



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:54 am BST

PDB ID : 3KZF
Title : Structure of Giardia Carbamate Kinase
Authors : Galkin, A.; Herzberg, O.
Deposited on : 2009-12-08
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

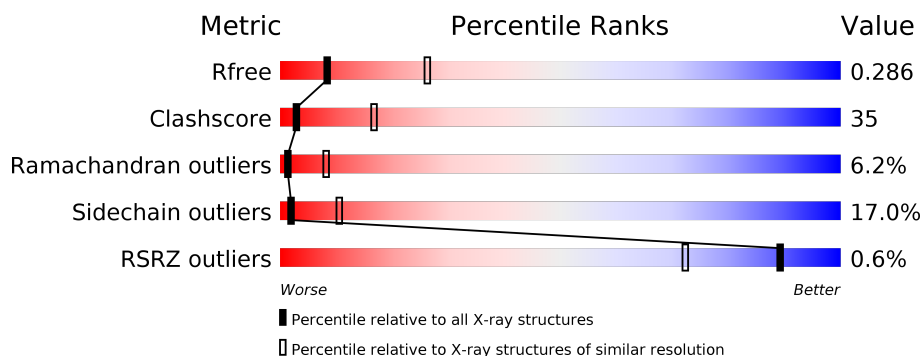
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	317	<div> <div>%</div> <div> <div></div> <div>38%</div> <div>41%</div> <div>9%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	317	<div> <div>%</div> <div> <div></div> <div>38%</div> <div>44%</div> <div>10%</div> <div>•</div> <div>6%</div> </div> </div>
1	C	317	<div> <div></div> <div> <div>36%</div> <div>41%</div> <div>12%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	317	<div> <div></div> <div> <div>38%</div> <div>41%</div> <div>12%</div> <div>•</div> <div>8%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8725 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 Carbamate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2127	1337	363	410	17			
1	B	298	Total	C	N	O	S	0	0	0
			2234	1402	385	430	17			
1	C	287	Total	C	N	O	S	0	0	0
			2147	1352	368	410	17			
1	D	293	Total	C	N	O	S	0	0	0
			2193	1375	378	423	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP A8BB85
B	0	GLY	-	EXPRESSION TAG	UNP A8BB85
C	0	GLY	-	EXPRESSION TAG	UNP A8BB85
D	0	GLY	-	EXPRESSION TAG	UNP A8BB85

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

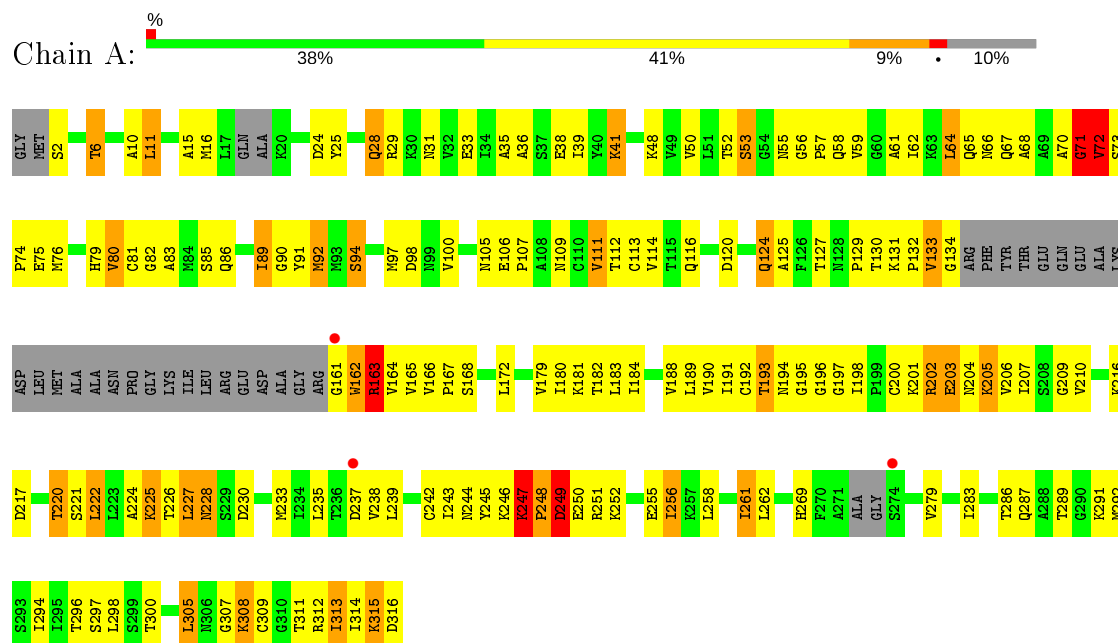


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

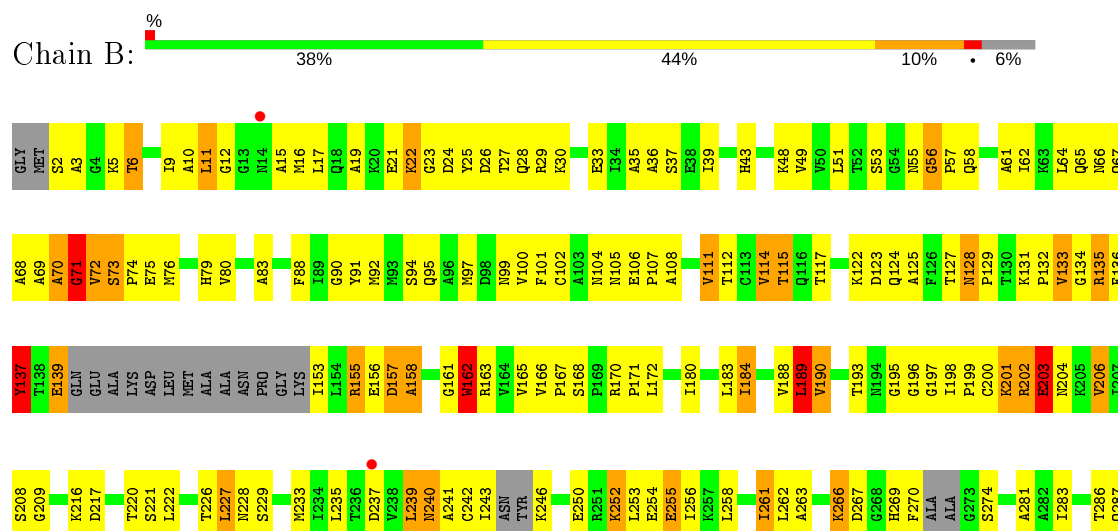
3 Residue-property plots

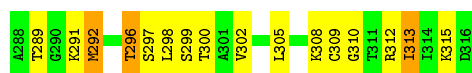
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



