



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 07:37 PM EDT

PDB ID : 3BLV
Title : Yeast Isocitrate Dehydrogenase with Citrate Bound in the Regulatory Subunits
Authors : Taylor, A.B.; Hu, G.; Hart, P.J.; McAlister-Henn, L.
Deposited on : 2007-12-11
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

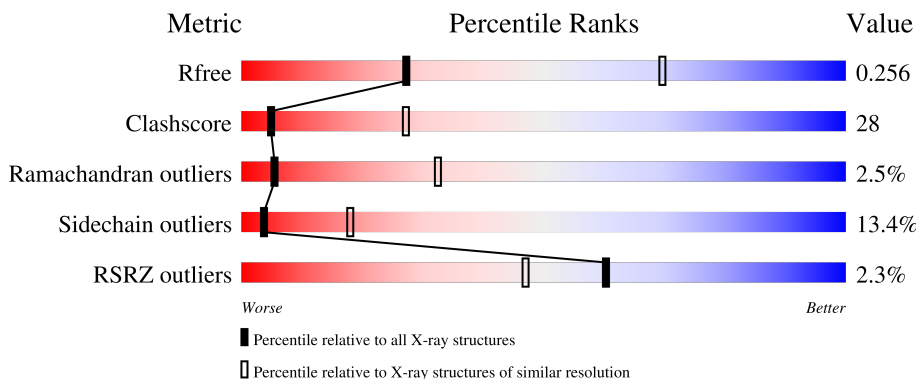
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


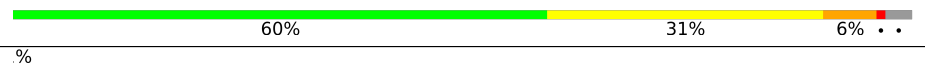

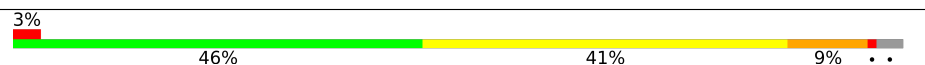

The reported resolution of this entry is 3.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	354	
1	C	354	
1	E	354	
1	G	354	
2	B	354	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	354	<p>%</p> <p>49% 39% 10% ..</p>
2	F	354	<p>3%</p> <p>46% 40% 11% ..</p>
2	H	354	<p>9%</p> <p>46% 42% 9% ..</p>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLC	G	1004	-	-	X	-

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 20849 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 Isocitrate dehydrogenase [NAD] subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	331	2538	1605	442	484	7	0	0	0
1	C	344	2634	1664	461	502	7	0	0	0
1	E	344	2634	1664	461	502	7	0	0	0
1	G	331	2538	1605	442	484	7	0	0	0

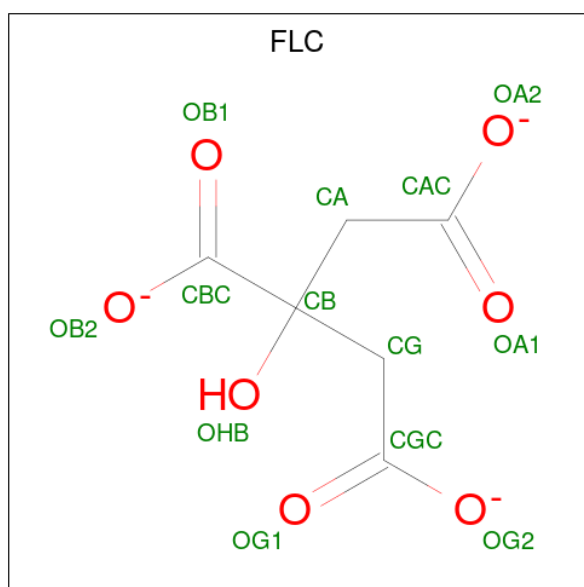
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	HIS	-	expression tag	UNP P28834
A	351	HIS	-	expression tag	UNP P28834
A	352	HIS	-	expression tag	UNP P28834
A	353	HIS	-	expression tag	UNP P28834
A	354	HIS	-	expression tag	UNP P28834
C	350	HIS	-	expression tag	UNP P28834
C	351	HIS	-	expression tag	UNP P28834
C	352	HIS	-	expression tag	UNP P28834
C	353	HIS	-	expression tag	UNP P28834
C	354	HIS	-	expression tag	UNP P28834
E	350	HIS	-	expression tag	UNP P28834
E	351	HIS	-	expression tag	UNP P28834
E	352	HIS	-	expression tag	UNP P28834
E	353	HIS	-	expression tag	UNP P28834
E	354	HIS	-	expression tag	UNP P28834
G	350	HIS	-	expression tag	UNP P28834
G	351	HIS	-	expression tag	UNP P28834
G	352	HIS	-	expression tag	UNP P28834
G	353	HIS	-	expression tag	UNP P28834
G	354	HIS	-	expression tag	UNP P28834

- Molecule 2 is a protein called Isocitrate dehydrogenase [NAD] subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	S				Se
2	B	345	Total 2600	C 1641	N 445	O 508	S 3	Se 3	0	0	0
2	D	347	Total 2617	C 1652	N 449	O 510	S 3	Se 3	0	0	0
2	F	347	Total 2617	C 1652	N 449	O 510	S 3	Se 3	0	0	0
2	H	348	Total 2619	C 1654	N 448	O 511	S 3	Se 3	0	0	0

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).

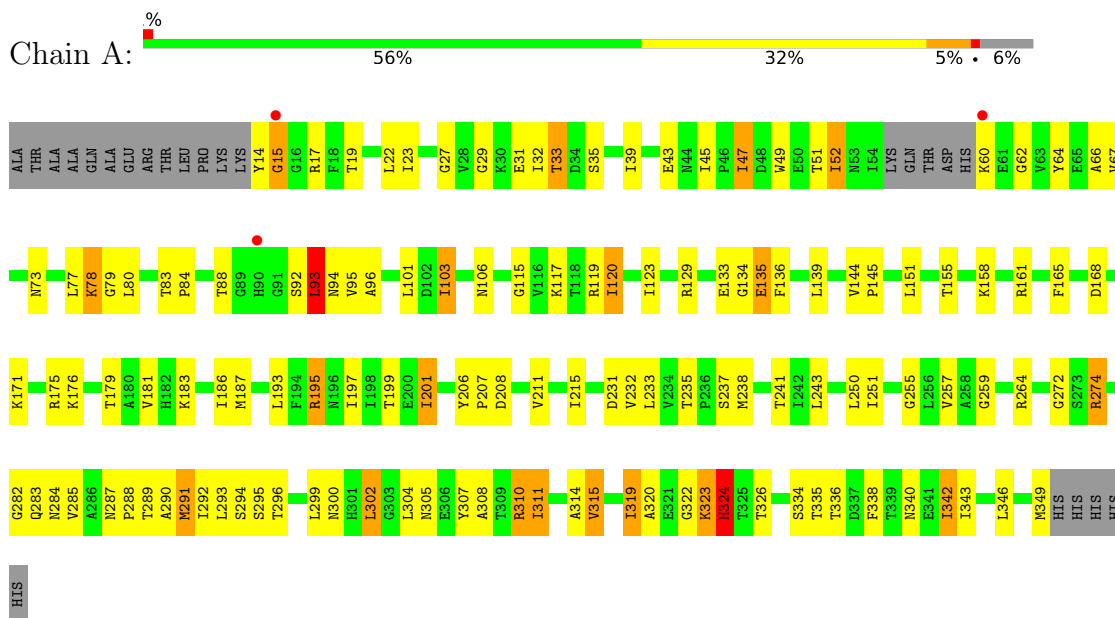


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C O		
3	A	1	Total 13	C O 6 7	0	0
3	C	1	Total 13	C O 6 7	0	0
3	E	1	Total 13	C O 6 7	0	0
3	G	1	Total 13	C O 6 7	0	0

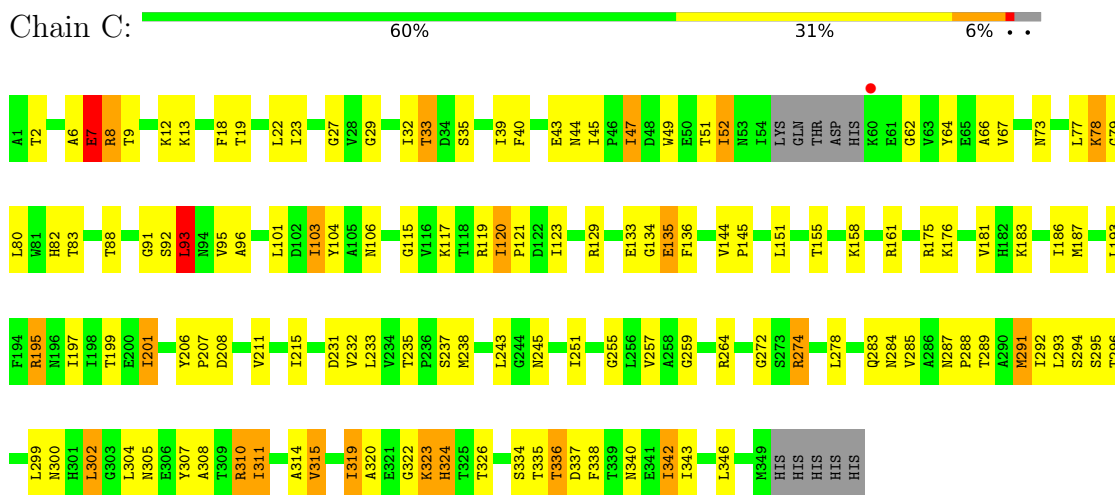
3 Residue-property plots

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

- Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1



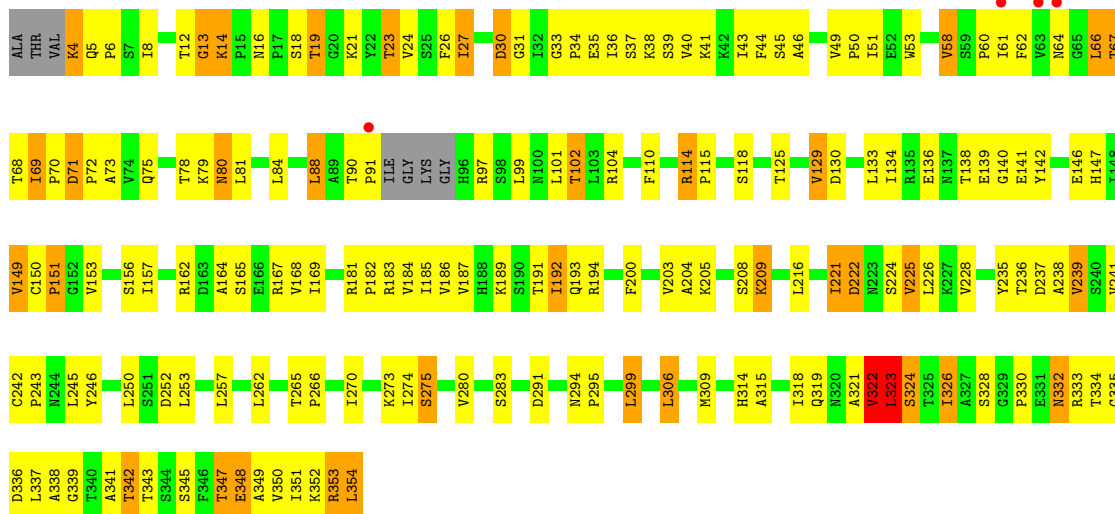
- Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1



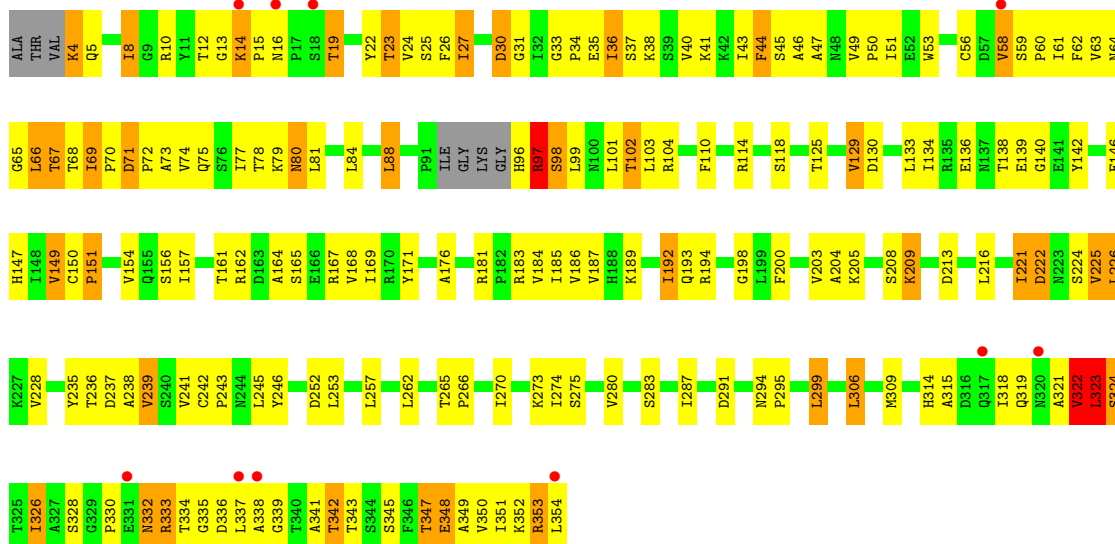
- Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1



• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

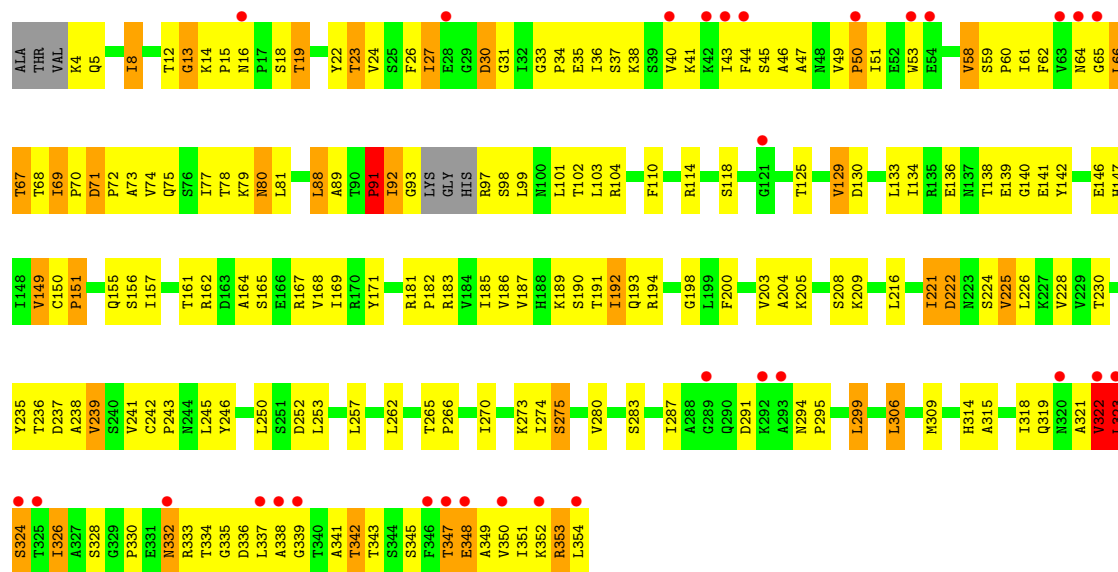


• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2



• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	256.90Å 112.95Å 125.62Å 90.00° 106.67° 90.00°	Depositor
Resolution (Å)	49.35 – 3.20 49.34 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.35-3.20) 95.8 (49.34-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.84 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.221 , 0.265 0.210 , 0.256	Depositor DCC
R_{free} test set	2772 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtrriage
Anisotropy	0.659	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20849	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.40	0/2574	0.76	4/3469 (0.1%)
1	C	0.41	0/2671	0.62	3/3600 (0.1%)
1	E	0.39	0/2671	0.63	3/3600 (0.1%)
1	G	0.41	0/2574	0.61	3/3469 (0.1%)
2	B	0.37	0/2641	0.57	0/3585
2	D	0.39	0/2660	0.56	0/3612
2	F	0.38	0/2660	0.57	0/3612
2	H	0.39	0/2661	0.59	1/3613 (0.0%)
All	All	0.39	0/21112	0.61	14/28560 (0.0%)

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	E	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ARG	NE-CZ-NH1	-19.14	110.73	120.30
1	A	264	ARG	NE-CZ-NH2	18.22	129.41	120.30
1	A	264	ARG	CD-NE-CZ	8.81	135.94	123.60
1	C	264	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	C	264	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	G	264	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	E	264	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	G	93	LEU	CA-CB-CG	5.92	128.92	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	93	LEU	CA-CB-CG	5.67	128.34	115.30
1	E	264	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	93	LEU	CA-CB-CG	5.49	127.92	115.30
1	E	93	LEU	CA-CB-CG	5.44	127.82	115.30
1	G	264	ARG	NE-CZ-NH1	5.13	122.87	120.30
2	H	93	GLY	N-CA-C	5.00	125.61	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	1	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	2538	0	2571	119	0
1	C	2634	0	2679	120	0
1	E	2634	0	2679	135	0
1	G	2538	0	2571	121	0
2	B	2600	0	2648	168	0
2	D	2617	0	2662	174	0
2	F	2617	0	2662	188	0
2	H	2619	0	2669	186	0
3	A	13	0	5	3	0
3	C	13	0	5	3	0
3	E	13	0	5	3	0
3	G	13	0	5	4	0
All	All	20849	0	21161	1156	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 28.

