



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:25 AM UTC

PDB ID : 8POO / pdb_00008poo
Title : Low resolution structure of inactive conformation of the Ktr cation channel in presence of ATP and c-di-AMP
Authors : Cereija, T.B.; Teixeira-Duarte, C.M.; Morais-Cabral, J.H.
Deposited on : 2023-07-05
Resolution : 5.77 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

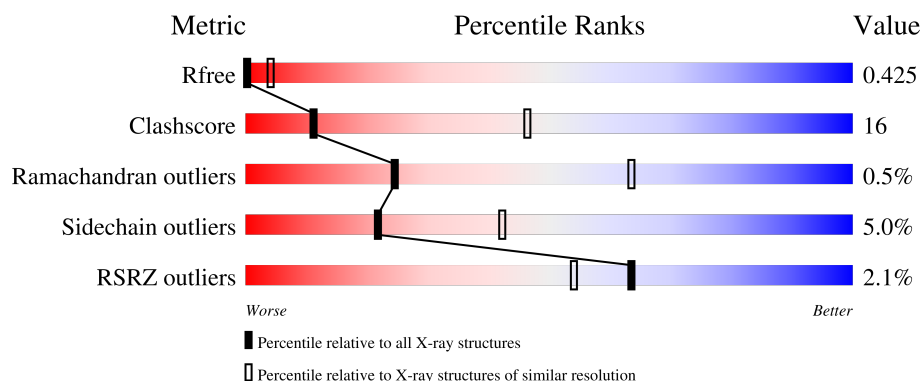
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.77 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1122 (7.56-4.00)
Clashscore	190562	1187 (7.56-4.00)
Ramachandran outliers	187476	1016 (7.54-4.00)
Sidechain outliers	187428	1007 (7.58-3.98)
RSRZ outliers	180081	1115 (7.56-4.00)

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 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	445	
1	B	445	
1	I	445	
1	J	445	
2	C	288	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	288	% 63% 30% 7%
2	E	288	3% 67% 26% 7%
2	G	288	% 69% 23% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20736 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 Ktr system potassium uptake protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	406	Total	C	N	O	S	0	0	0
			3088	2064	474	536	14			
1	J	406	Total	C	N	O	S	0	0	0
			3088	2064	474	536	14			
1	A	406	Total	C	N	O	S	0	0	0
			3088	2064	474	536	14			
1	B	406	Total	C	N	O	S	0	0	0
			3088	2064	474	536	14			

- Molecule 2 is a protein called Ktr system potassium uptake protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	268	Total	C	N	O	S	0	0	0
			2096	1336	362	394	4			
2	D	268	Total	C	N	O	S	0	0	0
			2096	1336	362	394	4			
2	E	268	Total	C	N	O	S	0	0	0
			2096	1336	362	394	4			
2	G	268	Total	C	N	O	S	0	0	0
			2096	1336	362	394	4			

There are 48 discrepancies between the modelled and reference sequences:

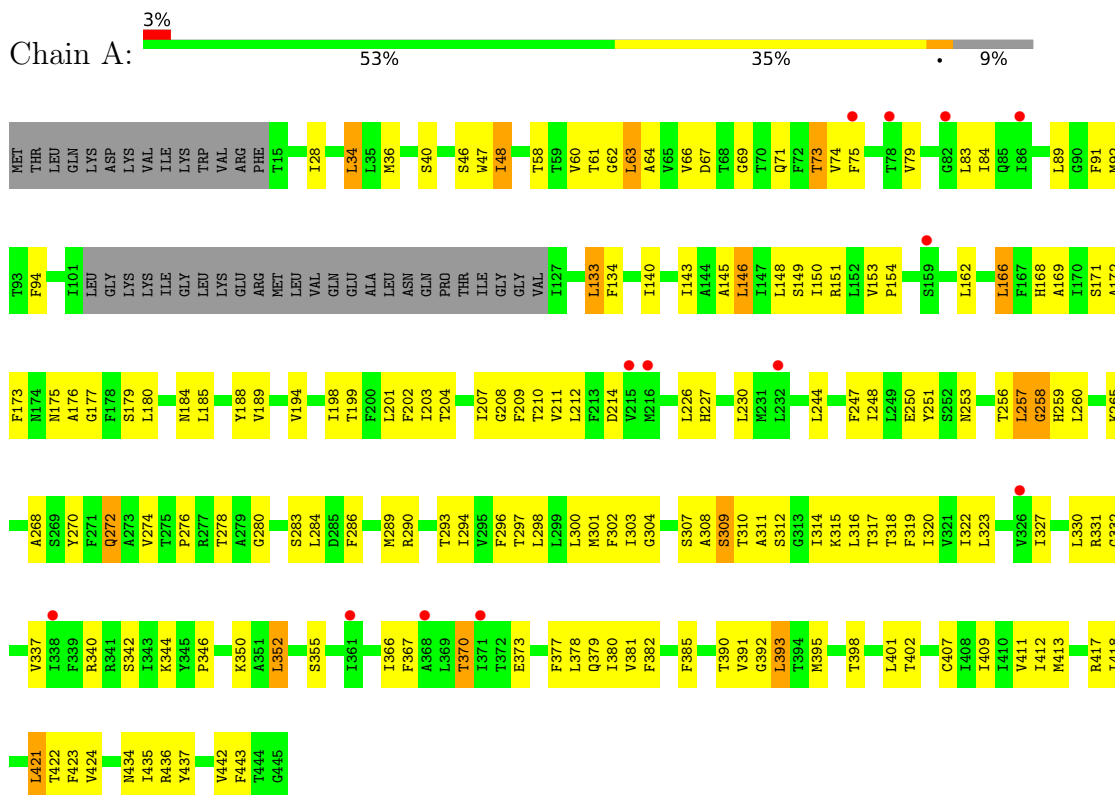
Chain	Residue	Modelled	Actual	Comment	Reference
C	22	VAL	CYS	engineered mutation	UNP O32080
C	145	LEU	-	linker	UNP O32080
C	146	GLU	-	linker	UNP O32080
C	147	GLY	-	linker	UNP O32080
C	148	SER	-	linker	UNP O32080
C	164	VAL	CYS	engineered mutation	UNP O32080
C	283	LEU	-	expression tag	UNP O32080
C	284	GLU	-	expression tag	UNP O32080

Continued on next page...

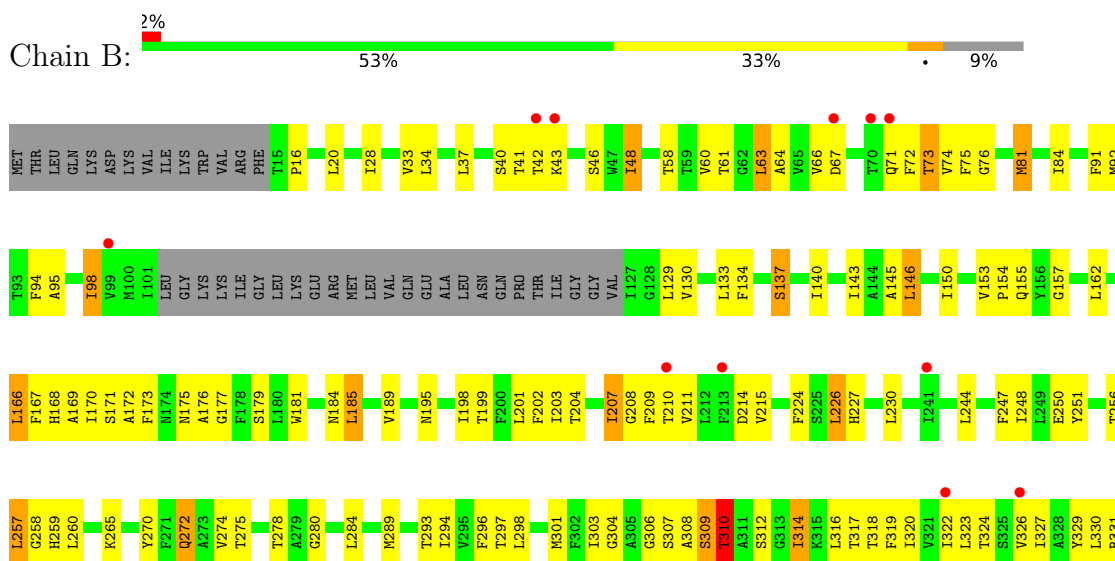
Continued from previous page...

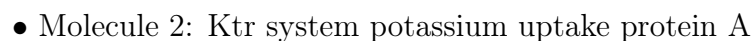
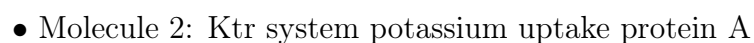
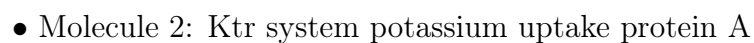
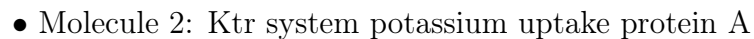
Chain	Residue	Modelled	Actual	Comment	Reference
C	285	LEU	-	expression tag	UNP O32080
C	286	VAL	-	expression tag	UNP O32080
C	287	PRO	-	expression tag	UNP O32080
C	288	ARG	-	expression tag	UNP O32080
D	22	VAL	CYS	engineered mutation	UNP O32080
D	145	LEU	-	linker	UNP O32080
D	146	GLU	-	linker	UNP O32080
D	147	GLY	-	linker	UNP O32080
D	148	SER	-	linker	UNP O32080
D	164	VAL	CYS	engineered mutation	UNP O32080
D	283	LEU	-	expression tag	UNP O32080
D	284	GLU	-	expression tag	UNP O32080
D	285	LEU	-	expression tag	UNP O32080
D	286	VAL	-	expression tag	UNP O32080
D	287	PRO	-	expression tag	UNP O32080
D	288	ARG	-	expression tag	UNP O32080
E	22	VAL	CYS	engineered mutation	UNP O32080
E	145	LEU	-	linker	UNP O32080
E	146	GLU	-	linker	UNP O32080
E	147	GLY	-	linker	UNP O32080
E	148	SER	-	linker	UNP O32080
E	164	VAL	CYS	engineered mutation	UNP O32080
E	283	LEU	-	expression tag	UNP O32080
E	284	GLU	-	expression tag	UNP O32080
E	285	LEU	-	expression tag	UNP O32080
E	286	VAL	-	expression tag	UNP O32080
E	287	PRO	-	expression tag	UNP O32080
E	288	ARG	-	expression tag	UNP O32080
G	22	VAL	CYS	engineered mutation	UNP O32080
G	145	LEU	-	linker	UNP O32080
G	146	GLU	-	linker	UNP O32080
G	147	GLY	-	linker	UNP O32080
G	148	SER	-	linker	UNP O32080
G	164	VAL	CYS	engineered mutation	UNP O32080
G	283	LEU	-	expression tag	UNP O32080
G	284	GLU	-	expression tag	UNP O32080
G	285	LEU	-	expression tag	UNP O32080
G	286	VAL	-	expression tag	UNP O32080
G	287	PRO	-	expression tag	UNP O32080
G	288	ARG	-	expression tag	UNP O32080

