91	0
1	D	285/303 (94%)	-0.33	3 (1%)	80	84	15, 41, 78, 112	0
All	All	1152/1212 (95%)	-0.39	8 (0%)	87	89	15, 39, 72, 144	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	98	GLU	5.8
1	D	212	TRP	3.9
1	B	1	MET	3.1
1	B	131	ASN	2.9
1	B	134	GLU	2.7
1	B	211	ARG	2.6
1	A	1	MET	2.3
1	D	213	PRO	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PLP	A	320	15/16	0.98	0.09	19,28,38,44	0
2	PLP	B	320	15/16	0.98	0.10	25,39,48,50	0
2	PLP	C	320	15/16	0.98	0.10	16,32,41,46	0
2	PLP	D	320	15/16	0.99	0.10	14,38,55,56	0

6.5 Other polymers

There are no such residues in this entry.