All (1156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:GLU:HG3	1:C:238:MSE:HB2	1.36	1.07
1:E:7:GLU:HB3	1:E:10:LEU:HD11	1.37	1.04
1:G:135:GLU:HG3	1:G:238:MSE:HB2	1.36	1.03
1:A:135:GLU:HG3	1:A:238:MSE:HB2	1.38	1.01
1:E:135:GLU:HG3	1:E:238:MSE:HB2	1.38	1.01
1:C:187:MSE:HE2	2:D:156:SER:HB3	1.45	0.98
2:B:342:THR:HG23	2:B:345:SER:H	1.28	0.98
2:H:342:THR:HG23	2:H:345:SER:H	1.29	0.97
1:E:187:MSE:HE2	2:F:156:SER:HB3	1.42	0.96
2:D:342:THR:HG23	2:D:345:SER:H	1.28	0.96
2:F:342:THR:HG23	2:F:345:SER:H	1.27	0.95
2:B:322:VAL:HG12	2:B:350:VAL:HG13	1.49	0.94
2:D:150:CYS:HB2	2:D:151:PRO:HD2	1.51	0.93
2:H:322:VAL:HG12	2:H:350:VAL:HG13	1.51	0.92
1:E:151:LEU:CD1	2:H:147:HIS:CD2	2.52	0.92
2:F:322:VAL:HG12	2:F:350:VAL:HG13	1.52	0.92
1:G:151:LEU:HD23	2:H:157:ILE:HG12	1.51	0.91
2:H:136:GLU:HG2	2:H:168:VAL:HG21	1.51	0.91
2:H:69:ILE:HD12	2:H:70:PRO:HD2	1.52	0.90
2:B:136:GLU:HG2	2:B:168:VAL:HG21	1.54	0.90
2:B:150:CYS:HB2	2:B:151:PRO:HD2	1.54	0.89
2:D:322:VAL:HG12	2:D:350:VAL:HG13	1.52	0.89
1:A:187:MSE:HE2	2:B:156:SER:HB3	1.52	0.89
2:F:150:CYS:HB2	2:F:151:PRO:HD2	1.55	0.89
2:F:69:ILE:HD12	2:F:70:PRO:HD2	1.54	0.89
2:B:58:VAL:HG12	2:B:69:ILE:HD13	1.55	0.88
2:F:58:VAL:HG12	2:F:69:ILE:HD13	1.56	0.87
2:H:150:CYS:HB2	2:H:151:PRO:HD2	1.55	0.87
2:F:136:GLU:HG2	2:F:168:VAL:HG21	1.53	0.87
1:A:195:ARG:HG2	1:A:195:ARG:HH11	1.40	0.86
2:B:69:ILE:HD12	2:B:70:PRO:HD2	1.56	0.86
2:D:69:ILE:HD12	2:D:70:PRO:HD2	1.56	0.86
2:H:58:VAL:HG12	2:H:69:ILE:HD13	1.54	0.86
2:D:58:VAL:HG12	2:D:69:ILE:HD13	1.56	0.86
2:D:136:GLU:HG2	2:D:168:VAL:HG21	1.57	0.86
1:E:119:ARG:HG2	2:F:125:THR:HG22	1.57	0.86
1:E:300:ASN:HA	1:E:305:ASN:HB3	1.57	0.86
1:G:300:ASN:HA	1:G:305:ASN:HB3	1.57	0.86
1:E:195:ARG:HG2	1:E:195:ARG:HH11	1.40	0.86
1:A:300:ASN:HA	1:A:305:ASN:HB3	1.58	0.85
2:F:221:ILE:O	2:F:225:VAL:HG12	1.75	0.85
1:C:300:ASN:HA	1:C:305:ASN:HB3	1.58	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:ILE:HG22	2:H:62:PHE:H	1.43	0.84
2:B:221:ILE:O	2:B:225:VAL:HG12	1.79	0.83
1:E:7:GLU:HB3	1:E:10:LEU:CD1	2.08	0.83
1:G:93:LEU:HA	1:G:96:ALA:HB3	1.61	0.83
1:G:323:LYS:HE3	1:G:323:LYS:H	1.43	0.83
1:G:195:ARG:HG2	1:G:195:ARG:HH11	1.43	0.83
1:C:92:SER:HB3	1:C:95:VAL:HG22	1.59	0.81
2:H:333:ARG:HB2	2:H:339:GLY:HA3	1.62	0.81
1:C:323:LYS:HE3	1:C:323:LYS:H	1.43	0.81
1:E:314:ALA:HB2	1:E:346:LEU:HD13	1.62	0.81
2:D:221:ILE:O	2:D:225:VAL:HG12	1.80	0.81
2:B:318:ILE:HA	2:B:322:VAL:HG21	1.61	0.81
2:D:333:ARG:HB2	2:D:339:GLY:HA3	1.62	0.81
2:B:333:ARG:HB2	2:B:339:GLY:HA3	1.63	0.81
1:E:195:ARG:HH11	1:E:195:ARG:CG	1.93	0.81
1:C:195:ARG:HG2	1:C:195:ARG:HH11	1.42	0.81
1:C:195:ARG:HH11	1:C:195:ARG:CG	1.94	0.81
1:A:93:LEU:HA	1:A:96:ALA:HB3	1.63	0.80
2:F:318:ILE:HA	2:F:322:VAL:HG21	1.64	0.80
1:G:92:SER:HB3	1:G:95:VAL:HG22	1.63	0.80
2:F:67:THR:HG21	2:F:96:HIS:N	1.96	0.80
1:A:323:LYS:HE3	1:A:323:LYS:H	1.46	0.80
2:B:130:ASP:HB3	2:B:236:THR:HG23	1.63	0.80
1:E:92:SER:HB3	1:E:95:VAL:HG22	1.63	0.80
2:H:318:ILE:HA	2:H:322:VAL:HG21	1.64	0.80
1:G:314:ALA:HB2	1:G:346:LEU:HD13	1.64	0.79
1:E:93:LEU:HA	1:E:96:ALA:HB3	1.64	0.79
1:A:92:SER:HB3	1:A:95:VAL:HG22	1.64	0.79
2:F:71:ASP:O	2:F:75:GLN:HG2	1.82	0.79
2:D:318:ILE:HA	2:D:322:VAL:HG21	1.64	0.79
2:F:333:ARG:HB2	2:F:339:GLY:HA3	1.63	0.78
2:F:61:ILE:HG22	2:F:62:PHE:H	1.47	0.78
1:A:195:ARG:HH11	1:A:195:ARG:CG	1.96	0.78
1:A:314:ALA:HB2	1:A:346:LEU:HD13	1.64	0.77
1:C:314:ALA:HB2	1:C:346:LEU:HD13	1.64	0.77
1:G:195:ARG:HH11	1:G:195:ARG:CG	1.97	0.77
2:H:221:ILE:O	2:H:225:VAL:HG12	1.85	0.76
2:F:97:ARG:HG3	2:F:102:THR:HG23	1.68	0.76
1:A:259:GLY:H	1:A:294:SER:HB3	1.51	0.76
1:E:151:LEU:HD11	2:H:147:HIS:CD2	2.20	0.76
3:C:1002:FLC:CBC	3:C:1002:FLC:OA1	2.33	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:130:ASP:HB3	2:D:236:THR:HG23	1.68	0.75
1:E:151:LEU:CD1	2:H:147:HIS:HD2	1.98	0.75
1:E:323:LYS:HE3	1:E:323:LYS:H	1.50	0.75
2:F:130:ASP:HB3	2:F:236:THR:HG23	1.67	0.74
1:G:274:ARG:HG2	3:G:1004:FLC:OB1	1.87	0.74
1:C:93:LEU:HA	1:C:96:ALA:HB3	1.69	0.74
2:H:130:ASP:HB3	2:H:236:THR:HG23	1.68	0.74
2:F:41:LYS:HG2	2:F:53:TRP:CD1	2.23	0.74
2:F:351:ILE:O	2:F:354:LEU:HB3	1.87	0.73
2:D:71:ASP:O	2:D:75:GLN:HG2	1.89	0.73
1:G:323:LYS:O	1:G:324:HIS:HB2	1.89	0.73
2:H:71:ASP:O	2:H:75:GLN:HG2	1.88	0.73
2:B:71:ASP:O	2:B:75:GLN:HG2	1.89	0.73
1:C:151:LEU:HD23	2:D:157:ILE:HG12	1.72	0.72
2:D:61:ILE:HG22	2:D:62:PHE:H	1.54	0.72
1:C:323:LYS:HE3	1:C:323:LYS:N	2.05	0.72
2:B:61:ILE:HG22	2:B:62:PHE:H	1.55	0.72
1:A:310:ARG:HG3	1:A:349:MSE:HE1	1.70	0.71
2:B:235:TYR:O	2:B:238:ALA:HB2	1.89	0.71
2:H:235:TYR:O	2:H:238:ALA:HB2	1.90	0.71
1:E:274:ARG:HG2	3:E:1003:FLC:OB1	1.90	0.71
2:H:66:LEU:HD23	2:H:97:ARG:HH11	1.55	0.71
1:A:310:ARG:HG3	1:A:349:MSE:CE	2.21	0.71
1:G:323:LYS:HE3	1:G:323:LYS:N	2.05	0.71
1:G:259:GLY:H	1:G:294:SER:HB3	1.55	0.71
1:A:323:LYS:O	1:A:324:HIS:HB2	1.90	0.70
2:H:60:PRO:HG3	2:H:99:LEU:HD13	1.73	0.70
1:G:305:ASN:HA	1:G:308:ALA:HB3	1.73	0.70
2:F:235:TYR:O	2:F:238:ALA:HB2	1.91	0.70
2:F:348:GLU:O	2:F:352:LYS:HG2	1.90	0.70
1:C:259:GLY:H	1:C:294:SER:HB3	1.55	0.70
1:A:119:ARG:HG2	2:B:125:THR:HG22	1.73	0.70
2:D:5:GLN:HG3	2:D:6:PRO:CD	2.22	0.70
1:C:52:ILE:HD12	1:C:66:ALA:HA	1.74	0.70
1:E:52:ILE:HD12	1:E:66:ALA:HA	1.75	0.69
1:E:187:MSE:HE2	2:F:156:SER:CB	2.19	0.69
2:F:322:VAL:HB	2:F:323:LEU:HD23	1.74	0.69
1:C:83:THR:HG21	2:D:191:THR:HG23	1.75	0.69
1:E:119:ARG:CG	2:F:125:THR:HG22	2.22	0.69
2:H:67:THR:HG23	2:H:97:ARG:HB3	1.75	0.69
2:D:326:ILE:HG21	2:D:350:VAL:HA	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:97:ARG:HG2	2:D:102:THR:HG23	1.74	0.68
1:E:305:ASN:HA	1:E:308:ALA:HB3	1.75	0.68
2:H:348:GLU:O	2:H:352:LYS:HG2	1.92	0.68
1:A:323:LYS:HE3	1:A:323:LYS:N	2.07	0.68
1:E:259:GLY:H	1:E:294:SER:HB3	1.58	0.68
2:H:326:ILE:HG21	2:H:350:VAL:HA	1.74	0.68
1:E:151:LEU:HD12	2:H:147:HIS:CD2	2.29	0.68
2:D:41:LYS:HG2	2:D:53:TRP:CD1	2.27	0.68
1:G:187:MSE:HE2	2:H:156:SER:HB3	1.75	0.68
1:A:305:ASN:HA	1:A:308:ALA:HB3	1.75	0.68
1:C:2:THR:O	1:C:6:ALA:HB2	1.93	0.68
2:F:274:ILE:HG22	2:F:275:SER:N	2.09	0.68
1:E:33:THR:HG23	1:E:291:MSE:HE3	1.75	0.68
1:A:195:ARG:HG2	1:A:195:ARG:NH1	2.09	0.68
1:C:195:ARG:HG2	1:C:195:ARG:NH1	2.09	0.68
2:D:235:TYR:O	2:D:238:ALA:HB2	1.92	0.68
2:H:41:LYS:HG2	2:H:53:TRP:CD1	2.29	0.68
2:H:150:CYS:CB	2:H:151:PRO:HD2	2.24	0.68
2:B:322:VAL:CG1	2:B:350:VAL:HG13	2.23	0.67
2:H:291:ASP:OD2	2:H:343:THR:HB	1.93	0.67
2:F:322:VAL:CG1	2:F:350:VAL:HG13	2.24	0.67
1:C:135:GLU:CG	1:C:238:MSE:HB2	2.19	0.67
1:E:323:LYS:HE3	1:E:323:LYS:N	2.09	0.67
1:C:33:THR:HG23	1:C:291:MSE:HE3	1.77	0.67
1:C:323:LYS:O	1:C:324:HIS:HB2	1.94	0.67
1:E:135:GLU:CG	1:E:238:MSE:HB2	2.22	0.67
2:F:40:VAL:HG22	2:F:299:LEU:HD13	1.77	0.67
2:B:326:ILE:HG21	2:B:350:VAL:HA	1.77	0.67
2:F:351:ILE:HG23	2:F:354:LEU:HD23	1.77	0.67
2:H:322:VAL:HB	2:H:323:LEU:HD23	1.77	0.67
1:A:52:ILE:HD12	1:A:66:ALA:HA	1.77	0.66
1:C:12:LYS:HE3	1:G:168:ASP:OD2	1.96	0.66
2:F:150:CYS:CB	2:F:151:PRO:HD2	2.25	0.66
2:B:60:PRO:HG3	2:B:99:LEU:HD13	1.78	0.66
1:G:52:ILE:HD12	1:G:66:ALA:HA	1.77	0.66
2:H:164:ALA:O	2:H:168:VAL:HG23	1.96	0.66
2:F:326:ILE:HG21	2:F:350:VAL:HA	1.77	0.66
2:D:40:VAL:HG22	2:D:299:LEU:HD13	1.78	0.65
2:H:322:VAL:CG1	2:H:350:VAL:HG13	2.25	0.65
2:F:147:HIS:CD2	1:G:151:LEU:CD1	2.79	0.65
2:F:291:ASP:OD2	2:F:343:THR:HB	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:ARG:HG2	1:G:195:ARG:NH1	2.11	0.65
2:B:164:ALA:O	2:B:168:VAL:HG23	1.97	0.65
1:E:323:LYS:O	1:E:324:HIS:HB2	1.96	0.65
2:F:333:ARG:O	2:F:341:ALA:HB3	1.96	0.65
2:F:164:ALA:O	2:F:168:VAL:HG23	1.95	0.65
1:G:181:VAL:HB	1:G:235:THR:HG22	1.79	0.65
1:A:307:TYR:O	1:A:311:ILE:HG23	1.97	0.65
2:B:322:VAL:HB	2:B:323:LEU:HD23	1.79	0.65
2:B:348:GLU:O	2:B:352:LYS:HG2	1.97	0.65
2:D:150:CYS:CB	2:D:151:PRO:HD2	2.25	0.65
1:G:33:THR:HG23	1:G:291:MSE:HE3	1.77	0.65
1:E:195:ARG:HG2	1:E:195:ARG:NH1	2.07	0.65
2:H:40:VAL:HG22	2:H:299:LEU:HD13	1.79	0.65
2:H:314:HIS:O	2:H:318:ILE:HG13	1.97	0.65
2:D:187:VAL:HB	2:D:242:CYS:HB3	1.79	0.64
1:C:35:SER:O	1:C:39:ILE:HG13	1.97	0.64
2:H:274:ILE:HG22	2:H:275:SER:N	2.13	0.64
1:A:151:LEU:HD23	2:B:157:ILE:HG12	1.78	0.64
2:D:322:VAL:HB	2:D:323:LEU:HD23	1.78	0.64
2:B:41:LYS:HG2	2:B:53:TRP:CD1	2.32	0.64
1:C:181:VAL:HB	1:C:235:THR:HG22	1.80	0.64
2:D:164:ALA:O	2:D:168:VAL:HG23	1.97	0.64
2:D:333:ARG:O	2:D:341:ALA:HB3	1.98	0.64
2:H:189:LYS:HD3	2:H:221:ILE:HD11	1.78	0.64
1:C:119:ARG:HG2	2:D:125:THR:HG22	1.78	0.64
2:F:97:ARG:HE	2:F:97:ARG:HA	1.62	0.64
2:H:12:THR:HB	2:H:81:LEU:HD12	1.79	0.64
2:B:323:LEU:HD23	2:B:323:LEU:H	1.62	0.64
2:D:322:VAL:HG11	2:D:354:LEU:HD13	1.80	0.64
2:H:58:VAL:HG12	2:H:69:ILE:CD1	2.27	0.64
1:A:45:ILE:HG22	1:A:47:ILE:HG22	1.80	0.64
2:D:60:PRO:HG3	2:D:99:LEU:HD13	1.80	0.64
1:G:135:GLU:CG	1:G:238:MSE:HB2	2.19	0.63
1:E:151:LEU:HD11	2:H:147:HIS:HD2	1.59	0.63
2:B:40:VAL:HG22	2:B:299:LEU:HD13	1.80	0.63
1:E:181:VAL:HB	1:E:235:THR:HG22	1.80	0.63
2:H:44:PHE:CD2	2:H:49:VAL:HG21	2.34	0.63
2:H:334:THR:HG22	2:H:335:GLY:H	1.63	0.63
2:F:43:ILE:HD13	2:F:350:VAL:HG11	1.81	0.63
2:F:60:PRO:HG3	2:F:99:LEU:HD13	1.81	0.63
1:C:307:TYR:O	1:C:311:ILE:HG23	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:VAL:O	1:E:319:ILE:HG23	1.99	0.63
2:H:61:ILE:HD11	2:H:70:PRO:HA	1.80	0.63
2:B:291:ASP:OD2	2:B:343:THR:HB	1.99	0.63
2:F:149:VAL:HA	1:G:139:LEU:HD11	1.81	0.63
2:H:333:ARG:O	2:H:341:ALA:HB3	1.98	0.63
1:A:135:GLU:CG	1:A:238:MSE:HB2	2.23	0.62
2:B:101:LEU:HD23	2:B:104:ARG:HH12	1.64	0.62
2:F:58:VAL:HG12	2:F:69:ILE:CD1	2.29	0.62
1:G:300:ASN:OD1	1:G:305:ASN:HB2	1.99	0.62
2:B:58:VAL:HG12	2:B:69:ILE:CD1	2.29	0.62
2:B:189:LYS:HD3	2:B:221:ILE:HD11	1.80	0.62
2:D:44:PHE:CD2	2:D:49:VAL:HG21	2.34	0.62
1:C:13:LYS:HD2	1:C:18:PHE:CE1	2.34	0.62
1:C:305:ASN:HA	1:C:308:ALA:HB3	1.79	0.62
2:D:291:ASP:OD2	2:D:343:THR:HB	1.98	0.62
1:A:315:VAL:O	1:A:319:ILE:HG23	1.99	0.62
2:D:322:VAL:CG1	2:D:350:VAL:HG13	2.25	0.62
2:D:101:LEU:HD23	2:D:104:ARG:HH12	1.64	0.62
2:B:150:CYS:CB	2:B:151:PRO:HD2	2.27	0.61
1:C:83:THR:CG2	2:D:191:THR:HG23	2.29	0.61
2:B:274:ILE:HG22	2:B:275:SER:N	2.14	0.61
2:B:333:ARG:O	2:B:341:ALA:HB3	2.00	0.61
2:D:23:THR:O	2:D:80:ASN:HB3	2.01	0.61
2:D:348:GLU:O	2:D:352:LYS:HG2	1.99	0.61
2:F:67:THR:CG2	2:F:96:HIS:N	2.62	0.61
2:H:23:THR:O	2:H:80:ASN:HB3	2.00	0.61
2:H:36:ILE:HG12	2:H:295:PRO:HA	1.82	0.61
2:D:5:GLN:HG3	2:D:6:PRO:HD3	1.82	0.61
2:D:274:ILE:HG22	2:D:275:SER:N	2.16	0.61
2:H:323:LEU:HD23	2:H:323:LEU:H	1.66	0.61
2:D:12:THR:HB	2:D:81:LEU:HD12	1.83	0.61
1:A:35:SER:O	1:A:39:ILE:HG13	2.00	0.60
1:A:274:ARG:HG2	3:A:1001:FLC:OB1	2.00	0.60
1:A:183:LYS:HE3	1:A:186:ILE:HD12	1.82	0.60
2:B:44:PHE:CD2	2:B:49:VAL:HG21	2.36	0.60
2:B:187:VAL:HB	2:B:242:CYS:HB3	1.83	0.60
2:F:36:ILE:HG12	2:F:295:PRO:HA	1.83	0.60
2:F:334:THR:HG22	2:F:335:GLY:H	1.65	0.60
1:G:35:SER:O	1:G:39:ILE:HG13	2.02	0.60
2:D:323:LEU:HD23	2:D:323:LEU:H	1.65	0.60
1:E:115:GLY:HA3	1:E:320:ALA:HA	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:186:VAL:HG23	2:F:216:LEU:HD11	1.83	0.60
1:A:181:VAL:HB	1:A:235:THR:HG22	1.82	0.60
1:C:115:GLY:HA3	1:C:320:ALA:HA	1.82	0.60
1:E:307:TYR:O	1:E:311:ILE:HG23	2.01	0.60
1:A:115:GLY:HA3	1:A:320:ALA:HA	1.83	0.60
1:C:45:ILE:HG22	1:C:47:ILE:HG22	1.84	0.60
1:A:33:THR:HG23	1:A:291:MSE:HE3	1.84	0.60
1:G:45:ILE:HG22	1:G:47:ILE:HG22	1.82	0.60
1:G:338:PHE:O	1:G:342:ILE:HG12	2.01	0.60
1:A:338:PHE:O	1:A:342:ILE:HG12	2.02	0.59
1:E:189:LEU:HB3	2:F:154:VAL:HG11	1.84	0.59
2:F:306:LEU:HD12	2:F:309:MSE:CE	2.32	0.59
1:E:35:SER:O	1:E:39:ILE:HG13	2.02	0.59
2:F:295:PRO:HB2	2:F:299:LEU:HD22	1.84	0.59
1:A:93:LEU:HA	1:A:96:ALA:CB	2.32	0.59
1:C:43:GLU:OE1	1:C:310:ARG:HD3	2.02	0.59
1:G:115:GLY:HA3	1:G:320:ALA:HA	1.82	0.59
1:G:315:VAL:O	1:G:319:ILE:HG23	2.02	0.59
2:H:165:SER:HG	2:H:200:PHE:HD1	1.49	0.59
1:A:45:ILE:HG12	1:A:307:TYR:CD2	2.37	0.59
2:F:12:THR:HB	2:F:81:LEU:HD12	1.83	0.59
2:F:44:PHE:CD2	2:F:49:VAL:HG21	2.37	0.59
2:F:351:ILE:HA	2:F:354:LEU:HB2	1.84	0.59
2:D:36:ILE:HG12	2:D:295:PRO:HA	1.85	0.59
2:D:97:ARG:HD2	2:D:101:LEU:HD12	1.85	0.59
1:E:300:ASN:OD1	1:E:305:ASN:HB2	2.02	0.59
1:G:129:ARG:CZ	1:G:274:ARG:HH12	2.14	0.59
2:H:295:PRO:HB2	2:H:299:LEU:HD22	1.84	0.59
2:F:67:THR:HG23	2:F:97:ARG:HB3	1.83	0.59
2:H:62:PHE:CE1	2:H:67:THR:HG22	2.36	0.59
2:H:101:LEU:HD23	2:H:104:ARG:HH12	1.67	0.59
1:G:80:LEU:HD11	1:G:274:ARG:HG3	1.85	0.59
2:H:186:VAL:HG23	2:H:216:LEU:HD11	1.84	0.59
2:D:186:VAL:HG23	2:D:216:LEU:HD11	1.84	0.59
2:F:314:HIS:O	2:F:318:ILE:HG13	2.02	0.59
2:B:334:THR:HG22	2:B:335:GLY:H	1.68	0.59
1:C:197:ILE:O	1:C:201:ILE:HG23	2.02	0.59
2:B:12:THR:HB	2:B:81:LEU:HD12	1.83	0.59
1:C:52:ILE:CD1	1:C:66:ALA:HA	2.33	0.58
2:H:306:LEU:HD12	2:H:309:MSE:CE	2.33	0.58
1:A:197:ILE:O	1:A:201:ILE:HG23	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:GLN:NE2	2:B:308:HIS:HA	2.19	0.58
