



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:11 PM UTC

PDB ID : 1EWV / pdb_00001ewv
Title : CRYSTAL STRUCTURE OF METABOTROPIC GLUTAMATE RECEPTOR SUBTYPE 1 LIGAND FREE FORM II
Authors : Kunishima, N.; Shimada, Y.; Tsuji, Y.; Jingami, H.; Morikawa, K.
Deposited on : 2000-04-27
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

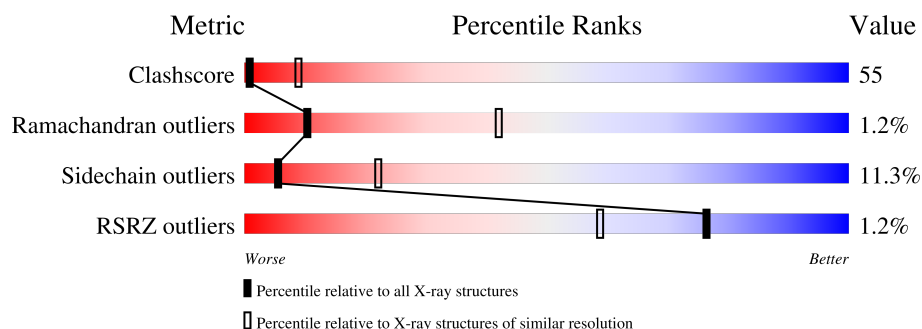
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	490	
1	B	490	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7120 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.

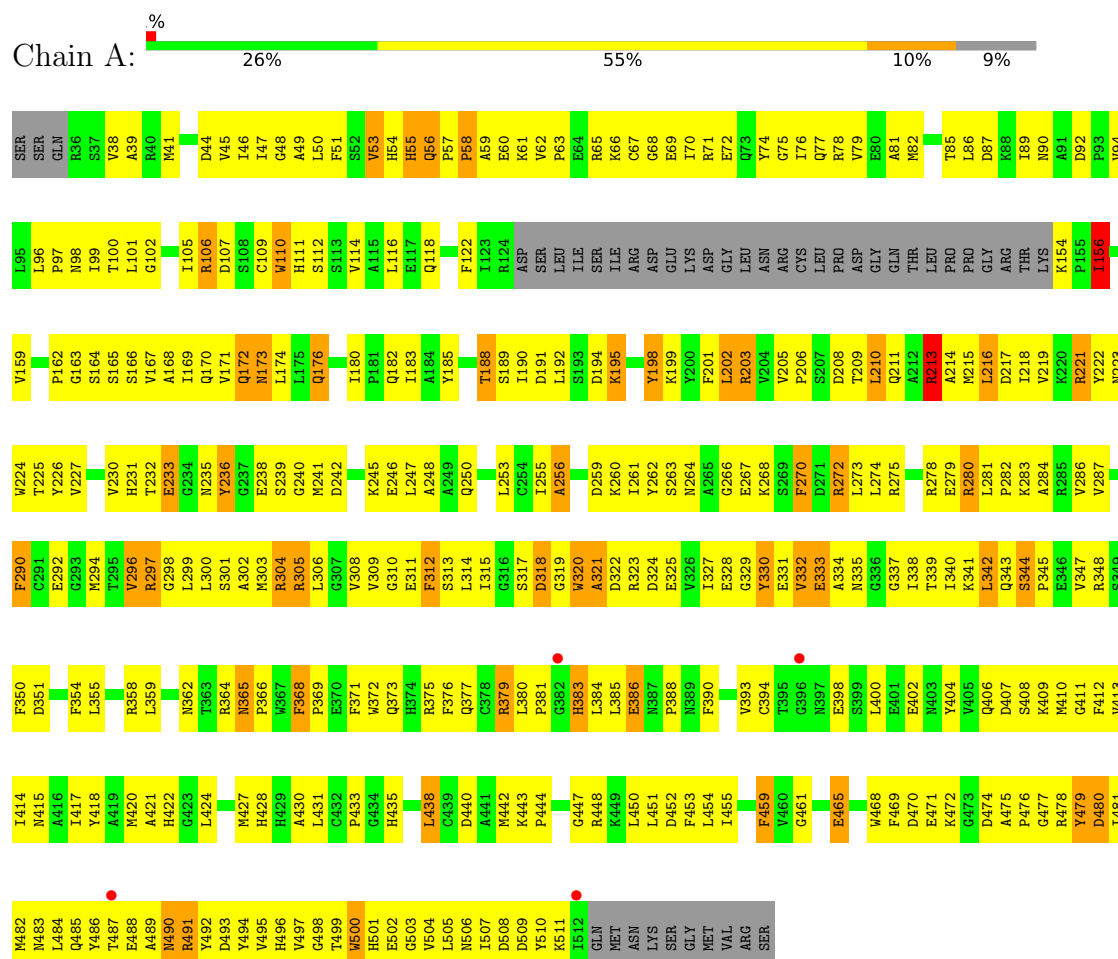
- Molecule 1 is a protein called METABOTROPIC GLUTAMATE RECEPTOR SUBTYPE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3560	2258	620	662	20			
1	B	448	Total	C	N	O	S	0	0	0
			3560	2258	620	662	20			

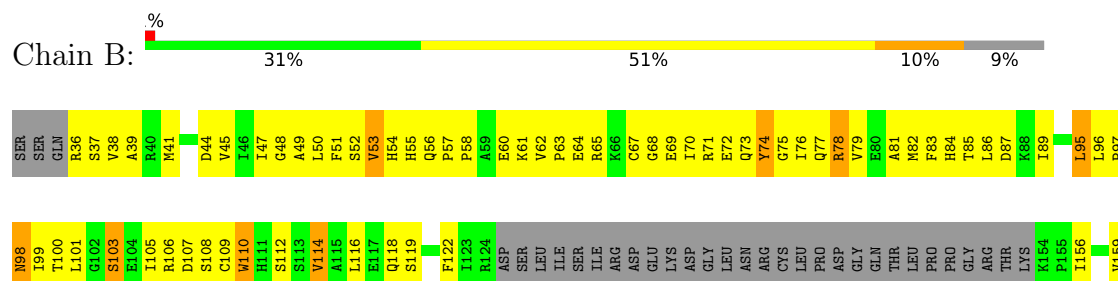
3 Residue-property plots

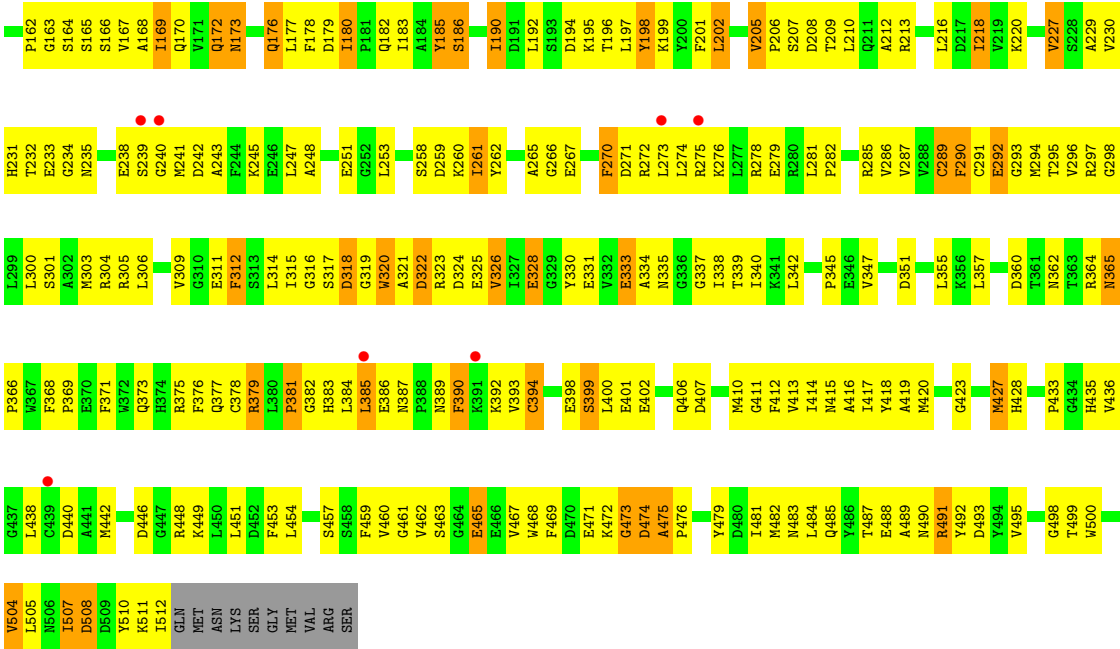
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: METABOTROPIC GLUTAMATE RECEPTOR SUBTYPE 1



• Molecule 1: METABOTROPIC GLUTAMATE RECEPTOR SUBTYPE 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.79Å 94.53Å 95.45Å 90.00° 113.20° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 20.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	89.1 (20.00-4.00) 88.8 (20.00-4.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 3.94Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.254 , 0.328 0.242 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	7120	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.92	6/3640 (0.2%)	1.32	24/4923 (0.5%)
1	B	0.84	2/3640 (0.1%)	1.30	15/4923 (0.3%)
All	All	0.88	8/7280 (0.1%)	1.31	39/9846 (0.4%)

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	B	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	TRP	NE1-CE2	10.49	1.49	1.37
1	A	500	TRP	NE1-CE2	10.41	1.49	1.37
1	A	372	TRP	NE1-CE2	10.40	1.48	1.37
1	A	468	TRP	NE1-CE2	10.40	1.48	1.37
1	B	110	TRP	NE1-CE2	10.39	1.48	1.37
1	A	320	TRP	NE1-CE2	10.37	1.48	1.37
1	B	320	TRP	NE1-CE2	10.37	1.48	1.37
1	A	110	TRP	NE1-CE2	10.32	1.48	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	VAL	N-CA-C	8.64	119.20	110.82
1	B	290	PHE	N-CA-C	-7.88	101.86	112.26
1	B	504	VAL	N-CA-C	7.40	118.78	108.12
1	B	292	GLU	N-CA-C	-6.78	99.55	110.32
1	A	154	LYS	CA-C-N	6.73	128.26	119.84
1	A	154	LYS	C-N-CA	6.73	128.26	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	VAL	CB-CA-C	-6.70	103.27	112.04
1	B	365	ASN	CA-C-N	6.62	126.32	119.56
1	B	365	ASN	C-N-CA	6.62	126.32	119.56
1	A	365	ASN	CA-C-N	6.33	126.01	119.56
1	A	365	ASN	C-N-CA	6.33	126.01	119.56
1	B	337	GLY	N-CA-C	5.99	119.69	111.54
1	A	180	ILE	N-CA-C	5.80	113.62	107.76
1	A	58	PRO	N-CA-CB	5.65	108.27	103.35
1	B	320	TRP	N-CA-C	-5.64	104.77	111.03
1	B	479	TYR	N-CA-C	5.56	118.53	109.24
1	B	37	SER	N-CA-C	5.54	118.27	109.96
1	A	180	ILE	CB-CA-C	-5.52	104.80	110.71
1	A	348	ARG	CD-NE-CZ	-5.33	116.93	124.40
1	B	103	SER	N-CA-C	5.30	117.45	109.23
1	A	297	ARG	N-CA-C	-5.30	105.19	110.97
1	B	491	ARG	CD-NE-CZ	-5.29	116.99	124.40
1	B	289	CYS	N-CA-C	5.29	117.04	108.26
1	A	106	ARG	CD-NE-CZ	-5.27	117.02	124.40
1	B	381	PRO	N-CA-CB	5.23	107.96	103.31
1	A	321	ALA	CB-CA-C	-5.21	110.15	117.23
1	A	213	ARG	CD-NE-CZ	-5.17	117.16	124.40
1	A	345	PRO	N-CA-CB	5.17	107.84	103.19
1	A	65	ARG	CD-NE-CZ	-5.15	117.19	124.40
1	A	203	ARG	CD-NE-CZ	-5.15	117.19	124.40
1	B	499	THR	N-CA-C	5.14	117.06	108.99
1	A	304	ARG	CD-NE-CZ	-5.13	117.21	124.40
1	A	272	ARG	CD-NE-CZ	-5.13	117.21	124.40
1	B	78	ARG	CD-NE-CZ	-5.11	117.25	124.40
1	A	379	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	A	221	ARG	CD-NE-CZ	-5.05	117.33	124.40
1	A	55	HIS	CA-CB-CG	-5.04	108.76	113.80
1	A	156	ILE	N-CA-C	5.03	116.87	109.63
1	A	305	ARG	CD-NE-CZ	-5.02	117.37	124.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	74	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	3560	0	3485	406	0
1	B	3560	0	3485	371	0
All	All	7120	0	6970	775	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 55.