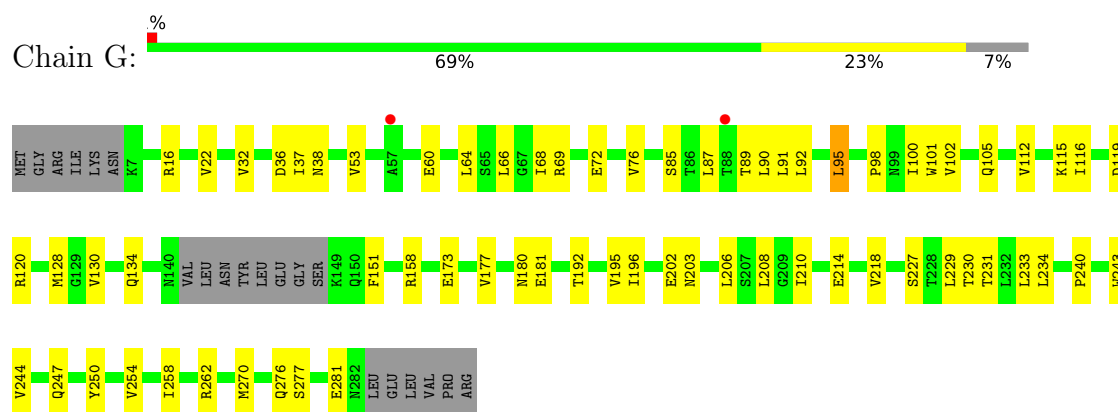
- Molecule 1: Ktr system potassium uptake protein B



- Molecule 1: Ktr system potassium uptake protein B







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	127.80Å 143.69Å 160.67Å 90.00° 112.37° 90.00°	Depositor
Resolution (Å)	48.00 – 5.77 48.00 – 5.77	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.00-5.77) 98.8 (48.00-5.77)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 5.73Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.405 , 0.426 0.411 , 0.425	Depositor DCC
R_{free} test set	1649 reflections (10.73%)	wwPDB-VP
Wilson B-factor (Å ²)	354.8	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 282.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	20736	wwPDB-VP
Average B, all atoms (Å ²)	362.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.19	0/3157	0.40	0/4297
1	B	0.20	0/3157	0.41	0/4297
1	I	0.20	0/3157	0.39	1/4297 (0.0%)
1	J	0.21	0/3157	0.43	1/4297 (0.0%)
2	C	0.17	0/2130	0.31	0/2882
2	D	0.16	0/2130	0.30	0/2882
2	E	0.17	0/2130	0.31	0/2882
2	G	0.15	0/2130	0.30	0/2882
All	All	0.18	0/21148	0.37	2/28716 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	274	VAL	N-CA-C	-7.11	106.95	113.71
1	I	309	SER	CB-CA-C	-5.54	109.20	115.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3088	0	3227	133	0
1	B	3088	0	3227	133	0
1	I	3088	0	3227	112	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	3088	0	3227	126	0
2	C	2096	0	2120	71	0
2	D	2096	0	2120	61	0
2	E	2096	0	2120	49	0
2	G	2096	0	2120	44	0
All	All	20736	0	21388	688	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 16.