2:B:61:ILE:HD11	2:B:70:PRO:HA	1.84	0.58
2:H:61:ILE:HG22	2:H:62:PHE:N	2.17	0.58
2:H:47:ALA:HB2	2:H:354:LEU:HD21	1.85	0.58
2:B:306:LEU:HD12	2:B:309:MSE:CE	2.33	0.58
2:F:322:VAL:O	2:F:324:SER:N	2.36	0.58
2:F:323:LEU:HD23	2:F:323:LEU:H	1.68	0.58
1:C:338:PHE:O	1:C:342:ILE:HG12	2.03	0.58
1:E:197:ILE:O	1:E:201:ILE:HG23	2.02	0.58
1:C:80:LEU:HD11	1:C:274:ARG:HG3	1.86	0.58
1:C:300:ASN:OD1	1:C:305:ASN:HB2	2.03	0.58
2:H:187:VAL:HB	2:H:242:CYS:HB3	1.86	0.58
2:F:189:LYS:HB2	2:F:221:ILE:HD11	1.85	0.57
2:B:23:THR:O	2:B:80:ASN:HB3	2.04	0.57
1:G:305:ASN:HA	1:G:308:ALA:CB	2.34	0.57
1:C:129:ARG:CZ	1:C:274:ARG:HH12	2.18	0.57
1:G:307:TYR:O	1:G:311:ILE:HG23	2.03	0.57
2:B:36:ILE:HG12	2:B:295:PRO:HA	1.87	0.57
2:D:189:LYS:HD3	2:D:221:ILE:HD11	1.85	0.57
2:F:101:LEU:HD23	2:F:104:ARG:HH12	1.70	0.57
2:H:16:ASN:O	2:H:19:THR:O	2.23	0.57
1:A:183:LYS:HE2	2:B:142:TYR:OH	2.05	0.57
2:D:314:HIS:O	2:D:318:ILE:HG13	2.04	0.57
2:D:334:THR:HG22	2:D:335:GLY:H	1.69	0.57
2:H:14:LYS:HD3	2:H:14:LYS:O	2.05	0.57
1:E:338:PHE:O	1:E:342:ILE:HG12	2.04	0.57
1:A:168:ASP:OD2	1:E:12:LYS:HE3	2.04	0.57
2:B:169:ILE:HD13	2:B:204:ALA:HB2	1.87	0.57
2:F:61:ILE:HG22	2:F:62:PHE:N	2.19	0.57
2:D:58:VAL:HG12	2:D:69:ILE:CD1	2.31	0.56
1:A:80:LEU:HD11	1:A:274:ARG:HG3	1.86	0.56
2:D:14:LYS:O	2:D:14:LYS:HD3	2.05	0.56
2:D:51:ILE:HD11	2:D:309:MSE:HE1	1.86	0.56
2:F:23:THR:O	2:F:80:ASN:HB3	2.05	0.56
2:F:51:ILE:HD11	2:F:309:MSE:HE1	1.87	0.56
1:G:93:LEU:HA	1:G:96:ALA:CB	2.32	0.56
2:H:43:ILE:HD13	2:H:350:VAL:HG11	1.86	0.56
2:H:253:LEU:C	2:H:253:LEU:HD23	2.26	0.56
2:F:16:ASN:O	2:F:19:THR:O	2.24	0.56
1:G:314:ALA:CB	1:G:346:LEU:HD13	2.35	0.56
1:G:183:LYS:HE3	1:G:186:ILE:HD12	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:CZ	1:A:274:ARG:HH12	2.18	0.56
1:E:45:ILE:HG12	1:E:307:TYR:CD2	2.41	0.56
2:F:181:ARG:HD3	2:F:238:ALA:N	2.21	0.56
2:B:243:PRO:HD2	2:B:246:TYR:HD2	1.71	0.56
1:E:93:LEU:HA	1:E:96:ALA:CB	2.34	0.56
2:F:68:THR:HG22	2:F:69:ILE:N	2.20	0.56
2:F:165:SER:HG	2:F:200:PHE:HD1	1.53	0.56
2:F:187:VAL:HB	2:F:242:CYS:HB3	1.86	0.56
1:A:206:TYR:N	1:A:207:PRO:HD3	2.21	0.56
1:C:315:VAL:O	1:C:319:ILE:HG23	2.06	0.56
1:G:43:GLU:OE1	1:G:310:ARG:HD3	2.05	0.56
2:B:165:SER:HG	2:B:200:PHE:HD1	1.54	0.56
1:C:45:ILE:HG12	1:C:307:TYR:CD2	2.41	0.56
1:E:129:ARG:CZ	1:E:274:ARG:HH12	2.18	0.56
1:G:144:VAL:HB	1:G:145:PRO:HD2	1.88	0.56
1:G:206:TYR:N	1:G:207:PRO:HD3	2.21	0.56
2:H:67:THR:CG2	2:H:97:ARG:HB3	2.35	0.56
2:H:322:VAL:O	2:H:324:SER:N	2.39	0.56
2:H:326:ILE:HG22	2:H:353:ARG:HG3	1.88	0.56
2:H:326:ILE:HG12	2:H:350:VAL:HG23	1.87	0.56
2:D:5:GLN:HG3	2:D:6:PRO:HD2	1.87	0.56
2:D:61:ILE:HD11	2:D:70:PRO:HA	1.87	0.56
2:D:322:VAL:O	2:D:324:SER:N	2.38	0.56
2:F:306:LEU:HB3	2:F:315:ALA:HB2	1.88	0.56
1:A:300:ASN:OD1	1:A:305:ASN:HB2	2.06	0.56
1:E:144:VAL:HB	1:E:145:PRO:HD2	1.88	0.56
2:F:14:LYS:O	2:F:14:LYS:HD3	2.06	0.56
1:A:305:ASN:HA	1:A:308:ALA:CB	2.36	0.55
2:D:151:PRO:HG2	1:E:5:GLN:NE2	2.21	0.55
1:G:197:ILE:O	1:G:201:ILE:HG23	2.06	0.55
1:C:83:THR:HG21	2:D:191:THR:CG2	2.36	0.55
1:C:144:VAL:HB	1:C:145:PRO:HD2	1.88	0.55
1:A:52:ILE:CD1	1:A:66:ALA:HA	2.36	0.55
2:B:43:ILE:HD13	2:B:350:VAL:HG11	1.87	0.55
2:F:189:LYS:HD3	2:F:221:ILE:HD11	1.87	0.55
1:G:45:ILE:HG12	1:G:307:TYR:CD2	2.42	0.55
2:H:243:PRO:HD2	2:H:246:TYR:HD2	1.70	0.55
2:D:43:ILE:HD13	2:D:350:VAL:HG11	1.87	0.55
1:G:187:MSE:HE3	2:H:141:GLU:O	2.06	0.55
2:B:5:GLN:HG3	2:B:6:PRO:HD2	1.88	0.55
1:C:195:ARG:HH11	1:C:195:ARG:CB	2.20	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ILE:CG1	1:A:288:PRO:HA	2.36	0.55
1:C:183:LYS:HE3	1:C:186:ILE:HD12	1.89	0.55
2:D:101:LEU:HD23	2:D:104:ARG:NH1	2.22	0.55
1:E:52:ILE:CD1	1:E:66:ALA:HA	2.36	0.55
2:F:274:ILE:HG22	2:F:275:SER:H	1.71	0.55
1:G:310:ARG:NH2	1:G:349:MSE:HB2	2.21	0.55
2:B:314:HIS:O	2:B:318:ILE:HG13	2.06	0.55
2:D:326:ILE:HG22	2:D:353:ARG:HG3	1.87	0.55
2:B:133:LEU:HD23	2:B:133:LEU:C	2.27	0.55
1:E:80:LEU:HD11	1:E:274:ARG:HG3	1.87	0.55
2:H:51:ILE:HD11	2:H:309:MSE:HE1	1.89	0.55
2:B:14:LYS:O	2:B:14:LYS:HD3	2.07	0.55
1:C:323:LYS:H	1:C:323:LYS:CE	2.18	0.55
2:D:306:LEU:HD12	2:D:309:MSE:CE	2.37	0.55
1:E:183:LYS:HE3	1:E:186:ILE:HD12	1.87	0.55
1:E:195:ARG:HH11	1:E:195:ARG:CB	2.19	0.55
2:H:68:THR:HG22	2:H:69:ILE:N	2.22	0.55
2:D:133:LEU:C	2:D:133:LEU:HD23	2.27	0.55
2:F:253:LEU:HD23	2:F:253:LEU:C	2.28	0.55
2:B:323:LEU:HD23	2:B:323:LEU:N	2.22	0.54
1:G:52:ILE:CD1	1:G:66:ALA:HA	2.37	0.54
2:H:273:LYS:HG3	2:H:274:ILE:HD12	1.88	0.54
1:A:22:LEU:HD11	1:A:33:THR:HG22	1.89	0.54
2:B:149:VAL:HG21	2:D:149:VAL:HG21	1.89	0.54
2:D:330:PRO:HA	2:D:333:ARG:HG3	1.90	0.54
2:D:351:ILE:O	2:D:354:LEU:HB2	2.07	0.54
2:F:133:LEU:C	2:F:133:LEU:HD23	2.28	0.54
1:C:93:LEU:HA	1:C:96:ALA:CB	2.36	0.54
2:D:136:GLU:OE2	2:D:138:THR:HB	2.08	0.54
2:B:326:ILE:HG12	2:B:350:VAL:HG23	1.90	0.54
1:C:183:LYS:HE2	2:D:142:TYR:OH	2.08	0.54
2:B:186:VAL:HG23	2:B:216:LEU:HD11	1.88	0.54
2:D:4:LYS:HD3	2:D:5:GLN:H	1.73	0.54
1:E:305:ASN:HA	1:E:308:ALA:CB	2.38	0.54
2:H:36:ILE:CG1	2:H:295:PRO:HA	2.38	0.54
2:D:68:THR:HG22	2:D:69:ILE:N	2.23	0.54
2:D:295:PRO:HB2	2:D:299:LEU:HD22	1.89	0.54
1:E:314:ALA:CB	1:E:346:LEU:HD13	2.35	0.54
2:H:181:ARG:HD3	2:H:238:ALA:N	2.23	0.54
1:A:119:ARG:CG	2:B:125:THR:HG22	2.38	0.54
2:D:243:PRO:HD2	2:D:246:TYR:HD2	1.71	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:GLU:OE1	1:E:310:ARG:HD3	2.08	0.54
2:F:326:ILE:HG12	2:F:350:VAL:HG23	1.88	0.54
2:B:322:VAL:O	2:B:324:SER:N	2.41	0.53
2:D:181:ARG:HD3	2:D:238:ALA:N	2.23	0.53
2:F:273:LYS:HG3	2:F:274:ILE:HD12	1.91	0.53
1:E:45:ILE:HG22	1:E:47:ILE:HG22	1.90	0.53
1:A:187:MSE:HE3	2:B:141:GLU:O	2.08	0.53
2:B:101:LEU:HD23	2:B:104:ARG:NH1	2.23	0.53
2:B:295:PRO:HB2	2:B:299:LEU:HD22	1.90	0.53
2:B:253:LEU:C	2:B:253:LEU:HD23	2.29	0.53
2:F:31:GLY:O	2:F:34:PRO:HD2	2.09	0.53
2:F:69:ILE:HD12	2:F:70:PRO:CD	2.34	0.53
2:F:318:ILE:HA	2:F:322:VAL:CG2	2.38	0.53
2:H:189:LYS:HD3	2:H:221:ILE:CD1	2.39	0.53
1:E:106:ASN:HB3	1:E:129:ARG:HG2	1.91	0.53
2:F:323:LEU:N	2:F:326:ILE:HG23	2.23	0.53
2:F:326:ILE:HG22	2:F:353:ARG:HG3	1.90	0.53
3:G:1004:FLC:CBC	3:G:1004:FLC:OA1	2.55	0.53
2:H:133:LEU:C	2:H:133:LEU:HD23	2.29	0.53
1:A:323:LYS:H	1:A:323:LYS:CE	2.21	0.53
1:E:32:ILE:CG1	1:E:288:PRO:HA	2.38	0.53
1:G:32:ILE:CG1	1:G:288:PRO:HA	2.39	0.53
1:C:283:GLN:HB3	1:C:285:VAL:HG13	1.90	0.53
1:E:5:GLN:NE2	1:E:5:GLN:H	2.07	0.53
2:F:326:ILE:HG12	2:F:350:VAL:CG2	2.39	0.53
2:B:33:GLY:O	2:B:36:ILE:HG22	2.07	0.53
2:B:68:THR:HG22	2:B:69:ILE:N	2.24	0.53
2:B:224:SER:O	2:B:228:VAL:HG23	2.09	0.53
2:D:169:ILE:HD13	2:D:204:ALA:HB2	1.91	0.53
1:A:144:VAL:HB	1:A:145:PRO:HD2	1.90	0.53
2:D:16:ASN:O	2:D:19:THR:O	2.27	0.53
2:D:36:ILE:CG1	2:D:295:PRO:HA	2.39	0.53
2:H:136:GLU:OE2	2:H:138:THR:HB	2.08	0.53
2:B:306:LEU:HB3	2:B:315:ALA:HB2	1.89	0.52
2:B:326:ILE:HG22	2:B:353:ARG:HG3	1.89	0.52
1:C:32:ILE:CG1	1:C:288:PRO:HA	2.40	0.52
2:F:97:ARG:CG	2:F:102:THR:HG23	2.39	0.52
1:A:133:GLU:HG2	1:A:134:GLY:H	1.74	0.52
2:B:189:LYS:CG	2:B:192:ILE:HD13	2.39	0.52
1:C:187:MSE:HE3	2:D:141:GLU:O	2.08	0.52
2:F:4:LYS:HE3	2:F:10:ARG:HH22	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:LEU:HD11	1:G:33:THR:HG22	1.89	0.52
1:G:323:LYS:H	1:G:323:LYS:CE	2.18	0.52
2:H:326:ILE:HG12	2:H:350:VAL:CG2	2.39	0.52
2:B:16:ASN:O	2:B:19:THR:O	2.27	0.52
2:F:64:ASN:C	2:F:66:LEU:H	2.12	0.52
2:D:62:PHE:CE1	2:D:67:THR:HG22	2.44	0.52
2:D:326:ILE:HG12	2:D:350:VAL:HG23	1.91	0.52
1:A:232:VAL:O	1:A:233:LEU:HD23	2.09	0.52
2:H:295:PRO:O	2:H:299:LEU:HB2	2.09	0.52
2:B:51:ILE:HD11	2:B:309:MSE:HE1	1.90	0.52
2:B:69:ILE:HD11	2:B:73:ALA:HB3	1.91	0.52
2:F:118:SER:OG	2:F:129:VAL:HG13	2.10	0.52
2:F:330:PRO:HA	2:F:333:ARG:HG3	1.91	0.52
2:H:253:LEU:HD23	2:H:253:LEU:O	2.09	0.52
1:A:43:GLU:OE1	1:A:310:ARG:HD3	2.10	0.52
2:H:69:ILE:HD12	2:H:70:PRO:CD	2.33	0.52
2:D:97:ARG:CG	2:D:102:THR:HG23	2.37	0.52
1:E:5:GLN:H	1:E:5:GLN:HE21	1.58	0.52
1:G:151:LEU:HD13	2:H:155:GLN:NE2	2.24	0.52
2:H:323:LEU:N	2:H:326:ILE:HG23	2.25	0.52
1:A:133:GLU:OE1	1:A:158:LYS:HD2	2.10	0.52
2:B:273:LYS:HG3	2:B:274:ILE:HD12	1.90	0.52
2:B:274:ILE:HG22	2:B:275:SER:H	1.74	0.52
2:B:330:PRO:HA	2:B:333:ARG:HG3	1.91	0.52
2:F:147:HIS:CD2	1:G:151:LEU:HD12	2.45	0.52
2:H:334:THR:HB	2:H:336:ASP:OD1	2.10	0.52
1:C:342:ILE:O	1:C:346:LEU:HB2	2.10	0.51
2:H:330:PRO:HA	2:H:333:ARG:HG3	1.92	0.51
1:A:101:LEU:HB2	1:A:103:ILE:HG13	1.91	0.51
1:A:314:ALA:CB	1:A:346:LEU:HD13	2.37	0.51
1:C:299:LEU:HB2	1:C:308:ALA:HB2	1.93	0.51
2:D:306:LEU:HB3	2:D:315:ALA:HB2	1.92	0.51
2:H:323:LEU:HD23	2:H:323:LEU:N	2.25	0.51
2:D:323:LEU:HD23	2:D:323:LEU:N	2.25	0.51
2:D:69:ILE:HD11	2:D:73:ALA:HB3	1.91	0.51
2:H:46:ALA:HB2	2:H:351:ILE:HD13	1.92	0.51
1:E:206:TYR:N	1:E:207:PRO:HD3	2.25	0.51
2:F:323:LEU:HD23	2:F:323:LEU:N	2.26	0.51
2:B:181:ARG:HD3	2:B:238:ALA:N	2.25	0.51
1:C:119:ARG:CG	2:D:125:THR:HG22	2.40	0.51
1:E:193:LEU:HD11	1:E:197:ILE:HD11	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:14:TYR:CG	1:G:15:GLY:N	2.77	0.51
2:F:189:LYS:HD3	2:F:221:ILE:CD1	2.41	0.51
2:H:69:ILE:HD11	2:H:73:ALA:HB3	1.92	0.51
1:A:14:TYR:CD2	1:A:15:GLY:N	2.79	0.51
2:B:337:LEU:O	2:B:338:ALA:HB3	2.11	0.51
2:D:341:ALA:HB1	2:D:345:SER:OG	2.11	0.51
2:F:36:ILE:CG1	2:F:295:PRO:HA	2.40	0.51
2:H:33:GLY:O	2:H:36:ILE:HG22	2.11	0.51
2:B:326:ILE:HG12	2:B:350:VAL:CG2	2.40	0.51
2:B:318:ILE:HA	2:B:322:VAL:CG2	2.36	0.51
1:E:119:ARG:HD2	2:F:125:THR:O	2.11	0.51
2:B:36:ILE:CG1	2:B:295:PRO:HA	2.41	0.50
1:C:22:LEU:HD11	1:C:33:THR:HG22	1.93	0.50
1:E:7:GLU:OE1	1:E:7:GLU:HA	2.10	0.50
2:B:31:GLY:O	2:B:34:PRO:HD2	2.11	0.50
2:B:189:LYS:HG2	2:B:192:ILE:HD13	1.93	0.50
1:E:151:LEU:HD23	2:F:157:ILE:HG12	1.93	0.50
1:G:224:VAL:HG11	2:H:257:LEU:HG	1.93	0.50
2:H:101:LEU:HD23	2:H:104:ARG:NH1	2.25	0.50
2:H:326:ILE:C	2:H:328:SER:H	2.14	0.50
2:F:69:ILE:HD11	2:F:73:ALA:HB3	1.94	0.50
1:C:305:ASN:HA	1:C:308:ALA:CB	2.40	0.50
3:C:1002:FLC:OA1	3:C:1002:FLC:OB1	2.30	0.50
2:D:224:SER:O	2:D:228:VAL:HG23	2.12	0.50
2:D:319:GLN:O	2:D:321:ALA:O	2.30	0.50
2:F:349:ALA:O	2:F:353:ARG:HD3	2.12	0.50
2:H:134:ILE:HD13	2:H:239:VAL:HG13	1.94	0.50
2:H:274:ILE:HG22	2:H:275:SER:H	1.76	0.50
2:B:169:ILE:HD12	2:B:203:VAL:HG12	1.94	0.50
2:B:334:THR:HB	2:B:336:ASP:OD1	2.11	0.50
2:F:243:PRO:HD2	2:F:246:TYR:HD2	1.77	0.50
2:H:64:ASN:C	2:H:66:LEU:H	2.15	0.50
2:H:224:SER:O	2:H:228:VAL:HG23	2.11	0.50
2:H:306:LEU:HB3	2:H:315:ALA:HB2	1.93	0.50
2:B:136:GLU:OE2	2:B:138:THR:HB	2.10	0.50
1:C:206:TYR:N	1:C:207:PRO:HD3	2.26	0.50
2:D:323:LEU:N	2:D:326:ILE:HG23	2.26	0.50
1:E:176:LYS:HE3	1:E:208:ASP:O	2.12	0.50
2:F:4:LYS:CE	2:F:10:ARG:HH22	2.25	0.50
2:F:46:ALA:HB2	2:F:351:ILE:HD13	1.94	0.50
1:G:175:ARG:NH1	1:G:231:ASP:OD1	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLY:C	1:A:29:GLY:H	2.15	0.50
2:B:62:PHE:CE1	2:B:67:THR:HG22	2.47	0.50
1:C:47:ILE:HD11	1:C:49:TRP:CE3	2.47	0.50
2:D:26:PHE:HE2	2:D:37:SER:OG	1.95	0.50
2:D:64:ASN:C	2:D:66:LEU:H	2.16	0.50
2:D:189:LYS:HB2	2:D:221:ILE:HD11	1.93	0.50
1:E:104:TYR:CE2	1:E:161:ARG:HG2	2.47	0.50
1:E:257:VAL:HG12	1:E:272:GLY:HA3	1.94	0.50
1:E:299:LEU:HB2	1:E:308:ALA:HB2	1.94	0.50
2:F:101:LEU:HD23	2:F:104:ARG:NH1	2.27	0.50
1:C:133:GLU:HG2	1:C:134:GLY:H	1.76	0.49
3:E:1003:FLC:OG1	3:E:1003:FLC:OHB	2.30	0.49
2:F:71:ASP:N	2:F:72:PRO:HD2	2.27	0.49
2:F:334:THR:HB	2:F:336:ASP:OD1	2.12	0.49
1:A:340:ASN:O	1:A:343:ILE:HG13	2.11	0.49
2:D:319:GLN:O	2:D:324:SER:HB2	2.12	0.49
2:D:326:ILE:HG12	2:D:350:VAL:CG2	2.42	0.49
2:F:97:ARG:O	2:F:98:SER:C	2.50	0.49
2:H:189:LYS:HB2	2:H:221:ILE:HD11	1.93	0.49
1:C:7:GLU:O	1:C:9:THR:N	2.46	0.49
1:C:67:VAL:HG13	1:C:101:LEU:HD21	1.95	0.49
2:F:274:ILE:CG2	2:F:275:SER:N	2.75	0.49
1:G:133:GLU:OE1	1:G:158:LYS:HD2	2.12	0.49
2:H:8:ILE:HG21	2:H:171:TYR:HB2	1.93	0.49
2:H:31:GLY:O	2:H:34:PRO:HD2	2.12	0.49
2:H:221:ILE:HD12	2:H:221:ILE:N	2.28	0.49
2:B:64:ASN:C	2:B:66:LEU:H	2.15	0.49
1:G:195:ARG:HH11	1:G:195:ARG:CB	2.25	0.49
2:H:189:LYS:HG2	2:H:192:ILE:HD13	1.95	0.49
1:C:314:ALA:CB	1:C:346:LEU:HD13	2.38	0.49
2:D:33:GLY:O	2:D:36:ILE:HG22	2.12	0.49
2:D:165:SER:HG	2:D:200:PHE:HD1	1.60	0.49
2:D:318:ILE:HA	2:D:322:VAL:CG2	2.39	0.49
2:D:334:THR:HB	2:D:336:ASP:OD1	2.12	0.49
2:H:322:VAL:HG13	2:H:354:LEU:HA	1.94	0.49
2:B:189:LYS:HD3	2:B:221:ILE:CD1	2.42	0.49
2:B:326:ILE:C	2:B:328:SER:H	2.15	0.49
2:D:337:LEU:O	2:D:338:ALA:HB3	2.13	0.49
2:F:61:ILE:HD11	2:F:70:PRO:HA	1.94	0.49
1:G:299:LEU:HB2	1:G:308:ALA:HB2	1.94	0.49
2:H:349:ALA:O	2:H:353:ARG:HD3	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:VAL:HG12	1:A:272:GLY:HA3	1.94	0.49
2:B:46:ALA:HB2	2:B:351:ILE:HD13	1.94	0.49
2:B:189:LYS:HE2	2:B:192:ILE:HD12	1.94	0.49
1:E:67:VAL:HG13	1:E:101:LEU:HD21	1.94	0.49
2:F:169:ILE:HD13	2:F:204:ALA:HB2	1.95	0.49
2:B:69:ILE:HD12	2:B:70:PRO:CD	2.35	0.49