All (775) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:PRO:CG	1:A:477:GLY:HA3	1.69	1.21
1:A:206:PRO:HG3	1:A:477:GLY:CA	1.74	1.17
1:B:190:ILE:H	1:B:190:ILE:HD12	1.04	1.14
1:A:162:PRO:HG3	1:A:171:VAL:HG21	1.29	1.10
1:B:240:GLY:C	1:B:290:PHE:CE1	2.32	1.07
1:A:475:ALA:HB1	1:A:476:PRO:HD2	1.23	1.07
1:B:475:ALA:HB1	1:B:476:PRO:HD2	1.30	1.07
1:A:195:LYS:HG3	1:A:199:LYS:HA	1.41	1.03
1:A:236:TYR:HD2	1:A:236:TYR:C	1.68	1.01
1:A:192:LEU:HD13	1:A:201:PHE:CZ	1.98	0.98
1:A:280:ARG:HH22	1:A:283:LYS:HB2	1.29	0.97
1:A:461:GLY:HA3	1:A:465:GLU:HG2	1.48	0.96
1:B:240:GLY:HA3	1:B:290:PHE:CZ	2.02	0.94
1:A:236:TYR:C	1:A:236:TYR:CD2	2.41	0.92
1:A:162:PRO:HG3	1:A:171:VAL:CG2	1.99	0.92
1:A:475:ALA:HB1	1:A:476:PRO:CD	1.99	0.92
1:B:475:ALA:HB1	1:B:476:PRO:CD	2.00	0.91
1:B:400:LEU:H	1:B:400:LEU:HD12	1.35	0.90
1:B:240:GLY:CA	1:B:290:PHE:CE1	2.55	0.90
1:B:109:CYS:SG	1:B:114:VAL:HG11	2.11	0.90
1:B:240:GLY:HA3	1:B:290:PHE:CE1	2.08	0.89
1:A:206:PRO:HG3	1:A:477:GLY:HA3	0.91	0.89
1:A:162:PRO:CG	1:A:171:VAL:HG21	2.02	0.88
1:A:381:PRO:HA	1:A:386:GLU:HG3	1.56	0.87
1:B:190:ILE:HD12	1:B:190:ILE:N	1.89	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLN:HA	1:B:172:GLN:HE21	1.39	0.86
1:B:185:TYR:CD2	1:B:185:TYR:N	2.42	0.86
1:B:185:TYR:HB2	1:B:412:PHE:HB3	1.58	0.86
1:B:287:VAL:HB	1:B:314:LEU:HD23	1.57	0.85
1:B:190:ILE:H	1:B:190:ILE:CD1	1.82	0.85
1:B:180:ILE:HD12	1:B:180:ILE:N	1.90	0.85
1:A:301:SER:HA	1:A:330:TYR:HE2	1.38	0.84
1:A:227:VAL:O	1:A:255:ILE:HG23	1.77	0.84
1:A:301:SER:HA	1:A:330:TYR:CE2	2.13	0.84
1:A:188:THR:O	1:A:208:ASP:CG	2.20	0.83
1:A:188:THR:HB	1:A:208:ASP:OD1	1.79	0.83
1:A:287:VAL:HB	1:A:314:LEU:HD23	1.60	0.83
1:B:205:VAL:HG23	1:B:206:PRO:HD2	1.60	0.83
1:A:236:TYR:HD2	1:A:236:TYR:O	1.60	0.82
1:B:379:ARG:NH2	1:B:381:PRO:HA	1.95	0.82
1:A:45:VAL:HB	1:A:101:LEU:HD23	1.59	0.81
1:B:192:LEU:HA	1:B:198:TYR:CE2	2.15	0.81
1:A:461:GLY:HA3	1:A:465:GLU:CG	2.09	0.81
1:A:116:LEU:HD23	1:B:177:LEU:HD11	1.62	0.81
1:B:192:LEU:HA	1:B:198:TYR:CD2	2.16	0.81
1:B:261:ILE:HG21	1:B:295:THR:HG23	1.63	0.81
1:B:415:ASN:HD22	1:B:467:VAL:HG21	1.45	0.80
1:A:488:GLU:CD	1:A:488:GLU:H	1.89	0.80
1:B:285:ARG:HG2	1:B:312:PHE:HA	1.63	0.80
1:A:122:PHE:O	1:A:156:ILE:HD11	1.81	0.80
1:A:334:ALA:O	1:A:484:LEU:HD23	1.81	0.80
1:A:383:HIS:CD2	1:A:384:LEU:N	2.50	0.80
1:B:300:LEU:O	1:B:303:MET:HB2	1.82	0.80
1:A:375:ARG:O	1:A:375:ARG:HG3	1.82	0.79
1:B:119:SER:HA	1:B:122:PHE:HD2	1.48	0.79
1:B:227:VAL:HG12	1:B:286:VAL:HB	1.64	0.78
1:B:362:ASN:HD21	1:B:365:ASN:HB3	1.45	0.78
1:A:172:GLN:HB2	1:A:182:GLN:OE1	1.83	0.78
1:A:383:HIS:HD2	1:A:384:LEU:N	1.80	0.78
1:B:293:GLY:O	1:B:296:VAL:HB	1.84	0.78
1:B:508:ASP:HB3	1:B:511:LYS:HB3	1.64	0.77
1:A:309:VAL:HG12	1:A:310:GLY:H	1.48	0.77
1:A:236:TYR:CD2	1:A:236:TYR:O	2.36	0.77
1:B:178:PHE:HB2	1:B:180:ILE:HD11	1.65	0.77
1:A:195:LYS:HD2	1:A:472:LYS:O	1.85	0.77
1:A:195:LYS:HE3	1:A:195:LYS:HA	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLN:HE22	1:A:386:GLU:HA	1.50	0.76
1:A:109:CYS:SG	1:A:114:VAL:HG11	2.26	0.76
1:B:185:TYR:H	1:B:185:TYR:HD2	1.31	0.75
1:B:270:PHE:CE1	1:B:298:GLY:HA3	2.20	0.75
1:B:185:TYR:CE1	1:B:413:VAL:HG22	2.23	0.74
1:B:185:TYR:N	1:B:185:TYR:HD2	1.80	0.74
1:B:190:ILE:HD11	1:B:239:SER:O	1.87	0.74
1:B:230:VAL:HG11	1:B:273:LEU:HD21	1.69	0.74
1:B:379:ARG:NH1	1:B:379:ARG:HB2	2.01	0.74
1:A:359:LEU:HD21	1:A:380:LEU:HD13	1.70	0.74
1:B:169:ILE:O	1:B:173:ASN:HB2	1.86	0.73
1:A:189:SER:HA	1:A:208:ASP:OD2	1.88	0.73
1:A:270:PHE:O	1:A:273:LEU:HB3	1.88	0.73
1:B:67:CYS:SG	1:B:114:VAL:HG21	2.29	0.73
1:A:156:ILE:HD13	1:A:156:ILE:H	1.53	0.73
1:B:285:ARG:CG	1:B:312:PHE:HA	2.19	0.72
1:A:210:LEU:N	1:A:210:LEU:HD23	2.03	0.72
1:B:357:LEU:HD13	1:B:368:PHE:HZ	1.54	0.72
1:A:500:TRP:HD1	1:A:505:LEU:HD13	1.53	0.72
1:B:172:GLN:HE21	1:B:172:GLN:CA	2.01	0.72
1:B:183:ILE:HA	1:B:202:LEU:O	1.89	0.72
1:A:55:HIS:CD2	1:A:71:ARG:HD2	2.24	0.72
1:B:373:GLN:O	1:B:377:GLN:N	2.22	0.71
1:A:192:LEU:HD23	1:A:198:TYR:CD2	2.26	0.71
1:B:95:LEU:HD11	1:B:96:LEU:HG	1.72	0.71
1:B:231:HIS:CE1	1:B:260:LYS:HG2	2.25	0.71
1:B:85:THR:HG21	1:B:417:ILE:HG21	1.72	0.71
1:A:248:ALA:HB1	1:A:253:LEU:HB3	1.72	0.70
1:B:85:THR:O	1:B:89:ILE:HG13	1.90	0.70
1:A:270:PHE:CE1	1:A:298:GLY:HA3	2.27	0.70
1:B:84:HIS:O	1:B:87:ASP:HB2	1.90	0.70
1:B:483:ASN:OD1	1:B:512:ILE:HG23	1.92	0.70
1:A:507:ILE:HG22	1:A:508:ASP:N	2.05	0.70
1:B:229:ALA:HB1	1:B:241:MET:CE	2.21	0.70
1:B:261:ILE:CG2	1:B:295:THR:HG23	2.21	0.70
1:A:451:LEU:O	1:A:454:LEU:N	2.20	0.70
1:B:375:ARG:HG3	1:B:375:ARG:HH11	1.55	0.69
1:B:274:LEU:HG	1:B:278:ARG:HD2	1.72	0.69
1:B:58:PRO:O	1:B:62:VAL:HG23	1.92	0.69
1:B:301:SER:HA	1:B:330:TYR:HE2	1.57	0.69
1:A:227:VAL:O	1:A:255:ILE:HD12	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LEU:HD22	1:B:201:PHE:CZ	2.28	0.69
1:B:240:GLY:C	1:B:290:PHE:CD1	2.70	0.69
1:B:369:PRO:HB2	1:B:385:LEU:HD12	1.75	0.69
1:A:76:ILE:HG13	1:A:371:PHE:CG	2.28	0.69
1:A:376:PHE:CE2	1:A:398:GLU:HB3	2.28	0.69
1:B:112:SER:O	1:B:116:LEU:HB2	1.93	0.69
1:A:475:ALA:CB	1:A:476:PRO:HD2	2.13	0.69
1:A:461:GLY:N	1:A:465:GLU:O	2.26	0.69
1:B:210:LEU:HD11	1:B:500:TRP:HH2	1.58	0.68
1:A:375:ARG:HG2	1:A:376:PHE:CZ	2.29	0.68