All (688) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:278:THR:HA	1:I:391:VAL:HA	1.46	0.95
1:A:278:THR:HA	1:A:391:VAL:HA	1.51	0.93
1:J:278:THR:HA	1:J:391:VAL:HA	1.51	0.92
1:B:278:THR:HA	1:B:391:VAL:HA	1.60	0.83
1:J:61:THR:HG23	1:J:390:THR:HA	1.60	0.82
1:I:208:GLY:HA2	1:I:309:SER:H	1.46	0.80
1:I:309:SER:OG	1:I:310:THR:N	2.09	0.80
1:I:61:THR:HG23	1:I:390:THR:HA	1.63	0.78
1:A:208:GLY:HA2	1:A:309:SER:H	1.49	0.77
1:A:61:THR:HG23	1:A:390:THR:HA	1.67	0.76
1:B:61:THR:HG23	1:B:390:THR:HA	1.65	0.76
1:A:28:ILE:HG12	1:A:58:THR:HG21	1.67	0.75
1:I:28:ILE:HG12	1:I:58:THR:HG21	1.67	0.75
1:B:378:LEU:HG	1:B:395:MET:HE1	1.70	0.74
1:B:324:THR:HG21	1:B:338:ILE:HD11	1.68	0.74
2:D:134:GLN:NE2	2:D:170:MET:SD	2.60	0.73
1:I:304:GLY:HA3	1:I:312:SER:HB3	1.69	0.73
1:I:378:LEU:HG	1:I:395:MET:HE1	1.72	0.71
2:D:258:ILE:HD11	2:G:254:VAL:HG23	1.72	0.71
2:C:195:VAL:HG21	2:C:208:LEU:HD11	1.74	0.70
1:J:202:PHE:HE1	1:J:274:VAL:HG12	1.56	0.69
1:A:92:MET:HG2	1:A:133:LEU:HB2	1.74	0.69
2:C:90:LEU:HD21	2:D:115:LYS:HB2	1.73	0.69
1:J:43:LYS:HD3	1:B:42:THR:HG22	1.73	0.69
1:J:304:GLY:HA3	1:J:312:SER:HB3	1.74	0.69
2:G:181:GLU:HB3	2:G:196:ILE:HD13	1.74	0.69
1:I:304:GLY:N	1:I:314:ILE:O	2.26	0.69
2:E:53:VAL:HG21	2:E:66:LEU:HD11	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:28:ILE:HG12	1:J:58:THR:HG21	1.75	0.68
1:J:378:LEU:HG	1:J:395:MET:HE1	1.74	0.68
1:J:92:MET:HA	1:J:209:PHE:HE2	1.59	0.68
2:D:195:VAL:HG21	2:D:208:LEU:HD11	1.75	0.68
2:E:195:VAL:HG21	2:E:208:LEU:HD11	1.75	0.68
1:B:304:GLY:HA3	1:B:312:SER:HB3	1.76	0.68
2:C:53:VAL:HG21	2:C:66:LEU:HD11	1.77	0.67
2:C:115:LYS:HB2	2:D:90:LEU:HD21	1.75	0.67
1:J:92:MET:HA	1:J:209:PHE:CE2	2.30	0.67
1:A:378:LEU:HG	1:A:395:MET:HE1	1.74	0.67
1:A:58:THR:HB	1:A:83:LEU:HG	1.76	0.67
1:A:257:LEU:O	1:A:259:HIS:N	2.27	0.67
1:B:304:GLY:N	1:B:314:ILE:O	2.25	0.66
1:B:250:GLU:OE2	1:B:293:THR:OG1	2.07	0.66
2:E:208:LEU:HB3	2:E:210:ILE:HG13	1.77	0.66
1:B:133:LEU:O	1:B:137:SER:OG	2.12	0.66
1:I:257:LEU:HD13	1:I:268:ALA:HB3	1.76	0.66
1:J:304:GLY:N	1:J:314:ILE:O	2.26	0.66
2:E:66:LEU:HB3	2:E:68:ILE:HG13	1.78	0.66
2:G:53:VAL:HG21	2:G:66:LEU:HD11	1.78	0.66
2:G:105:GLN:O	2:G:158:ARG:NH1	2.29	0.66
1:B:301:MET:HB2	1:B:391:VAL:HG11	1.76	0.65
1:J:370:THR:HA	1:J:380:ILE:HD13	1.78	0.65
1:A:301:MET:HB2	1:A:391:VAL:HG11	1.78	0.65
1:B:171:SER:HB2	1:B:176:ALA:HB3	1.78	0.65
1:B:257:LEU:O	1:B:259:HIS:N	2.30	0.65
1:A:304:GLY:N	1:A:314:ILE:O	2.29	0.65
1:B:181:TRP:HE1	1:B:185:LEU:HA	1.61	0.65
2:C:20:SER:HA	2:C:23:LYS:HE2	1.78	0.65
1:J:301:MET:HB2	1:J:391:VAL:HG11	1.78	0.65
1:B:61:THR:HA	1:B:390:THR:HB	1.78	0.64
1:J:60:VAL:HG23	1:J:84:ILE:HG23	1.79	0.64
2:C:208:LEU:HB3	2:C:210:ILE:HG13	1.79	0.64
1:A:352:LEU:HD23	1:B:352:LEU:HD23	1.79	0.64
1:A:370:THR:HG23	1:A:380:ILE:HG21	1.79	0.64
2:G:128:MET:HE2	2:G:270:MET:HE2	1.79	0.64
1:I:150:ILE:HD11	1:I:162:LEU:HD23	1.79	0.63
1:J:72:PHE:HB3	1:J:76:GLY:HA3	1.81	0.63
1:A:150:ILE:HD11	1:A:162:LEU:HD23	1.81	0.63
2:C:105:GLN:O	2:C:158:ARG:NH1	2.31	0.63
1:J:297:THR:HG22	1:J:301:MET:HE2	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:ILE:HD13	1:B:412:ILE:HD12	1.81	0.63
2:E:128:MET:HE2	2:E:270:MET:HE2	1.80	0.63
2:E:20:SER:HA	2:E:23:LYS:HE2	1.80	0.63
1:A:297:THR:HG22	1:A:301:MET:HE2	1.80	0.63
1:B:28:ILE:HG12	1:B:58:THR:HG21	1.81	0.63
1:I:34:LEU:HB3	1:I:79:VAL:HG11	1.81	0.62
1:I:61:THR:HA	1:I:390:THR:HB	1.80	0.62
1:J:150:ILE:HD11	1:J:162:LEU:HD23	1.80	0.62
1:I:352:LEU:HD23	1:J:352:LEU:HD23	1.80	0.62
1:I:202:PHE:HE1	1:I:274:VAL:HG12	1.64	0.62
2:E:90:LEU:HD21	2:G:115:LYS:HB2	1.80	0.62
1:I:370:THR:HG23	1:I:380:ILE:HG21	1.82	0.62
2:G:195:VAL:HG21	2:G:208:LEU:HD11	1.81	0.62
1:A:247:PHE:O	1:A:251:TYR:HB2	1.99	0.62
1:J:171:SER:HB2	1:J:176:ALA:HB3	1.82	0.62
2:D:53:VAL:HG21	2:D:66:LEU:HD11	1.82	0.62
1:I:92:MET:HG2	1:I:133:LEU:HB2	1.81	0.62
1:J:140:ILE:HD12	1:J:143:ILE:HD11	1.82	0.62
1:A:189:VAL:HG11	1:A:260:LEU:HD21	1.82	0.62
1:B:140:ILE:HD12	1:B:143:ILE:HD11	1.82	0.61
1:B:150:ILE:HD11	1:B:162:LEU:HD23	1.81	0.61
1:A:272:GLN:HG2	1:A:289:MET:HE1	1.83	0.61
1:A:434:ASN:HD22	2:G:203:ASN:HD22	1.47	0.61
2:C:128:MET:HE2	2:C:270:MET:HE2	1.82	0.61
1:A:304:GLY:HA3	1:A:312:SER:HB3	1.80	0.61
2:C:66:LEU:HB3	2:C:68:ILE:HG13	1.82	0.61
2:D:208:LEU:HB3	2:D:210:ILE:HG13	1.81	0.61
1:A:202:PHE:HE1	1:A:274:VAL:HG12	1.65	0.61
1:A:330:LEU:HD13	1:B:424:VAL:HG11	1.84	0.60
2:D:128:MET:HE2	2:D:270:MET:HE2	1.83	0.60
1:J:61:THR:HA	1:J:390:THR:HB	1.82	0.60
1:B:370:THR:HG23	1:B:380:ILE:HG21	1.83	0.60
1:A:307:SER:HA	1:A:315:LYS:HG3	1.83	0.60
2:G:69:ARG:HG2	2:G:95:LEU:HB3	1.84	0.60
1:B:210:THR:O	1:B:214:ASP:N	2.30	0.60
1:I:173:PHE:HB2	1:I:201:LEU:HD22	1.83	0.60
1:J:309:SER:OG	1:J:310:THR:N	2.33	0.60
1:B:60:VAL:HG23	1:B:84:ILE:HG23	1.84	0.60
1:I:60:VAL:HG23	1:I:84:ILE:HG23	1.83	0.60
1:A:140:ILE:HD12	1:A:143:ILE:HD11	1.84	0.59
1:B:297:THR:HG22	1:B:301:MET:HE2	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:THR:HA	1:A:390:THR:HB	1.85	0.59
1:I:370:THR:HA	1:I:380:ILE:HD13	1.84	0.58
1:B:272:GLN:OE1	1:B:284:LEU:N	2.37	0.58
1:J:202:PHE:CE1	1:J:274:VAL:HG12	2.37	0.58
1:I:140:ILE:HD12	1:I:143:ILE:HD11	1.85	0.58
1:I:298:LEU:HA	1:I:301:MET:HE3	1.86	0.58
1:J:247:PHE:HE1	1:J:265:LYS:HB3	1.68	0.58
1:A:409:ILE:HD13	1:A:412:ILE:HD12	1.86	0.58
1:B:272:GLN:HA	1:B:275:THR:HG22	1.85	0.58
1:J:298:LEU:HA	1:J:301:MET:HE3	1.85	0.58
1:A:168:HIS:O	1:A:172:ALA:N	2.35	0.58
1:A:256:THR:HG22	1:A:257:LEU:H	1.69	0.58
1:B:309:SER:OG	1:B:310:THR:N	2.35	0.58
2:C:76:VAL:HG21	2:C:89:THR:HG22	1.84	0.58
2:E:115:LYS:HB2	2:G:90:LEU:HD21	1.85	0.58
1:B:173:PHE:HB2	1:B:201:LEU:HD22	1.84	0.58
1:B:92:MET:HA	1:B:209:PHE:CE2	2.39	0.57
1:J:370:THR:HG23	1:J:380:ILE:HG21	1.86	0.57
1:B:227:HIS:CE1	1:B:317:THR:HG21	2.40	0.57
2:C:115:LYS:HD2	2:D:90:LEU:HG	1.85	0.57
2:D:180:ASN:OD1	2:D:181:GLU:N	2.32	0.57
1:B:322:ILE:HD13	1:B:355:SER:HB2	1.87	0.57
1:I:409:ILE:HD13	1:I:412:ILE:HD12	1.86	0.57
1:I:433:SER:HB2	1:J:333:LYS:HG2	1.86	0.57
1:J:246:VAL:HG11	1:J:272:GLN:HB3	1.86	0.57
1:B:247:PHE:O	1:B:251:TYR:HB2	2.05	0.57
1:B:92:MET:HA	1:B:209:PHE:HE2	1.70	0.57
1:J:208:GLY:HA2	1:J:309:SER:H	1.69	0.56