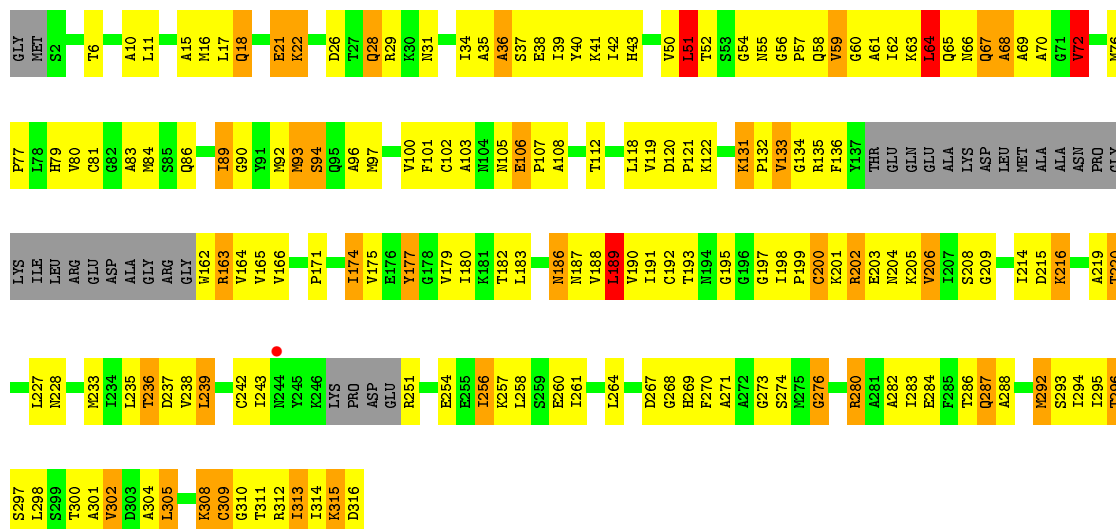
• Molecule 1: Carbamate kinase





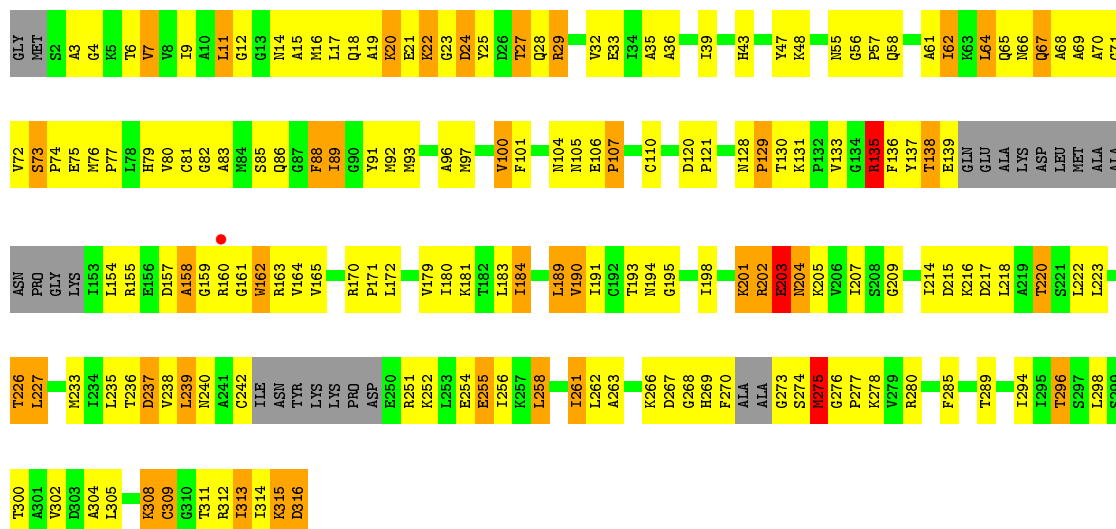
• Molecule 1: Carbamate kinase

Chain C: 36% 41% 12% 9%



• Molecule 1: Carbamate kinase

Chain D: 38% 41% 12% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.77Å 85.41Å 102.10Å 90.00° 106.80° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 10.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.4 (10.00-3.00) 88.4 (10.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 2.99Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.227 , 0.283 0.224 , 0.286	Depositor DCC
R_{free} test set	998 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8725	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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 48.91 % 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 8.0396e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.87	2/2153 (0.1%)	1.04	9/2908 (0.3%)
1	B	0.82	0/2261	0.95	4/3051 (0.1%)
1	C	0.81	1/2175 (0.0%)	0.99	4/2939 (0.1%)
1	D	0.89	1/2219 (0.0%)	0.97	1/2995 (0.0%)
All	All	0.85	4/8808 (0.0%)	0.99	18/11893 (0.2%)

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	2
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	GLY	C-N	-6.95	1.18	1.34
1	C	200	CYS	CB-SG	-5.91	1.72	1.81
1	A	200	CYS	CB-SG	-5.73	1.72	1.81
1	D	110	CYS	CB-SG	-5.14	1.73	1.81

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	LEU	CA-CB-CG	7.88	133.42	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	51	LEU	CB-CG-CD1	-7.28	98.63	111.00
1	A	72	VAL	O-C-N	7.03	133.95	122.70
1	A	247	LYS	C-N-CD	-6.70	105.86	120.60
1	A	11	LEU	CA-CB-CG	6.53	130.32	115.30
1	A	249	ASP	N-CA-C	6.45	128.40	111.00
1	A	227	LEU	CA-CB-CG	6.14	129.41	115.30
1	A	72	VAL	CA-C-N	-5.86	104.31	117.20
1	B	162	TRP	N-CA-C	5.70	126.38	111.00
1	A	111	VAL	CB-CA-C	-5.67	100.63	111.40
1	C	64	LEU	CA-CB-CG	5.62	128.22	115.30
1	C	189	LEU	CA-CB-CG	5.52	127.99	115.30
1	B	155	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	C	227	LEU	CA-CB-CG	5.50	127.94	115.30
1	D	314	ILE	N-CA-C	5.46	125.74	111.00
1	A	71	GLY	C-N-CA	5.39	135.16	121.70
1	A	11	LEU	CB-CG-CD1	-5.21	102.14	111.00
1	B	71	GLY	N-CA-C	-5.17	100.17	113.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	308	LYS	Peptide
1	A	71	GLY	Mainchain
1	B	68	ALA	Peptide
1	C	54	GLY	Peptide
1	D	138	THR	Peptide
1	D	70	ALA	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	2127	0	2188	161	0
1	B	2234	0	2295	160	0
1	C	2147	0	2209	149	0
1	D	2193	0	2247	169	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	6	0	8	0	0
2	B	6	0	8	1	0
2	C	6	0	8	0	0
2	D	6	0	8	1	0
All	All	8725	0	8971	618	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 35.