1:B:240:GLY:O	1:B:290:PHE:HE1	1.76	0.68
1:A:230:VAL:HA	1:A:259:ASP:O	1.92	0.68
1:A:240:GLY:HA3	1:A:290:PHE:CE2	2.28	0.68
1:A:278:ARG:HB3	1:A:278:ARG:NH1	2.08	0.68
1:A:62:VAL:N	1:A:63:PRO:CD	2.57	0.68
1:A:183:ILE:HA	1:A:202:LEU:O	1.94	0.68
1:B:163:GLY:HA2	1:B:186:SER:OG	1.94	0.68
1:B:304:ARG:HG2	1:B:304:ARG:HH11	1.58	0.68
1:B:119:SER:HA	1:B:122:PHE:CD2	2.29	0.67
1:B:427:MET:SD	1:B:442:MET:HE3	2.34	0.67
1:B:162:PRO:HG3	1:B:167:VAL:HG12	1.76	0.67
1:A:342:LEU:HA	1:A:479:TYR:HB3	1.77	0.67
1:B:275:ARG:O	1:B:279:GLU:HG3	1.95	0.67
1:A:47:ILE:HD13	1:A:420:MET:HG3	1.77	0.67
1:A:280:ARG:HH22	1:A:283:LYS:CB	2.07	0.67
1:B:73:GLN:H	1:B:73:GLN:NE2	1.92	0.67
1:A:110:TRP:CZ2	1:A:164:SER:HB2	2.30	0.67
1:B:172:GLN:HG2	1:B:198:TYR:HB3	1.77	0.67
1:A:164:SER:HB3	1:A:167:VAL:HG23	1.77	0.67
1:A:76:ILE:HG13	1:A:371:PHE:CD1	2.30	0.66
1:A:383:HIS:CD2	1:A:383:HIS:C	2.74	0.66
1:B:266:GLY:O	1:B:270:PHE:HB2	1.95	0.66
1:B:301:SER:HA	1:B:330:TYR:CE2	2.31	0.66
1:B:454:LEU:O	1:B:457:SER:HB2	1.95	0.66
1:A:459:PHE:N	1:A:459:PHE:CD2	2.61	0.66
1:B:82:MET:HG2	1:B:105:ILE:HD11	1.77	0.66
1:A:188:THR:O	1:A:208:ASP:OD1	2.14	0.66
1:A:202:LEU:N	1:A:202:LEU:HD23	2.11	0.66
1:B:322:ASP:CG	1:B:322:ASP:O	2.38	0.66
1:A:206:PRO:CB	1:A:477:GLY:HA3	2.25	0.66
1:A:281:LEU:HB3	1:A:282:PRO:HA	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ASP:C	1:A:470:ASP:OD2	2.38	0.66
1:B:342:LEU:HD21	1:B:412:PHE:HE2	1.60	0.66
1:A:60:GLU:CD	1:A:60:GLU:H	2.04	0.65
1:A:290:PHE:CD1	1:A:317:SER:HB3	2.31	0.65
1:A:491:ARG:HD2	1:A:492:TYR:O	1.96	0.65
1:B:48:GLY:H	1:B:156:ILE:HG23	1.60	0.65
1:A:45:VAL:HG11	1:A:424:LEU:HD11	1.78	0.65
1:B:109:CYS:HB2	1:B:114:VAL:HG11	1.79	0.65
1:B:312:PHE:CD2	1:B:312:PHE:N	2.60	0.65
1:A:62:VAL:N	1:A:63:PRO:HD3	2.12	0.65
1:A:309:VAL:HG12	1:A:310:GLY:N	2.10	0.65
1:A:339:THR:OG1	1:A:482:MET:HB2	1.96	0.65
1:A:491:ARG:NH1	1:A:492:TYR:O	2.28	0.65
1:A:347:VAL:HG12	1:A:350:PHE:H	1.61	0.65
1:B:109:CYS:CB	1:B:114:VAL:HG11	2.25	0.65
1:A:278:ARG:HB3	1:A:278:ARG:HH11	1.58	0.65
1:B:281:LEU:HB3	1:B:282:PRO:HA	1.77	0.65
1:A:483:ASN:HD22	1:A:484:LEU:H	1.45	0.65
1:A:195:LYS:HE2	1:A:198:TYR:O	1.96	0.64
1:B:216:LEU:C	1:B:216:LEU:HD23	2.22	0.64
1:A:54:HIS:HD2	1:A:70:ILE:HD12	1.62	0.64
1:A:270:PHE:CZ	1:A:298:GLY:HA3	2.33	0.64
1:B:202:LEU:HD23	1:B:202:LEU:N	2.11	0.64
1:B:240:GLY:C	1:B:290:PHE:HE1	2.01	0.64
1:B:95:LEU:CD1	1:B:96:LEU:HG	2.26	0.64
1:A:327:ILE:HD12	1:A:328:GLU:N	2.12	0.64
1:A:332:VAL:HB	1:A:333:GLU:OE2	1.97	0.64
1:B:216:LEU:HD23	1:B:216:LEU:O	1.98	0.64
1:B:240:GLY:O	1:B:290:PHE:CE1	2.50	0.64
1:A:211:GLN:HG3	1:A:340:ILE:HG21	1.80	0.64
1:A:218:ILE:HD11	1:A:481:ILE:HD12	1.79	0.64
1:A:51:PHE:CD1	1:A:78:ARG:HB3	2.34	0.63
1:B:306:LEU:O	1:B:306:LEU:HD12	1.97	0.63
1:B:510:TYR:CD1	1:B:510:TYR:C	2.76	0.63
1:A:210:LEU:HB2	1:A:479:TYR:OH	1.97	0.63
1:B:72:GLU:H	1:B:73:GLN:NE2	1.96	0.63
1:A:327:ILE:HD12	1:A:327:ILE:C	2.23	0.63
1:A:169:ILE:O	1:A:173:ASN:HB2	1.99	0.63
1:A:305:ARG:NH1	1:A:305:ARG:HG3	2.14	0.63
1:A:500:TRP:CZ2	1:A:503:GLY:HA2	2.33	0.63
1:B:300:LEU:HD13	1:B:334:ALA:HB2	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:HE3	1:A:195:LYS:CA	2.24	0.63
1:A:309:VAL:HG11	1:A:333:GLU:HA	1.81	0.63
1:B:362:ASN:ND2	1:B:365:ASN:HB3	2.12	0.63
1:B:382:GLY:N	1:B:386:GLU:OE1	2.32	0.63
1:A:300:LEU:O	1:A:303:MET:HB2	1.99	0.62
1:B:312:PHE:H	1:B:312:PHE:HD2	1.46	0.62
1:B:65:ARG:HG3	1:B:65:ARG:HH11	1.64	0.62
1:B:199:LYS:NZ	1:B:448:ARG:HH12	1.97	0.62
1:B:261:ILE:HD11	1:B:265:ALA:HB3	1.80	0.62
1:B:400:LEU:HD12	1:B:400:LEU:N	2.13	0.62
1:B:508:ASP:HB3	1:B:511:LYS:CB	2.30	0.62
1:B:82:MET:CG	1:B:105:ILE:HD11	2.30	0.62
1:B:85:THR:CG2	1:B:417:ILE:HG21	2.29	0.61
1:A:306:LEU:O	1:A:308:VAL:HG13	2.00	0.61
1:A:483:ASN:HD22	1:A:484:LEU:N	1.98	0.61
1:B:508:ASP:CB	1:B:511:LYS:HB3	2.30	0.61
1:A:71:ARG:O	1:A:76:ILE:HG12	1.99	0.61
1:B:47:ILE:CG2	1:B:420:MET:HG2	2.31	0.61
1:B:195:LYS:HG3	1:B:472:LYS:O	1.99	0.61
1:A:89:ILE:HD11	1:A:418:TYR:CD2	2.35	0.61
1:A:342:LEU:H	1:A:342:LEU:HD12	1.66	0.61
1:B:50:LEU:HD21	1:B:122:PHE:HE2	1.64	0.61
1:A:275:ARG:HG2	1:A:279:GLU:OE1	2.00	0.61
1:A:232:THR:HG21	1:A:292:GLU:HB2	1.82	0.61
1:A:451:LEU:O	1:A:452:ASP:C	2.43	0.61
1:A:85:THR:O	1:A:89:ILE:HG13	2.00	0.60
1:A:414:ILE:O	1:A:417:ILE:HB	2.00	0.60
1:A:485:GLN:HE21	1:A:495:VAL:HG21	1.66	0.60
1:B:65:ARG:HG3	1:B:65:ARG:NH1	2.16	0.60
1:B:73:GLN:H	1:B:73:GLN:CD	2.09	0.60
1:A:82:MET:CG	1:A:105:ILE:HD11	2.31	0.60
1:A:156:ILE:H	1:A:156:ILE:CD1	2.11	0.60
1:A:459:PHE:N	1:A:459:PHE:HD2	1.98	0.60
1:A:497:VAL:O	1:A:507:ILE:HG23	2.01	0.60
1:A:213:ARG:CG	1:A:213:ARG:HH11	2.14	0.60
1:A:89:ILE:CG1	1:A:418:TYR:HE2	2.15	0.60
1:A:226:TYR:HE2	1:A:280:ARG:NH2	1.99	0.60
1:A:471:GLU:HG3	1:A:472:LYS:N	2.17	0.60
1:A:280:ARG:HH21	1:A:284:ALA:HB2	1.66	0.60
1:B:178:PHE:HB2	1:B:180:ILE:CD1	2.31	0.60
1:B:241:MET:N	1:B:290:PHE:CD1	2.69	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:ARG:NH1	1:B:379:ARG:CB	2.65	0.60
1:A:185:TYR:O	1:A:205:VAL:HG11	2.01	0.60
1:A:172:GLN:NE2	1:A:201:PHE:HB2	2.17	0.59
1:A:240:GLY:HA3	1:A:290:PHE:HE2	1.66	0.59
1:B:393:VAL:HG12	1:B:394:CYS:N	2.18	0.59
1:A:215:MET:O	1:A:219:VAL:HG23	2.03	0.59
1:B:240:GLY:CA	1:B:290:PHE:CZ	2.79	0.59