2:F:33:GLY:O	2:F:36:ILE:HG22	2.13	0.49
2:B:134:ILE:HD13	2:B:239:VAL:HG13	1.95	0.49
1:E:22:LEU:HD11	1:E:33:THR:HG22	1.95	0.49
1:G:255:GLY:O	1:G:289:THR:HB	2.13	0.49
2:H:341:ALA:HB1	2:H:345:SER:OG	2.13	0.49
1:A:195:ARG:HH11	1:A:195:ARG:CB	2.25	0.49
2:D:321:ALA:O	2:D:322:VAL:O	2.31	0.49
1:E:255:GLY:O	1:E:289:THR:HB	2.12	0.49
1:G:119:ARG:HG2	2:H:125:THR:HG22	1.95	0.49
1:A:299:LEU:HA	1:A:302:LEU:CD1	2.44	0.48
1:C:155:THR:HG22	2:D:153:VAL:HG13	1.95	0.48
2:D:31:GLY:O	2:D:34:PRO:HD2	2.13	0.48
2:D:253:LEU:C	2:D:253:LEU:HD23	2.33	0.48
2:B:253:LEU:HD23	2:B:253:LEU:O	2.13	0.48
2:B:322:VAL:O	2:B:323:LEU:C	2.51	0.48
1:C:175:ARG:NH1	1:C:231:ASP:OD1	2.47	0.48
1:E:10:LEU:HB3	1:E:11:PRO:CD	2.43	0.48
1:E:133:GLU:HG2	1:E:134:GLY:H	1.78	0.48
1:E:133:GLU:OE1	1:E:158:LYS:HD2	2.13	0.48
1:G:29:GLY:O	1:G:33:THR:OG1	2.31	0.48
1:G:340:ASN:O	1:G:343:ILE:HG13	2.13	0.48
1:A:255:GLY:O	1:A:289:THR:HB	2.12	0.48
2:B:265:THR:O	2:B:280:VAL:HG22	2.13	0.48
1:C:27:GLY:C	1:C:29:GLY:H	2.15	0.48
1:E:175:ARG:NH1	1:E:231:ASP:OD1	2.47	0.48
1:G:199:THR:HA	1:G:211:VAL:HG11	1.95	0.48
2:B:323:LEU:N	2:B:326:ILE:HG23	2.28	0.48
2:B:341:ALA:HB1	2:B:345:SER:OG	2.12	0.48
2:D:273:LYS:HG3	2:D:274:ILE:HD12	1.94	0.48
1:E:342:ILE:O	1:E:346:LEU:HB2	2.12	0.48
2:F:189:LYS:CG	2:F:192:ILE:HD13	2.44	0.48
1:C:245:ASN:ND2	2:D:222:ASP:HA	2.29	0.48
1:C:288:PRO:HG3	1:C:335:THR:HG23	1.95	0.48
1:E:62:GLY:C	1:E:64:TYR:N	2.65	0.48
2:F:134:ILE:HD13	2:F:239:VAL:HG13	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:195:ARG:HH11	1:E:195:ARG:HB3	1.78	0.48
1:E:199:THR:HA	1:E:211:VAL:HG11	1.96	0.48
2:F:147:HIS:CD2	1:G:151:LEU:HD11	2.48	0.48
1:A:175:ARG:NH1	1:A:231:ASP:OD1	2.46	0.48
2:B:189:LYS:HB2	2:B:221:ILE:HD11	1.96	0.48
2:F:189:LYS:HE2	2:F:192:ILE:HD12	1.95	0.48
2:F:228:VAL:HG12	2:F:257:LEU:CD1	2.44	0.48
2:F:253:LEU:HD23	2:F:253:LEU:O	2.14	0.48
1:G:151:LEU:CD2	2:H:157:ILE:HG12	2.35	0.48
2:D:69:ILE:HD12	2:D:70:PRO:CD	2.35	0.48
2:D:189:LYS:CG	2:D:192:ILE:HD13	2.44	0.48
2:H:47:ALA:HB2	2:H:354:LEU:HD11	1.95	0.48
1:C:106:ASN:HB3	1:C:129:ARG:HG2	1.96	0.48
2:D:181:ARG:HH11	2:D:238:ALA:H	1.60	0.48
1:E:283:GLN:HB3	1:E:285:VAL:HG13	1.94	0.48
2:H:319:GLN:O	2:H:321:ALA:O	2.32	0.48
1:A:151:LEU:CD1	2:D:147:HIS:CD2	2.97	0.48
2:F:337:LEU:O	2:F:338:ALA:HB3	2.14	0.48
1:G:310:ARG:HG3	1:G:349:MSE:HE1	1.95	0.48
2:H:189:LYS:CG	2:H:192:ILE:HD13	2.44	0.48
1:A:106:ASN:HB3	1:A:129:ARG:HG2	1.95	0.47
2:B:270:ILE:HA	2:B:275:SER:OG	2.14	0.47
2:D:189:LYS:HD3	2:D:221:ILE:CD1	2.43	0.47
1:E:27:GLY:C	1:E:29:GLY:H	2.17	0.47
1:E:189:LEU:HB3	2:F:154:VAL:CG1	2.44	0.47
1:E:292:ILE:O	1:E:296:THR:HG23	2.13	0.47
1:A:139:LEU:HD22	2:D:147:HIS:HB3	1.96	0.47
2:D:134:ILE:HD13	2:D:239:VAL:HG13	1.95	0.47
1:E:19:THR:O	1:E:73:ASN:HB3	2.14	0.47
2:H:270:ILE:HA	2:H:275:SER:OG	2.14	0.47
2:H:337:LEU:O	2:H:338:ALA:HB3	2.14	0.47
1:A:176:LYS:HE3	1:A:208:ASP:O	2.14	0.47
2:B:147:HIS:CD2	1:C:151:LEU:CD1	2.98	0.47
1:C:255:GLY:O	1:C:289:THR:HB	2.13	0.47
2:F:319:GLN:O	2:F:324:SER:HB2	2.14	0.47
1:G:323:LYS:O	1:G:324:HIS:CB	2.61	0.47
2:B:351:ILE:O	2:B:354:LEU:HB2	2.14	0.47
1:C:257:VAL:HG12	1:C:272:GLY:HA3	1.96	0.47
2:D:274:ILE:HG22	2:D:275:SER:H	1.78	0.47
1:E:104:TYR:CZ	1:E:161:ARG:HG2	2.49	0.47
2:F:169:ILE:HD12	2:F:203:VAL:HG12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:181:ARG:HH11	2:F:238:ALA:H	1.62	0.47
2:F:228:VAL:HG12	2:F:257:LEU:HD11	1.96	0.47
1:G:288:PRO:HG3	1:G:335:THR:HG23	1.97	0.47
2:H:169:ILE:HD13	2:H:204:ALA:HB2	1.95	0.47
1:A:47:ILE:HD11	1:A:49:TRP:CE3	2.50	0.47
2:D:118:SER:OG	2:D:129:VAL:HG13	2.14	0.47
1:E:205:GLU:HB2	1:E:206:TYR:CD1	2.49	0.47
1:C:12:LYS:HB2	1:C:73:ASN:HA	1.95	0.47
2:F:319:GLN:O	2:F:321:ALA:O	2.32	0.47
1:G:18:PHE:CD1	1:G:19:THR:N	2.82	0.47
1:G:251:ILE:HD11	1:G:257:VAL:HG22	1.96	0.47
2:H:24:VAL:HG11	2:H:53:TRP:HZ3	1.78	0.47
2:H:265:THR:O	2:H:280:VAL:HG22	2.15	0.47
1:A:288:PRO:HG3	1:A:335:THR:HG23	1.97	0.47
1:A:342:ILE:O	1:A:346:LEU:HB2	2.14	0.47
2:B:118:SER:OG	2:B:129:VAL:HG13	2.15	0.47
2:B:228:VAL:HG12	2:B:257:LEU:CD1	2.45	0.47
2:B:319:GLN:O	2:B:324:SER:HB2	2.14	0.47
2:D:270:ILE:HA	2:D:275:SER:OG	2.15	0.47
2:F:136:GLU:OE2	2:F:138:THR:HB	2.13	0.47
2:F:326:ILE:C	2:F:328:SER:H	2.17	0.47
1:G:342:ILE:O	1:G:346:LEU:HB2	2.15	0.47
2:H:319:GLN:O	2:H:324:SER:HB2	2.15	0.47
1:A:283:GLN:HB3	1:A:285:VAL:HG13	1.97	0.47
1:A:299:LEU:HB2	1:A:308:ALA:HB2	1.95	0.47
2:D:46:ALA:HB2	2:D:351:ILE:HD13	1.97	0.47
2:D:326:ILE:C	2:D:328:SER:H	2.17	0.47
1:E:60:LYS:O	1:E:60:LYS:HG2	2.15	0.47
2:F:341:ALA:HB1	2:F:345:SER:OG	2.15	0.47
1:A:251:ILE:HD11	1:A:257:VAL:HG22	1.97	0.47
1:C:78:LYS:HE2	1:C:79:GLY:O	2.15	0.47
1:C:104:TYR:CE2	1:C:161:ARG:HG2	2.50	0.47
2:D:295:PRO:O	2:D:299:LEU:HB2	2.15	0.47
2:D:349:ALA:O	2:D:353:ARG:HD3	2.15	0.47
1:E:29:GLY:O	1:E:33:THR:OG1	2.33	0.47
2:F:224:SER:O	2:F:228:VAL:HG23	2.15	0.47
2:F:295:PRO:O	2:F:299:LEU:HB2	2.14	0.47
2:D:221:ILE:HD12	2:D:221:ILE:N	2.29	0.46
2:D:322:VAL:O	2:D:323:LEU:C	2.53	0.46
1:E:47:ILE:HD11	1:E:49:TRP:CE3	2.50	0.46
1:E:254:PRO:HG3	2:F:226:LEU:HD11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:26:PHE:HE2	2:F:37:SER:OG	1.98	0.46
2:H:46:ALA:CB	2:H:351:ILE:HD13	2.45	0.46
2:H:287:ILE:HG23	2:H:287:ILE:O	2.14	0.46
1:A:158:LYS:HG2	1:A:161:ARG:NH2	2.30	0.46
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.68	0.46
1:A:323:LYS:O	1:A:324:HIS:CB	2.60	0.46
2:B:142:TYR:N	2:B:142:TYR:CD1	2.84	0.46
2:B:319:GLN:O	2:B:321:ALA:O	2.32	0.46
2:F:318:ILE:HG22	2:F:323:LEU:HD21	1.97	0.46
1:G:183:LYS:HE2	2:H:142:TYR:OH	2.15	0.46
2:F:189:LYS:O	2:F:189:LYS:HG3	2.15	0.46
1:A:19:THR:O	1:A:73:ASN:HB3	2.16	0.46
1:C:176:LYS:HE3	1:C:208:ASP:O	2.15	0.46
1:C:340:ASN:O	1:C:343:ILE:HG13	2.16	0.46
1:E:12:LYS:HB2	1:E:73:ASN:HA	1.97	0.46
2:F:110:PHE:CE1	2:F:167:ARG:HG3	2.50	0.46
2:B:26:PHE:HE2	2:B:37:SER:OG	1.99	0.46
2:B:70:PRO:O	2:B:74:VAL:HG23	2.15	0.46
2:F:189:LYS:HG2	2:F:192:ILE:HD13	1.98	0.46
2:F:322:VAL:O	2:F:323:LEU:C	2.53	0.46
2:H:142:TYR:N	2:H:142:TYR:CD1	2.82	0.46
2:H:306:LEU:HD12	2:H:309:MSE:HE1	1.97	0.46
2:H:321:ALA:O	2:H:322:VAL:O	2.33	0.46
1:A:310:ARG:HG3	1:A:349:MSE:HE2	1.96	0.46
2:B:221:ILE:N	2:B:221:ILE:HD12	2.31	0.46
2:B:306:LEU:HD12	2:B:309:MSE:HE1	1.98	0.46
1:C:62:GLY:C	1:C:64:TYR:N	2.68	0.46
1:C:284:ASN:O	1:C:334:SER:HB2	2.16	0.46
3:C:1002:FLC:OG1	3:C:1002:FLC:OHB	2.30	0.46
2:D:30:ASP:OD2	2:D:88:LEU:HA	2.16	0.46
1:E:323:LYS:H	1:E:323:LYS:CE	2.23	0.46
2:F:26:PHE:O	2:F:27:ILE:HB	2.15	0.46
2:H:24:VAL:CG1	2:H:53:TRP:HZ3	2.29	0.46
2:H:189:LYS:O	2:H:189:LYS:HG3	2.15	0.46
1:A:199:THR:HA	1:A:211:VAL:HG11	1.97	0.46
1:C:195:ARG:HH11	1:C:195:ARG:HB3	1.79	0.46
1:C:232:VAL:O	1:C:233:LEU:HD23	2.15	0.46
2:D:265:THR:HA	2:D:266:PRO:HD3	1.63	0.46
1:G:62:GLY:C	1:G:64:TYR:N	2.68	0.46
2:H:294:ASN:HA	2:H:295:PRO:HD2	1.75	0.46
1:C:7:GLU:C	1:C:9:THR:H	2.19	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:ASP:N	2:B:72:PRO:HD2	2.31	0.46
2:B:77:ILE:O	2:B:80:ASN:O	2.33	0.46
2:B:194:ARG:O	2:B:198:GLY:HA3	2.16	0.46
2:H:67:THR:HG23	2:H:97:ARG:CB	2.42	0.46
2:B:67:THR:HG23	2:B:97:ARG:HB3	1.99	0.45
2:B:349:ALA:O	2:B:353:ARG:HD3	2.16	0.45
2:D:12:THR:HB	2:D:81:LEU:CD1	2.46	0.45
1:G:101:LEU:HB2	1:G:103:ILE:HG13	1.96	0.45
1:G:115:GLY:CA	1:G:320:ALA:HA	2.45	0.45
2:H:12:THR:HB	2:H:81:LEU:CD1	2.43	0.45
2:H:265:THR:HA	2:H:266:PRO:HD3	1.64	0.45
2:H:318:ILE:HA	2:H:322:VAL:CG2	2.38	0.45
1:A:283:GLN:CB	1:A:285:VAL:HG13	2.47	0.45
1:A:62:GLY:C	1:A:64:TYR:N	2.69	0.45
1:A:115:GLY:CA	1:A:320:ALA:HA	2.45	0.45
1:C:29:GLY:O	1:C:33:THR:OG1	2.35	0.45
2:D:189:LYS:HG2	2:D:192:ILE:HD13	1.98	0.45
2:D:265:THR:O	2:D:280:VAL:HG22	2.16	0.45
2:F:44:PHE:O	2:F:49:VAL:HG22	2.16	0.45
1:G:299:LEU:HA	1:G:302:LEU:CD1	2.46	0.45
2:B:287:ILE:O	2:B:287:ILE:HG23	2.15	0.45
2:B:295:PRO:O	2:B:299:LEU:HB2	2.16	0.45
1:C:293:LEU:HD23	1:C:293:LEU:HA	1.65	0.45
2:D:183:ARG:O	2:D:238:ALA:O	2.35	0.45
1:E:101:LEU:HB2	1:E:103:ILE:HG13	1.97	0.45
1:E:120:ILE:HA	1:E:121:PRO:HD3	1.76	0.45
1:E:251:ILE:HD11	1:E:257:VAL:HG22	1.99	0.45
1:E:288:PRO:HG3	1:E:335:THR:HG23	1.97	0.45
2:F:64:ASN:O	2:F:66:LEU:N	2.48	0.45
2:H:274:ILE:CG2	2:H:275:SER:N	2.79	0.45
1:A:67:VAL:HG13	1:A:101:LEU:HD21	1.98	0.45
2:F:189:LYS:HE2	2:F:192:ILE:CD1	2.47	0.45
2:F:209:LYS:HE3	2:F:209:LYS:HB3	1.36	0.45
1:G:176:LYS:HE3	1:G:208:ASP:O	2.17	0.45
1:A:136:PHE:CD1	1:A:237:SER:HB2	2.52	0.45
1:C:136:PHE:CD1	1:C:237:SER:HB2	2.52	0.45
1:E:179:THR:HB	1:E:233:LEU:HD22	1.98	0.45
1:E:232:VAL:O	1:E:233:LEU:HD23	2.16	0.45
2:F:24:VAL:HG11	2:F:53:TRP:HZ3	1.82	0.45
1:G:133:GLU:HG2	1:G:134:GLY:H	1.80	0.45
1:G:283:GLN:HB3	1:G:285:VAL:HG13	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:26:PHE:HE2	2:H:37:SER:OG	1.99	0.45
2:H:169:ILE:HD12	2:H:203:VAL:HG12	1.97	0.45
2:H:221:ILE:O	2:H:222:ASP:C	2.53	0.45
2:D:181:ARG:HD3	2:D:238:ALA:H	1.81	0.45
2:D:189:LYS:HE2	2:D:192:ILE:HD12	1.98	0.45
1:E:340:ASN:O	1:E:343:ILE:HG13	2.17	0.45
2:H:44:PHE:O	2:H:49:VAL:HG22	2.17	0.45
2:B:30:ASP:OD2	2:B:88:LEU:HA	2.17	0.45
2:D:228:VAL:HG12	2:D:257:LEU:HD11	1.98	0.45
1:E:32:ILE:HG13	1:E:288:PRO:HA	1.99	0.45
2:F:43:ILE:HD12	2:F:299:LEU:HD21	1.99	0.45
2:F:97:ARG:HG3	2:F:102:THR:CG2	2.44	0.45
1:G:27:GLY:C	1:G:29:GLY:H	2.19	0.45
2:H:44:PHE:HD2	2:H:49:VAL:HG21	1.81	0.45
2:B:43:ILE:HD12	2:B:299:LEU:HD21	1.99	0.45
2:B:103:LEU:HD12	2:B:103:LEU:HA	1.73	0.45
1:C:193:LEU:O	1:C:197:ILE:HG13	2.16	0.45
1:E:136:PHE:CD1	1:E:237:SER:HB2	2.52	0.45
1:E:233:LEU:HD12	1:E:243:LEU:HD13	1.98	0.45
2:F:265:THR:O	2:F:280:VAL:HG22	2.17	0.45
2:H:189:LYS:HE2	2:H:192:ILE:HD12	1.99	0.45
1:A:32:ILE:HG13	1:A:288:PRO:HA	1.98	0.45
1:E:101:LEU:HD12	1:E:103:ILE:HD11	1.99	0.45
2:F:287:ILE:HG23	2:F:287:ILE:O	2.17	0.45
1:G:158:LYS:HG2	1:G:161:ARG:NH2	2.31	0.45
2:H:181:ARG:HH11	2:H:238:ALA:H	1.65	0.45
1:A:195:ARG:O	1:A:199:THR:HG23	2.17	0.44
2:B:265:THR:HA	2:B:266:PRO:HD3	1.64	0.44
2:B:274:ILE:CG2	2:B:275:SER:N	2.80	0.44
1:C:12:LYS:HE3	1:G:168:ASP:CG	2.38	0.44
1:C:193:LEU:HD11	1:C:197:ILE:HD11	1.98	0.44
2:D:169:ILE:HD12	2:D:203:VAL:HG12	1.98	0.44
2:F:146:GLU:HB3	2:F:156:SER:HA	1.99	0.44
2:F:321:ALA:O	2:F:322:VAL:O	2.34	0.44
2:H:194:ARG:HG3	2:H:194:ARG:HH11	1.82	0.44
1:A:60:LYS:O	1:A:60:LYS:HG2	2.16	0.44
2:D:43:ILE:HD12	2:D:299:LEU:HD21	1.99	0.44
2:D:189:LYS:O	2:D:189:LYS:HG3	2.18	0.44
2:D:205:LYS:O	2:D:208:SER:HB3	2.18	0.44
1:G:78:LYS:HE2	1:G:79:GLY:O	2.17	0.44
1:G:287:ASN:HA	1:G:288:PRO:HD3	1.87	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1004:FLC:OB1	3:G:1004:FLC:OA1	2.34	0.44
2:H:299:LEU:HD12	2:H:299:LEU:HA	1.85	0.44
1:C:133:GLU:OE1	1:C:158:LYS:HD2	2.17	0.44
2:D:146:GLU:HB3	2:D:156:SER:HA	2.00	0.44
2:D:182:PRO:HD2	2:D:237:ASP:HB2	2.00	0.44
2:D:228:VAL:HG12	2:D:257:LEU:CD1	2.47	0.44
2:F:186:VAL:CG2	2:F:216:LEU:HD11	2.46	0.44
2:F:273:LYS:HE3	2:F:274:ILE:HD11	1.98	0.44
1:G:47:ILE:HD11	1:G:49:TRP:CE3	2.52	0.44
1:G:257:VAL:HG12	1:G:272:GLY:HA3	2.00	0.44
2:H:89:ALA:O	2:H:91:PRO:HD3	2.17	0.44
1:A:232:VAL:C	1:A:233:LEU:HD23	2.37	0.44
1:A:288:PRO:O	1:A:292:ILE:HG13	2.17	0.44
2:B:326:ILE:HG21	2:B:350:VAL:HG22	2.00	0.44
1:C:101:LEU:HB2	1:C:103:ILE:HG13	2.00	0.44
2:D:186:VAL:CG2	2:D:216:LEU:HD11	2.46	0.44
1:G:241:THR:OG1	3:G:1004:FLC:OA2	2.21	0.44
2:H:186:VAL:CG2	2:H:216:LEU:HD11	2.47	0.44
1:A:284:ASN:O	1:A:334:SER:HB2	2.17	0.44
2:B:321:ALA:O	2:B:322:VAL:O	2.34	0.44
2:F:326:ILE:HG21	2:F:350:VAL:HG22	1.98	0.44
2:H:326:ILE:HG21	2:H:350:VAL:HG22	2.00	0.44
1:A:95:VAL:HG23	1:A:96:ALA:N	2.33	0.44
1:A:299:LEU:HA	1:A:302:LEU:HD11	1.99	0.44
2:B:12:THR:HB	2:B:81:LEU:CD1	2.47	0.44
2:B:169:ILE:HG21	2:B:204:ALA:HA	2.00	0.44
2:B:273:LYS:HE3	2:B:274:ILE:HD11	1.98	0.44
2:D:139:GLU:HB2	2:D:140:GLY:H	1.61	0.44
2:F:62:PHE:CE1	2:F:67:THR:HG22	2.52	0.44
2:F:265:THR:HA	2:F:266:PRO:HD3	1.63	0.44
1:G:60:LYS:O	1:G:60:LYS:HG2	2.16	0.44
2:B:181:ARG:HH11	2:B:238:ALA:H	1.66	0.44
1:E:43:GLU:OE1	1:E:310:ARG:NH1	2.51	0.44
1:E:119:ARG:HG2	2:F:125:THR:CG2	2.39	0.44
2:H:89:ALA:C	2:H:91:PRO:HD3	2.38	0.44
2:H:142:TYR:N	2:H:142:TYR:HD1	2.15	0.44
1:A:155:THR:HG22	2:B:153:VAL:HG13	1.99	0.44
2:B:189:LYS:HG2	2:B:192:ILE:CD1	2.48	0.44
1:C:199:THR:HA	1:C:211:VAL:HG11	1.99	0.44
2:D:24:VAL:HG11	2:D:53:TRP:HZ3	1.83	0.44
2:D:26:PHE:O	2:D:27:ILE:HB	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:194:ARG:HG3	2:D:194:ARG:HH11	1.83	0.44
2:F:8:ILE:HG21	2:F:171:TYR:HB2	2.00	0.44
1:G:310:ARG:HG3	1:G:349:MSE:CE	2.48	0.44
2:H:228:VAL:HG12	2:H:257:LEU:CD1	2.48	0.44
1:A:340:ASN:HA	1:A:343:ILE:CG1	2.48	0.44
2:B:61:ILE:HG22	2:B:62:PHE:N	2.27	0.44
2:B:110:PHE:CE1	2:B:167:ARG:HG3	2.52	0.44
2:B:146:GLU:HB3	2:B:156:SER:HA	2.00	0.44
1:C:40:PHE:CD1	1:C:45:ILE:HD12	2.53	0.44
2:F:139:GLU:HB2	2:F:140:GLY:H	1.58	0.44
2:B:189:LYS:C	2:B:191:THR:H	2.20	0.43