1:I:301:MET:HB2	1:I:391:VAL:HG11	1.87	0.56
2:D:66:LEU:HB3	2:D:68:ILE:HG13	1.85	0.56
1:J:379:GLN:HG3	1:J:395:MET:HB2	1.87	0.56
1:A:92:MET:HA	1:A:209:PHE:CE2	2.40	0.56
1:B:168:HIS:O	1:B:172:ALA:N	2.37	0.56
1:I:424:VAL:HG11	1:J:330:LEU:HD13	1.88	0.56
1:B:370:THR:HA	1:B:380:ILE:HD13	1.87	0.56
1:B:418:ILE:HG23	1:B:423:PHE:HB2	1.88	0.56
2:C:72:GLU:HA	2:C:98:PRO:HD2	1.87	0.56
1:I:297:THR:HG22	1:I:301:MET:HE2	1.86	0.56
1:A:294:ILE:HG23	1:A:382:PHE:HD2	1.71	0.56
1:A:322:ILE:HD13	1:A:355:SER:HB2	1.88	0.56
2:G:37:ILE:HG13	2:G:38:ASN:N	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:209:PHE:HA	1:I:212:LEU:HB2	1.87	0.56
1:I:256:THR:HB	1:I:284:LEU:HB3	1.87	0.56
1:J:145:ALA:HA	1:J:149:SER:HB2	1.88	0.56
2:C:175:LEU:HD21	2:C:208:LEU:HG	1.87	0.56
1:I:330:LEU:HD13	1:J:424:VAL:HG11	1.88	0.55
1:A:173:PHE:HB2	1:A:201:LEU:HD22	1.89	0.55
2:D:218:VAL:HB	2:D:244:VAL:HG13	1.87	0.55
1:J:250:GLU:HG3	1:J:289:MET:HE2	1.87	0.55
1:A:370:THR:HA	1:A:380:ILE:HD13	1.88	0.55
1:B:72:PHE:HB3	1:B:76:GLY:HA3	1.89	0.55
1:B:202:PHE:HE1	1:B:274:VAL:HG12	1.70	0.55
2:C:258:ILE:HD11	2:E:254:VAL:HG23	1.87	0.55
2:D:181:GLU:HB3	2:D:196:ILE:HD13	1.88	0.55
1:J:210:THR:O	1:J:214:ASP:N	2.32	0.55
1:A:340:ARG:HD3	2:C:193:HIS:NE2	2.22	0.55
2:D:231:THR:HA	2:D:234:LEU:HD12	1.88	0.55
2:G:208:LEU:HB3	2:G:210:ILE:HG13	1.88	0.55
1:I:307:SER:HA	1:I:315:LYS:HG3	1.89	0.55
1:A:417:ARG:O	1:A:417:ARG:NH1	2.39	0.55
1:I:247:PHE:O	1:I:251:TYR:HB2	2.07	0.55
1:I:322:ILE:HD13	1:I:355:SER:HB2	1.89	0.55
1:J:168:HIS:O	1:J:172:ALA:N	2.37	0.55
2:G:101:TRP:CD2	2:G:120:ARG:HD3	2.41	0.55
1:J:344:LYS:HG3	1:J:346:PRO:HD2	1.88	0.55
1:A:145:ALA:HA	1:A:149:SER:HB2	1.88	0.55
1:B:294:ILE:HG23	1:B:382:PHE:HD2	1.72	0.54
1:J:398:THR:HA	1:J:401:LEU:HG	1.90	0.54
1:B:337:VAL:HA	1:B:342:SER:HA	1.90	0.54
1:I:67:ASP:O	1:I:71:GLN:HB3	2.07	0.54
1:I:227:HIS:CE1	1:I:317:THR:HG21	2.42	0.54
1:I:294:ILE:HG23	1:I:382:PHE:HD2	1.71	0.54
1:B:175:ASN:ND2	1:B:202:PHE:HB2	2.23	0.54
1:B:270:TYR:O	1:B:274:VAL:HG23	2.08	0.54
2:C:231:THR:HA	2:C:234:LEU:HD12	1.89	0.54
1:J:257:LEU:HD13	1:J:268:ALA:HB3	1.90	0.54
2:C:202:GLU:O	2:C:206:LEU:HG	2.08	0.54
1:J:303:ILE:HA	1:J:314:ILE:HG23	1.90	0.54
2:E:231:THR:HA	2:E:234:LEU:HD12	1.90	0.54
1:I:247:PHE:HE1	1:I:265:LYS:HB3	1.72	0.54
1:J:175:ASN:ND2	1:J:202:PHE:HB2	2.23	0.54
1:A:175:ASN:ND2	1:A:202:PHE:HB2	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:218:VAL:HB	2:C:244:VAL:HG13	1.90	0.54
1:A:209:PHE:HD1	1:A:212:LEU:HD12	1.73	0.53
2:D:218:VAL:HG21	2:D:231:THR:HG22	1.91	0.53
1:I:443:PHE:O	1:J:307:SER:OG	2.25	0.53
1:J:294:ILE:HG23	1:J:382:PHE:HD2	1.74	0.53
1:A:298:LEU:HA	1:A:301:MET:HE3	1.89	0.53
1:A:64:ALA:H	1:A:398:THR:HG21	1.74	0.53
1:A:247:PHE:HE1	1:A:265:LYS:HB3	1.72	0.53
1:A:344:LYS:HG3	1:A:346:PRO:HD2	1.91	0.53
1:A:146:LEU:HD13	1:A:166:LEU:HD23	1.90	0.53
1:A:204:THR:O	1:A:207:ILE:HG12	2.08	0.53
1:J:64:ALA:H	1:J:398:THR:HG21	1.73	0.53
1:A:60:VAL:HG12	1:A:84:ILE:HG23	1.88	0.53
1:B:257:LEU:O	1:B:260:LEU:N	2.34	0.53
2:C:33:LEU:HD21	2:C:66:LEU:HG	1.90	0.53
2:E:218:VAL:HG21	2:E:231:THR:HG22	1.90	0.53
1:I:227:HIS:HA	1:I:230:LEU:HD12	1.91	0.53
1:J:407:CYS:O	1:J:411:VAL:HG23	2.09	0.53
1:J:409:ILE:HD13	1:J:412:ILE:HD12	1.91	0.53
1:B:250:GLU:HG3	1:B:289:MET:HE2	1.90	0.52
1:I:337:VAL:HA	1:I:342:SER:HA	1.90	0.52
1:B:179:SER:HB3	1:B:184:ASN:HA	1.92	0.52
1:J:95:ALA:HA	1:J:98:ILE:HB	1.91	0.52
2:E:202:GLU:O	2:E:206:LEU:HG	2.09	0.52
1:A:36:MET:HE1	1:A:47:TRP:CD1	2.45	0.52
1:I:73:THR:HG22	1:I:74:VAL:H	1.75	0.52
2:D:89:THR:HA	2:D:92:LEU:HD12	1.91	0.52
2:D:181:GLU:CB	2:D:196:ILE:HD13	2.40	0.52
1:I:209:PHE:HD1	1:I:212:LEU:HD12	1.74	0.52
1:I:204:THR:O	1:I:207:ILE:HG12	2.10	0.52
1:I:256:THR:HB	1:I:284:LEU:HD13	1.91	0.52
2:D:151:PHE:HB2	2:D:173:GLU:O	2.10	0.52
1:I:146:LEU:HD13	1:I:166:LEU:HD23	1.92	0.52
1:I:92:MET:HA	1:I:209:PHE:CE2	2.45	0.51
1:J:67:ASP:O	1:J:71:GLN:HB3	2.10	0.51
1:A:270:TYR:O	1:A:274:VAL:HG23	2.10	0.51
1:B:314:ILE:HD12	1:B:355:SER:HA	1.92	0.51
1:B:204:THR:O	1:B:207:ILE:HG12	2.11	0.51
2:C:90:LEU:HG	2:D:115:LYS:HD2	1.91	0.51
1:A:350:LYS:HE3	1:A:421:LEU:HD12	1.91	0.51
1:A:424:VAL:HG11	1:B:330:LEU:HD13	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:227:SER:O	2:D:231:THR:HG23	2.10	0.51
2:G:16:ARG:NH1	2:G:247:GLN:O	2.43	0.51
1:A:227:HIS:HA	1:A:230:LEU:HD12	1.92	0.51
1:B:67:ASP:O	1:B:71:GLN:HB3	2.09	0.51
2:C:192:THR:HG22	2:C:193:HIS:HD1	1.75	0.51
2:G:69:ARG:HD3	2:G:95:LEU:HD12	1.92	0.51
2:G:202:GLU:O	2:G:206:LEU:HG	2.10	0.51
1:A:67:ASP:O	1:A:71:GLN:HB3	2.10	0.51
1:B:353:ALA:O	1:B:357:THR:OG1	2.21	0.51
2:E:87:LEU:O	2:E:91:LEU:HG	2.11	0.51
1:I:92:MET:HG2	1:I:133:LEU:HD13	1.93	0.51
1:I:168:HIS:O	1:I:172:ALA:N	2.42	0.51
1:J:227:HIS:HA	1:J:230:LEU:HD12	1.92	0.51
2:D:169:ARG:NH1	2:D:170:MET:HG2	2.25	0.51
1:A:171:SER:HB2	1:A:176:ALA:HB3	1.93	0.51
1:B:208:GLY:HA2	1:B:309:SER:H	1.76	0.51
1:B:294:ILE:HG23	1:B:382:PHE:CD2	2.46	0.51
1:B:298:LEU:HA	1:B:301:MET:HE3	1.93	0.51
1:I:302:PHE:HB2	1:I:385:PHE:HD2	1.76	0.51
2:G:66:LEU:HB3	2:G:68:ILE:HG13	1.92	0.51
2:G:277:SER:O	2:G:281:GLU:HB2	2.10	0.51
1:J:257:LEU:HD11	1:J:265:LYS:HA	1.92	0.51
1:A:337:VAL:HA	1:A:342:SER:HA	1.93	0.51
2:E:227:SER:O	2:E:231:THR:HG23	2.11	0.51
1:J:146:LEU:HD13	1:J:166:LEU:HD23	1.92	0.51
2:D:23:LYS:HG2	2:D:48:TYR:HD2	1.76	0.51
2:D:101:TRP:CD2	2:D:120:ARG:HD3	2.45	0.51
2:E:218:VAL:HB	2:E:244:VAL:HG13	1.93	0.50
2:C:60:GLU:O	2:C:64:LEU:HG	2.11	0.50
1:I:314:ILE:HD12	1:I:355:SER:HA	1.93	0.50
1:J:61:THR:HG21	1:J:413:MET:HG2	1.93	0.50
1:B:92:MET:HE2	1:B:209:PHE:HZ	1.76	0.50
2:C:85:SER:O	2:C:89:THR:HG23	2.11	0.50
1:J:173:PHE:HB2	1:J:201:LEU:HD22	1.93	0.50
1:B:195:ASN:O	1:B:199:THR:OG1	2.23	0.50
1:B:64:ALA:H	1:B:398:THR:HG21	1.77	0.50
1:B:227:HIS:HA	1:B:230:LEU:HD12	1.93	0.50
2:E:151:PHE:HB2	2:E:173:GLU:O	2.12	0.50
2:D:214:GLU:HA	2:D:240:PRO:HD2	1.93	0.50
1:J:247:PHE:O	1:J:251:TYR:HB2	2.11	0.49
2:E:180:ASN:OD1	2:E:181:GLU:N	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:36:MET:HE1	1:I:47:TRP:CD1	2.47	0.49
1:J:63:LEU:HB3	1:J:398:THR:HG21	1.94	0.49
1:B:81:MET:SD	1:B:167:PHE:HA	2.52	0.49