1:B:330:TYR:N	1:B:330:TYR:CD1	2.70	0.59
1:B:71:ARG:NH2	1:B:74:TYR:CD2	2.69	0.59
1:B:210:LEU:HD11	1:B:500:TRP:CH2	2.37	0.59
1:B:492:TYR:N	1:B:492:TYR:CD2	2.69	0.59
1:A:198:TYR:CD1	1:A:198:TYR:N	2.70	0.59
1:A:227:VAL:HG23	1:A:255:ILE:CD1	2.33	0.59
1:B:179:ASP:C	1:B:180:ILE:HD12	2.27	0.59
1:A:54:HIS:CD2	1:A:70:ILE:HD12	2.38	0.58
1:B:270:PHE:CZ	1:B:298:GLY:HA3	2.37	0.58
1:A:47:ILE:HD13	1:A:420:MET:CG	2.32	0.58
1:B:60:GLU:HG2	1:B:61:LYS:N	2.16	0.58
1:B:248:ALA:HB1	1:B:253:LEU:HB3	1.86	0.58
1:A:375:ARG:NH2	1:A:402:GLU:O	2.36	0.58
1:B:36:ARG:HD2	1:B:118:GLN:NE2	2.19	0.58
1:B:162:PRO:HG3	1:B:167:VAL:CG1	2.33	0.58
1:B:194:ASP:OD2	1:B:194:ASP:C	2.45	0.58
1:A:59:ALA:O	1:A:62:VAL:HG23	2.04	0.58
1:A:488:GLU:HG2	1:A:489:ALA:N	2.19	0.58
1:B:376:PHE:CE1	1:B:398:GLU:HB2	2.38	0.58
1:B:233:GLU:HB3	1:B:262:TYR:CD2	2.38	0.57
1:B:232:THR:HG21	1:B:292:GLU:HG3	1.87	0.57
1:B:379:ARG:HH22	1:B:381:PRO:HA	1.68	0.57
1:A:226:TYR:O	1:A:227:VAL:HG13	2.04	0.57
1:B:47:ILE:HD13	1:B:420:MET:CG	2.33	0.57
1:A:427:MET:O	1:A:430:ALA:N	2.35	0.57
1:A:55:HIS:N	1:A:69:GLU:O	2.35	0.57
1:B:351:ASP:O	1:B:355:LEU:HG	2.03	0.57
1:B:412:PHE:O	1:B:413:VAL:C	2.46	0.57
1:B:320:TRP:CD1	1:B:320:TRP:C	2.80	0.57
1:A:305:ARG:HG3	1:A:305:ARG:HH11	1.70	0.57
1:B:375:ARG:HG3	1:B:375:ARG:NH1	2.19	0.57
1:B:483:ASN:HD22	1:B:484:LEU:H	1.53	0.57
1:A:218:ILE:CD1	1:A:481:ILE:HD12	2.35	0.57
1:B:86:LEU:HA	1:B:89:ILE:HD12	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:PHE:CB	1:B:180:ILE:HD11	2.34	0.56
1:B:192:LEU:HA	1:B:198:TYR:HE2	1.68	0.56
1:A:110:TRP:CE2	1:A:164:SER:HB2	2.40	0.56
1:B:321:ALA:HB3	1:B:323:ARG:HG3	1.87	0.56
1:B:510:TYR:HD1	1:B:510:TYR:O	1.87	0.56
1:A:213:ARG:HG3	1:A:213:ARG:NH1	2.19	0.56
1:A:301:SER:CB	1:A:305:ARG:HH22	2.19	0.56
1:A:317:SER:C	1:A:319:GLY:N	2.63	0.56
1:A:317:SER:O	1:A:319:GLY:N	2.37	0.56
1:B:172:GLN:CG	1:B:198:TYR:HB3	2.34	0.56
1:B:379:ARG:CB	1:B:379:ARG:HH11	2.18	0.56
1:A:507:ILE:CG2	1:A:508:ASP:N	2.68	0.56
1:A:211:GLN:N	1:A:479:TYR:OH	2.38	0.56
1:B:54:HIS:HD1	1:B:70:ILE:HA	1.69	0.56
1:B:471:GLU:HG3	1:B:472:LYS:H	1.70	0.56
1:A:192:LEU:HD13	1:A:201:PHE:CE2	2.41	0.56
1:A:499:THR:N	1:A:506:ASN:O	2.36	0.56
1:B:453:PHE:O	1:B:457:SER:OG	2.22	0.56
1:A:214:ALA:O	1:A:218:ILE:HG13	2.06	0.56
1:B:85:THR:HG22	1:B:89:ILE:HD11	1.88	0.56
1:A:54:HIS:HB3	1:A:68:GLY:O	2.05	0.56
1:A:188:THR:O	1:A:208:ASP:OD2	2.24	0.56
1:A:215:MET:HE3	1:A:340:ILE:HG13	1.88	0.56
1:B:197:LEU:C	1:B:198:TYR:CD1	2.84	0.56
1:A:82:MET:HG2	1:A:105:ILE:HD11	1.87	0.55
1:A:451:LEU:O	1:A:454:LEU:HB2	2.05	0.55
1:B:407:ASP:HB3	1:B:410:MET:HE2	1.88	0.55
1:A:233:GLU:HG2	1:A:260:LYS:HD2	1.88	0.55
1:A:359:LEU:HD21	1:A:380:LEU:CD1	2.37	0.55
1:B:71:ARG:O	1:B:75:GLY:HA3	2.07	0.55
1:B:304:ARG:HG2	1:B:304:ARG:NH1	2.22	0.55
1:B:507:ILE:HG23	1:B:508:ASP:N	2.22	0.55
1:A:167:VAL:O	1:A:171:VAL:HG23	2.06	0.55
1:A:203:ARG:NE	1:A:474:ASP:OD1	2.39	0.55
1:A:480:ASP:OD1	1:A:499:THR:HG22	2.06	0.55
1:B:48:GLY:O	1:B:159:VAL:HA	2.07	0.55
1:B:206:PRO:HB3	1:B:210:LEU:HD23	1.88	0.55
1:B:427:MET:HB2	1:B:453:PHE:CD2	2.42	0.55
1:A:45:VAL:O	1:A:102:GLY:N	2.36	0.55
1:A:256:ALA:HB1	1:A:280:ARG:HE	1.72	0.55
1:A:351:ASP:O	1:A:355:LEU:HG	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:GLY:HA3	1:A:507:ILE:HA	1.87	0.55
1:B:50:LEU:HD21	1:B:122:PHE:CE2	2.42	0.55
1:A:379:ARG:NH1	1:A:381:PRO:HG3	2.22	0.55
1:A:482:MET:SD	1:A:496:HIS:HA	2.47	0.55
1:A:317:SER:C	1:A:319:GLY:H	2.15	0.54
1:B:192:LEU:HA	1:B:198:TYR:HD2	1.70	0.54
1:B:379:ARG:O	1:B:393:VAL:HG13	2.07	0.54
1:B:165:SER:O	1:B:166:SER:C	2.50	0.54
1:B:71:ARG:NH2	1:B:74:TYR:HD2	2.05	0.54
1:B:78:ARG:O	1:B:82:MET:N	2.38	0.54
1:A:210:LEU:N	1:A:210:LEU:CD2	2.70	0.54
1:B:192:LEU:O	1:B:195:LYS:HE3	2.08	0.54
1:A:375:ARG:NH2	1:A:400:LEU:O	2.40	0.54
1:B:97:PRO:HB2	1:B:98:ASN:OD1	2.07	0.54
1:B:47:ILE:HG21	1:B:420:MET:HG2	1.90	0.54
1:A:67:CYS:SG	1:A:114:VAL:HG11	2.48	0.54
1:A:422:HIS:NE2	1:A:459:PHE:CD1	2.76	0.53
1:A:480:ASP:HB3	1:A:496:HIS:NE2	2.23	0.53
1:B:216:LEU:HD21	1:B:220:LYS:HD2	1.89	0.53
1:B:234:GLY:O	1:B:238:GLU:CB	2.56	0.53
1:A:266:GLY:C	1:A:268:LYS:N	2.66	0.53
1:B:261:ILE:CG2	1:B:295:THR:CG2	2.87	0.53
1:B:481:ILE:HG12	1:B:498:GLY:O	2.08	0.53
1:A:341:LYS:C	1:A:479:TYR:HB3	2.34	0.53
1:A:48:GLY:O	1:A:159:VAL:HA	2.08	0.53
1:A:491:ARG:HD2	1:A:492:TYR:C	2.33	0.53
1:B:232:THR:H	1:B:291:CYS:HA	1.73	0.53
1:A:169:ILE:HD12	1:A:192:LEU:HD21	1.89	0.53
1:A:315:ILE:HA	1:A:338:ILE:O	2.08	0.53
1:B:301:SER:O	1:B:305:ARG:HB2	2.07	0.53
1:B:235:ASN:O	1:B:239:SER:HB2	2.08	0.53
1:B:475:ALA:CB	1:B:476:PRO:HD2	2.20	0.53
1:B:467:VAL:HG12	1:B:468:TRP:N	2.24	0.53
1:A:259:ASP:OD1	1:A:260:LYS:N	2.42	0.52
1:B:207:SER:HB2	1:B:474:ASP:OD2	2.09	0.52
1:A:75:GLY:O	1:A:79:VAL:HG23	2.10	0.52
1:A:383:HIS:HD2	1:A:384:LEU:H	1.56	0.52
1:B:491:ARG:HG2	1:B:492:TYR:N	2.22	0.52
1:A:461:GLY:CA	1:A:465:GLU:HG2	2.31	0.52
1:B:276:LYS:O	1:B:279:GLU:HB2	2.10	0.52
1:B:483:ASN:HD22	1:B:484:LEU:N	2.06	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASP:OD2	1:A:364:ARG:NH1	2.36	0.52
1:B:79:VAL:HG13	1:B:105:ILE:HG21	1.92	0.52
1:A:213:ARG:CG	1:A:213:ARG:NH1	2.67	0.52
1:A:214:ALA:HB2	1:A:500:TRP:CE2	2.45	0.52