2:B:189:LYS:C	2:B:191:THR:N	2.71	0.43
2:D:61:ILE:HG22	2:D:62:PHE:N	2.26	0.43
2:F:25:SER:HB3	2:F:56:CYS:SG	2.58	0.43
1:G:19:THR:O	1:G:73:ASN:HB3	2.18	0.43
2:H:118:SER:OG	2:H:129:VAL:HG13	2.18	0.43
1:A:29:GLY:O	1:A:33:THR:OG1	2.36	0.43
2:F:181:ARG:HD3	2:F:238:ALA:H	1.83	0.43
2:F:322:VAL:C	2:F:326:ILE:HG23	2.39	0.43
1:G:193:LEU:HD11	1:G:197:ILE:HD11	1.98	0.43
2:H:77:ILE:O	2:H:80:ASN:O	2.37	0.43
2:H:273:LYS:HE3	2:H:274:ILE:HD11	1.99	0.43
2:B:189:LYS:HG3	2:B:189:LYS:O	2.17	0.43
1:C:27:GLY:C	1:C:29:GLY:N	2.72	0.43
1:C:195:ARG:O	1:C:199:THR:HG23	2.17	0.43
1:E:283:GLN:CB	1:E:285:VAL:HG13	2.47	0.43
1:E:336:THR:HG22	1:E:337:ASP:N	2.33	0.43
2:F:149:VAL:O	2:F:150:CYS:HB3	2.18	0.43
2:H:66:LEU:HD13	2:H:66:LEU:O	2.19	0.43
2:H:146:GLU:HB3	2:H:156:SER:HA	2.00	0.43
1:A:241:THR:OG1	3:A:1001:FCL:OA2	2.24	0.43
2:B:12:THR:O	2:B:13:GLY:O	2.36	0.43
1:C:292:ILE:O	1:C:296:THR:HG23	2.18	0.43
1:E:195:ARG:O	1:E:199:THR:HG23	2.19	0.43
2:F:299:LEU:HD12	2:F:299:LEU:HA	1.86	0.43
2:H:205:LYS:O	2:H:208:SER:HB3	2.19	0.43
2:B:228:VAL:HG12	2:B:257:LEU:HD11	2.00	0.43
1:C:19:THR:O	1:C:73:ASN:HB3	2.19	0.43
1:C:115:GLY:CA	1:C:320:ALA:HA	2.46	0.43
2:F:59:SER:HA	2:F:60:PRO:HD3	1.86	0.43
1:A:193:LEU:HD11	1:A:197:ILE:HD11	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ILE:HA	1:C:121:PRO:HD3	1.77	0.43
1:C:283:GLN:CB	1:C:285:VAL:HG13	2.49	0.43
1:C:299:LEU:HA	1:C:302:LEU:CD1	2.49	0.43
1:G:101:LEU:HD12	1:G:103:ILE:HD11	2.00	0.43
2:H:139:GLU:HB2	2:H:140:GLY:H	1.61	0.43
2:H:169:ILE:HG21	2:H:204:ALA:HA	2.00	0.43
1:A:255:GLY:O	1:A:290:ALA:N	2.51	0.43
2:B:183:ARG:NH1	2:B:237:ASP:OD2	2.52	0.43
2:D:299:LEU:HD12	2:D:299:LEU:HA	1.84	0.43
1:G:340:ASN:HA	1:G:343:ILE:HG13	2.01	0.43
1:C:201:ILE:HG13	1:C:201:ILE:O	2.18	0.43
1:C:251:ILE:HD11	1:C:257:VAL:HG22	2.01	0.43
2:D:253:LEU:HD23	2:D:253:LEU:O	2.19	0.43
2:D:336:ASP:O	2:D:337:LEU:HD23	2.19	0.43
1:E:14:TYR:O	1:E:15:GLY:C	2.56	0.43
1:E:158:LYS:HG2	1:E:161:ARG:NH2	2.33	0.43
2:F:77:ILE:O	2:F:80:ASN:O	2.37	0.43
1:G:83:THR:HB	2:H:191:THR:HG23	2.00	0.43
2:H:66:LEU:HD22	2:H:67:THR:N	2.34	0.43
2:H:250:LEU:HD23	2:H:250:LEU:HA	1.86	0.43
1:A:193:LEU:O	1:A:197:ILE:HG13	2.19	0.43
2:B:142:TYR:N	2:B:142:TYR:HD1	2.17	0.43
2:D:67:THR:CG2	2:D:97:ARG:H	2.32	0.43
2:D:90:THR:HG22	2:D:91:PRO:O	2.19	0.43
2:D:189:LYS:C	2:D:191:THR:H	2.22	0.43
2:D:221:ILE:O	2:D:222:ASP:C	2.58	0.43
1:E:342:ILE:HG12	1:E:342:ILE:H	1.62	0.43
2:F:46:ALA:CB	2:F:351:ILE:HD13	2.49	0.43
2:F:183:ARG:O	2:F:238:ALA:O	2.36	0.43
1:G:292:ILE:O	1:G:296:THR:HG23	2.19	0.43
2:H:26:PHE:O	2:H:27:ILE:HB	2.19	0.43
2:H:71:ASP:N	2:H:72:PRO:HD2	2.34	0.43
2:H:322:VAL:O	2:H:323:LEU:C	2.57	0.43
1:A:92:SER:C	1:A:94:ASN:H	2.22	0.43
1:C:287:ASN:HA	1:C:288:PRO:HD3	1.87	0.43
2:D:294:ASN:HA	2:D:295:PRO:HD2	1.71	0.43
2:D:326:ILE:HD12	2:D:332:ASN:HB3	2.00	0.43
2:F:326:ILE:HD12	2:F:332:ASN:HB3	2.01	0.43
2:H:194:ARG:O	2:H:198:GLY:HA3	2.19	0.43
2:F:47:ALA:HB2	2:F:354:LEU:HD11	2.01	0.42
1:G:288:PRO:O	1:G:292:ILE:HG13	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:15:PRO:HG3	2:H:22:TYR:CZ	2.54	0.42
2:H:142:TYR:OH	2:H:245:LEU:HD12	2.19	0.42
1:A:171:LYS:HZ2	1:E:72:ARG:CZ	2.32	0.42
1:E:245:ASN:ND2	2:F:222:ASP:HA	2.34	0.42
1:G:106:ASN:HB3	1:G:129:ARG:HG2	2.01	0.42
2:H:189:LYS:C	2:H:191:THR:N	2.73	0.42
2:H:318:ILE:HG22	2:H:323:LEU:HD21	2.00	0.42
1:A:296:THR:HA	1:A:299:LEU:HD12	1.99	0.42
1:A:342:ILE:HG12	1:A:342:ILE:H	1.62	0.42
1:C:78:LYS:C	1:C:291:MSE:HE1	2.40	0.42
1:C:158:LYS:HG2	1:C:161:ARG:NH2	2.34	0.42
2:D:236:THR:HG22	2:D:236:THR:O	2.20	0.42
2:D:273:LYS:HE3	2:D:274:ILE:HD11	2.02	0.42
1:E:5:GLN:O	1:E:6:ALA:O	2.38	0.42
3:E:1003:FLC:OB1	3:E:1003:FLC:OA1	2.36	0.42
2:F:46:ALA:HB3	2:F:354:LEU:CD2	2.49	0.42
2:F:142:TYR:N	2:F:142:TYR:CD1	2.86	0.42
2:F:348:GLU:H	2:F:348:GLU:HG2	1.63	0.42
1:G:119:ARG:NH2	2:H:230:THR:O	2.52	0.42
1:G:284:ASN:O	1:G:334:SER:HB2	2.20	0.42
2:B:15:PRO:HG3	2:B:22:TYR:CZ	2.54	0.42
2:B:176:ALA:HA	2:B:239:VAL:HG21	2.02	0.42
2:F:30:ASP:OD2	2:F:88:LEU:HA	2.17	0.42
2:F:213:ASP:OD1	2:F:213:ASP:N	2.50	0.42
1:G:92:SER:C	1:G:94:ASN:H	2.23	0.42
2:H:30:ASP:OD2	2:H:88:LEU:HA	2.20	0.42
2:D:189:LYS:HE2	2:D:192:ILE:CD1	2.50	0.42
1:E:284:ASN:O	1:E:334:SER:HB2	2.19	0.42
2:F:221:ILE:HD12	2:F:221:ILE:N	2.33	0.42
1:G:201:ILE:HG13	1:G:201:ILE:O	2.19	0.42
2:H:43:ILE:HD12	2:H:299:LEU:HD21	2.01	0.42
2:H:66:LEU:HD23	2:H:97:ARG:NH1	2.30	0.42
1:A:78:LYS:C	1:A:291:MSE:HE1	2.40	0.42
1:A:83:THR:HA	1:A:84:PRO:HD3	1.80	0.42
2:D:274:ILE:CG2	2:D:275:SER:N	2.82	0.42
1:G:293:LEU:HA	1:G:293:LEU:HD23	1.63	0.42
2:H:12:THR:O	2:H:13:GLY:O	2.37	0.42
2:B:236:THR:HG22	2:B:236:THR:O	2.19	0.42
2:B:326:ILE:HD12	2:B:332:ASN:HB3	2.01	0.42
1:C:104:TYR:CZ	1:C:161:ARG:HG2	2.54	0.42
1:E:115:GLY:CA	1:E:320:ALA:HA	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:194:ARG:O	2:F:198:GLY:HA3	2.19	0.42
1:G:47:ILE:C	1:G:47:ILE:HD13	2.40	0.42
2:H:181:ARG:HD3	2:H:238:ALA:H	1.84	0.42
1:A:78:LYS:HE2	1:A:79:GLY:O	2.19	0.42
2:D:142:TYR:CD1	2:D:142:TYR:N	2.87	0.42
1:E:340:ASN:HA	1:E:343:ILE:HG13	2.02	0.42
1:A:22:LEU:HD11	1:A:33:THR:CG2	2.50	0.42
2:B:44:PHE:O	2:B:49:VAL:HG22	2.20	0.42
2:B:348:GLU:H	2:B:348:GLU:HG2	1.60	0.42
1:C:232:VAL:C	1:C:233:LEU:HD23	2.40	0.42
2:D:250:LEU:HD23	2:D:250:LEU:HA	1.85	0.42
2:F:142:TYR:OH	2:F:245:LEU:HD12	2.20	0.42
2:F:347:THR:O	2:F:351:ILE:HG13	2.20	0.42
2:H:49:VAL:HA	2:H:50:PRO:HD3	1.87	0.42
2:H:149:VAL:O	2:H:150:CYS:HB3	2.20	0.42
1:A:287:ASN:HA	1:A:288:PRO:HD3	1.89	0.42
2:B:39:SER:OG	2:B:347:THR:HG23	2.19	0.42
1:E:193:LEU:O	1:E:197:ILE:HG13	2.20	0.42
2:F:294:ASN:HA	2:F:295:PRO:HD2	1.74	0.42
1:G:340:ASN:HA	1:G:343:ILE:CG1	2.49	0.42
2:H:182:PRO:HD2	2:H:237:ASP:HB2	2.02	0.42
1:A:27:GLY:C	1:A:29:GLY:N	2.73	0.41
2:B:13:GLY:O	2:B:14:LYS:HB3	2.19	0.41
2:B:59:SER:HA	2:B:60:PRO:HD3	1.85	0.41
2:B:347:THR:O	2:B:351:ILE:HG13	2.20	0.41
1:C:47:ILE:HD11	1:C:49:TRP:CD2	2.55	0.41
1:E:40:PHE:CD1	1:E:45:ILE:HD12	2.55	0.41
1:E:47:ILE:HD11	1:E:49:TRP:CD2	2.55	0.41
2:F:306:LEU:HD12	2:F:309:MSE:HE1	2.00	0.41
1:G:33:THR:HG23	1:G:291:MSE:CE	2.48	0.41
1:G:195:ARG:O	1:G:199:THR:HG23	2.20	0.41
1:G:278:LEU:HD23	1:G:278:LEU:HA	1.85	0.41
2:B:26:PHE:CE1	2:B:84:LEU:HD23	2.55	0.41
2:B:142:TYR:OH	2:B:245:LEU:HD12	2.19	0.41
1:C:336:THR:HG22	1:C:337:ASP:N	2.35	0.41
1:E:7:GLU:O	1:E:10:LEU:HD12	2.20	0.41
1:E:27:GLY:C	1:E:29:GLY:N	2.73	0.41
1:E:181:VAL:HG21	1:E:243:LEU:CD1	2.49	0.41
1:E:299:LEU:HA	1:E:302:LEU:CD1	2.49	0.41
2:F:15:PRO:HG3	2:F:22:TYR:CZ	2.55	0.41
2:F:236:THR:O	2:F:236:THR:HG22	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:306:LEU:HD23	2:F:315:ALA:HA	2.02	0.41
2:F:336:ASP:O	2:F:337:LEU:HD23	2.21	0.41
2:H:59:SER:HA	2:H:60:PRO:HD3	1.81	0.41
2:H:70:PRO:O	2:H:74:VAL:HG23	2.20	0.41
2:H:322:VAL:C	2:H:326:ILE:HG23	2.40	0.41
1:C:82:HIS:CG	1:C:83:THR:N	2.89	0.41
2:D:24:VAL:CG1	2:D:53:TRP:HZ3	2.34	0.41
2:D:26:PHE:CE1	2:D:84:LEU:HD23	2.55	0.41
1:E:13:LYS:HD2	1:E:18:PHE:CE1	2.54	0.41
1:E:47:ILE:C	1:E:47:ILE:HD13	2.40	0.41
2:F:322:VAL:HG13	2:F:354:LEU:HA	2.02	0.41
1:A:101:LEU:HD12	1:A:103:ILE:HD11	2.02	0.41
2:B:43:ILE:CD1	2:B:299:LEU:HD21	2.51	0.41
1:C:278:LEU:HD23	1:C:278:LEU:HA	1.90	0.41
1:G:67:VAL:HG13	1:G:101:LEU:HD21	2.02	0.41
1:G:205:GLU:HB2	1:G:206:TYR:CD1	2.55	0.41
1:A:165:PHE:HA	1:E:14:TYR:OH	2.20	0.41
1:A:181:VAL:HG21	1:A:243:LEU:CD1	2.50	0.41
1:A:292:ILE:O	1:A:296:THR:HG23	2.20	0.41
2:B:142:TYR:HB2	2:B:244:ASN:ND2	2.36	0.41
2:B:189:LYS:HE2	2:B:192:ILE:CD1	2.51	0.41
2:B:250:LEU:HD23	2:B:250:LEU:HA	1.84	0.41
1:C:47:ILE:C	1:C:47:ILE:HD13	2.40	0.41
1:C:340:ASN:HA	1:C:343:ILE:HG13	2.03	0.41
2:D:142:TYR:OH	2:D:245:LEU:HD12	2.20	0.41
1:G:232:VAL:O	1:G:233:LEU:HD23	2.21	0.41
2:H:189:LYS:C	2:H:191:THR:H	2.22	0.41
2:H:336:ASP:O	2:H:337:LEU:HD23	2.21	0.41
2:D:209:LYS:HB3	2:D:209:LYS:HE3	1.36	0.41
2:D:318:ILE:HG22	2:D:323:LEU:HD21	2.03	0.41
2:F:24:VAL:CG1	2:F:53:TRP:HZ3	2.33	0.41
1:G:43:GLU:OE1	1:G:310:ARG:NH1	2.52	0.41
1:G:283:GLN:CB	1:G:285:VAL:HG13	2.49	0.41
2:H:183:ARG:O	2:H:238:ALA:O	2.39	0.41
2:B:306:LEU:CB	2:B:315:ALA:HB2	2.50	0.41
2:D:44:PHE:O	2:D:49:VAL:HG22	2.20	0.41
1:E:146:GLY:O	2:F:161:THR:HA	2.20	0.41
1:E:201:ILE:O	1:E:201:ILE:HG13	2.20	0.41
2:F:205:LYS:O	2:F:208:SER:HB3	2.21	0.41
2:F:253:LEU:C	2:F:253:LEU:CD2	2.89	0.41
1:G:22:LEU:HD11	1:G:33:THR:CG2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:296:THR:HA	1:G:299:LEU:HD12	2.02	0.41
2:H:326:ILE:HD12	2:H:332:ASN:HB3	2.02	0.41
1:A:47:ILE:HD13	1:A:47:ILE:C	2.41	0.41
3:A:1001:FLC:OG1	3:A:1001:FLC:OHB	2.32	0.41
1:C:32:ILE:HG13	1:C:288:PRO:HA	2.02	0.41
1:C:43:GLU:OE1	1:C:310:ARG:NH1	2.54	0.41
2:D:114:ARG:HA	2:D:115:PRO:HD3	1.85	0.41
2:D:326:ILE:HG21	2:D:350:VAL:HG22	2.01	0.41
1:E:78:LYS:C	1:E:291:MSE:HE1	2.41	0.41
2:F:176:ALA:HA	2:F:239:VAL:HG21	2.01	0.41
2:F:183:ARG:NH1	2:F:237:ASP:OD2	2.51	0.41
1:G:104:TYR:CZ	1:G:161:ARG:HG2	2.56	0.41
2:H:253:LEU:C	2:H:253:LEU:CD2	2.88	0.41
1:A:120:ILE:HD13	1:A:250:LEU:HD22	2.02	0.41
1:A:340:ASN:HA	1:A:343:ILE:HG13	2.02	0.41
2:B:46:ALA:CB	2:B:351:ILE:HD13	2.51	0.41
2:B:253:LEU:C	2:B:253:LEU:CD2	2.90	0.41
1:C:23:ILE:HB	1:C:78:LYS:HB2	2.03	0.41
1:C:44:ASN:HD21	1:G:303:GLY:HA3	1.86	0.41
2:D:43:ILE:CD1	2:D:299:LEU:HD21	2.51	0.41
2:D:350:VAL:HG12	2:D:351:ILE:N	2.36	0.41
1:E:202:GLY:HA3	1:E:211:VAL:HG21	2.03	0.41
2:F:70:PRO:O	2:F:74:VAL:HG23	2.21	0.41
1:G:27:GLY:HA3	1:G:276:VAL:O	2.21	0.41
2:H:103:LEU:HD12	2:H:103:LEU:HA	1.69	0.41
2:H:189:LYS:HE2	2:H:192:ILE:CD1	2.51	0.41
2:B:25:SER:HB3	2:B:56:CYS:SG	2.61	0.41
2:B:318:ILE:HG22	2:B:323:LEU:HD21	2.03	0.41
1:C:91:GLY:O	1:C:92:SER:C	2.59	0.41
1:C:187:MSE:CE	2:D:156:SER:HB3	2.33	0.41
2:D:322:VAL:C	2:D:326:ILE:HG23	2.41	0.41
1:E:101:LEU:HB2	1:E:103:ILE:CG1	2.51	0.41
1:A:47:ILE:HD11	1:A:49:TRP:CD2	2.56	0.40
1:A:95:VAL:CG2	1:A:96:ALA:N	2.85	0.40
2:B:8:ILE:HG21	2:B:171:TYR:HB2	2.01	0.40
2:B:26:PHE:O	2:B:27:ILE:HB	2.21	0.40
2:B:221:ILE:O	2:B:222:ASP:C	2.58	0.40
2:B:306:LEU:HD23	2:B:315:ALA:HA	2.02	0.40
1:C:195:ARG:CG	1:C:195:ARG:NH1	2.64	0.40
2:D:49:VAL:HA	2:D:50:PRO:HD3	1.88	0.40
2:D:71:ASP:N	2:D:72:PRO:HD2	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:110:PHE:CE1	2:D:167:ARG:HG3	2.57	0.40
1:E:92:SER:C	1:E:94:ASN:H	2.25	0.40
1:E:232:VAL:C	1:E:233:LEU:HD23	2.41	0.40
1:E:288:PRO:O	1:E:292:ILE:HG13	2.20	0.40
2:F:63:VAL:HG12	2:F:64:ASN:ND2	2.36	0.40
2:F:169:ILE:HG21	2:F:204:ALA:HA	2.02	0.40
1:G:27:GLY:C	1:G:29:GLY:N	2.74	0.40
1:G:83:THR:HA	1:G:84:PRO:HD3	1.82	0.40
1:G:193:LEU:O	1:G:197:ILE:HG13	2.21	0.40
2:H:306:LEU:CB	2:H:315:ALA:HB2	2.51	0.40
2:H:348:GLU:H	2:H:348:GLU:HG2	1.61	0.40
1:A:23:ILE:HB	1:A:78:LYS:HB2	2.03	0.40
1:A:179:THR:HB	1:A:233:LEU:HD22	2.03	0.40
2:B:186:VAL:CG2	2:B:216:LEU:HD11	2.51	0.40
2:B:299:LEU:HD12	2:B:299:LEU:HA	1.86	0.40
1:C:299:LEU:HA	1:C:302:LEU:HD11	2.04	0.40
1:C:342:ILE:HG12	1:C:342:ILE:H	1.64	0.40
2:D:46:ALA:CB	2:D:351:ILE:HD13	2.51	0.40
1:E:2:THR:O	1:E:3:ALA:HB2	2.21	0.40
1:E:156:ARG:N	1:E:157:PRO:CD	2.84	0.40
2:H:189:LYS:HG2	2:H:192:ILE:CD1	2.51	0.40
2:H:347:THR:O	2:H:351:ILE:HG13	2.20	0.40
1:C:181:VAL:HG21	1:C:243:LEU:CD1	2.51	0.40
1:C:186:ILE:HD13	2:D:142:TYR:CD2	2.56	0.40
2:D:19:THR:C	2:D:21:LYS:H	2.24	0.40
2:D:39:SER:OG	2:D:347:THR:HG23	2.21	0.40
1:G:95:VAL:HG23	1:G:96:ALA:N	2.35	0.40
1:A:31:GLU:OE1	1:A:282:GLY:N	2.49	0.40
2:B:39:SER:OG	2:B:347:THR:CG2	2.69	0.40
2:B:119:ILE:HD13	2:B:119:ILE:HA	1.88	0.40
2:D:149:VAL:O	2:D:150:CYS:HB3	2.21	0.40
1:E:323:LYS:O	1:E:324:HIS:CB	2.67	0.40
2:F:150:CYS:CB	2:F:151:PRO:CD	2.97	0.40
2:F:242:CYS:HA	2:F:243:PRO:HD3	1.93	0.40
2:F:270:ILE:HA	2:F:275:SER:OG	2.22	0.40
2:F:343:THR:O	2:F:347:THR:OG1	2.38	0.40
1:G:23:ILE:HB	1:G:78:LYS:HB2	2.03	0.40
1:G:146:GLY:O	2:H:161:THR:HA	2.22	0.40
1:G:342:ILE:HG12	1:G:342:ILE:H	1.66	0.40
2:H:44:PHE:CZ	2:H:306:LEU:HD11	2.57	0.40
2:H:69:ILE:HA	2:H:70:PRO:HD3	1.95	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:VAL:O	2:B:150:CYS:HB3	2.21	0.40
2:D:12:THR:O	2:D:13:GLY:O	2.39	0.40
1:E:223:ALA:O	1:E:227:PRO:HG3	2.21	0.40
2:F:26:PHE:CE1	2:F:84:LEU:HD23	2.56	0.40
2:F:103:LEU:HD12	2:F:103:LEU:HA	1.69	0.40
2:H:64:ASN:O	2:H:66:LEU:N	2.51	0.40
2:H:110:PHE:CE1	2:H:167:ARG:HG3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	327/354 (92%)	296 (90%)	26 (8%)	5 (2%)	10	44
1	C	340/354 (96%)	307 (90%)	28 (8%)	5 (2%)	10	44
1	E	340/354 (96%)	304 (89%)	31 (9%)	5 (2%)	10	44
1	G	327/354 (92%)	296 (90%)	27 (8%)	4 (1%)	13	49
2	B	341/354 (96%)	288 (84%)	40 (12%)	13 (4%)	3	22
2	D	343/354 (97%)	291 (85%)	43 (12%)	9 (3%)	5	31
2	F	343/354 (97%)	289 (84%)	41 (12%)	13 (4%)	3	22
2	H	344/354 (97%)	290 (84%)	40 (12%)	14 (4%)	3	21
All	All	2705/2832 (96%)	2361 (87%)	276 (10%)	68 (2%)	5	32