All (618) 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:A:248:PRO:HA	1:A:250:GLU:N	1.49	1.24
1:C:216:LYS:O	1:C:220:THR:HG22	1.37	1.23
1:D:315:LYS:O	1:D:316:ASP:HB2	1.43	1.19
1:D:135:ARG:HG3	1:D:135:ARG:HH11	1.08	1.15
1:D:216:LYS:O	1:D:220:THR:HG22	1.46	1.13
1:B:17:LEU:HD23	1:B:57:PRO:HB3	1.18	1.12
1:A:85:SER:O	1:A:89:ILE:HG12	1.50	1.11
1:A:248:PRO:CA	1:A:250:GLU:H	1.63	1.10
1:C:90:GLY:O	1:C:94:SER:HB2	1.47	1.09
1:C:21:GLU:HB3	1:C:22:LYS:HA	1.37	1.05
1:A:64:LEU:HD11	1:B:72:VAL:HG22	1.38	1.05
1:A:161:GLY:O	1:A:162:TRP:HB2	1.48	1.04
1:A:216:LYS:O	1:A:220:THR:HG22	1.58	1.02
1:B:28:GLN:HE22	1:B:58:GLN:NE2	1.56	1.02
1:A:62:ILE:HA	1:A:65:GLN:HE21	1.27	0.99
1:A:216:LYS:HE3	1:A:217:ASP:OD1	1.61	0.99
1:A:246:LYS:O	1:A:247:LYS:HG3	1.62	0.97
1:C:17:LEU:HD23	1:C:57:PRO:HB3	1.46	0.97
1:A:247:LYS:O	1:A:250:GLU:HB2	1.66	0.96
1:C:42:ILE:HG12	1:C:302:VAL:HG13	1.49	0.94
1:B:66:ASN:ND2	1:B:76:MET:H	1.64	0.94
1:D:28:GLN:HE22	1:D:58:GLN:HE21	0.97	0.93
1:D:28:GLN:HE22	1:D:58:GLN:NE2	1.66	0.93
1:C:233:MET:HE2	1:C:294:ILE:HG21	1.50	0.92
1:D:97:MET:O	1:D:100:VAL:HG12	1.70	0.92
1:D:7:VAL:HG13	1:D:48:LYS:O	1.69	0.92
1:B:66:ASN:HD22	1:B:76:MET:H	0.94	0.92
1:C:296:THR:HG23	1:C:310:GLY:HA2	1.52	0.91
1:C:66:ASN:HD22	1:C:76:MET:H	1.12	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:MET:HB3	1:D:191:ILE:HD13	1.51	0.91
1:C:17:LEU:CD2	1:C:57:PRO:HB3	2.01	0.90
1:D:135:ARG:CG	1:D:136:PHE:H	1.85	0.89
1:B:235:LEU:HD13	1:B:298:LEU:HD12	1.55	0.89
1:C:42:ILE:CG1	1:C:302:VAL:HG13	2.03	0.88
1:C:256:ILE:HD13	1:C:261:ILE:HG21	1.56	0.88
1:D:135:ARG:HG2	1:D:136:PHE:H	1.39	0.87
1:A:11:LEU:HD13	1:A:15:ALA:HB1	1.56	0.86
1:C:28:GLN:HE22	1:C:58:GLN:HE21	1.20	0.86
1:A:161:GLY:O	1:A:162:TRP:CB	2.23	0.85
1:D:135:ARG:HG3	1:D:135:ARG:NH1	1.88	0.84
1:C:105:ASN:O	1:C:107:PRO:HD3	1.77	0.83
1:B:28:GLN:HE22	1:B:58:GLN:HE21	1.22	0.83
1:C:282:ALA:HB1	1:C:293:SER:OG	1.76	0.83
1:C:315:LYS:HD2	1:C:316:ASP:H	1.44	0.83
1:C:66:ASN:ND2	1:C:76:MET:H	1.77	0.83
1:A:235:LEU:HA	1:A:296:THR:O	1.76	0.82
1:A:28:GLN:HE22	1:A:58:GLN:HE21	1.25	0.82
1:D:273:GLY:HA3	1:D:274:SER:C	1.99	0.82
1:C:296:THR:CG2	1:C:310:GLY:HA2	2.09	0.82
1:B:252:LYS:H	1:B:252:LYS:NZ	1.78	0.82
1:B:101:PHE:HD2	1:B:108:ALA:HB3	1.44	0.81
1:C:216:LYS:O	1:C:220:THR:CG2	2.26	0.81
1:C:21:GLU:HB3	1:C:22:LYS:CA	2.10	0.81
1:D:28:GLN:NE2	1:D:58:GLN:HE21	1.78	0.81
1:A:163:ARG:CG	1:A:163:ARG:HH11	1.95	0.80
1:D:263:ALA:HA	1:D:266:LYS:HD3	1.63	0.80
1:C:61:ALA:O	1:C:65:GLN:HG3	1.81	0.80
1:B:156:GLU:O	1:B:162:TRP:HA	1.81	0.79
1:C:62:ILE:HA	1:C:65:GLN:HE21	1.47	0.79
1:A:163:ARG:NH1	1:A:163:ARG:HG3	1.97	0.79
1:C:199:PRO:HG3	1:C:214:ILE:HD12	1.65	0.78
1:C:296:THR:HG23	1:C:310:GLY:CA	2.14	0.78
1:D:203:GLU:O	1:D:204:ASN:HB2	1.81	0.78
1:D:296:THR:HG22	1:D:300:THR:OG1	1.83	0.78
1:D:62:ILE:HA	1:D:65:GLN:HE21	1.48	0.78
1:D:121:PRO:HG3	1:D:201:LYS:HD2	1.65	0.77
1:D:17:LEU:HD23	1:D:57:PRO:HB3	1.66	0.77
1:A:61:ALA:O	1:A:65:GLN:HG3	1.84	0.77
1:B:17:LEU:HD13	1:B:23:GLY:HA2	1.66	0.77
1:B:43:HIS:HE1	1:B:106:GLU:OE1	1.68	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ILE:HD12	1:A:315:LYS:O	1.85	0.77
1:D:315:LYS:O	1:D:316:ASP:CB	2.26	0.77
1:C:243:ILE:HD13	1:C:264:LEU:HD21	1.65	0.76
1:B:243:ILE:O	1:B:250:GLU:HA	1.84	0.76
1:B:252:LYS:H	1:B:252:LYS:HZ2	1.29	0.76
1:A:132:PRO:HA	1:A:165:VAL:HG12	1.67	0.76
1:B:256:ILE:HD13	1:B:261:ILE:CG2	2.16	0.76
1:A:86:GLN:NE2	1:A:197:GLY:HA2	2.00	0.76
1:D:24:ASP:HB3	1:D:27:THR:OG1	1.86	0.76
1:A:90:GLY:O	1:A:94:SER:HB2	1.86	0.75
1:A:296:THR:HG22	1:A:297:SER:O	1.85	0.75
1:A:315:LYS:HB3	1:A:315:LYS:NZ	2.02	0.75
1:A:216:LYS:CE	1:A:217:ASP:OD1	2.33	0.74
1:C:239:LEU:CD1	1:C:309:CYS:SG	2.76	0.74
1:B:157:ASP:O	1:B:158:ALA:CB	2.35	0.74
1:C:43:HIS:HE1	1:C:106:GLU:OE1	1.68	0.74
1:D:29:ARG:HH11	1:D:29:ARG:CG	2.00	0.74
1:A:203:GLU:O	1:A:204:ASN:HB2	1.88	0.74
1:C:308:LYS:O	1:C:309:CYS:HB2	1.86	0.73
1:C:308:LYS:O	1:C:309:CYS:CB	2.35	0.73
1:B:157:ASP:O	1:B:158:ALA:HB3	1.88	0.73
1:A:203:GLU:O	1:A:204:ASN:CB	2.34	0.73
1:D:273:GLY:CA	1:D:274:SER:C	2.57	0.72
1:A:256:ILE:HD13	1:A:261:ILE:HG21	1.71	0.72
1:B:101:PHE:CD2	1:B:108:ALA:HB3	2.24	0.72
1:B:201:LYS:HG3	1:B:203:GLU:HG3	1.71	0.72
1:A:11:LEU:HD13	1:A:15:ALA:CB	2.20	0.71
1:A:105:ASN:O	1:A:107:PRO:HD3	1.91	0.71
1:D:154:LEU:HD12	1:D:155:ARG:H	1.56	0.71
1:B:17:LEU:HD23	1:B:57:PRO:CB	2.10	0.70
1:A:64:LEU:CD1	1:B:72:VAL:HG22	2.18	0.69
1:A:163:ARG:O	1:A:163:ARG:CG	2.40	0.69
1:D:66:ASN:HD22	1:D:76:MET:H	1.40	0.69
1:B:28:GLN:NE2	1:B:58:GLN:NE2	2.36	0.69
1:D:29:ARG:HH11	1:D:29:ARG:CB	2.06	0.69
1:D:135:ARG:CG	1:D:135:ARG:HH11	1.97	0.69
1:A:163:ARG:CG	1:A:163:ARG:NH1	2.52	0.69
1:A:64:LEU:HD11	1:B:72:VAL:CG2	2.20	0.69
1:D:203:GLU:O	1:D:203:GLU:HG3	1.91	0.69
1:A:105:ASN:C	1:A:107:PRO:HD3	2.14	0.69
1:A:247:LYS:O	1:A:250:GLU:CB	2.40	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:GLY:H	1:D:277:PRO:HD2	1.58	0.68
1:C:39:ILE:HD13	1:C:51:LEU:HD11	1.75	0.68
1:C:43:HIS:CE1	1:C:106:GLU:OE1	2.46	0.68
1:D:61:ALA:O	1:D:65:GLN:HG3	1.93	0.68
1:D:100:VAL:CG1	1:D:101:PHE:N	2.56	0.68
1:C:309:CYS:O	1:C:312:ARG:HD3	1.94	0.68
1:C:239:LEU:HD12	1:C:309:CYS:SG	2.34	0.68
1:A:11:LEU:CD1	1:A:15:ALA:HB1	2.25	0.67
1:B:70:ALA:O	1:B:72:VAL:N	2.27	0.67
1:D:29:ARG:HG2	1:D:29:ARG:HH11	1.58	0.67
1:D:66:ASN:ND2	1:D:76:MET:H	1.92	0.67
1:A:25:TYR:CE1	1:A:92:MET:HE3	2.30	0.67
1:C:296:THR:CG2	1:C:310:GLY:CA	2.72	0.67
1:A:10:ALA:CB	1:A:220:THR:HG21	2.24	0.67
1:A:6:THR:HB	1:A:48:LYS:HB2	1.77	0.66
1:D:203:GLU:CG	1:D:203:GLU:O	2.42	0.66
1:A:90:GLY:HA3	1:A:112:THR:HG21	1.78	0.66
1:B:256:ILE:HD13	1:B:261:ILE:HG21	1.76	0.66
1:C:189:LEU:HD12	1:C:189:LEU:O	1.96	0.66
1:C:64:LEU:HA	1:C:67:GLN:HG3	1.77	0.66
1:A:294:ILE:HA	1:A:311:THR:O	1.95	0.66
1:B:28:GLN:HB2	1:B:92:MET:HE1	1.77	0.66
1:A:25:TYR:CD1	1:A:92:MET:HE1	2.31	0.66
1:B:79:HIS:CD2	1:B:209:GLY:HA3	2.31	0.66
1:B:66:ASN:HD22	1:B:76:MET:N	1.80	0.65
1:D:72:VAL:O	1:D:72:VAL:HG23	1.96	0.65
1:B:132:PRO:HB2	1:B:163:ARG:HH11	1.60	0.65
1:A:247:LYS:H	1:A:248:PRO:HD3	1.60	0.65
1:A:193:THR:HG22	1:A:196:GLY:HA2	1.79	0.65
1:A:97:MET:HA	1:A:100:VAL:HG12	1.79	0.65
1:C:309:CYS:SG	1:C:310:GLY:N	2.70	0.65
1:D:138:THR:OG1	1:D:139:GLU:O	2.15	0.65
1:D:29:ARG:HA	1:D:92:MET:HE2	1.79	0.65
1:B:66:ASN:O	1:B:69:ALA:HB2	1.96	0.65
1:A:71:GLY:O	1:A:73:SER:N	2.30	0.64
1:B:216:LYS:NZ	1:B:217:ASP:OD1	2.26	0.64
1:C:112:THR:HA	1:C:191:ILE:O	1.97	0.64
1:D:29:ARG:HB3	1:D:29:ARG:HH11	1.61	0.64
1:C:180:ILE:HG23	1:C:190:VAL:HG11	1.79	0.64
1:B:258:LEU:HD22	1:B:286:THR:HG22	1.79	0.64
1:D:24:ASP:CB	1:D:27:THR:OG1	2.46	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ASP:OD2	1:A:249:ASP:N	2.30	0.64
1:B:61:ALA:O	1:B:65:GLN:HG3	1.98	0.64
1:C:288:ALA:HA	1:D:263:ALA:HB1	1.79	0.64
1:D:135:ARG:CG	1:D:136:PHE:N	2.57	0.63
1:C:119:VAL:HG22	1:C:200:CYS:O	1.98	0.63
1:C:35:ALA:HA	1:C:298:LEU:HD21	1.80	0.63
1:A:52:THR:HG22	1:A:192:CYS:O	1.98	0.63
1:B:256:ILE:HD13	1:B:261:ILE:HG23	1.80	0.63
1:D:80:VAL:O	1:D:83:ALA:HB3	1.99	0.63
1:B:136:PHE:O	1:B:137:TYR:HB3	1.98	0.63
1:A:133:VAL:CG1	1:A:134:GLY:H	2.12	0.62
1:D:66:ASN:C	1:D:68:ALA:H	2.03	0.62
1:A:112:THR:HB	1:B:114:VAL:HG13	1.81	0.62
1:A:83:ALA:HA	1:A:198:ILE:HD11	1.81	0.62
1:A:205:LYS:HB3	1:B:102:CYS:SG	2.39	0.62
1:C:235:LEU:HA	1:C:296:THR:O	1.99	0.62
1:C:52:THR:HG22	1:C:192:CYS:O	1.99	0.62
1:D:86:GLN:HG2	1:D:194:ASN:HB2	1.81	0.62
1:C:42:ILE:HG13	1:C:302:VAL:HG13	1.81	0.62
1:B:193:THR:HG22	1:B:196:GLY:HA2	1.82	0.62
1:A:261:ILE:HD11	1:A:313:ILE:HD12	1.81	0.62
1:D:25:TYR:CE1	1:D:92:MET:HE3	2.35	0.62
1:D:28:GLN:NE2	1:D:58:GLN:NE2	2.40	0.61
1:C:257:LYS:HG2	1:C:316:ASP:HB3	1.81	0.61
1:D:19:ALA:O	1:D:20:LYS:HB2	1.98	0.61
1:A:35:ALA:HA	1:A:298:LEU:HD21	1.81	0.61
1:C:243:ILE:HD11	1:C:251:ARG:HD3	1.82	0.61
1:C:66:ASN:HD22	1:C:76:MET:N	1.92	0.61
1:D:43:HIS:HE1	1:D:106:GLU:OE1	1.84	0.61
1:C:179:VAL:HG12	1:C:183:LEU:HD12	1.82	0.61
1:D:104:ASN:O	1:D:105:ASN:C	2.38	0.61
1:B:133:VAL:HG12	1:B:133:VAL:O	2.00	0.61
1:B:24:ASP:HB3	1:B:27:THR:OG1	1.99	0.61
1:A:86:GLN:HE22	1:A:197:GLY:HA2	1.62	0.61
1:D:16:MET:SD	1:D:89:ILE:HG23	2.41	0.61
1:A:66:ASN:HD22	1:A:76:MET:N	1.98	0.60
1:B:105:ASN:C	1:B:107:PRO:HD3	2.21	0.60
1:B:80:VAL:O	1:B:83:ALA:HB3	2.01	0.60
1:A:25:TYR:CE1	1:A:92:MET:CE	2.84	0.60
1:B:235:LEU:HD22	1:B:298:LEU:HA	1.84	0.60
1:C:239:LEU:HD11	1:C:309:CYS:SG	2.41	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:ILE:HD13	1:C:261:ILE:CG2	2.31	0.60
1:B:261:ILE:HD11	1:B:313:ILE:HD12	1.83	0.60
1:A:163:ARG:HH11	1:A:163:ARG:HG3	1.62	0.60
1:C:79:HIS:ND1	1:C:209:GLY:HA3	2.16	0.60
1:D:66:ASN:HB3	1:D:75:GLU:HG3	1.83	0.60
1:B:115:THR:O	1:B:198:ILE:HG12	2.01	0.59
1:A:198:ILE:HG21	1:B:91:TYR:CZ	2.37	0.59
1:B:127:THR:O	1:B:128:ASN:HB2	2.02	0.59
1:D:129:PRO:O	1:D:165:VAL:CG2	2.50	0.59
1:D:129:PRO:HB2	1:D:165:VAL:HG23	1.83	0.59
1:A:10:ALA:HB1	1:A:220:THR:HG21	1.83	0.59
1:A:221:SER:O	1:A:222:LEU:C	2.41	0.59
1:D:239:LEU:HD23	1:D:296:THR:HA	1.85	0.59