1:A:329:GLY:C	1:A:331:GLU:H	2.17	0.52
1:B:178:PHE:C	1:B:180:ILE:HD12	2.35	0.52
1:B:320:TRP:CD1	1:B:321:ALA:O	2.63	0.52
1:A:172:GLN:HG3	1:A:172:GLN:O	2.07	0.52
1:A:309:VAL:CG1	1:A:333:GLU:HA	2.39	0.52
1:A:428:HIS:HA	1:A:442:MET:HE1	1.91	0.52
1:A:480:ASP:HA	1:A:499:THR:HA	1.92	0.52
1:B:54:HIS:ND1	1:B:70:ILE:HA	2.24	0.52
1:A:45:VAL:O	1:A:46:ILE:HD13	2.09	0.52
1:A:164:SER:OG	1:A:165:SER:N	2.41	0.52
1:A:490:ASN:HD22	1:A:490:ASN:C	2.17	0.52
1:B:109:CYS:HB2	1:B:114:VAL:CG1	2.39	0.52
1:B:490:ASN:C	1:B:490:ASN:HD22	2.16	0.52
1:A:79:VAL:HG13	1:A:105:ILE:HG21	1.90	0.52
1:A:281:LEU:CB	1:A:282:PRO:HA	2.37	0.52
1:A:480:ASP:HB3	1:A:499:THR:HG22	1.92	0.52
1:A:221:ARG:HG3	1:A:222:TYR:CE2	2.45	0.51
1:A:318:ASP:HA	1:A:340:ILE:O	2.09	0.51
1:B:55:HIS:CE1	1:B:71:ARG:NE	2.78	0.51
1:B:345:PRO:HG2	1:B:463:SER:HB3	1.91	0.51
1:A:327:ILE:C	1:A:327:ILE:CD1	2.83	0.51
1:B:231:HIS:O	1:B:231:HIS:ND1	2.43	0.51
1:B:446:ASP:OD1	1:B:446:ASP:C	2.52	0.51
1:A:383:HIS:CD2	1:A:385:LEU:H	2.28	0.51
1:A:475:ALA:CB	1:A:476:PRO:CD	2.74	0.51
1:B:52:SER:O	1:B:75:GLY:HA2	2.10	0.51
1:B:475:ALA:CB	1:B:476:PRO:CD	2.79	0.51
1:A:301:SER:OG	1:A:305:ARG:NH2	2.40	0.51
1:A:162:PRO:HG3	1:A:167:VAL:HG12	1.92	0.51
1:A:164:SER:HB3	1:A:167:VAL:CG2	2.40	0.51
1:A:172:GLN:C	1:A:174:LEU:N	2.68	0.51
1:A:270:PHE:CE2	1:A:299:LEU:N	2.78	0.51
1:A:438:LEU:HD11	1:A:442:MET:HG2	1.92	0.51
1:B:315:ILE:HA	1:B:338:ILE:O	2.11	0.51
1:A:41:MET:HE1	1:A:364:ARG:HH11	1.75	0.51
1:A:319:GLY:O	1:A:323:ARG:NH1	2.44	0.51
1:B:261:ILE:HG23	1:B:261:ILE:O	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:LEU:CD1	1:B:334:ALA:HB2	2.40	0.51
1:A:61:LYS:C	1:A:63:PRO:HD2	2.35	0.50
1:B:119:SER:O	1:B:122:PHE:HB2	2.11	0.50
1:A:320:TRP:HZ2	1:A:327:ILE:CG2	2.24	0.50
1:B:399:SER:OG	1:B:401:GLU:HG3	2.10	0.50
1:B:462:VAL:HG22	1:B:462:VAL:O	2.12	0.50
1:A:45:VAL:HG11	1:A:424:LEU:CD1	2.42	0.50
1:A:489:ALA:O	1:A:491:ARG:N	2.44	0.50
1:B:393:VAL:HG12	1:B:394:CYS:H	1.77	0.50
1:A:172:GLN:O	1:A:176:GLN:HG2	2.12	0.50
1:A:227:VAL:HG12	1:A:286:VAL:HB	1.93	0.50
1:B:216:LEU:HD13	1:B:247:LEU:HB3	1.93	0.50
1:A:162:PRO:HG2	1:A:167:VAL:HB	1.94	0.50
1:A:331:GLU:HB3	1:A:492:TYR:CD2	2.46	0.50
1:B:201:PHE:C	1:B:202:LEU:HD23	2.37	0.50
1:A:343:GLN:O	1:A:343:GLN:HG2	2.12	0.50
1:B:428:HIS:HB2	1:B:442:MET:SD	2.52	0.50
1:A:44:ASP:OD2	1:A:100:THR:HG23	2.11	0.50
1:A:347:VAL:HG21	1:A:414:ILE:CD1	2.42	0.50
1:B:400:LEU:H	1:B:400:LEU:CD1	2.11	0.50
1:A:347:VAL:HG21	1:A:414:ILE:HD11	1.94	0.50
1:B:36:ARG:CD	1:B:118:GLN:NE2	2.75	0.50
1:B:347:VAL:H	1:B:406:GLN:HE22	1.60	0.50
1:A:393:VAL:HG12	1:A:394:CYS:H	1.77	0.49
1:B:86:LEU:HD23	1:B:89:ILE:HD12	1.94	0.49
1:A:85:THR:OG1	1:A:414:ILE:HG23	2.12	0.49
1:A:241:MET:O	1:A:245:LYS:HG3	2.13	0.49
1:A:324:ASP:HA	1:A:327:ILE:HD11	1.94	0.49
1:A:447:GLY:O	1:A:450:LEU:N	2.46	0.49
1:B:47:ILE:HG13	1:B:101:LEU:HD22	1.95	0.49
1:B:78:ARG:HA	1:B:81:ALA:HB3	1.94	0.49
1:B:270:PHE:HZ	1:B:295:THR:HA	1.77	0.49
1:B:481:ILE:HG12	1:B:498:GLY:C	2.37	0.49
1:A:61:LYS:C	1:A:63:PRO:CD	2.85	0.49
1:A:106:ARG:HD3	1:A:118:GLN:OE1	2.13	0.49
1:B:369:PRO:HB2	1:B:385:LEU:CD1	2.42	0.49
1:A:407:ASP:HB3	1:A:410:MET:HB2	1.95	0.49
1:A:486:TYR:OH	1:A:490:ASN:ND2	2.45	0.49
1:A:216:LEU:HD13	1:A:247:LEU:HB3	1.93	0.49
1:A:226:TYR:CD2	1:A:283:LYS:HB3	2.47	0.49
1:A:438:LEU:HG	1:A:442:MET:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:TYR:CE1	1:A:511:LYS:HG3	2.47	0.49
1:B:413:VAL:O	1:B:416:ALA:HB3	2.13	0.49
1:A:280:ARG:HH21	1:A:284:ALA:CB	2.26	0.49
1:A:450:LEU:HD12	1:A:450:LEU:O	2.12	0.49
1:A:201:PHE:C	1:A:202:LEU:HD23	2.37	0.49
1:A:322:ASP:HA	1:A:494:TYR:CE2	2.48	0.49
1:A:427:MET:HE3	1:A:450:LEU:HA	1.95	0.48
1:B:51:PHE:C	1:B:108:SER:OG	2.56	0.48
1:B:95:LEU:HD12	1:B:96:LEU:N	2.27	0.48
1:B:208:ASP:HB3	1:B:240:GLY:HA2	1.95	0.48
1:B:241:MET:C	1:B:243:ALA:N	2.70	0.48
1:B:484:LEU:HD12	1:B:493:ASP:O	2.13	0.48
1:A:56:GLN:HG3	1:A:57:PRO:O	2.14	0.48
1:A:74:TYR:O	1:A:78:ARG:HD2	2.13	0.48
1:A:156:ILE:HD13	1:A:156:ILE:N	2.26	0.48
1:A:221:ARG:HH12	1:A:507:ILE:HB	1.78	0.48
1:A:480:ASP:CB	1:A:499:THR:HG22	2.44	0.48
1:B:38:VAL:HG21	1:B:106:ARG:NH1	2.27	0.48
1:A:398:GLU:N	1:A:398:GLU:OE1	2.46	0.48
1:A:256:ALA:HB1	1:A:280:ARG:NE	2.29	0.48
1:B:53:VAL:HG23	1:B:107:ASP:OD2	2.13	0.48
1:A:57:PRO:HB3	1:A:66:LYS:O	2.12	0.48
1:A:225:THR:HA	1:A:253:LEU:CD1	2.44	0.48
1:B:190:ILE:CD1	1:B:239:SER:O	2.58	0.48
1:A:500:TRP:CH2	1:A:503:GLY:N	2.74	0.48
1:B:180:ILE:N	1:B:180:ILE:CD1	2.61	0.48
1:B:383:HIS:CD2	1:B:384:LEU:N	2.82	0.48
1:B:459:PHE:CD1	1:B:459:PHE:C	2.91	0.48
1:A:49:ALA:CB	1:A:82:MET:HE2	2.44	0.48
1:A:192:LEU:HD23	1:A:198:TYR:HD2	1.73	0.48
1:B:169:ILE:HG13	1:B:198:TYR:CZ	2.49	0.48
1:B:172:GLN:OE1	1:B:201:PHE:HB2	2.13	0.48
1:A:213:ARG:HA	1:A:247:LEU:CD1	2.44	0.47
1:B:233:GLU:HG2	1:B:262:TYR:CE2	2.49	0.47
1:B:47:ILE:HG23	1:B:420:MET:HG2	1.95	0.47
1:B:78:ARG:O	1:B:81:ALA:N	2.46	0.47
1:B:461:GLY:N	1:B:465:GLU:O	2.46	0.47
1:A:362:ASN:HD21	1:A:365:ASN:HB3	1.79	0.47
1:A:393:VAL:HG12	1:A:394:CYS:N	2.28	0.47
1:A:447:GLY:O	1:A:448:ARG:C	2.55	0.47
1:A:320:TRP:NE1	1:A:494:TYR:OH	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:HIS:CA	1:A:442:MET:HE1	2.45	0.47
1:B:55:HIS:ND1	1:B:71:ARG:HD2	2.29	0.47