2:C:218:VAL:HG21	2:C:231:THR:HG22	1.93	0.49
1:I:417:ARG:O	1:I:417:ARG:NH1	2.45	0.49
1:A:209:PHE:HA	1:A:212:LEU:HB2	1.93	0.49
2:E:214:GLU:HA	2:E:240:PRO:HD2	1.94	0.49
1:I:294:ILE:HG23	1:I:382:PHE:CD2	2.47	0.49
1:J:174:ASN:HA	1:J:310:THR:HG21	1.95	0.49
2:C:242:ILE:HG13	2:C:261:ASP:H	1.78	0.49
2:D:100:ILE:HG13	2:D:119:ASP:H	1.76	0.49
1:A:294:ILE:HG23	1:A:382:PHE:CD2	2.48	0.49
1:A:303:ILE:HA	1:A:314:ILE:HG23	1.94	0.49
1:I:60:VAL:O	1:I:60:VAL:HG13	2.12	0.49
1:I:303:ILE:HA	1:I:314:ILE:HG23	1.95	0.49
2:D:60:GLU:O	2:D:64:LEU:HG	2.13	0.49
2:D:85:SER:O	2:D:89:THR:HG23	2.13	0.49
2:E:156:LEU:N	2:E:178:ASP:OD2	2.37	0.49
1:I:175:ASN:ND2	1:I:310:THR:OG1	2.46	0.49
1:I:270:TYR:O	1:I:274:VAL:HG23	2.12	0.49
1:J:272:GLN:HE22	1:J:284:LEU:HB2	1.78	0.49
1:J:322:ILE:HD13	1:J:355:SER:HB2	1.94	0.49
2:E:229:LEU:O	2:E:233:LEU:HG	2.12	0.49
1:J:37:LEU:O	1:J:41:THR:HG22	2.12	0.48
1:A:209:PHE:CD2	1:A:308:ALA:HB1	2.48	0.48
1:A:418:ILE:HG23	1:A:423:PHE:HB2	1.94	0.48
1:B:203:ILE:HD11	1:B:274:VAL:HG11	1.96	0.48
2:D:112:VAL:O	2:D:116:ILE:HG12	2.13	0.48
2:D:243:TRP:CE2	2:D:262:ARG:HG3	2.48	0.48
1:I:418:ILE:HG23	1:I:423:PHE:HB2	1.95	0.48
1:A:434:ASN:ND2	2:G:203:ASN:HD22	2.11	0.48
2:D:72:GLU:HA	2:D:98:PRO:HD2	1.96	0.48
1:J:20:LEU:HD13	1:J:94:PHE:HE1	1.78	0.48
1:J:199:THR:HG21	1:J:270:TYR:HE2	1.78	0.48
1:J:294:ILE:HG23	1:J:382:PHE:CD2	2.49	0.48
1:A:379:GLN:HG3	1:A:395:MET:HB2	1.95	0.48
1:B:421:LEU:HD23	1:B:421:LEU:HA	1.70	0.48
2:C:83:GLN:NE2	2:D:108:TYR:HB2	2.29	0.48
2:C:112:VAL:O	2:C:116:ILE:HG12	2.14	0.48
2:G:243:TRP:CE2	2:G:262:ARG:HG3	2.49	0.48
1:I:129:LEU:HG	1:I:133:LEU:HD23	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:354:VAL:HG13	1:J:420:PRO:HG2	1.96	0.48
1:B:303:ILE:HA	1:B:314:ILE:HG23	1.96	0.48
1:J:81:MET:SD	1:J:170:ILE:HD12	2.53	0.48
1:B:322:ILE:CD1	1:B:355:SER:HB2	2.43	0.48
1:B:436:ARG:HB2	2:C:196:ILE:HB	1.96	0.48
1:A:227:HIS:CE1	1:A:317:THR:HG21	2.48	0.48
2:G:227:SER:O	2:G:231:THR:HG23	2.14	0.48
1:B:20:LEU:HD13	1:B:94:PHE:HE1	1.78	0.48
2:C:87:LEU:O	2:C:91:LEU:HG	2.14	0.48
1:J:81:MET:SD	1:J:167:PHE:HA	2.54	0.47
1:A:188:TYR:CG	1:A:194:VAL:HG21	2.49	0.47
1:A:268:ALA:HB1	1:A:284:LEU:HD11	1.96	0.47
1:B:146:LEU:HD13	1:B:166:LEU:HD23	1.94	0.47
1:B:407:CYS:O	1:B:411:VAL:HG23	2.14	0.47
1:B:438:PRO:HD3	2:C:194:ALA:O	2.14	0.47
2:D:202:GLU:O	2:D:206:LEU:HG	2.13	0.47
2:E:72:GLU:HA	2:E:98:PRO:HD2	1.96	0.47
2:C:198:ASN:OD1	2:C:200:THR:OG1	2.21	0.47
2:G:36:ASP:OD1	2:G:37:ILE:N	2.47	0.47
1:B:60:VAL:HG22	1:B:176:ALA:HA	1.95	0.47
2:D:76:VAL:HG21	2:D:89:THR:HG22	1.96	0.47
2:D:87:LEU:O	2:D:91:LEU:HG	2.14	0.47
2:E:27:ARG:HH12	2:E:28:MET:HG2	1.80	0.47
2:G:254:VAL:O	2:G:258:ILE:HG12	2.15	0.47
1:J:418:ILE:HG23	1:J:423:PHE:HB2	1.96	0.47
1:B:247:PHE:HE1	1:B:265:LYS:HB3	1.79	0.47
2:G:250:TYR:O	2:G:254:VAL:HG12	2.15	0.47
1:B:73:THR:HG22	1:B:74:VAL:H	1.79	0.47
1:I:208:GLY:HA2	1:I:308:ALA:HB3	1.97	0.47
1:I:407:CYS:O	1:I:411:VAL:HG23	2.15	0.47
1:J:29:ILE:HD13	1:J:51:LEU:HD11	1.96	0.47
1:A:34:LEU:HB3	1:A:79:VAL:HG11	1.96	0.47
1:A:296:PHE:HB2	1:B:367:PHE:CE2	2.50	0.47
1:B:92:MET:SD	1:B:133:LEU:HB2	2.55	0.47
1:B:323:LEU:O	1:B:327:ILE:HG13	2.15	0.47
2:C:76:VAL:HB	2:C:102:VAL:HG13	1.96	0.47
2:C:89:THR:HA	2:C:92:LEU:HD12	1.95	0.47
2:C:108:TYR:HB2	2:D:83:GLN:NE2	2.30	0.47
2:C:150:GLN:HG3	2:C:213:PHE:CE2	2.49	0.47
1:J:153:VAL:N	1:J:154:PRO:CD	2.78	0.47
1:J:208:GLY:HA2	1:J:308:ALA:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:SER:HB3	1:B:48:ILE:HD12	1.96	0.47
1:B:81:MET:SD	1:B:170:ILE:HD12	2.54	0.47
2:G:180:ASN:OD1	2:G:181:GLU:N	2.44	0.47
1:J:204:THR:O	1:J:207:ILE:HG12	2.14	0.47
1:J:302:PHE:HB2	1:J:385:PHE:HD2	1.80	0.47
2:C:227:SER:O	2:C:231:THR:HG23	2.15	0.47
2:E:202:GLU:HG2	2:E:203:ASN:N	2.30	0.47
1:A:208:GLY:HA2	1:A:308:ALA:HB3	1.95	0.47
1:I:257:LEU:HD11	1:I:265:LYS:HA	1.96	0.46
1:A:443:PHE:O	1:B:307:SER:OG	2.32	0.46
1:B:133:LEU:HD12	1:B:134:PHE:N	2.30	0.46
2:C:22:VAL:HG13	2:C:49:ALA:HB2	1.97	0.46
2:G:76:VAL:HB	2:G:102:VAL:HG13	1.97	0.46
1:B:175:ASN:HB3	1:B:278:THR:O	2.14	0.46
2:C:135:SER:O	2:C:139:GLU:HB2	2.16	0.46
2:C:214:GLU:HA	2:C:240:PRO:HD2	1.97	0.46
1:I:64:ALA:H	1:I:398:THR:HG21	1.79	0.46
1:I:379:GLN:HE21	1:I:397:LEU:HB2	1.80	0.46
1:A:46:SER:HB3	1:A:48:ILE:HD12	1.97	0.46
1:A:199:THR:HA	1:A:202:PHE:CE2	2.50	0.46
1:I:318:THR:HG22	1:I:322:ILE:HD11	1.98	0.46
1:I:323:LEU:O	1:I:327:ILE:HG13	2.15	0.46
1:A:63:LEU:HB3	1:A:398:THR:HG21	1.96	0.46
1:A:253:ASN:HD22	1:A:290:ARG:HG3	1.79	0.46
1:A:153:VAL:N	1:A:154:PRO:CD	2.78	0.46
1:B:257:LEU:HA	1:B:260:LEU:HD13	1.98	0.46
2:D:178:ASP:OD1	2:D:179:ILE:N	2.48	0.46
1:I:322:ILE:CD1	1:I:355:SER:HB2	2.46	0.46
2:E:60:GLU:O	2:E:64:LEU:HG	2.16	0.46
1:J:314:ILE:HD12	1:J:355:SER:HA	1.97	0.46
1:B:145:ALA:HB2	1:B:169:ALA:CB	2.46	0.46
1:B:199:THR:HG21	1:B:270:TYR:HE2	1.81	0.46
1:B:379:GLN:HG3	1:B:395:MET:HB2	1.96	0.46
2:C:100:ILE:HG13	2:C:119:ASP:H	1.80	0.46
1:J:91:PHE:HB2	1:J:417:ARG:NH2	2.31	0.46
2:E:89:THR:HA	2:E:92:LEU:HD12	1.97	0.46
1:I:153:VAL:N	1:I:154:PRO:CD	2.79	0.46
1:J:133:LEU:HD12	1:J:134:PHE:N	2.31	0.46
1:J:145:ALA:HB2	1:J:169:ALA:CB	2.45	0.46
2:C:202:GLU:HG2	2:C:203:ASN:N	2.31	0.46
1:A:208:GLY:CA	1:A:308:ALA:HB3	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:GLY:O	1:B:309:SER:HB3	2.16	0.46
1:B:437:TYR:HB3	1:B:438:PRO:HD2	1.98	0.46
2:C:199:ALA:HA	2:C:205:LEU:HD11	1.98	0.46
2:G:89:THR:HA	2:G:92:LEU:HD12	1.98	0.46
1:I:133:LEU:HD12	1:I:134:PHE:N	2.31	0.45
1:I:199:THR:HA	1:I:202:PHE:CE2	2.51	0.45
1:J:60:VAL:O	1:J:60:VAL:HG13	2.15	0.45
1:J:242:ALA:CB	1:J:273:ALA:HB1	2.46	0.45
1:B:153:VAL:N	1:B:154:PRO:CD	2.79	0.45
1:B:209:PHE:H	1:B:308:ALA:HB3	1.81	0.45
1:B:417:ARG:O	1:B:417:ARG:NH1	2.49	0.45
2:G:87:LEU:O	2:G:91:LEU:HG	2.16	0.45
1:J:36:MET:HA	1:J:45:LEU:HD23	1.96	0.45
1:A:94:PHE:HE1	1:A:422:THR:OG1	2.00	0.45
1:A:442:VAL:HG13	1:B:347:ILE:HG21	1.99	0.45
1:B:272:GLN:HE22	1:B:284:LEU:HD12	1.80	0.45
2:G:112:VAL:O	2:G:116:ILE:HG12	2.16	0.45
1:I:171:SER:HB3	1:I:176:ALA:HB3	1.97	0.45
1:J:172:ALA:O	1:J:202:PHE:HB3	2.16	0.45
1:J:257:LEU:HA	1:J:260:LEU:HD22	1.97	0.45
1:A:150:ILE:O	1:A:154:PRO:HD3	2.17	0.45