1:D:273:GLY:HA3	1:D:274:SER:O	2.03	0.59
1:D:308:LYS:O	1:D:309:CYS:HB3	2.02	0.59
1:B:76:MET:HB3	1:B:80:VAL:HG11	1.84	0.58
1:C:35:ALA:O	1:C:36:ALA:C	2.41	0.58
1:C:283:ILE:O	1:C:287:GLN:HB2	2.03	0.58
1:B:202:ARG:O	1:B:206:VAL:O	2.21	0.58
1:C:233:MET:HE1	1:C:301:ALA:O	2.02	0.58
1:C:62:ILE:HD13	1:C:84:MET:HB3	1.85	0.58
1:B:43:HIS:CE1	1:B:106:GLU:OE1	2.54	0.58
1:C:237:ASP:OD1	1:C:238:VAL:HG13	2.04	0.58
1:C:21:GLU:CB	1:C:22:LYS:HA	2.25	0.58
1:B:139:GLU:HG2	1:B:139:GLU:O	2.04	0.57
1:A:73:SER:HB2	1:B:64:LEU:HD13	1.85	0.57
1:D:88:PHE:O	1:D:89:ILE:C	2.42	0.57
1:B:254:GLU:O	1:B:255:GLU:C	2.43	0.57
1:D:55:ASN:HB2	1:D:195:GLY:CA	2.34	0.57
1:D:57:PRO:HB2	1:D:58:GLN:OE1	2.04	0.57
1:A:70:ALA:O	1:A:72:VAL:N	2.38	0.57
1:A:246:LYS:O	1:A:247:LYS:CG	2.45	0.57
1:B:137:TYR:HD2	1:B:137:TYR:O	1.86	0.57
1:B:9:ILE:HA	1:B:233:MET:O	2.05	0.57
1:D:202:ARG:O	1:D:203:GLU:C	2.43	0.57
1:A:82:GLY:O	1:A:85:SER:OG	2.21	0.57
1:D:258:LEU:O	1:D:261:ILE:HD12	2.04	0.57
1:C:268:GLY:O	1:C:271:ALA:HB2	2.04	0.57
1:D:100:VAL:HG13	1:D:101:PHE:N	2.18	0.57
1:A:255:GLU:HG3	1:A:312:ARG:HB2	1.87	0.56
1:D:256:ILE:O	1:D:313:ILE:HA	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ILE:CD1	1:A:313:ILE:HD12	2.36	0.56
1:C:56:GLY:HA2	1:C:133:VAL:CG2	2.36	0.56
1:B:28:GLN:NE2	1:B:58:GLN:HE21	1.97	0.56
1:A:233:MET:HG2	1:A:235:LEU:HD21	1.87	0.56
1:C:199:PRO:HG3	1:C:214:ILE:CD1	2.36	0.56
1:C:17:LEU:HD22	1:C:57:PRO:HB3	1.86	0.56
1:D:29:ARG:HG2	1:D:29:ARG:NH1	2.21	0.56
1:C:136:PHE:CD1	1:C:163:ARG:HG3	2.41	0.55
1:C:42:ILE:HG12	1:C:302:VAL:CG1	2.32	0.55
1:C:55:ASN:HB2	1:C:195:GLY:HA2	1.89	0.55
1:C:297:SER:OG	1:C:300:THR:OG1	2.20	0.55
1:C:66:ASN:ND2	1:C:76:MET:HB2	2.22	0.55
1:D:216:LYS:NZ	1:D:217:ASP:OD1	2.38	0.55
1:A:233:MET:CE	1:A:294:ILE:HG21	2.36	0.55
1:B:3:ALA:HB2	1:D:47:TYR:CE1	2.42	0.55
1:B:222:LEU:O	1:B:226:THR:OG1	2.23	0.55
1:B:97:MET:O	1:B:100:VAL:HG12	2.06	0.55
1:D:193:THR:O	1:D:193:THR:HG22	2.05	0.55
1:B:267:ASP:HB3	1:B:269:HIS:CE1	2.42	0.55
1:C:42:ILE:HD11	1:C:301:ALA:CB	2.37	0.55
1:D:16:MET:HG2	1:D:32:VAL:CG2	2.37	0.55
1:A:66:ASN:HD22	1:A:76:MET:H	1.54	0.55
1:D:129:PRO:O	1:D:165:VAL:HG21	2.07	0.55
1:D:135:ARG:HG2	1:D:136:PHE:N	2.16	0.55
1:D:171:PRO:HB3	1:D:214:ILE:HG21	1.88	0.55
1:B:70:ALA:C	1:B:72:VAL:N	2.61	0.55
1:D:254:GLU:O	1:D:255:GLU:C	2.45	0.55
1:D:158:ALA:O	1:D:160:ARG:N	2.39	0.55
1:C:186:ASN:N	1:C:186:ASN:HD22	2.04	0.54
1:A:133:VAL:HG13	1:A:134:GLY:H	1.72	0.54
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.08	0.54
1:A:237:ASP:OD2	1:A:238:VAL:N	2.39	0.54
1:C:280:ARG:NH2	1:C:284:GLU:OE2	2.38	0.54
1:D:29:ARG:HB3	1:D:29:ARG:NH1	2.23	0.54
1:B:76:MET:HB3	1:B:80:VAL:CG1	2.38	0.54
1:C:28:GLN:HE22	1:C:58:GLN:NE2	1.99	0.54
1:B:49:VAL:HB	1:B:189:LEU:HD22	1.89	0.54
1:C:100:VAL:HA	1:C:103:ALA:HB3	1.90	0.54
1:B:136:PHE:O	1:B:137:TYR:CB	2.55	0.54
1:C:171:PRO:HG3	1:C:214:ILE:CG2	2.38	0.54
1:D:86:GLN:NE2	1:D:198:ILE:HG13	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ILE:HG22	1:C:177:TYR:H	1.72	0.53
1:B:222:LEU:HG	1:B:222:LEU:O	2.06	0.53
1:C:120:ASP:OD1	1:C:121:PRO:HD2	2.08	0.53
1:C:42:ILE:HD11	1:C:301:ALA:HB1	1.91	0.53
1:C:34:ILE:O	1:C:37:SER:HB2	2.09	0.53
1:C:89:ILE:O	1:C:93:MET:HG3	2.09	0.53
1:C:43:HIS:HE1	1:C:106:GLU:CD	2.11	0.53
1:C:63:LYS:O	1:C:67:GLN:HG2	2.09	0.53
1:C:179:VAL:HG12	1:C:183:LEU:CD1	2.38	0.53
1:A:248:PRO:CA	1:A:250:GLU:N	2.42	0.53
1:C:134:GLY:H	1:C:164:VAL:HB	1.74	0.53
1:C:70:ALA:O	1:C:72:VAL:N	2.42	0.53
1:D:17:LEU:HB2	1:D:28:GLN:NE2	2.24	0.53
1:D:223:LEU:HG	1:D:227:LEU:HD22	1.91	0.53
1:A:16:MET:HB3	1:A:28:GLN:HE21	1.73	0.53
1:D:55:ASN:HB2	1:D:195:GLY:HA2	1.90	0.53
1:B:258:LEU:HD21	1:B:287:GLN:HA	1.91	0.53
1:A:283:ILE:O	1:A:287:GLN:HB2	2.09	0.52
1:B:104:ASN:O	1:B:105:ASN:HB2	2.09	0.52
1:B:289:THR:O	1:B:291:LYS:HG2	2.10	0.52
1:B:6:THR:O	1:B:229:SER:OG	2.27	0.52
1:A:64:LEU:CD1	1:B:72:VAL:CG2	2.85	0.52
1:B:289:THR:C	1:B:291:LYS:H	2.11	0.52
1:D:101:PHE:HZ	1:D:189:LEU:HD23	1.74	0.52
1:B:308:LYS:O	1:B:309:CYS:HB3	2.09	0.52
1:A:25:TYR:HE1	1:A:92:MET:HE3	1.74	0.52
1:D:101:PHE:CZ	1:D:189:LEU:HD23	2.45	0.52
1:A:233:MET:HE1	1:A:305:LEU:HD22	1.90	0.52
1:A:315:LYS:HG2	1:A:316:ASP:H	1.74	0.52
1:C:233:MET:CE	1:C:305:LEU:HD22	2.40	0.52
1:B:134:GLY:O	1:B:163:ARG:NH2	2.43	0.52
1:A:248:PRO:HA	1:A:250:GLU:H	0.66	0.52
1:D:88:PHE:O	1:D:91:TYR:N	2.43	0.52
1:A:133:VAL:CG1	1:A:134:GLY:N	2.74	0.51
1:A:163:ARG:O	1:A:163:ARG:HG2	2.11	0.51
1:A:230:ASP:HA	1:A:291:LYS:HE2	1.91	0.51
1:A:243:ILE:HG22	1:A:269:HIS:HB3	1.91	0.51
1:C:286:THR:HG21	1:C:313:ILE:HD13	1.92	0.51
1:B:55:ASN:ND2	1:B:195:GLY:HA3	2.25	0.51
1:A:233:MET:HE3	1:A:294:ILE:HG21	1.92	0.51
1:A:62:ILE:HA	1:A:65:GLN:NE2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:THR:HB	1:B:291:LYS:HG2	1.93	0.51
1:C:101:PHE:HD2	1:C:108:ALA:HB3	1.75	0.51
1:B:184:ILE:HD11	1:B:227:LEU:HG	1.91	0.51
1:B:3:ALA:O	1:D:4:GLY:HA2	2.11	0.51
1:D:238:VAL:O	1:D:238:VAL:CG2	2.59	0.51
1:B:197:GLY:O	1:B:199:PRO:HD3	2.10	0.51
1:B:200:CYS:HB3	1:B:208:SER:O	2.11	0.51
1:A:127:THR:O	1:A:129:PRO:HD3	2.11	0.51
1:B:156:GLU:O	1:B:157:ASP:O	2.29	0.51
1:C:186:ASN:N	1:C:186:ASN:ND2	2.59	0.51
1:D:201:LYS:O	1:D:207:ILE:HA	2.11	0.51
1:D:180:ILE:O	1:D:184:ILE:HG12	2.10	0.51
1:A:245:TYR:O	1:A:246:LYS:HB2	2.11	0.50
1:C:120:ASP:OD1	1:C:122:LYS:HG2	2.11	0.50
1:C:65:GLN:O	1:C:68:ALA:HB3	2.11	0.50
1:C:77:PRO:HB2	1:C:79:HIS:CD2	2.46	0.50
1:B:240:ASN:HD21	1:B:310:GLY:HA2	1.76	0.50
1:A:80:VAL:C	1:A:82:GLY:N	2.63	0.50
1:B:286:THR:HG21	1:B:313:ILE:HG13	1.92	0.50
1:A:64:LEU:HD13	1:B:71:GLY:O	2.12	0.50
1:C:50:VAL:HG13	1:C:190:VAL:HG13	1.94	0.50
1:D:294:ILE:HA	1:D:311:THR:O	2.11	0.50
1:A:10:ALA:HB2	1:A:220:THR:HG21	1.92	0.50
1:A:315:LYS:HB3	1:A:315:LYS:HZ2	1.75	0.50
1:C:239:LEU:HD13	1:C:300:THR:HG21	1.94	0.50
1:C:315:LYS:HD2	1:C:316:ASP:N	2.19	0.50
1:D:136:PHE:CE1	1:D:163:ARG:HD2	2.47	0.50
1:D:79:HIS:ND1	1:D:209:GLY:HA3	2.26	0.50
1:A:133:VAL:HG13	1:A:134:GLY:N	2.27	0.50
1:B:170:ARG:HG3	1:B:171:PRO:HD2	1.94	0.50
1:B:296:THR:CG2	1:B:300:THR:OG1	2.60	0.50
1:A:52:THR:O	1:A:53:SER:HB3	2.12	0.50
1:D:25:TYR:HE1	1:D:92:MET:HE3	1.76	0.50
1:A:179:VAL:HG11	1:B:111:VAL:CG1	2.42	0.49
1:B:66:ASN:ND2	1:B:76:MET:N	2.46	0.49
1:C:254:GLU:HA	1:C:254:GLU:OE1	2.11	0.49
1:D:160:ARG:HB3	1:D:160:ARG:NH1	2.27	0.49
1:D:82:GLY:O	1:D:85:SER:OG	2.22	0.49
1:A:53:SER:OG	1:A:194:ASN:OD1	2.30	0.49
1:B:135:ARG:NH1	1:B:135:ARG:HG2	2.28	0.49
1:A:16:MET:SD	1:A:89:ILE:HG23	2.53	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:PRO:O	1:B:165:VAL:HG21	2.11	0.49
1:D:83:ALA:HA	1:D:198:ILE:HD11	1.93	0.49
1:B:221:SER:HB2	1:B:281:ALA:HB1	1.95	0.49
1:B:25:TYR:CD1	1:B:92:MET:HE3	2.47	0.49
1:B:125:ALA:HB1	1:B:168:SER:H	1.78	0.49
1:B:246:LYS:HA	1:B:250:GLU:OE2	2.13	0.49
1:C:29:ARG:N	1:C:92:MET:HE1	2.28	0.49
1:D:217:ASP:OD2	1:D:278:LYS:HE2	2.11	0.49
1:C:182:THR:O	1:C:186:ASN:ND2	2.45	0.49
1:B:241:ALA:HB3	1:B:270:PHE:HE1	1.77	0.49
1:B:25:TYR:CD1	1:B:92:MET:CE	2.96	0.49
1:B:183:LEU:O	1:B:188:VAL:HB	2.13	0.48
1:D:240:ASN:O	1:D:275:MET:SD	2.71	0.48
1:B:3:ALA:HB2	1:D:47:TYR:CZ	2.47	0.48
1:D:85:SER:OG	1:D:86:GLN:N	2.44	0.48
1:A:233:MET:HE3	1:A:294:ILE:HD13	1.95	0.48
1:B:292:MET:SD	1:B:312:ARG:HB3	2.53	0.48
1:A:79:HIS:CD2	1:A:209:GLY:HA3	2.48	0.48
1:B:253:LEU:HD22	1:B:256:ILE:HG12	1.94	0.48
1:B:67:GLN:HA	1:B:75:GLU:OE2	2.13	0.48
1:D:11:LEU:HD12	1:D:15:ALA:HB1	1.95	0.48
1:A:247:LYS:C	1:A:250:GLU:HB2	2.32	0.48
1:C:101:PHE:CD2	1:C:108:ALA:HB3	2.48	0.48
1:D:17:LEU:HD23	1:D:57:PRO:CB	2.41	0.48
1:D:275:MET:HA	1:D:278:LYS:HB2	1.94	0.48
1:D:25:TYR:CE1	1:D:92:MET:CE	2.97	0.48
1:D:275:MET:HG2	1:D:275:MET:H	1.52	0.48
1:D:58:GLN:OE1	1:D:58:GLN:N	2.43	0.48
1:A:258:LEU:HD22	1:A:286:THR:HG22	1.95	0.48
1:B:296:THR:HG21	1:B:300:THR:OG1	2.14	0.48
1:B:5:LYS:HG3	1:D:3:ALA:O	2.14	0.47
1:A:204:ASN:O	1:A:206:VAL:N	2.48	0.47
1:A:97:MET:O	1:A:98:ASP:C	2.50	0.47
1:B:267:ASP:HB3	1:B:269:HIS:ND1	2.29	0.47
1:C:59:VAL:CG1	1:C:60:GLY:N	2.77	0.47
1:B:129:PRO:O	1:B:165:VAL:CG2	2.62	0.47
1:C:187:ASN:O	1:C:187:ASN:CG	2.53	0.47
1:A:55:ASN:CG	1:A:195:GLY:HA3	2.34	0.47
1:A:62:ILE:HG22	1:A:81:CYS:HB3	1.95	0.47
1:B:139:GLU:CG	1:B:139:GLU:O	2.62	0.47
1:D:201:LYS:NZ	1:D:203:GLU:OE1	2.32	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LYS:HE2	1:A:210:VAL:CG1	2.45	0.47
1:C:131:LYS:HA	1:C:132:PRO:HD2	1.75	0.47
1:B:216:LYS:HZ1	1:B:217:ASP:CG	2.15	0.47
1:C:239:LEU:HA	1:C:297:SER:H	1.80	0.47
1:A:25:TYR:HD1	1:A:92:MET:HE1	1.77	0.47
1:B:136:PHE:CD2	1:B:136:PHE:N	2.81	0.47
1:D:9:ILE:HA	1:D:233:MET:O	2.15	0.47
1:A:242:CYS:HA	1:A:252:LYS:HA	1.97	0.46
1:A:247:LYS:O	1:A:250:GLU:N	2.48	0.46
1:B:131:LYS:HB3	1:B:168:SER:HB2	1.97	0.46
1:D:267:ASP:HB2	1:D:269:HIS:CE1	2.51	0.46
1:C:171:PRO:HG2	1:C:219:ALA:N	2.30	0.46
1:C:31:ASN:HA	1:C:34:ILE:HD12	1.98	0.46
1:D:170:ARG:HG2	1:D:172:LEU:HD21	1.97	0.46
1:A:112:THR:HA	1:A:191:ILE:O	2.15	0.46
1:A:113:CYS:HA	1:B:112:THR:O	2.16	0.46
1:C:11:LEU:HB3	1:C:15:ALA:HB2	1.98	0.46