1:B:82:MET:HG2	1:B:105:ILE:CD1	2.43	0.47
1:B:199:LYS:HZ1	1:B:448:ARG:HH12	1.63	0.47
1:B:207:SER:O	1:B:210:LEU:HB3	2.14	0.47
1:A:209:THR:O	1:A:213:ARG:HB2	2.14	0.47
1:B:281:LEU:HB3	1:B:282:PRO:CA	2.44	0.47
1:A:305:ARG:HH11	1:A:305:ARG:CG	2.26	0.47
1:A:431:LEU:C	1:A:433:PRO:HD3	2.39	0.47
1:A:329:GLY:O	1:A:331:GLU:N	2.46	0.47
1:A:369:PRO:CB	1:A:383:HIS:HE1	2.27	0.47
1:A:379:ARG:O	1:A:381:PRO:HD3	2.15	0.47
1:A:406:GLN:O	1:A:407:ASP:C	2.58	0.47
1:B:74:TYR:O	1:B:78:ARG:HD2	2.14	0.47
1:B:243:ALA:C	1:B:245:LYS:N	2.73	0.47
1:B:339:THR:OG1	1:B:482:MET:HB2	2.14	0.47
1:B:387:ASN:OD1	1:B:387:ASN:C	2.58	0.47
1:A:216:LEU:HD23	1:A:217:ASP:OD1	2.14	0.47
1:B:38:VAL:HG12	1:B:39:ALA:N	2.29	0.47
1:B:72:GLU:HB2	1:B:371:PHE:CE1	2.49	0.47
1:B:112:SER:O	1:B:116:LEU:CB	2.63	0.47
1:B:197:LEU:HB3	1:B:198:TYR:CE1	2.50	0.47
1:B:297:ARG:HG3	1:B:326:VAL:O	2.15	0.47
1:B:330:TYR:N	1:B:330:TYR:HD1	2.10	0.47
1:B:459:PHE:CE1	1:B:467:VAL:HB	2.50	0.47
1:A:89:ILE:HG12	1:A:418:TYR:HE2	1.80	0.47
1:A:270:PHE:CE2	1:A:298:GLY:C	2.93	0.47
1:A:507:ILE:CG2	1:A:508:ASP:H	2.28	0.47
1:B:234:GLY:O	1:B:238:GLU:HB3	2.15	0.47
1:B:345:PRO:HG2	1:B:463:SER:CB	2.45	0.47
1:A:500:TRP:CZ2	1:A:503:GLY:CA	2.98	0.46
1:B:54:HIS:HA	1:B:69:GLU:O	2.15	0.46
1:B:212:ALA:HB2	1:B:290:PHE:CE1	2.50	0.46
1:B:364:ARG:O	1:B:366:PRO:HD3	2.15	0.46
1:B:379:ARG:HB2	1:B:379:ARG:CZ	2.44	0.46
1:B:415:ASN:ND2	1:B:467:VAL:HG21	2.23	0.46
1:A:49:ALA:HB2	1:A:82:MET:HE2	1.95	0.46
1:A:38:VAL:HG12	1:A:39:ALA:N	2.29	0.46
1:A:364:ARG:O	1:A:366:PRO:HD3	2.16	0.46
1:A:452:ASP:C	1:A:454:LEU:H	2.23	0.46
1:A:280:ARG:NH2	1:A:284:ALA:H	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:GLU:CD	1:A:488:GLU:N	2.62	0.46
1:B:294:MET:SD	1:B:294:MET:N	2.89	0.46
1:B:196:THR:OG1	1:B:197:LEU:N	2.48	0.46
1:B:383:HIS:O	1:B:386:GLU:HB2	2.15	0.46
1:B:387:ASN:CG	1:B:390:PHE:CE1	2.93	0.46
1:B:469:PHE:N	1:B:469:PHE:CD1	2.82	0.46
1:A:47:ILE:CD1	1:A:420:MET:HG3	2.44	0.46
1:B:47:ILE:HD13	1:B:420:MET:HG3	1.97	0.46
1:A:384:LEU:C	1:A:384:LEU:HD23	2.41	0.46
1:B:62:VAL:HB	1:B:63:PRO:HD3	1.97	0.46
1:B:65:ARG:HH11	1:B:65:ARG:CG	2.28	0.46
1:B:70:ILE:HD13	1:B:371:PHE:HA	1.98	0.46
1:B:468:TRP:N	1:B:468:TRP:CD1	2.84	0.46
1:A:264:ASN:N	1:A:264:ASN:OD1	2.48	0.46
1:A:278:ARG:NH2	1:A:311:GLU:OE1	2.34	0.46
1:A:304:ARG:HG2	1:A:304:ARG:HH11	1.80	0.46
1:B:55:HIS:CE1	1:B:71:ARG:HD2	2.50	0.46
1:B:99:ILE:HD13	1:B:438:LEU:CD2	2.46	0.46
1:A:53:VAL:HG23	1:A:107:ASP:OD2	2.16	0.46
1:A:318:ASP:N	1:A:318:ASP:OD1	2.49	0.46
1:A:335:ASN:C	1:A:337:GLY:H	2.24	0.46
1:A:400:LEU:O	1:A:404:TYR:HB2	2.16	0.46
1:A:415:ASN:O	1:A:418:TYR:HB2	2.16	0.46
1:A:433:PRO:O	1:A:435:HIS:HD2	1.99	0.46
1:B:355:LEU:C	1:B:357:LEU:H	2.24	0.46
1:B:387:ASN:OD1	1:B:389:ASN:N	2.49	0.46
1:B:411:GLY:O	1:B:412:PHE:C	2.57	0.46
1:A:272:ARG:HG3	1:A:275:ARG:NH2	2.31	0.45
1:A:469:PHE:CD1	1:A:469:PHE:N	2.82	0.45
1:B:45:VAL:HB	1:B:101:LEU:HD23	1.97	0.45
1:A:210:LEU:O	1:A:213:ARG:HB3	2.16	0.45
1:A:221:ARG:HG3	1:A:222:TYR:CD2	2.51	0.45
1:A:450:LEU:O	1:A:454:LEU:HG	2.15	0.45
1:A:507:ILE:HG22	1:A:508:ASP:H	1.76	0.45
1:B:276:LYS:HD3	1:B:279:GLU:OE2	2.16	0.45
1:B:410:MET:HE2	1:B:410:MET:HB2	1.66	0.45
1:B:428:HIS:O	1:B:428:HIS:CG	2.68	0.45
1:A:162:PRO:HD2	1:A:168:ALA:HB2	1.98	0.45
1:A:162:PRO:CD	1:A:171:VAL:HG21	2.46	0.45
1:B:199:LYS:HZ3	1:B:448:ARG:HH12	1.64	0.45
1:B:323:ARG:HH21	1:B:325:GLU:CD	2.25	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:LYS:HD3	1:B:198:TYR:O	2.16	0.45
1:B:387:ASN:HD21	1:B:389:ASN:HB2	1.79	0.45
1:B:500:TRP:HA	1:B:504:VAL:O	2.16	0.45
1:A:488:GLU:CG	1:A:489:ALA:N	2.79	0.45
1:B:206:PRO:HB3	1:B:476:PRO:O	2.16	0.45
1:A:278:ARG:HH11	1:A:278:ARG:CB	2.28	0.45
1:A:347:VAL:HG12	1:A:347:VAL:O	2.16	0.45
1:B:471:GLU:HG3	1:B:472:LYS:N	2.31	0.45
1:A:172:GLN:O	1:A:173:ASN:C	2.59	0.45
1:A:490:ASN:C	1:A:490:ASN:ND2	2.75	0.45
1:A:72:GLU:HG3	1:A:371:PHE:CZ	2.52	0.45
1:A:438:LEU:CD1	1:A:442:MET:HG2	2.46	0.45
1:B:234:GLY:O	1:B:238:GLU:HB2	2.17	0.45
1:B:320:TRP:C	1:B:320:TRP:HD1	2.24	0.45
1:A:341:LYS:O	1:A:479:TYR:HB3	2.16	0.45
1:A:350:PHE:CE2	1:A:354:PHE:HB2	2.52	0.45
1:B:505:LEU:HD21	1:B:507:ILE:HD13	1.99	0.45
1:A:167:VAL:O	1:A:170:GLN:HB3	2.17	0.45
1:B:96:LEU:N	1:B:97:PRO:HD3	2.32	0.45
1:B:285:ARG:HG3	1:B:312:PHE:HA	1.99	0.45
1:B:449:LYS:C	1:B:451:LEU:N	2.75	0.45
1:A:344:SER:HB2	1:A:412:PHE:CE2	2.52	0.44
1:B:208:ASP:C	1:B:210:LEU:N	2.75	0.44
1:B:301:SER:HB3	1:B:305:ARG:NH2	2.32	0.44
1:A:192:LEU:C	1:A:194:ASP:N	2.76	0.44
1:A:300:LEU:HD13	1:A:334:ALA:HB2	1.98	0.44
1:A:471:GLU:CG	1:A:472:LYS:N	2.80	0.44
1:B:39:ALA:HB3	1:B:105:ILE:HB	2.00	0.44
1:B:316:GLY:O	1:B:339:THR:HA	2.16	0.44
1:A:300:LEU:CD1	1:A:334:ALA:HB2	2.48	0.44
1:A:302:ALA:O	1:A:303:MET:C	2.61	0.44
1:B:61:LYS:O	1:B:64:GLU:HG2	2.17	0.44
1:B:168:ALA:O	1:B:172:GLN:HB3	2.17	0.44
1:B:272:ARG:O	1:B:272:ARG:HG2	2.17	0.44
1:A:263:SER:HB2	1:A:292:GLU:OE2	2.17	0.44
1:A:78:ARG:NE	1:A:407:ASP:OD1	2.50	0.44
1:A:110:TRP:CD1	1:A:110:TRP:O	2.71	0.44
1:A:232:THR:OG1	1:A:292:GLU:N	2.44	0.44
1:A:266:GLY:O	1:A:267:GLU:C	2.59	0.44
1:A:342:LEU:CA	1:A:479:TYR:HB3	2.44	0.44
1:A:376:PHE:CD2	1:A:398:GLU:HG2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ASP:O	1:B:209:THR:C	2.58	0.44