1:A:437:TYR:N	2:G:196:ILE:HD12	2.31	0.45
2:E:242:ILE:HG13	2:E:261:ASP:H	1.82	0.45
1:J:46:SER:HB3	1:J:48:ILE:HD12	1.98	0.45
2:G:151:PHE:HB2	2:G:173:GLU:O	2.16	0.45
1:I:91:PHE:HB2	1:I:417:ARG:NH2	2.32	0.45
1:J:199:THR:HG21	1:J:270:TYR:CE2	2.51	0.45
1:A:421:LEU:HD21	1:B:329:TYR:CE1	2.51	0.45
1:I:175:ASN:OD1	1:I:202:PHE:HB2	2.16	0.45
1:A:366:ILE:HD13	1:A:381:VAL:HG13	1.99	0.45
1:B:199:THR:HA	1:B:202:PHE:CE2	2.52	0.45
2:D:130:VAL:HB	2:D:166:GLU:HG3	1.98	0.45
2:G:100:ILE:HG13	2:G:119:ASP:H	1.80	0.45
1:A:327:ILE:O	1:A:331:ARG:HG3	2.16	0.45
1:B:350:LYS:HE3	1:B:421:LEU:HD12	1.98	0.45
2:D:230:THR:O	2:D:234:LEU:HG	2.17	0.45
1:J:227:HIS:CE1	1:J:317:THR:HG21	2.51	0.45
1:B:319:PHE:CZ	1:B:323:LEU:HD22	2.52	0.45
2:D:242:ILE:HG13	2:D:261:ASP:H	1.82	0.45
1:J:92:MET:SD	1:J:133:LEU:HB2	2.57	0.45
1:J:226:LEU:O	1:J:230:LEU:HG	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:THR:HA	1:A:401:LEU:HG	1.99	0.45
1:B:256:THR:HG22	1:B:289:MET:HG2	1.97	0.45
2:C:69:ARG:HG2	2:C:95:LEU:HB3	1.98	0.45
2:G:60:GLU:O	2:G:64:LEU:HG	2.17	0.45
2:E:135:SER:O	2:E:139:GLU:HB2	2.18	0.44
2:E:250:TYR:O	2:E:254:VAL:HG12	2.17	0.44
1:I:301:MET:HB2	1:I:391:VAL:HG21	1.99	0.44
1:J:209:PHE:H	1:J:308:ALA:HB3	1.82	0.44
1:J:323:LEU:O	1:J:327:ILE:HG13	2.17	0.44
1:A:316:LEU:O	1:A:320:ILE:HG13	2.16	0.44
2:C:106:ASN:CG	2:D:83:GLN:HE22	2.22	0.44
1:J:133:LEU:O	1:J:137:SER:OG	2.33	0.44
1:J:206:GLY:HA2	1:J:310:THR:OG1	2.16	0.44
2:E:230:THR:O	2:E:234:LEU:HG	2.18	0.44
2:C:277:SER:O	2:C:281:GLU:HB2	2.17	0.44
2:G:231:THR:HA	2:G:234:LEU:HD12	1.99	0.44
1:I:210:THR:O	1:I:214:ASP:N	2.41	0.44
1:J:91:PHE:HE2	1:J:308:ALA:HB1	1.83	0.44
1:I:379:GLN:NE2	1:I:397:LEU:HB2	2.32	0.44
1:J:337:VAL:HA	1:J:342:SER:HA	1.99	0.44
2:D:229:LEU:O	2:D:233:LEU:HG	2.18	0.44
1:A:61:THR:HG21	1:A:413:MET:HG2	1.99	0.44
1:A:296:PHE:HB2	1:B:367:PHE:HE2	1.83	0.44
1:B:16:PRO:O	1:B:20:LEU:HG	2.17	0.44
2:C:27:ARG:HH12	2:C:28:MET:HG2	1.81	0.44
2:D:21:ILE:HG13	2:D:275:ALA:HB2	1.99	0.44
2:D:135:SER:O	2:D:139:GLU:HB2	2.17	0.44
1:A:179:SER:HB3	1:A:184:ASN:HA	1.99	0.44
1:A:436:ARG:HA	1:A:436:ARG:HD3	1.87	0.44
2:G:72:GLU:N	2:G:72:GLU:OE1	2.50	0.44
1:I:29:ILE:HD13	1:I:51:LEU:HD11	1.99	0.44
1:I:305:ALA:O	1:I:309:SER:HB2	2.18	0.44
1:J:60:VAL:HG22	1:J:176:ALA:HA	1.99	0.44
1:J:322:ILE:CD1	1:J:355:SER:HB2	2.48	0.44
1:J:353:ALA:O	1:J:357:THR:OG1	2.27	0.44
1:A:210:THR:O	1:A:214:ASP:N	2.46	0.44
1:A:286:PHE:CZ	1:A:393:LEU:HG	2.53	0.44
1:A:373:GLU:CD	1:A:402:THR:H	2.25	0.44
1:B:189:VAL:HG11	1:B:260:LEU:HD21	2.00	0.44
2:D:59:GLU:HB2	2:D:62:GLU:HG3	1.99	0.44
2:E:199:ALA:HB1	2:E:230:THR:HG23	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:179:SER:HB3	1:J:184:ASN:HA	1.99	0.43
1:J:294:ILE:O	1:J:298:LEU:HD13	2.18	0.43
1:J:377:PHE:O	1:J:381:VAL:HG23	2.18	0.43
1:B:42:THR:OG1	1:B:43:LYS:N	2.43	0.43
2:C:83:GLN:HE22	2:D:106:ASN:CG	2.26	0.43
2:C:214:GLU:OE1	2:C:214:GLU:N	2.48	0.43
2:E:112:VAL:O	2:E:116:ILE:HG12	2.17	0.43
1:A:298:LEU:HD12	1:A:301:MET:HE3	2.00	0.43
1:A:322:ILE:CD1	1:A:355:SER:HB2	2.48	0.43
2:C:60:GLU:HG2	2:C:61:ASN:N	2.33	0.43
1:I:94:PHE:HE1	1:I:422:THR:OG1	2.00	0.43
1:I:208:GLY:CA	1:I:308:ALA:HB3	2.48	0.43
1:I:276:PRO:HB2	1:I:300:LEU:HG	2.01	0.43
1:A:145:ALA:HB2	1:A:169:ALA:CB	2.48	0.43
1:A:189:VAL:CG1	1:A:260:LEU:HD21	2.47	0.43
1:A:203:ILE:O	1:A:207:ILE:HG23	2.18	0.43
1:B:226:LEU:O	1:B:230:LEU:HG	2.18	0.43
1:B:322:ILE:HD11	1:B:351:ALA:O	2.18	0.43
2:C:153:VAL:HG22	2:C:217:ILE:HB	2.00	0.43
2:C:156:LEU:HD21	2:C:176:ALA:HB1	1.99	0.43
2:D:205:LEU:HA	2:D:210:ILE:HD12	2.00	0.43
1:I:203:ILE:O	1:I:207:ILE:HG23	2.18	0.43
1:A:177:GLY:HA3	1:A:280:GLY:HA3	1.99	0.43
1:A:268:ALA:O	1:A:272:GLN:HB2	2.18	0.43
2:C:101:TRP:CD2	2:C:120:ARG:HD2	2.53	0.43
2:E:243:TRP:CE2	2:E:262:ARG:HG3	2.53	0.43
2:G:85:SER:O	2:G:89:THR:HG23	2.18	0.43
2:G:202:GLU:HG2	2:G:203:ASN:N	2.33	0.43
1:A:373:GLU:OE2	1:A:402:THR:N	2.48	0.43
2:C:178:ASP:OD1	2:C:179:ILE:N	2.51	0.43
2:D:174:VAL:H	2:D:192:THR:HB	1.83	0.43
2:E:205:LEU:HA	2:E:210:ILE:HD12	2.01	0.43
2:G:214:GLU:HA	2:G:240:PRO:HD2	1.99	0.43
1:I:60:VAL:HG22	1:I:176:ALA:HA	2.00	0.43
1:I:146:LEU:HD12	1:I:146:LEU:HA	1.89	0.43
1:I:81:MET:HG3	1:I:170:ILE:HD12	2.00	0.43
1:J:388:PHE:O	1:J:416:GLY:HA3	2.18	0.43
1:J:390:THR:HG21	1:J:417:ARG:HB2	2.01	0.43
1:A:73:THR:HG22	1:A:74:VAL:H	1.83	0.43
1:A:199:THR:HG21	1:A:270:TYR:HE2	1.82	0.43
1:A:203:ILE:HD11	1:A:274:VAL:HG11	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ILE:O	1:B:154:PRO:HD3	2.19	0.43
1:B:388:PHE:O	1:B:416:GLY:HA3	2.19	0.43
2:C:208:LEU:HD23	2:C:210:ILE:HD11	2.00	0.43
1:I:244:LEU:O	1:I:248:ILE:HG12	2.17	0.43
1:I:417:ARG:HA	1:I:417:ARG:HD2	1.87	0.43
1:J:297:THR:HA	1:J:300:LEU:HB3	2.01	0.43
1:A:294:ILE:O	1:A:298:LEU:HD13	2.19	0.43
1:B:316:LEU:O	1:B:320:ILE:HG13	2.18	0.43
2:C:27:ARG:NH1	2:C:28:MET:HG2	2.34	0.43
2:C:174:VAL:H	2:C:192:THR:HB	1.84	0.43
2:D:199:ALA:HB1	2:D:230:THR:HG23	2.00	0.43
2:E:217:ILE:HA	2:E:243:TRP:O	2.19	0.43
1:I:92:MET:HG3	1:I:133:LEU:HD22	2.01	0.43
1:J:62:GLY:HA3	1:J:392:GLY:HA2	2.01	0.43
1:A:60:VAL:CG1	1:A:84:ILE:HG23	2.49	0.43
1:A:382:PHE:HE1	1:A:393:LEU:O	2.02	0.43
2:G:72:GLU:HA	2:G:98:PRO:HD2	2.00	0.43
1:A:40:SER:HB3	1:A:75:PHE:CD2	2.54	0.43
1:A:146:LEU:HD12	1:A:146:LEU:HA	1.90	0.43
1:A:257:LEU:O	1:A:260:LEU:N	2.39	0.43
1:J:369:LEU:HD11	1:J:409:ILE:HD11	2.01	0.42
1:A:302:PHE:HB2	1:A:385:PHE:HD2	1.83	0.42
1:B:63:LEU:HB3	1:B:398:THR:HG21	2.00	0.42
1:B:320:ILE:O	1:B:324:THR:HG22	2.18	0.42
2:C:63:LEU:HG	2:C:68:ILE:HD12	2.01	0.42
1:A:307:SER:HA	1:A:315:LYS:CG	2.48	0.42
1:B:40:SER:HB3	1:B:75:PHE:CD2	2.54	0.42
2:C:72:GLU:OE1	2:C:72:GLU:N	2.51	0.42
1:I:316:LEU:O	1:I:320:ILE:HG13	2.18	0.42
1:I:322:ILE:HD11	1:I:351:ALA:O	2.19	0.42
1:J:383:GLU:HG3	1:J:397:LEU:HD23	2.01	0.42
1:B:418:ILE:CG2	1:B:423:PHE:HB2	2.49	0.42
2:C:229:LEU:O	2:C:233:LEU:HG	2.18	0.42
2:E:66:LEU:HD12	2:E:66:LEU:HA	1.91	0.42
1:A:407:CYS:O	1:A:411:VAL:HG23	2.20	0.42
1:B:294:ILE:O	1:B:298:LEU:HD13	2.20	0.42
2:C:151:PHE:HB2	2:C:173:GLU:O	2.20	0.42
2:D:60:GLU:HG2	2:D:61:ASN:N	2.34	0.42
2:E:198:ASN:HD21	2:E:200:THR:HG23	1.84	0.42
1:I:153:VAL:N	1:I:154:PRO:HD2	2.35	0.42