1:C:189:LEU:C	1:C:189:LEU:HD12	2.35	0.46
1:B:261:ILE:H	1:B:261:ILE:HD13	1.81	0.46
1:D:62:ILE:HG22	1:D:81:CYS:SG	2.56	0.46
1:D:85:SER:O	1:D:88:PHE:HB3	2.15	0.46
1:A:203:GLU:HG2	1:A:203:GLU:O	2.14	0.46
1:B:73:SER:HA	1:B:74:PRO:HD2	1.71	0.46
1:B:228:ASN:HD21	1:C:122:LYS:HA	1.81	0.46
1:D:66:ASN:O	1:D:68:ALA:N	2.39	0.46
1:A:41:LYS:HE3	1:A:41:LYS:HB3	1.40	0.46
1:B:90:GLY:HA3	1:B:112:THR:HG21	1.98	0.46
1:C:214:ILE:HG22	1:C:215:ASP:N	2.31	0.46
1:D:21:GLU:O	1:D:135:ARG:NH2	2.49	0.46
1:D:276:GLY:N	1:D:277:PRO:HD2	2.23	0.46
1:A:242:CYS:HB3	1:A:252:LYS:HA	1.97	0.46
1:B:131:LYS:HA	1:B:132:PRO:HD2	1.75	0.46
1:D:100:VAL:HG12	1:D:101:PHE:N	2.31	0.46
1:D:14:ASN:CG	1:D:237:ASP:HB3	2.37	0.46
1:A:279:VAL:O	1:A:283:ILE:HD12	2.16	0.45
1:C:258:LEU:HD22	1:C:286:THR:HG22	1.97	0.45
1:C:56:GLY:HA2	1:C:133:VAL:HG23	1.97	0.45
1:A:239:LEU:HA	1:A:297:SER:H	1.81	0.45
1:A:71:GLY:C	1:A:73:SER:N	2.69	0.45
1:B:123:ASP:OD1	1:B:124:GLN:N	2.48	0.45
1:B:26:ASP:HB3	1:B:30:LYS:HE3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:VAL:HA	1:C:103:ALA:CB	2.46	0.45
1:A:307:GLY:HA2	1:A:312:ARG:CZ	2.46	0.45
1:A:66:ASN:ND2	1:A:76:MET:HB2	2.31	0.45
1:B:261:ILE:H	1:B:261:ILE:CD1	2.29	0.45
1:C:315:LYS:HD3	1:C:315:LYS:HA	1.86	0.45
1:D:222:LEU:O	1:D:226:THR:OG1	2.30	0.45
1:A:25:TYR:CD1	1:A:92:MET:CE	2.97	0.45
1:C:304:ALA:O	1:C:305:LEU:C	2.54	0.45
1:D:135:ARG:HG3	1:D:136:PHE:H	1.75	0.45
1:B:25:TYR:HD1	1:B:92:MET:HE3	1.81	0.45
1:D:128:ASN:O	1:D:130:THR:HG23	2.16	0.45
1:D:76:MET:HB3	1:D:80:VAL:CG1	2.46	0.45
1:B:10:ALA:HB2	1:B:220:THR:HG21	1.98	0.45
1:B:258:LEU:CD2	1:B:287:GLN:HA	2.47	0.45
1:A:247:LYS:N	1:A:248:PRO:HD3	2.25	0.45
1:B:21:GLU:O	1:B:22:LYS:C	2.55	0.45
1:A:16:MET:HB3	1:A:28:GLN:NE2	2.32	0.45
1:C:171:PRO:HG3	1:C:214:ILE:HG21	1.99	0.45
1:C:214:ILE:CG2	1:C:215:ASP:N	2.80	0.45
1:D:55:ASN:HB2	1:D:195:GLY:HA3	1.98	0.45
1:D:235:LEU:HD13	1:D:298:LEU:CD1	2.47	0.45
1:D:131:LYS:NZ	2:D:322:GOL:O1	2.50	0.45
1:A:97:MET:HA	1:A:100:VAL:CG1	2.46	0.45
1:A:57:PRO:HD2	1:A:58:GLN:OE1	2.17	0.44
1:B:166:VAL:HG23	1:B:167:PRO:O	2.17	0.44
1:C:83:ALA:HA	1:C:198:ILE:HD11	1.98	0.44
1:D:18:GLN:O	1:D:21:GLU:HB2	2.18	0.44
1:B:243:ILE:CD1	1:B:269:HIS:HB3	2.47	0.44
1:D:276:GLY:H	1:D:277:PRO:CD	2.27	0.44
1:A:55:ASN:O	1:A:58:GLN:N	2.50	0.44
1:D:274:SER:O	1:D:277:PRO:HD2	2.18	0.44
1:D:16:MET:HG2	1:D:32:VAL:HG22	1.97	0.44
1:D:67:GLN:HG3	1:D:67:GLN:H	1.55	0.44
1:A:180:ILE:O	1:A:184:ILE:HG12	2.17	0.44
1:A:247:LYS:O	1:A:250:GLU:CA	2.65	0.44
1:A:36:ALA:O	1:A:39:ILE:N	2.50	0.44
1:B:97:MET:O	1:B:101:PHE:CD1	2.70	0.44
1:B:239:LEU:HB3	1:B:297:SER:HB3	1.99	0.44
1:D:100:VAL:HG12	1:D:101:PHE:H	1.82	0.44
1:D:106:GLU:O	1:D:107:PRO:C	2.54	0.44
1:D:66:ASN:HD22	1:D:75:GLU:HA	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:MET:HB3	1:D:80:VAL:HG11	1.99	0.44
1:D:88:PHE:O	1:D:91:TYR:HB3	2.17	0.44
1:A:50:VAL:HG13	1:A:190:VAL:HG13	1.99	0.44
1:A:76:MET:HB3	1:A:80:VAL:CG1	2.47	0.44
1:B:62:ILE:HA	1:B:65:GLN:NE2	2.32	0.44
1:D:11:LEU:HD11	1:D:35:ALA:HB1	2.00	0.44
1:D:205:LYS:HE3	1:D:205:LYS:HB2	1.79	0.44
1:A:131:LYS:HB3	1:A:168:SER:HB2	2.00	0.44
1:A:201:LYS:HE2	1:A:210:VAL:HG12	1.98	0.44
1:C:183:LEU:O	1:C:188:VAL:HB	2.18	0.44
1:D:12:GLY:C	1:D:14:ASN:H	2.21	0.44
1:A:125:ALA:O	1:A:167:PRO:HB3	2.17	0.44
1:B:12:GLY:O	1:B:15:ALA:HB3	2.17	0.44
1:B:263:ALA:O	1:B:266:LYS:HG2	2.18	0.44
1:B:55:ASN:O	1:B:56:GLY:C	2.55	0.44
1:D:155:ARG:HA	1:D:164:VAL:HA	1.99	0.44
1:A:109:ASN:ND2	1:A:188:VAL:HG22	2.33	0.44
1:A:179:VAL:O	1:A:182:THR:HB	2.18	0.44
1:A:28:GLN:O	1:A:31:ASN:N	2.51	0.44
1:C:189:LEU:C	1:C:189:LEU:CD1	2.86	0.44
1:C:233:MET:HE3	1:C:305:LEU:HD22	1.98	0.44
1:D:270:PHE:HB3	1:D:275:MET:O	2.17	0.44
1:A:239:LEU:HA	1:A:297:SER:HB3	1.99	0.44
1:C:118:LEU:HG	1:C:175:VAL:HG23	1.98	0.44
1:C:56:GLY:HA2	1:C:133:VAL:HG22	2.00	0.44
1:C:236:THR:HB	1:C:238:VAL:H	1.83	0.43
1:D:238:VAL:HG22	1:D:238:VAL:O	2.18	0.43
1:D:17:LEU:CD1	1:D:23:GLY:HA2	2.48	0.43
1:D:276:GLY:N	1:D:277:PRO:CD	2.80	0.43
1:D:64:LEU:HD22	1:D:64:LEU:O	2.19	0.43
1:C:256:ILE:HD12	1:C:313:ILE:HB	2.00	0.43
1:D:36:ALA:HB2	1:D:96:ALA:HB1	2.00	0.43
1:D:21:GLU:O	1:D:22:LYS:C	2.57	0.43
1:A:132:PRO:CA	1:A:165:VAL:HG12	2.44	0.43
1:B:11:LEU:O	1:B:53:SER:HA	2.19	0.43
1:D:171:PRO:O	1:D:172:LEU:HD23	2.19	0.43
1:B:137:TYR:OH	1:B:155:ARG:NH2	2.52	0.43
1:C:296:THR:HG23	1:C:310:GLY:HA3	1.98	0.43
1:D:66:ASN:C	1:D:68:ALA:N	2.71	0.43
1:A:205:LYS:HG2	1:B:102:CYS:SG	2.58	0.43
1:B:117:THR:HG21	1:B:171:PRO:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:MET:HB2	1:C:314:ILE:HG22	2.01	0.43
1:A:289:THR:OG1	1:A:291:LYS:HB2	2.19	0.43
1:C:260:GLU:O	1:C:264:LEU:HB2	2.18	0.43
1:A:225:LYS:HG2	1:A:226:THR:N	2.34	0.43
1:C:43:HIS:CE1	1:C:106:GLU:OE2	2.72	0.43
1:C:86:GLN:NE2	1:C:198:ILE:HD12	2.34	0.43
1:D:129:PRO:O	1:D:165:VAL:HG23	2.19	0.43
1:A:197:GLY:O	1:A:198:ILE:C	2.57	0.42
1:B:21:GLU:O	1:B:22:LYS:O	2.37	0.42
1:B:9:ILE:HG23	1:B:233:MET:HG2	2.01	0.42
1:B:35:ALA:O	1:B:36:ALA:C	2.57	0.42
1:A:198:ILE:HG21	1:B:91:TYR:CE1	2.53	0.42
1:A:181:LYS:O	1:A:184:ILE:HG13	2.19	0.42
1:B:171:PRO:O	1:B:172:LEU:HD23	2.18	0.42
1:C:274:SER:C	1:C:276:GLY:H	2.22	0.42
1:C:66:ASN:HD21	1:C:76:MET:HB2	1.84	0.42
1:D:138:THR:HA	1:D:162:TRP:HB2	2.00	0.42
1:A:233:MET:HG2	1:A:235:LEU:CD2	2.49	0.42
1:B:6:THR:HG22	1:B:48:LYS:HG3	2.01	0.42
1:C:106:GLU:O	1:C:106:GLU:HG2	2.19	0.42
1:C:202:ARG:HE	1:C:202:ARG:HB3	1.54	0.42
1:D:14:ASN:OD1	1:D:237:ASP:HB3	2.19	0.42
1:D:285:PHE:O	1:D:289:THR:HG23	2.19	0.42
1:A:224:ALA:O	1:A:228:ASN:N	2.53	0.42
1:C:51:LEU:HB2	1:C:191:ILE:HG12	2.01	0.42
1:C:62:ILE:HD13	1:C:84:MET:CB	2.49	0.42
1:C:183:LEU:HD22	1:C:188:VAL:HG11	2.02	0.42
1:D:89:ILE:O	1:D:92:MET:N	2.53	0.42
1:A:163:ARG:O	1:A:163:ARG:HG3	2.19	0.42
1:A:179:VAL:HG12	1:A:183:LEU:CD1	2.50	0.42
1:B:80:VAL:O	1:B:83:ALA:N	2.52	0.42
1:C:38:GLU:HG3	1:C:298:LEU:HG	2.01	0.42
1:C:81:CYS:O	1:C:84:MET:HB2	2.19	0.42
1:C:40:TYR:O	1:C:41:LYS:C	2.58	0.42
1:D:179:VAL:HG12	1:D:183:LEU:CD1	2.50	0.42
1:D:235:LEU:HD13	1:D:298:LEU:HD13	2.02	0.42
1:A:134:GLY:O	1:A:164:VAL:HB	2.20	0.42
1:A:120:ASP:HB2	1:A:172:LEU:HD11	2.01	0.42
1:C:136:PHE:CZ	1:C:163:ARG:HD2	2.55	0.42
1:D:189:LEU:HD12	1:D:190:VAL:N	2.35	0.42
1:A:243:ILE:CG1	1:A:251:ARG:HB3	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:GLN:OE1	1:B:95:GLN:HB2	2.20	0.41
1:B:180:ILE:HG13	1:B:180:ILE:H	1.70	0.41
1:B:180:ILE:HG23	1:B:190:VAL:HG21	2.02	0.41
1:B:246:LYS:HD3	1:B:246:LYS:N	2.34	0.41
1:B:29:ARG:NH1	1:B:33:GLU:OE1	2.53	0.41
1:A:206:VAL:HG23	1:B:99:ASN:ND2	2.35	0.41
1:C:55:ASN:ND2	1:C:59:VAL:HB	2.35	0.41
1:A:202:ARG:HG3	1:A:207:ILE:HG13	2.01	0.41
1:A:71:GLY:O	1:A:72:VAL:C	2.59	0.41
1:B:235:LEU:CD1	1:B:298:LEU:HD12	2.37	0.41
1:B:283:ILE:O	1:B:287:GLN:HB2	2.20	0.41
1:B:66:ASN:HD21	1:B:76:MET:CG	2.32	0.41
1:C:105:ASN:O	1:C:107:PRO:CD	2.58	0.41
1:C:10:ALA:HB2	1:C:220:THR:HG21	2.01	0.41
1:B:104:ASN:O	1:B:105:ASN:CB	2.68	0.41
1:C:55:ASN:HD21	1:C:59:VAL:HG21	1.85	0.41
1:D:236:THR:HG21	1:D:275:MET:CE	2.51	0.41
1:D:11:LEU:HD21	1:D:39:ILE:HD11	2.02	0.41
1:B:129:PRO:HA	1:B:166:VAL:O	2.20	0.41
1:B:6:THR:HA	1:B:48:LYS:HB2	2.02	0.41
1:B:66:ASN:HD21	1:B:76:MET:HG2	1.86	0.41
1:C:233:MET:CE	1:C:294:ILE:HD13	2.50	0.41
1:C:295:ILE:HB	1:C:311:THR:HB	2.03	0.41
1:C:96:ALA:O	1:C:97:MET:C	2.57	0.41
1:B:242:CYS:HB3	1:B:250:GLU:OE2	2.21	0.41
1:A:91:TYR:OH	1:B:79:HIS:HD2	2.03	0.41
1:D:180:ILE:O	1:D:181:LYS:C	2.57	0.41
1:D:266:LYS:C	1:D:268:GLY:H	2.24	0.41
1:C:237:ASP:CG	1:C:238:VAL:N	2.74	0.41
1:D:11:LEU:HD13	1:D:15:ALA:HB2	2.02	0.41
1:A:35:ALA:O	1:A:38:GLU:HB2	2.21	0.41
1:D:296:THR:CG2	1:D:300:THR:OG1	2.62	0.41
1:A:66:ASN:HD22	1:A:75:GLU:HA	1.86	0.41
1:A:73:SER:HA	1:A:74:PRO:HD3	1.50	0.41
1:C:286:THR:HG21	1:C:313:ILE:CD1	2.50	0.41
1:C:80:VAL:O	1:C:81:CYS:C	2.56	0.41
1:D:128:ASN:HA	1:D:129:PRO:HD2	1.77	0.41
1:D:73:SER:HA	1:D:74:PRO:HD3	1.93	0.41
1:A:16:MET:O	1:A:28:GLN:HA	2.21	0.41
1:B:240:ASN:N	1:B:240:ASN:ND2	2.69	0.41
1:D:17:LEU:HD11	1:D:23:GLY:HA2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:LEU:HA	1:D:305:LEU:HD12	1.88	0.41
1:A:29:ARG:N	1:A:92:MET:HE2	2.36	0.40
1:B:204:ASN:CG	1:B:204:ASN:O	2.59	0.40
2:B:321:GOL:O1	2:B:321:GOL:O3	2.30	0.40
1:C:101:PHE:O	1:C:102:CYS:C	2.59	0.40
1:C:197:GLY:O	1:C:199:PRO:HD3	2.22	0.40
1:D:294:ILE:HG21	1:D:304:ALA:HB1	2.01	0.40
1:D:71:GLY:N	1:D:72:VAL:HA	2.34	0.40
1:D:77:PRO:HD2	1:D:80:VAL:HG21	2.02	0.40
1:D:29:ARG:CA	1:D:92:MET:HE2	2.50	0.40
1:B:100:VAL:CG1	1:B:101:PHE:N	2.83	0.40
1:D:11:LEU:HD12	1:D:15:ALA:CB	2.51	0.40
1:B:51:LEU:HD23	1:B:51:LEU:HA	1.80	0.40
1:B:71:GLY:O	1:B:73:SER:N	2.55	0.40
1:D:215:ASP:OD1	1:D:218:LEU:N	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	277/317 (87%)	225 (81%)	36 (13%)	16 (6%)	1	10
1	B	290/317 (92%)	233 (80%)	42 (14%)	15 (5%)	2	12
1	C	281/317 (89%)	208 (74%)	58 (21%)	15 (5%)	2	11
1	D	285/317 (90%)	222 (78%)	39 (14%)	24 (8%)	1	4
All	All	1133/1268 (89%)	888 (78%)	175 (15%)	70 (6%)	1	8