1:B:230:VAL:O	1:B:291:CYS:SG	2.76	0.44
1:B:109:CYS:O	1:B:110:TRP:C	2.61	0.44
1:B:206:PRO:CB	1:B:210:LEU:HD23	2.48	0.44
1:B:414:ILE:O	1:B:417:ILE:HB	2.18	0.44
1:A:89:ILE:HD11	1:A:418:TYR:HD2	1.80	0.44
1:A:306:LEU:O	1:A:306:LEU:HG	2.18	0.44
1:A:327:ILE:HG22	1:A:334:ALA:CB	2.48	0.44
1:B:49:ALA:O	1:B:50:LEU:HD23	2.17	0.44
1:B:281:LEU:CB	1:B:282:PRO:HA	2.43	0.44
1:A:478:ARG:HE	1:A:501:HIS:CE1	2.36	0.43
1:B:70:ILE:HD13	1:B:371:PHE:CA	2.47	0.43
1:A:58:PRO:O	1:A:59:ALA:C	2.60	0.43
1:A:111:HIS:C	1:A:111:HIS:ND1	2.76	0.43
1:A:226:TYR:CE2	1:A:280:ARG:NH2	2.84	0.43
1:B:300:LEU:HA	1:B:303:MET:HG3	2.00	0.43
1:B:427:MET:HE3	1:B:453:PHE:HD2	1.83	0.43
1:A:39:ALA:HB3	1:A:105:ILE:HB	2.00	0.43
1:A:206:PRO:HB3	1:A:477:GLY:HA3	2.00	0.43
1:A:410:MET:O	1:A:411:GLY:C	2.59	0.43
1:B:230:VAL:CG1	1:B:273:LEU:HD21	2.44	0.43
1:B:365:ASN:OD1	1:B:365:ASN:C	2.61	0.43
1:A:373:GLN:NE2	1:A:386:GLU:HA	2.23	0.43
1:A:116:LEU:HD23	1:B:177:LEU:CD1	2.40	0.43
1:A:379:ARG:HB2	1:A:386:GLU:OE2	2.18	0.43
1:B:55:HIS:CG	1:B:71:ARG:HD2	2.53	0.43
1:B:76:ILE:HG21	1:B:371:PHE:CE2	2.54	0.43
1:B:176:GLN:HE21	1:B:176:GLN:HB2	1.35	0.43
1:A:51:PHE:CE1	1:A:78:ARG:HB3	2.54	0.43
1:A:304:ARG:HG2	1:A:304:ARG:NH1	2.33	0.43
1:B:57:PRO:HG3	1:B:67:CYS:N	2.34	0.43
1:B:83:PHE:HD2	1:B:83:PHE:HA	1.70	0.43
1:B:164:SER:HB3	1:B:167:VAL:HG23	2.01	0.43
1:B:232:THR:HG21	1:B:292:GLU:CG	2.48	0.43
1:B:357:LEU:HD13	1:B:368:PHE:CZ	2.41	0.43
1:B:229:ALA:O	1:B:258:SER:HA	2.19	0.43
1:B:387:ASN:ND2	1:B:390:PHE:CZ	2.87	0.43
1:B:423:GLY:HA3	1:B:454:LEU:HD23	2.01	0.43
1:A:90:ASN:OD1	1:A:101:LEU:N	2.41	0.43
1:A:484:LEU:HD12	1:A:493:ASP:O	2.18	0.43
1:B:41:MET:HB3	1:B:103:SER:H	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ASN:OD1	1:B:365:ASN:O	2.36	0.43
1:A:82:MET:HG2	1:A:105:ILE:CD1	2.49	0.43
1:A:388:PRO:C	1:A:390:PHE:H	2.27	0.43
1:B:56:GLN:HB3	1:B:109:CYS:O	2.19	0.43
1:B:317:SER:C	1:B:319:GLY:H	2.26	0.43
1:A:165:SER:O	1:A:166:SER:C	2.62	0.43
1:A:281:LEU:HD21	1:A:284:ALA:O	2.19	0.43
1:A:438:LEU:CG	1:A:442:MET:HG2	2.49	0.43
1:A:211:GLN:CG	1:A:340:ILE:HG21	2.45	0.42
1:B:52:SER:O	1:B:75:GLY:CA	2.66	0.42
1:B:483:ASN:O	1:B:495:VAL:N	2.51	0.42
1:A:376:PHE:O	1:A:377:GLN:C	2.61	0.42
1:A:488:GLU:HG2	1:A:489:ALA:H	1.84	0.42
1:A:508:ASP:O	1:A:509:ASP:C	2.62	0.42
1:B:335:ASN:OD1	1:B:485:GLN:HA	2.18	0.42
1:A:74:TYR:N	1:A:74:TYR:CD1	2.88	0.42
1:A:195:LYS:HA	1:A:195:LYS:CE	2.43	0.42
1:A:409:LYS:O	1:A:410:MET:C	2.62	0.42
1:B:195:LYS:NZ	1:B:473:GLY:HA3	2.34	0.42
1:B:285:ARG:HG3	1:B:311:GLU:O	2.18	0.42
1:B:471:GLU:O	1:B:472:LYS:C	2.62	0.42
1:A:49:ALA:O	1:A:50:LEU:HD23	2.19	0.42
1:A:272:ARG:HH11	1:A:272:ARG:HD3	1.60	0.42
1:A:342:LEU:H	1:A:342:LEU:CD1	2.26	0.42
1:B:205:VAL:HG23	1:B:206:PRO:CD	2.41	0.42
1:B:342:LEU:HD21	1:B:412:PHE:CE2	2.46	0.42
1:A:77:GLN:O	1:A:81:ALA:HB2	2.19	0.42
1:A:365:ASN:OD1	1:A:365:ASN:C	2.63	0.42
1:B:261:ILE:HG12	1:B:270:PHE:CE2	2.55	0.42
1:B:427:MET:HG3	1:B:453:PHE:CE2	2.54	0.42
1:A:41:MET:HE1	1:A:364:ARG:NH1	2.34	0.42
1:A:226:TYR:C	1:A:227:VAL:HG13	2.44	0.42
1:A:235:ASN:OD1	1:A:235:ASN:O	2.38	0.42
1:A:368:PHE:HB3	1:A:369:PRO:HD3	2.01	0.42
1:A:510:TYR:CD1	1:A:511:LYS:HG3	2.55	0.42
1:B:253:LEU:HD12	1:B:253:LEU:HA	1.89	0.42
1:B:400:LEU:C	1:B:402:GLU:N	2.76	0.42
1:A:394:CYS:HB3	1:A:398:GLU:OE2	2.19	0.42
1:B:44:ASP:N	1:B:100:THR:OG1	2.53	0.42
1:B:202:LEU:N	1:B:202:LEU:CD2	2.79	0.42
1:A:38:VAL:HG21	1:A:106:ARG:NH1	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:LEU:O	1:A:455:ILE:C	2.62	0.42
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.77	0.42
1:A:191:ASP:OD2	1:A:235:ASN:OD1	2.38	0.42
1:A:226:TYR:CE2	1:A:283:LYS:HB3	2.54	0.42
1:A:443:LYS:HA	1:A:444:PRO:HA	1.78	0.42
1:B:49:ALA:CB	1:B:82:MET:HE2	2.49	0.42
1:B:53:VAL:O	1:B:70:ILE:HA	2.20	0.42
1:B:77:GLN:O	1:B:81:ALA:HB2	2.19	0.42
1:B:379:ARG:NH2	1:B:381:PRO:CA	2.77	0.42
1:A:96:LEU:HB3	1:A:99:ILE:HB	2.02	0.42
1:A:172:GLN:HB2	1:A:172:GLN:HE21	1.49	0.42
1:A:176:GLN:HE21	1:A:176:GLN:HB2	1.49	0.42
1:A:221:ARG:NH1	1:A:507:ILE:HB	2.34	0.42
1:A:231:HIS:CE1	1:A:260:LYS:HB3	2.55	0.42
1:A:296:VAL:O	1:A:300:LEU:HG	2.20	0.42
1:B:278:ARG:NH1	1:B:278:ARG:HB3	2.35	0.42
1:B:317:SER:C	1:B:319:GLY:N	2.77	0.42
1:A:172:GLN:HE22	1:A:201:PHE:CA	2.33	0.41
1:A:335:ASN:C	1:A:337:GLY:N	2.77	0.41
1:B:58:PRO:HB2	1:B:60:GLU:OE1	2.20	0.41
1:B:267:GLU:O	1:B:271:ASP:HB2	2.20	0.41
1:A:77:GLN:O	1:A:81:ALA:CB	2.68	0.41
1:A:202:LEU:N	1:A:202:LEU:CD2	2.79	0.41
1:A:222:TYR:O	1:A:223:ASN:HB2	2.19	0.41
1:B:101:LEU:HD23	1:B:101:LEU:HA	1.91	0.41
1:B:106:ARG:HD3	1:B:118:GLN:OE1	2.20	0.41
1:B:393:VAL:CG1	1:B:394:CYS:N	2.81	0.41
1:A:278:ARG:HE	1:A:311:GLU:CD	2.27	0.41
1:A:329:GLY:C	1:A:331:GLU:OE1	2.63	0.41
1:A:502:GLU:C	1:A:504:VAL:H	2.28	0.41
1:B:169:ILE:HG22	1:B:170:GLN:N	2.35	0.41
1:B:241:MET:O	1:B:243:ALA:N	2.53	0.41
1:B:317:SER:HA	1:B:340:ILE:HB	2.02	0.41
1:B:378:CYS:HB2	1:B:392:LYS:O	2.21	0.41
1:A:342:LEU:HD11	1:A:409:LYS:HE3	2.03	0.41
1:B:98:ASN:OD1	1:B:98:ASN:N	2.52	0.41
1:B:320:TRP:O	1:B:321:ALA:HB3	2.20	0.41
1:B:368:PHE:HA	1:B:371:PHE:HB3	2.02	0.41
1:B:375:ARG:NH1	1:B:375:ARG:CG	2.81	0.41
1:B:459:PHE:HD1	1:B:460:VAL:O	2.03	0.41