1:I:388:PHE:O	1:I:416:GLY:HA3	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:306:GLY:O	1:J:309:SER:HB3	2.18	0.42
1:I:424:VAL:HG11	1:J:330:LEU:HD22	2.00	0.42
1:B:95:ALA:HA	1:B:98:ILE:HB	2.00	0.42
2:C:36:ASP:OD1	2:C:37:ILE:N	2.52	0.42
1:I:188:TYR:CG	1:I:194:VAL:HG21	2.55	0.42
1:J:256:THR:HB	1:J:284:LEU:HB3	2.01	0.42
1:B:37:LEU:O	1:B:41:THR:HG22	2.19	0.42
1:B:42:THR:HG23	1:B:71:GLN:O	2.20	0.42
1:B:215:VAL:HG22	1:B:224:PHE:CE2	2.55	0.42
1:I:226:LEU:O	1:I:230:LEU:HG	2.20	0.42
1:J:199:THR:HA	1:J:202:PHE:CE2	2.55	0.42
1:A:148:LEU:HG	1:A:151:ARG:CZ	2.50	0.42
1:A:251:TYR:O	1:A:258:GLY:HA2	2.19	0.42
1:A:367:PHE:HE2	1:B:296:PHE:HB2	1.84	0.42
1:B:322:ILE:O	1:B:326:VAL:HG23	2.19	0.42
2:C:32:VAL:H	2:C:50:THR:HB	1.83	0.42
2:E:199:ALA:HA	2:E:205:LEU:HD11	2.02	0.42
1:I:204:THR:O	1:I:212:LEU:HD21	2.20	0.42
1:I:250:GLU:HG3	1:I:289:MET:HE2	2.00	0.42
1:I:291:GLU:O	1:I:295:VAL:HG23	2.20	0.42
1:J:436:ARG:HA	1:J:436:ARG:HD3	1.90	0.42
1:A:133:LEU:HD12	1:A:134:PHE:N	2.35	0.42
2:E:72:GLU:N	2:E:72:GLU:OE1	2.52	0.42
2:E:153:VAL:HG22	2:E:217:ILE:HB	2.01	0.42
1:J:92:MET:HE2	1:J:209:PHE:HZ	1.85	0.42
2:E:11:VAL:HG22	2:E:75:ILE:HB	2.02	0.42
2:E:254:VAL:O	2:E:258:ILE:HG12	2.19	0.42
1:I:40:SER:HB3	1:I:75:PHE:CD2	2.55	0.41
1:I:317:THR:HA	1:I:320:ILE:HD12	2.02	0.41
2:C:83:GLN:HE22	2:D:106:ASN:ND2	2.18	0.41
2:D:128:MET:HG3	2:D:159:PHE:HE1	1.85	0.41
2:D:202:GLU:HG2	2:D:203:ASN:N	2.34	0.41
2:E:154:ILE:N	2:E:217:ILE:O	2.33	0.41
1:J:230:LEU:HD23	1:J:339:PHE:CE2	2.56	0.41
1:A:421:LEU:HD23	1:A:421:LEU:HA	1.59	0.41
1:B:354:VAL:HG13	1:B:420:PRO:HG2	2.02	0.41
2:C:156:LEU:N	2:C:178:ASP:OD2	2.48	0.41
2:D:217:ILE:HA	2:D:243:TRP:O	2.20	0.41
2:D:254:VAL:O	2:D:258:ILE:HG12	2.19	0.41
2:E:27:ARG:NH1	2:E:28:MET:HG2	2.35	0.41
1:I:91:PHE:HD1	1:I:91:PHE:HA	1.70	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:379:GLN:HG3	1:I:395:MET:HB2	2.02	0.41
1:J:204:THR:O	1:J:212:LEU:HD21	2.21	0.41
1:B:244:LEU:O	1:B:248:ILE:HG12	2.20	0.41
2:C:83:GLN:OE1	2:D:82:ILE:HD13	2.20	0.41
2:C:230:THR:O	2:C:234:LEU:HG	2.20	0.41
2:E:36:ASP:OD1	2:E:37:ILE:N	2.54	0.41
1:J:89:LEU:HA	1:J:92:MET:HG3	2.01	0.41
1:B:91:PHE:CD1	1:B:310:THR:HA	2.56	0.41
1:B:145:ALA:HB2	1:B:169:ALA:HB3	2.02	0.41
1:J:203:ILE:HD11	1:J:274:VAL:HG11	2.02	0.41
1:I:48:ILE:HG22	1:I:406:LYS:HD3	2.02	0.41
1:J:148:LEU:HG	1:J:151:ARG:CZ	2.51	0.41
1:J:242:ALA:HB1	1:J:273:ALA:HB1	2.01	0.41
1:A:209:PHE:H	1:A:308:ALA:HB3	1.85	0.41
1:A:272:GLN:OE1	1:A:283:SER:HB3	2.20	0.41
1:B:155:GLN:C	1:B:157:GLY:H	2.29	0.41
1:B:327:ILE:O	1:B:331:ARG:HG3	2.21	0.41
2:D:175:LEU:HD22	2:D:213:PHE:CE1	2.56	0.41
1:J:45:LEU:HG	1:J:50:ALA:HB2	2.02	0.41
1:J:322:ILE:O	1:J:326:VAL:HG23	2.20	0.41
1:A:188:TYR:CD1	1:A:194:VAL:HG21	2.56	0.41
1:A:209:PHE:HA	1:A:212:LEU:HD12	2.02	0.41
1:A:276:PRO:HB2	1:A:300:LEU:HG	2.03	0.41
1:A:367:PHE:CE2	1:B:296:PHE:HB2	2.56	0.41
1:A:378:LEU:HD13	1:B:377:PHE:CE1	2.56	0.41
1:B:91:PHE:HE2	1:B:308:ALA:HB1	1.85	0.41
1:B:146:LEU:HD12	1:B:146:LEU:HA	1.89	0.41
1:B:177:GLY:HA3	1:B:280:GLY:HA3	2.02	0.41
1:B:419:GLY:O	1:B:423:PHE:HB3	2.19	0.41
2:G:229:LEU:O	2:G:233:LEU:HG	2.20	0.41
1:I:91:PHE:CB	1:I:417:ARG:HH22	2.34	0.41
1:J:40:SER:HB3	1:J:75:PHE:CD2	2.55	0.41
1:J:209:PHE:HA	1:J:212:LEU:HD12	2.03	0.41
1:J:286:PHE:CZ	1:J:393:LEU:HG	2.55	0.41
1:A:318:THR:HG22	1:A:322:ILE:HD11	2.02	0.41
1:B:130:VAL:HA	1:B:133:LEU:HG	2.02	0.41
2:G:22:VAL:HA	2:G:32:VAL:HG11	2.03	0.41
1:J:34:LEU:HD22	1:J:79:VAL:HG21	2.03	0.41
1:A:60:VAL:HB	1:A:176:ALA:HA	2.03	0.41
1:A:92:MET:HG3	1:A:133:LEU:HD22	2.02	0.41
1:A:319:PHE:CZ	1:A:323:LEU:HD22	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PHE:CE1	1:B:378:LEU:HD13	2.56	0.41
1:A:434:ASN:OD1	1:A:435:ILE:HG23	2.21	0.41
1:B:129:LEU:HG	1:B:133:LEU:HD23	2.03	0.41
1:B:318:THR:HG22	1:B:322:ILE:HD11	2.02	0.41
1:B:390:THR:HG21	1:B:417:ARG:HB2	2.03	0.41
2:E:8:GLN:HB2	2:E:71:PHE:HA	2.03	0.41
2:G:218:VAL:HB	2:G:244:VAL:HG13	2.02	0.41
2:G:230:THR:O	2:G:234:LEU:HG	2.20	0.41
1:I:230:LEU:HD23	1:I:339:PHE:CE2	2.56	0.41
1:J:34:LEU:HB3	1:J:79:VAL:HG11	2.02	0.41
1:A:62:GLY:HA3	1:A:392:GLY:HA2	2.02	0.41
2:D:63:LEU:HA	2:D:68:ILE:HD12	2.03	0.41
2:D:88:THR:O	2:D:92:LEU:HG	2.20	0.41
2:E:214:GLU:OE1	2:E:214:GLU:N	2.53	0.41
1:I:398:THR:HA	1:I:401:LEU:HG	2.03	0.40
1:A:69:GLY:HA3	1:A:180:LEU:O	2.20	0.40
1:A:227:HIS:HB2	1:B:442:VAL:HA	2.03	0.40
2:G:177:VAL:HA	2:G:195:VAL:O	2.21	0.40
1:J:318:THR:HG22	1:J:322:ILE:HD11	2.03	0.40
2:C:108:TYR:O	2:C:112:VAL:HG12	2.22	0.40
2:D:72:GLU:OE1	2:D:72:GLU:N	2.53	0.40
2:E:108:TYR:O	2:E:112:VAL:HG12	2.21	0.40
1:I:251:TYR:O	1:I:258:GLY:HA2	2.21	0.40
1:I:294:ILE:O	1:I:298:LEU:HD13	2.21	0.40
1:I:319:PHE:CZ	1:I:323:LEU:HD22	2.56	0.40
1:I:366:ILE:HD13	1:I:381:VAL:HG13	2.03	0.40
1:J:59:THR:O	1:J:60:VAL:HG12	2.22	0.40
1:J:322:ILE:HD11	1:J:351:ALA:O	2.21	0.40
2:C:12:ILE:HA	2:C:35:VAL:HG13	2.02	0.40
1:I:199:THR:HG21	1:I:270:TYR:HE2	1.86	0.40
1:J:270:TYR:O	1:J:274:VAL:HG23	2.21	0.40
1:J:361:ILE:HD13	1:J:415:ILE:HG21	2.03	0.40
1:A:250:GLU:OE2	1:A:293:THR:OG1	2.32	0.40
1:A:377:PHE:O	1:A:381:VAL:HG23	2.22	0.40
2:C:199:ALA:HB1	2:C:230:THR:HG23	2.02	0.40
2:D:16:ARG:NH1	2:D:247:GLN:O	2.55	0.40
2:E:85:SER:O	2:E:89:THR:HG23	2.21	0.40
2:E:175:LEU:HD21	2:E:208:LEU:HG	2.03	0.40
1:I:69:GLY:HA3	1:I:180:LEU:O	2.21	0.40
1:I:203:ILE:HD11	1:I:274:VAL:HG11	2.04	0.40
1:A:204:THR:O	1:A:212:LEU:HD21	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LEU:O	1:A:248:ILE:HG12	2.21	0.40
1:B:436:ARG:HA	1:B:436:ARG:HD3	1.89	0.40
2:C:83:GLN:HE22	2:D:106:ASN:HD21	1.70	0.40
2:C:235:LYS:HA	2:C:235:LYS:HD2	1.90	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	402/445 (90%)	355 (88%)	43 (11%)	4 (1%)	12	48
1	B	402/445 (90%)	351 (87%)	47 (12%)	4 (1%)	12	48
1	I	402/445 (90%)	354 (88%)	47 (12%)	1 (0%)	43	77
1	J	402/445 (90%)	358 (89%)	41 (10%)	3 (1%)	18	56
2	C	264/288 (92%)	243 (92%)	21 (8%)	0	100	100
2	D	264/288 (92%)	246 (93%)	18 (7%)	0	100	100
2	E	264/288 (92%)	244 (92%)	20 (8%)	0	100	100
2	G	264/288 (92%)	243 (92%)	21 (8%)	0	100	100
All	All	2664/2932 (91%)	2394 (90%)	258 (10%)	12 (0%)	24	63