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	GLY
1	A	71	GLY
1	A	162	TRP
1	A	247	LYS
1	A	249	ASP
1	B	22	LYS
1	B	72	VAL
1	B	128	ASN
1	B	157	ASP
1	C	68	ALA
1	C	106	GLU
1	C	177	TYR
1	C	203	GLU
1	C	309	CYS
1	D	67	GLN
1	D	88	PHE
1	D	135	ARG
1	D	157	ASP
1	D	159	GLY
1	D	203	GLU
1	D	204	ASN
1	D	275	MET
1	A	53	SER
1	A	68	ALA
1	A	163	ARG
1	A	205	LYS
1	A	244	ASN
1	A	309	CYS
1	B	19	ALA
1	B	56	GLY
1	B	70	ALA
1	B	71	GLY
1	B	137	TYR
1	B	158	ALA
1	C	18	GLN
1	C	72	VAL
1	C	163	ARG
1	D	69	ALA
1	D	89	ILE
1	D	161	GLY
1	B	202	ARG
1	B	203	GLU
1	C	69	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	273	GLY
1	D	24	ASP
1	D	158	ALA
1	D	251	ARG
1	D	255	GLU
1	D	258	LEU
1	D	309	CYS
1	A	72	VAL
1	A	222	LEU
1	A	248	PRO
1	B	88	PHE
1	B	162	TRP
1	C	21	GLU
1	C	206	VAL
1	D	22	LYS
1	D	162	TRP
1	A	106	GLU
1	C	36	ALA
1	C	204	ASN
1	D	129	PRO
1	A	124	GLN
1	B	161	GLY
1	D	62	ILE
1	D	107	PRO
1	D	315	LYS
1	C	276	GLY
1	D	56	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	235/257 (91%)	197 (84%)	38 (16%)	2	12
1	B	245/257 (95%)	205 (84%)	40 (16%)	2	11
1	C	235/257 (91%)	187 (80%)	48 (20%)	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	240/257 (93%)	204 (85%)	36 (15%)	3	14
All	All	955/1028 (93%)	793 (83%)	162 (17%)	2	10