1:A:350:PHE:HD2	1:A:351:ASP:OD2	2.04	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLY:O	1:B:186:SER:HB2	2.21	0.41
1:B:192:LEU:HD22	1:B:201:PHE:CE2	2.55	0.41
1:B:209:THR:O	1:B:213:ARG:HB2	2.20	0.41
1:B:229:ALA:HB1	1:B:241:MET:HE3	2.00	0.41
1:B:328:GLU:HA	1:B:331:GLU:OE2	2.21	0.41
1:B:487:THR:C	1:B:489:ALA:H	2.26	0.41
1:A:383:HIS:O	1:A:384:LEU:C	2.64	0.41
1:B:70:ILE:HD13	1:B:371:PHE:HB2	2.03	0.41
1:B:70:ILE:CD1	1:B:371:PHE:HB2	2.50	0.41
1:A:89:ILE:CG1	1:A:418:TYR:CE2	3.01	0.41
1:A:185:TYR:CD1	1:A:413:VAL:HG22	2.56	0.41
1:A:189:SER:CA	1:A:208:ASP:OD2	2.65	0.41
1:A:266:GLY:C	1:A:268:LYS:H	2.29	0.41
1:A:358:ARG:HG2	1:A:359:LEU:N	2.35	0.41
1:A:56:GLN:HG3	1:A:57:PRO:N	2.35	0.41
1:A:246:GLU:O	1:A:247:LEU:C	2.64	0.41
1:B:190:ILE:HD11	1:B:239:SER:C	2.46	0.41
1:A:190:ILE:O	1:A:191:ASP:C	2.64	0.41
1:A:232:THR:HG21	1:A:292:GLU:CB	2.51	0.41
1:A:232:THR:HG21	1:A:292:GLU:CG	2.51	0.41
1:A:294:MET:O	1:A:297:ARG:N	2.54	0.41
1:A:342:LEU:HD12	1:A:342:LEU:N	2.32	0.41
1:A:365:ASN:HA	1:A:366:PRO:HD2	1.90	0.41
1:A:435:HIS:CD2	1:A:435:HIS:N	2.89	0.41
1:B:198:TYR:CD1	1:B:198:TYR:N	2.87	0.41
1:B:205:VAL:CG2	1:B:206:PRO:HD2	2.39	0.41
1:B:373:GLN:OE1	1:B:387:ASN:HB3	2.21	0.41
1:A:96:LEU:N	1:A:97:PRO:HD3	2.36	0.41
1:A:261:ILE:HG12	1:A:262:TYR:N	2.36	0.41
1:A:274:LEU:HD11	1:A:312:PHE:CE2	2.56	0.41
1:A:347:VAL:O	1:A:406:GLN:NE2	2.54	0.41
1:B:172:GLN:HB2	1:B:182:GLN:OE1	2.21	0.41
1:A:232:THR:HG1	1:A:292:GLU:H	1.63	0.40
1:B:209:THR:HG22	1:B:243:ALA:CB	2.50	0.40
1:A:421:ALA:O	1:A:424:LEU:HB2	2.22	0.40
1:B:95:LEU:O	1:B:96:LEU:C	2.62	0.40
1:B:309:VAL:HG22	1:B:333:GLU:HB3	2.01	0.40
1:B:418:TYR:O	1:B:419:ALA:C	2.64	0.40
1:A:122:PHE:HB3	1:A:156:ILE:HG13	2.04	0.40
1:A:320:TRP:O	1:A:321:ALA:HB3	2.21	0.40
1:A:112:SER:HB3	1:A:170:GLN:HE21	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:SER:O	1:A:169:ILE:HB	2.22	0.40
1:A:329:GLY:C	1:A:331:GLU:N	2.79	0.40
1:A:452:ASP:C	1:A:454:LEU:N	2.79	0.40
1:A:483:ASN:ND2	1:A:484:LEU:N	2.67	0.40
1:B:72:GLU:OE2	1:B:375:ARG:HD2	2.22	0.40
1:B:229:ALA:HB1	1:B:241:MET:HE1	2.00	0.40
1:B:383:HIS:HD2	1:B:384:LEU:H	1.69	0.40
1:A:280:ARG:O	1:A:281:LEU:HG	2.22	0.40
1:A:411:GLY:O	1:A:412:PHE:C	2.65	0.40
1:B:218:ILE:HD13	1:B:338:ILE:HG21	2.04	0.40
1:B:318:ASP:O	1:B:321:ALA:HB2	2.22	0.40
1:B:433:PRO:C	1:B:435:HIS:H	2.28	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	444/490 (91%)	379 (85%)	58 (13%)	7 (2%)	7	37
1	B	444/490 (91%)	390 (88%)	50 (11%)	4 (1%)	14	48
All	All	888/980 (91%)	769 (87%)	108 (12%)	11 (1%)	10	42

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	ALA
1	B	68	GLY
1	A	330	TYR
1	A	490	ASN
1	B	385	LEU
1	A	318	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	453	PHE
1	A	487	THR
1	A	163	GLY
1	B	473	GLY
1	B	475	ALA

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	384/422 (91%)	340 (88%)	44 (12%)	5	22
1	B	384/422 (91%)	341 (89%)	43 (11%)	6	22
All	All	768/844 (91%)	681 (89%)	87 (11%)	5	22

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
1	A	56	GLN
1	A	86	LEU
1	A	92	ASP
1	A	98	ASN
1	A	156	ILE
1	A	172	GLN
1	A	173	ASN
1	A	176	GLN
1	A	188	THR
1	A	195	LYS
1	A	198	TYR
1	A	202	LEU
1	A	210	LEU
1	A	213	ARG
1	A	216	LEU
1	A	233	GLU
1	A	236	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	238	GLU
1	A	239	SER
1	A	242	ASP
1	A	250	GLN
1	A	270	PHE
1	A	280	ARG
1	A	290	PHE
1	A	296	VAL
1	A	312	PHE
1	A	313	SER
1	A	325	GLU
1	A	332	VAL
1	A	333	GLU
1	A	342	LEU
1	A	344	SER
1	A	368	PHE
1	A	383	HIS
1	A	386	GLU
1	A	408	SER
1	A	438	LEU
1	A	440	ASP
1	A	459	PHE
1	A	465	GLU
1	A	479	TYR
1	A	480	ASP
1	A	491	ARG
1	B	53	VAL
1	B	95	LEU
1	B	98	ASN
1	B	114	VAL
1	B	169	ILE
1	B	172	GLN
1	B	173	ASN
1	B	176	GLN
1	B	180	ILE
1	B	185	TYR
1	B	186	SER
1	B	190	ILE
1	B	198	TYR
1	B	202	LEU
1	B	205	VAL
1	B	218	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	227	VAL
1	B	242	ASP
1	B	251	GLU
1	B	259	ASP
1	B	261	ILE
1	B	270	PHE
1	B	289	CYS
1	B	312	PHE
1	B	318	ASP
1	B	322	ASP
1	B	324	ASP
1	B	326	VAL
1	B	328	GLU
1	B	333	GLU
1	B	360	ASP
1	B	379	ARG
1	B	390	PHE
1	B	394	CYS
1	B	399	SER
1	B	427	MET
1	B	436	VAL
1	B	440	ASP
1	B	465	GLU
1	B	474	ASP
1	B	488	GLU
1	B	507	ILE
1	B	508	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	173	ASN
1	A	176	GLN
1	A	211	GLN
1	A	362	ASN
1	A	383	HIS
1	A	406	GLN
1	A	426	ASN
1	A	435	HIS
1	A	483	ASN
1	A	485	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	490	ASN
1	B	55	HIS
1	B	73	GLN
1	B	84	HIS
1	B	170	GLN
1	B	173	ASN
1	B	176	GLN
1	B	235	ASN
1	B	250	GLN
1	B	264	ASN
1	B	362	ASN
1	B	383	HIS
1	B	406	GLN
1	B	415	ASN
1	B	422	HIS
1	B	483	ASN
1	B	490	ASN

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	448/490 (91%)	0.30	4 (0%) 81 64	21, 37, 69, 88	0
1	B	448/490 (91%)	0.21	7 (1%) 70 52	17, 30, 51, 67	0
All	All	896/980 (91%)	0.25	11 (1%) 76 59	17, 33, 59, 88	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	GLY	3.6
1	B	273	LEU	2.7
1	A	512	ILE	2.6
1	B	275	ARG	2.5
1	B	385	LEU	2.4
1	A	487	THR	2.3
1	A	396	GLY	2.3
1	A	382	GLY	2.3
1	B	391	LYS	2.2
1	B	239	SER	2.2
1	B	439	CYS	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 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.