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	LEU
2	B	13	GLY
2	B	98	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	151	PRO
2	B	322	VAL
2	B	323	LEU
1	C	8	ARG
1	C	304	LEU
2	D	13	GLY
2	D	151	PRO
2	D	322	VAL
2	D	323	LEU
1	E	3	ALA
1	E	6	ALA
1	E	304	LEU
2	F	97	ARG
2	F	151	PRO
2	F	322	VAL
2	F	323	LEU
1	G	304	LEU
2	H	13	GLY
2	H	91	PRO
2	H	98	SER
2	H	151	PRO
2	H	322	VAL
2	H	323	LEU
1	A	322	GLY
1	C	7	GLU
1	C	322	GLY
1	E	322	GLY
2	F	13	GLY
2	F	98	SER
1	G	322	GLY
2	H	92	ILE
2	B	79	LYS
1	A	310	ARG
1	C	310	ARG
2	D	79	LYS
1	E	310	ARG
2	F	79	LYS
2	F	332	ASN
2	H	79	LYS
2	H	190	SER
2	H	332	ASN
1	A	324	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	89	ALA
2	B	239	VAL
2	B	332	ASN
2	D	239	VAL
2	D	332	ASN
2	F	239	VAL
1	G	310	ARG
1	G	324	HIS
2	H	239	VAL
2	H	50	PRO
2	F	65	GLY
2	H	65	GLY
1	A	15	GLY
2	B	27	ILE
2	B	50	PRO
2	B	65	GLY
2	D	27	ILE
2	F	27	ILE
2	F	50	PRO
2	H	27	ILE
2	D	14	LYS
2	B	14	LYS
2	F	14	LYS