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	6	THR
1	A	24	ASP
1	A	28	GLN
1	A	33	GLU
1	A	41	LYS
1	A	59	VAL
1	A	64	LEU
1	A	67	GLN
1	A	72	VAL
1	A	80	VAL
1	A	89	ILE
1	A	92	MET
1	A	94	SER
1	A	111	VAL
1	A	114	VAL
1	A	124	GLN
1	A	130	THR
1	A	133	VAL
1	A	163	ARG
1	A	166	VAL
1	A	189	LEU
1	A	193	THR
1	A	202	ARG
1	A	203	GLU
1	A	220	THR
1	A	225	LYS
1	A	227	LEU
1	A	228	ASN
1	A	256	ILE
1	A	261	ILE
1	A	262	LEU
1	A	292	MET
1	A	300	THR
1	A	305	LEU
1	A	308	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	313	ILE
1	A	315	LYS
1	B	2	SER
1	B	6	THR
1	B	11	LEU
1	B	16	MET
1	B	37	SER
1	B	39	ILE
1	B	73	SER
1	B	94	SER
1	B	111	VAL
1	B	114	VAL
1	B	115	THR
1	B	122	LYS
1	B	133	VAL
1	B	135	ARG
1	B	137	TYR
1	B	139	GLU
1	B	153	ILE
1	B	184	ILE
1	B	189	LEU
1	B	190	VAL
1	B	201	LYS
1	B	203	GLU
1	B	206	VAL
1	B	227	LEU
1	B	237	ASP
1	B	239	LEU
1	B	240	ASN
1	B	252	LYS
1	B	255	GLU
1	B	261	ILE
1	B	262	LEU
1	B	266	LYS
1	B	274	SER
1	B	292	MET
1	B	296	THR
1	B	299	SER
1	B	302	VAL
1	B	305	LEU
1	B	313	ILE
1	B	315	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	6	THR
1	C	16	MET
1	C	18	GLN
1	C	22	LYS
1	C	26	ASP
1	C	28	GLN
1	C	51	LEU
1	C	59	VAL
1	C	64	LEU
1	C	67	GLN
1	C	72	VAL
1	C	89	ILE
1	C	93	MET
1	C	94	SER
1	C	131	LYS
1	C	133	VAL
1	C	135	ARG
1	C	162	TRP
1	C	165	VAL
1	C	166	VAL
1	C	174	ILE
1	C	186	ASN
1	C	189	LEU
1	C	193	THR
1	C	201	LYS
1	C	202	ARG
1	C	205	LYS
1	C	206	VAL
1	C	208	SER
1	C	216	LYS
1	C	220	THR
1	C	228	ASN
1	C	236	THR
1	C	239	LEU
1	C	242	CYS
1	C	256	ILE
1	C	267	ASP
1	C	269	HIS
1	C	270	PHE
1	C	280	ARG
1	C	287	GLN
1	C	292	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	296	THR
1	C	302	VAL
1	C	305	LEU
1	C	308	LYS
1	C	313	ILE
1	C	315	LYS
1	D	6	THR
1	D	7	VAL
1	D	11	LEU
1	D	20	LYS
1	D	27	THR
1	D	29	ARG
1	D	33	GLU
1	D	64	LEU
1	D	73	SER
1	D	100	VAL
1	D	133	VAL
1	D	135	ARG
1	D	137	TYR
1	D	184	ILE
1	D	189	LEU
1	D	190	VAL
1	D	201	LYS
1	D	202	ARG
1	D	203	GLU
1	D	220	THR
1	D	226	THR
1	D	227	LEU
1	D	237	ASP
1	D	239	LEU
1	D	242	CYS
1	D	252	LYS
1	D	261	ILE
1	D	262	LEU
1	D	275	MET
1	D	280	ARG
1	D	296	THR
1	D	302	VAL
1	D	308	LYS
1	D	312	ARG
1	D	313	ILE
1	D	316	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	65	GLN
1	A	66	ASN
1	A	79	HIS
1	A	269	HIS
1	B	14	ASN
1	B	31	ASN
1	B	43	HIS
1	B	58	GLN
1	B	65	GLN
1	B	66	ASN
1	B	79	HIS
1	B	128	ASN
1	B	194	ASN
1	B	228	ASN
1	B	240	ASN
1	C	14	ASN
1	C	28	GLN
1	C	31	ASN
1	C	43	HIS
1	C	55	ASN
1	C	65	GLN
1	C	66	ASN
1	C	79	HIS
1	C	244	ASN
1	C	269	HIS
1	C	287	GLN
1	D	28	GLN
1	D	43	HIS
1	D	65	GLN
1	D	66	ASN
1	D	116	GLN
1	D	128	ASN
1	D	306	ASN