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	GLY
1	A	309	SER
1	B	258	GLY
1	J	310	THR
1	J	311	ALA
1	B	310	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	309	SER
1	A	311	ALA
1	B	309	SER
1	I	332	GLY
1	A	332	GLY
1	B	332	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	335/374 (90%)	314 (94%)	21 (6%)	16	37
1	B	335/374 (90%)	312 (93%)	23 (7%)	14	36
1	I	335/374 (90%)	314 (94%)	21 (6%)	16	37
1	J	335/374 (90%)	312 (93%)	23 (7%)	14	36
2	C	222/240 (92%)	216 (97%)	6 (3%)	39	60
2	D	222/240 (92%)	215 (97%)	7 (3%)	34	55
2	E	222/240 (92%)	216 (97%)	6 (3%)	39	60
2	G	222/240 (92%)	217 (98%)	5 (2%)	44	63
All	All	2228/2456 (91%)	2116 (95%)	112 (5%)	22	42

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	34	LEU
1	I	48	ILE
1	I	60	VAL
1	I	63	LEU
1	I	66	VAL
1	I	73	THR
1	I	89	LEU
1	I	91	PHE
1	I	133	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	146	LEU
1	I	166	LEU
1	I	185	LEU
1	I	198	ILE
1	I	211	VAL
1	I	226	LEU
1	I	309	SER
1	I	310	THR
1	I	314	ILE
1	I	352	LEU
1	I	370	THR
1	I	421	LEU
1	J	33	VAL
1	J	34	LEU
1	J	48	ILE
1	J	60	VAL
1	J	63	LEU
1	J	66	VAL
1	J	73	THR
1	J	81	MET
1	J	92	MET
1	J	93	THR
1	J	137	SER
1	J	146	LEU
1	J	166	LEU
1	J	185	LEU
1	J	198	ILE
1	J	211	VAL
1	J	226	LEU
1	J	272	GLN
1	J	310	THR
1	J	314	ILE
1	J	352	LEU
1	J	370	THR
1	J	421	LEU
1	A	34	LEU
1	A	48	ILE
1	A	63	LEU
1	A	66	VAL
1	A	73	THR
1	A	89	LEU
1	A	91	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	133	LEU
1	A	146	LEU
1	A	166	LEU
1	A	185	LEU
1	A	198	ILE
1	A	211	VAL
1	A	226	LEU
1	A	257	LEU
1	A	272	GLN
1	A	310	THR
1	A	352	LEU
1	A	370	THR
1	A	393	LEU
1	A	421	LEU
1	B	33	VAL
1	B	34	LEU
1	B	48	ILE
1	B	63	LEU
1	B	66	VAL
1	B	73	THR
1	B	81	MET
1	B	98	ILE
1	B	137	SER
1	B	146	LEU
1	B	166	LEU
1	B	185	LEU
1	B	198	ILE
1	B	207	ILE
1	B	211	VAL
1	B	226	LEU
1	B	257	LEU
1	B	272	GLN
1	B	310	THR
1	B	314	ILE
1	B	352	LEU
1	B	370	THR
1	B	421	LEU
2	C	50	THR
2	C	95	LEU
2	C	134	GLN
2	C	192	THR
2	C	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	276	GLN
2	D	28	MET
2	D	50	THR
2	D	95	LEU
2	D	134	GLN
2	D	192	THR
2	D	237	LEU
2	D	276	GLN
2	E	50	THR
2	E	95	LEU
2	E	134	GLN
2	E	192	THR
2	E	237	LEU
2	E	276	GLN
2	G	95	LEU
2	G	130	VAL
2	G	134	GLN
2	G	192	THR
2	G	276	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	175	ASN
1	I	184	ASN
1	I	195	ASN
1	I	259	HIS
1	I	379	GLN
1	J	175	ASN
1	A	184	ASN
1	B	175	ASN
1	B	184	ASN
1	B	195	ASN
2	C	30	HIS
2	C	81	ASN
2	C	83	GLN
2	C	223	ASN
2	C	276	GLN
2	D	8	GLN
2	D	83	GLN
2	D	134	GLN
2	D	172	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	276	GLN
2	E	30	HIS
2	E	134	GLN
2	E	150	GLN
2	E	223	ASN
2	E	276	GLN
2	G	8	GLN
2	G	203	ASN
2	G	223	ASN
2	G	225	GLN
2	G	265	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	406/445 (91%)	-0.13	13 (3%)	50	45	356, 356, 356, 356	0
1	B	406/445 (91%)	-0.13	11 (2%)	56	48	356, 356, 356, 356	0
1	I	406/445 (91%)	-0.25	7 (1%)	69	58	357, 357, 357, 357	0
1	J	406/445 (91%)	-0.29	6 (1%)	72	60	357, 357, 357, 357	0
2	C	268/288 (93%)	-0.18	7 (2%)	57	48	371, 371, 371, 371	0
2	D	268/288 (93%)	-0.32	2 (0%)	84	73	371, 371, 371, 371	0
2	E	268/288 (93%)	-0.14	8 (2%)	52	45	371, 371, 371, 371	0
2	G	268/288 (93%)	-0.34	2 (0%)	84	73	371, 371, 371, 371	0
All	All	2696/2932 (91%)	-0.22	56 (2%)	63	54	356, 357, 371, 371	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	43	LYS	6.5
2	E	254	VAL	5.9
1	B	71	GLN	4.9
1	I	322	ILE	4.8
2	C	254	VAL	4.6
2	C	134	GLN	3.8
1	A	232	LEU	3.7
1	A	361	ILE	3.5
1	A	86	ILE	3.5
1	B	326	VAL	3.4
1	B	322	ILE	3.4
1	B	42	THR	3.3
1	B	210	THR	3.2
2	E	248	ASN	3.1
1	A	216	MET	3.1
1	A	338	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	78	THR	3.0
1	A	159	SER	3.0
2	C	130	VAL	2.9
2	C	127	ASP	2.9
2	C	131	LYS	2.9
2	D	60	GLU	2.9
1	B	241	ILE	2.8
1	A	75	PHE	2.8
1	B	70	THR	2.8
1	B	213	PHE	2.8
2	E	255	LEU	2.8
1	A	371	ILE	2.7
1	A	368	ALA	2.7
1	B	67	ASP	2.7
1	A	215	VAL	2.7
2	C	108	TYR	2.6
1	I	164	ALA	2.6
1	B	99	VAL	2.6
1	J	321	VAL	2.5
1	I	323	LEU	2.5
1	J	135	LEU	2.4
2	G	57	ALA	2.4
1	J	343	ILE	2.4
2	D	83	GLN	2.3
1	I	349	ILE	2.3
1	J	326	VAL	2.3
1	J	96	VAL	2.3
1	I	321	VAL	2.3
2	E	224	ILE	2.2
2	E	228	THR	2.2
2	C	132	ILE	2.2
1	J	129	LEU	2.2
1	A	326	VAL	2.2
2	G	88	THR	2.2
2	E	132	ILE	2.2
1	I	90	GLY	2.1
1	I	20	LEU	2.1
1	A	82	GLY	2.1
2	E	250	TYR	2.1
2	E	265	HIS	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.