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	275/287 (96%)	246 (90%)	29 (10%)	7 28
1	C	284/287 (99%)	254 (89%)	30 (11%)	6 27
1	E	284/287 (99%)	254 (89%)	30 (11%)	6 27
1	G	275/287 (96%)	248 (90%)	27 (10%)	8 31
2	B	291/294 (99%)	245 (84%)	46 (16%)	2 12
2	D	293/294 (100%)	246 (84%)	47 (16%)	2 11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	293/294 (100%)	244 (83%)	49 (17%)	2	10
2	H	293/294 (100%)	245 (84%)	48 (16%)	2	11
All	All	2288/2324 (98%)	1982 (87%)	306 (13%)	4	18

All (306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	33	THR
1	A	47	ILE
1	A	51	THR
1	A	52	ILE
1	A	77	LEU
1	A	78	LYS
1	A	88	THR
1	A	93	LEU
1	A	103	ILE
1	A	117	LYS
1	A	120	ILE
1	A	123	ILE
1	A	135	GLU
1	A	195	ARG
1	A	201	ILE
1	A	215	ILE
1	A	274	ARG
1	A	291	MSE
1	A	295	SER
1	A	302	LEU
1	A	311	ILE
1	A	315	VAL
1	A	319	ILE
1	A	323	LYS
1	A	324	HIS
1	A	326	THR
1	A	336	THR
1	A	342	ILE
2	B	4	LYS
2	B	8	ILE
2	B	18	SER
2	B	19	THR
2	B	23	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	30	ASP
2	B	35	GLU
2	B	38	LYS
2	B	45	SER
2	B	58	VAL
2	B	66	LEU
2	B	67	THR
2	B	69	ILE
2	B	71	ASP
2	B	78	THR
2	B	80	ASN
2	B	88	LEU
2	B	102	THR
2	B	114	ARG
2	B	129	VAL
2	B	149	VAL
2	B	162	ARG
2	B	185	ILE
2	B	192	ILE
2	B	193	GLN
2	B	209	LYS
2	B	221	ILE
2	B	222	ASP
2	B	225	VAL
2	B	226	LEU
2	B	241	VAL
2	B	252	ASP
2	B	262	LEU
2	B	275	SER
2	B	283	SER
2	B	299	LEU
2	B	306	LEU
2	B	322	VAL
2	B	323	LEU
2	B	324	SER
2	B	326	ILE
2	B	333	ARG
2	B	342	THR
2	B	347	THR
2	B	348	GLU
2	B	353	ARG
1	C	7	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	8	ARG
1	C	33	THR
1	C	47	ILE
1	C	51	THR
1	C	52	ILE
1	C	77	LEU
1	C	78	LYS
1	C	88	THR
1	C	93	LEU
1	C	103	ILE
1	C	117	LYS
1	C	120	ILE
1	C	123	ILE
1	C	135	GLU
1	C	195	ARG
1	C	201	ILE
1	C	215	ILE
1	C	274	ARG
1	C	291	MSE
1	C	295	SER
1	C	302	LEU
1	C	311	ILE
1	C	315	VAL
1	C	319	ILE
1	C	323	LYS
1	C	324	HIS
1	C	326	THR
1	C	336	THR
1	C	342	ILE
2	D	4	LYS
2	D	8	ILE
2	D	18	SER
2	D	19	THR
2	D	23	THR
2	D	30	ASP
2	D	35	GLU
2	D	38	LYS
2	D	45	SER
2	D	58	VAL
2	D	66	LEU
2	D	67	THR
2	D	69	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	71	ASP
2	D	78	THR
2	D	80	ASN
2	D	88	LEU
2	D	102	THR
2	D	114	ARG
2	D	129	VAL
2	D	149	VAL
2	D	162	ARG
2	D	184	VAL
2	D	185	ILE
2	D	192	ILE
2	D	193	GLN
2	D	209	LYS
2	D	221	ILE
2	D	222	ASP
2	D	225	VAL
2	D	226	LEU
2	D	241	VAL
2	D	252	ASP
2	D	262	LEU
2	D	275	SER
2	D	283	SER
2	D	299	LEU
2	D	306	LEU
2	D	322	VAL
2	D	323	LEU
2	D	324	SER
2	D	326	ILE
2	D	342	THR
2	D	347	THR
2	D	348	GLU
2	D	353	ARG
2	D	354	LEU
1	E	5	GLN
1	E	8	ARG
1	E	33	THR
1	E	47	ILE
1	E	51	THR
1	E	52	ILE
1	E	77	LEU
1	E	78	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	88	THR
1	E	93	LEU
1	E	103	ILE
1	E	119	ARG
1	E	120	ILE
1	E	135	GLU
1	E	195	ARG
1	E	201	ILE
1	E	215	ILE
1	E	274	ARG
1	E	285	VAL
1	E	291	MSE
1	E	295	SER
1	E	302	LEU
1	E	311	ILE
1	E	315	VAL
1	E	319	ILE
1	E	323	LYS
1	E	324	HIS
1	E	326	THR
1	E	336	THR
1	E	342	ILE
2	F	4	LYS
2	F	5	GLN
2	F	8	ILE
2	F	19	THR
2	F	23	THR
2	F	30	ASP
2	F	35	GLU
2	F	36	ILE
2	F	38	LYS
2	F	44	PHE
2	F	45	SER
2	F	58	VAL
2	F	66	LEU
2	F	67	THR
2	F	69	ILE
2	F	71	ASP
2	F	78	THR
2	F	80	ASN
2	F	88	LEU
2	F	97	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	102	THR
2	F	114	ARG
2	F	129	VAL
2	F	149	VAL
2	F	162	ARG
2	F	184	VAL
2	F	185	ILE
2	F	192	ILE
2	F	193	GLN
2	F	209	LYS
2	F	221	ILE
2	F	222	ASP
2	F	225	VAL
2	F	226	LEU
2	F	241	VAL
2	F	252	ASP
2	F	262	LEU
2	F	283	SER
2	F	299	LEU
2	F	306	LEU
2	F	322	VAL
2	F	323	LEU
2	F	324	SER
2	F	326	ILE
2	F	333	ARG
2	F	342	THR
2	F	347	THR
2	F	348	GLU
2	F	353	ARG
1	G	17	ARG
1	G	33	THR
1	G	47	ILE
1	G	51	THR
1	G	52	ILE
1	G	77	LEU
1	G	78	LYS
1	G	88	THR
1	G	93	LEU
1	G	103	ILE
1	G	119	ARG
1	G	120	ILE
1	G	135	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	195	ARG
1	G	201	ILE
1	G	274	ARG
1	G	291	MSE
1	G	295	SER
1	G	302	LEU
1	G	311	ILE
1	G	315	VAL
1	G	319	ILE
1	G	323	LYS
1	G	324	HIS
1	G	326	THR
1	G	336	THR
1	G	342	ILE
2	H	4	LYS
2	H	5	GLN
2	H	8	ILE
2	H	18	SER
2	H	19	THR
2	H	23	THR
2	H	30	ASP
2	H	35	GLU
2	H	38	LYS
2	H	45	SER
2	H	58	VAL
2	H	66	LEU
2	H	67	THR
2	H	69	ILE
2	H	71	ASP
2	H	78	THR
2	H	80	ASN
2	H	88	LEU
2	H	91	PRO
2	H	92	ILE
2	H	102	THR
2	H	114	ARG
2	H	129	VAL
2	H	149	VAL
2	H	162	ARG
2	H	185	ILE
2	H	192	ILE
2	H	193	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	209	LYS
2	H	221	ILE
2	H	222	ASP
2	H	225	VAL
2	H	226	LEU
2	H	241	VAL
2	H	252	ASP
2	H	262	LEU
2	H	275	SER
2	H	283	SER
2	H	299	LEU
2	H	306	LEU
2	H	322	VAL
2	H	323	LEU
2	H	324	SER
2	H	326	ILE
2	H	342	THR
2	H	347	THR
2	H	348	GLU
2	H	353	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
2	B	5	GLN
2	B	147	HIS
2	B	193	GLN
2	B	231	ASN
1	C	44	ASN
1	C	106	ASN
1	C	245	ASN
1	C	301	HIS
1	E	5	GLN
1	E	106	ASN
1	E	301	HIS
2	F	64	ASN
2	F	193	GLN
1	G	106	ASN
2	H	147	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	FLC	E	1003	-	12,12,12	3.51	8 (66%)	17,17,17	1.54	1 (5%)
3	FLC	A	1001	-	12,12,12	3.52	7 (58%)	17,17,17	1.92	2 (11%)
3	FLC	G	1004	-	12,12,12	3.51	8 (66%)	17,17,17	1.54	1 (5%)
3	FLC	C	1002	-	12,12,12	3.52	8 (66%)	17,17,17	1.54	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FLC	E	1003	-	-	8/16/16/16	-
3	FLC	A	1001	-	-	3/16/16/16	-
3	FLC	G	1004	-	-	3/16/16/16	-
3	FLC	C	1002	-	-	6/16/16/16	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	FLC	OB1-CBC	5.92	1.41	1.22
3	A	1001	FLC	OB1-CBC	5.91	1.41	1.22
3	G	1004	FLC	OB1-CBC	5.90	1.41	1.22
3	E	1003	FLC	OB1-CBC	5.89	1.41	1.22
3	C	1002	FLC	OA1-CAC	5.86	1.41	1.22
3	G	1004	FLC	OA1-CAC	5.85	1.41	1.22
3	E	1003	FLC	OG1-CGC	5.84	1.41	1.22
3	E	1003	FLC	OA1-CAC	5.84	1.41	1.22
3	G	1004	FLC	OG1-CGC	5.82	1.41	1.22
3	C	1002	FLC	OG1-CGC	5.82	1.41	1.22
3	A	1001	FLC	OG1-CGC	5.79	1.41	1.22
3	A	1001	FLC	OA1-CAC	5.78	1.41	1.22
3	A	1001	FLC	OA2-CAC	-3.51	1.18	1.30
3	A	1001	FLC	OG2-CGC	-3.39	1.19	1.30
3	G	1004	FLC	OG2-CGC	-3.36	1.19	1.30
3	C	1002	FLC	OG2-CGC	-3.36	1.19	1.30
3	E	1003	FLC	OG2-CGC	-3.35	1.19	1.30
3	C	1002	FLC	OA2-CAC	-3.31	1.19	1.30
3	E	1003	FLC	OA2-CAC	-3.31	1.19	1.30
3	G	1004	FLC	OA2-CAC	-3.29	1.19	1.30
3	A	1001	FLC	OB2-CBC	-3.07	1.18	1.30
3	G	1004	FLC	OB2-CBC	-2.90	1.19	1.30
3	C	1002	FLC	OB2-CBC	-2.90	1.19	1.30
3	E	1003	FLC	OB2-CBC	-2.89	1.19	1.30
3	C	1002	FLC	CA-CB	2.09	1.56	1.53
3	G	1004	FLC	CA-CB	2.09	1.56	1.53
3	E	1003	FLC	CG-CB	2.09	1.56	1.53
3	C	1002	FLC	CG-CB	2.08	1.56	1.53
3	E	1003	FLC	CA-CB	2.04	1.56	1.53
3	G	1004	FLC	CG-CB	2.01	1.56	1.53
3	A	1001	FLC	CA-CB	2.00	1.56	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FLC	OB2-CBC-CB	4.49	120.85	113.05
3	G	1004	FLC	OB2-CBC-CB	4.09	120.14	113.05
3	E	1003	FLC	OB2-CBC-CB	4.08	120.14	113.05
3	C	1002	FLC	OB2-CBC-CB	4.08	120.13	113.05
3	A	1001	FLC	OHB-CB-CBC	-3.88	103.41	108.86