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 carbohydrates 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	GOL	D	322	-	5,5,5	0.56	0	5,5,5	0.22	0
2	GOL	A	324	-	5,5,5	0.48	0	5,5,5	0.61	0
2	GOL	C	323	-	5,5,5	0.59	0	5,5,5	0.33	0
2	GOL	B	321	-	5,5,5	0.55	0	5,5,5	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	322	-	-	3/4/4/4	-
2	GOL	A	324	-	-	4/4/4/4	-
2	GOL	C	323	-	-	2/4/4/4	-
2	GOL	B	321	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	322	GOL	O1-C1-C2-C3
2	A	324	GOL	O1-C1-C2-O2
2	A	324	GOL	O1-C1-C2-C3
2	A	324	GOL	C1-C2-C3-O3
2	C	323	GOL	C1-C2-C3-O3
2	D	322	GOL	O1-C1-C2-O2
2	B	321	GOL	O2-C2-C3-O3
2	B	321	GOL	C1-C2-C3-O3
2	A	324	GOL	O2-C2-C3-O3
2	C	323	GOL	O2-C2-C3-O3
2	D	322	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	322	GOL	1	0
2	B	321	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	71:GLY	C	72:VAL	N	1.18

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	285/317 (89%)	-0.59	3 (1%) 80 56	13, 34, 66, 93	0
1	B	298/317 (94%)	-0.61	2 (0%) 87 69	12, 36, 70, 89	0
1	C	287/317 (90%)	-0.68	1 (0%) 94 84	10, 33, 71, 85	0
1	D	293/317 (92%)	-0.64	1 (0%) 94 84	10, 33, 71, 85	0
All	All	1163/1268 (91%)	-0.63	7 (0%) 89 72	10, 34, 71, 93	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	ASP	2.8
1	B	237	ASP	2.6
1	A	161	GLY	2.6
1	C	244	ASN	2.5
1	D	160	ARG	2.3
1	B	14	ASN	2.2
1	A	274	SER	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 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	C	323	6/6	0.74	0.24	43,43,43,43	0
2	GOL	B	321	6/6	0.76	0.32	53,53,53,53	0
2	GOL	D	322	6/6	0.81	0.26	43,43,43,43	0
2	GOL	A	324	6/6	0.93	0.18	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.