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	FLC	OHB-CB-CG-CGC
3	C	1002	FLC	CA-CB-CG-CGC
3	C	1002	FLC	CBC-CB-CG-CGC
3	E	1003	FLC	CA-CB-CG-CGC
3	E	1003	FLC	CBC-CB-CG-CGC
3	E	1003	FLC	OHB-CB-CG-CGC
3	G	1004	FLC	CA-CB-CG-CGC
3	G	1004	FLC	CBC-CB-CG-CGC
3	G	1004	FLC	OHB-CB-CG-CGC
3	A	1001	FLC	CA-CB-CG-CGC
3	C	1002	FLC	CAC-CA-CB-CBC
3	C	1002	FLC	CAC-CA-CB-OHB
3	A	1001	FLC	CBC-CB-CG-CGC
3	C	1002	FLC	OHB-CB-CG-CGC
3	E	1003	FLC	CAC-CA-CB-CBC
3	C	1002	FLC	CAC-CA-CB-CG
3	E	1003	FLC	CAC-CA-CB-OHB
3	E	1003	FLC	CA-CB-CBC-OB2
3	E	1003	FLC	CG-CB-CBC-OB2
3	E	1003	FLC	CAC-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1003	FLC	3	0
3	A	1001	FLC	3	0
3	G	1004	FLC	4	0
3	C	1002	FLC	3	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, 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	324/354 (91%)	-0.15	3 (0%) 84 75	48, 66, 95, 124	0
1	C	337/354 (95%)	-0.24	1 (0%) 94 92	48, 64, 93, 125	0
1	E	337/354 (95%)	-0.20	3 (0%) 84 75	47, 66, 95, 138	0
1	G	324/354 (91%)	-0.20	1 (0%) 94 92	47, 64, 91, 123	0
2	B	342/354 (96%)	-0.04	9 (2%) 56 40	43, 76, 108, 123	0
2	D	344/354 (97%)	-0.04	4 (1%) 79 67	43, 74, 103, 128	0
2	F	344/354 (97%)	0.16	10 (2%) 51 36	44, 76, 107, 122	0
2	H	345/354 (97%)	0.29	31 (8%) 9 5	43, 77, 109, 124	0
All	All	2697/2832 (95%)	-0.05	62 (2%) 60 47	43, 70, 103, 138	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	63	VAL	4.4
2	H	346	PHE	3.9
2	H	324	SER	3.9
2	H	348	GLU	3.7
2	H	64	ASN	3.7
1	E	347	SER	3.6
2	F	18	SER	3.6
2	H	42	LYS	3.5
2	B	18	SER	3.4
2	H	50	PRO	3.4
2	H	44	PHE	3.4
1	E	204	LYS	3.2
2	H	63	VAL	3.1
2	B	17	PRO	3.0
2	D	64	ASN	2.9
2	F	317	GLN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	91	PRO	2.9
2	B	64	ASN	2.9
2	H	53	TRP	2.8
1	A	60	LYS	2.8
2	H	16	ASN	2.8
2	H	40	VAL	2.8
2	H	323	LEU	2.8
2	H	354	LEU	2.8
2	B	320	ASN	2.8
2	F	320	ASN	2.8
2	D	61	ILE	2.7
2	H	352	LYS	2.7
2	D	63	VAL	2.7
2	H	350	VAL	2.7
1	E	87	GLN	2.6
2	H	332	ASN	2.6
2	H	320	ASN	2.6
2	H	43	ILE	2.6
2	B	354	LEU	2.6
2	F	331	GLU	2.5
2	F	14	LYS	2.5
2	H	347	THR	2.5
1	G	324	HIS	2.4
2	H	293	ALA	2.4
1	A	15	GLY	2.4
2	H	338	ALA	2.4
2	B	66	LEU	2.4
2	H	322	VAL	2.4
2	F	337	LEU	2.4
2	H	292	LYS	2.4
2	F	338	ALA	2.3
2	B	323	LEU	2.3
2	H	28	GLU	2.3
2	F	354	LEU	2.2
2	H	121	GLY	2.2
2	H	65	GLY	2.2
2	H	289	GLY	2.2
2	H	54	GLU	2.2
2	H	337	LEU	2.2
2	H	339	GLY	2.2
2	F	16	ASN	2.1
2	H	325	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	58	VAL	2.1
1	A	90	HIS	2.1
2	B	20	GLY	2.0
1	C	60	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
3	FLC	E	1003	13/13	0.91	0.23	62,86,94,96	0
3	FLC	A	1001	13/13	0.92	0.25	76,83,99,99	0
3	FLC	C	1002	13/13	0.94	0.21	71,82,94,94	0
3	FLC	G	1004	13/13	0.95	0.20	53,77,84,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.