



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:06 PM GMT

PDB ID : 1IPK
Title : CRYSTAL STRUCTURES OF RECOMBINANT AND NATIVE SOYBEAN BETA-CONGLYCININ BETA HOMOTRIMERS
Authors : Maruyama, N.; Adachi, M.; Takahashi, K.; Yagasaki, K.; Kohno, M.; Takenaka, Y.; Okuda, E.; Nakagawa, S.; Mikami, B.; Utsumi, S.
Deposited on : 2001-05-16
Resolution : 2.70 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

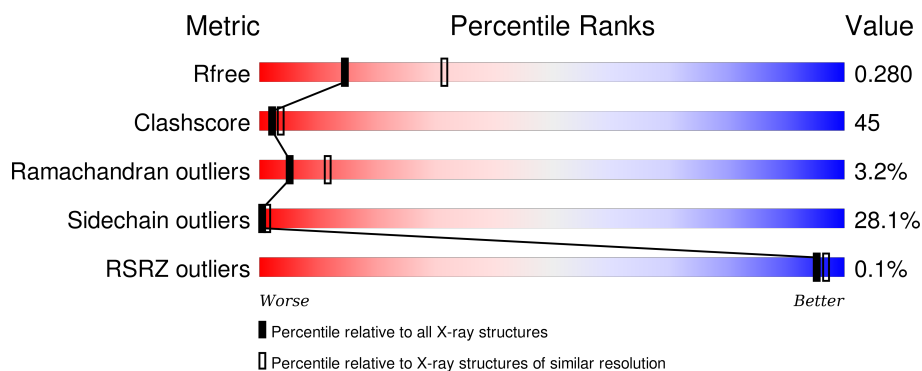
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	416	 28% 44% 17% 12%
1	B	416	 23% 46% 18% • 12%
1	C	416	 32% 43% 14% • 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9074 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 BETA-CONGLYCININ, BETA CHAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	0	0	0
			3001	1900	534	567			
1	B	365	Total	C	N	O	0	0	0
			2977	1886	529	562			
1	C	379	Total	C	N	O	0	0	0
			3096	1953	552	591			

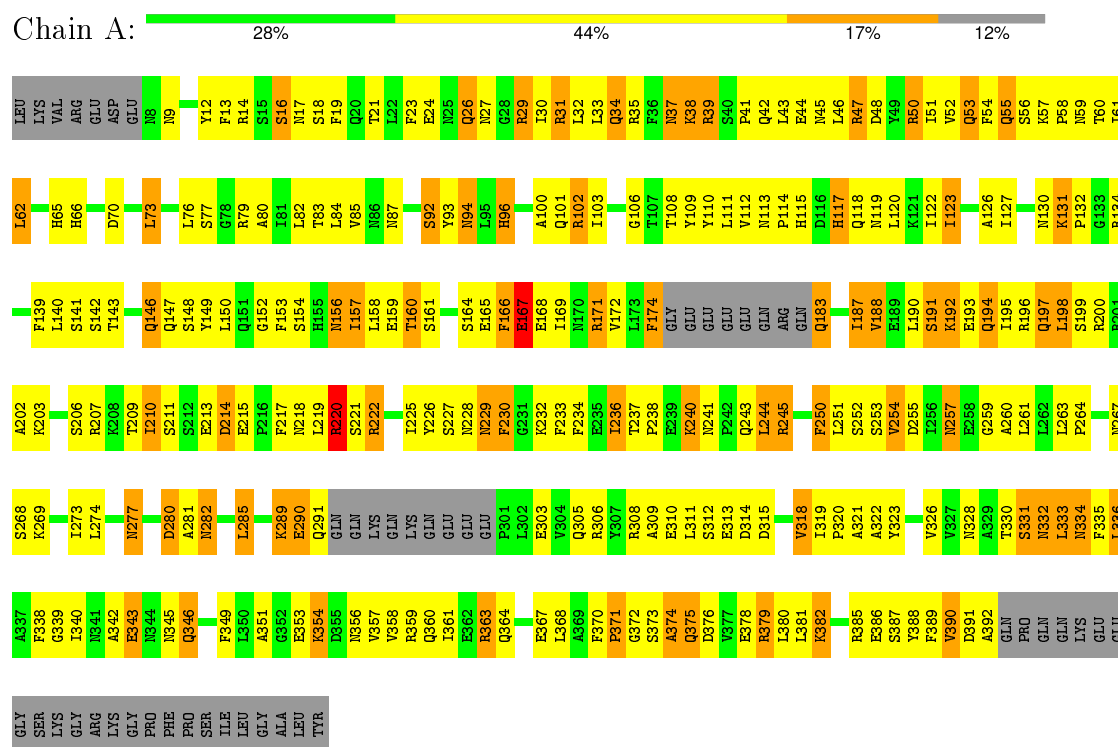
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLY	VAL	CONFLICT	UNP P25974
B	28	GLY	VAL	CONFLICT	UNP P25974
C	28	GLY	VAL	CONFLICT	UNP P25974

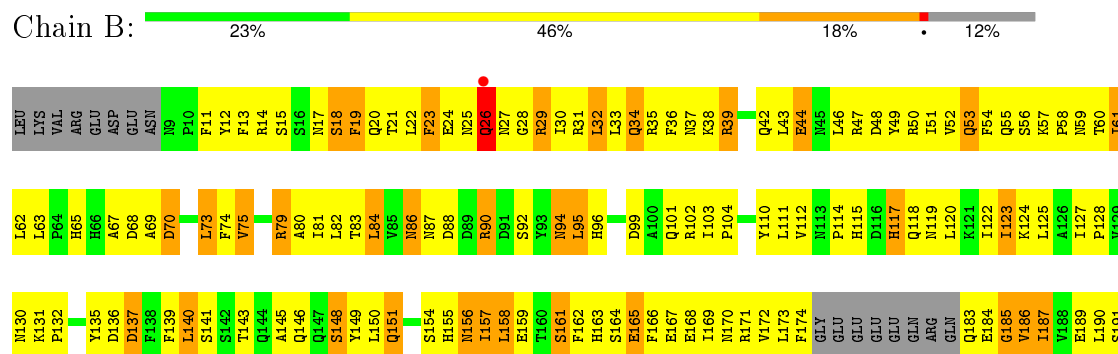
3 Residue-property plots

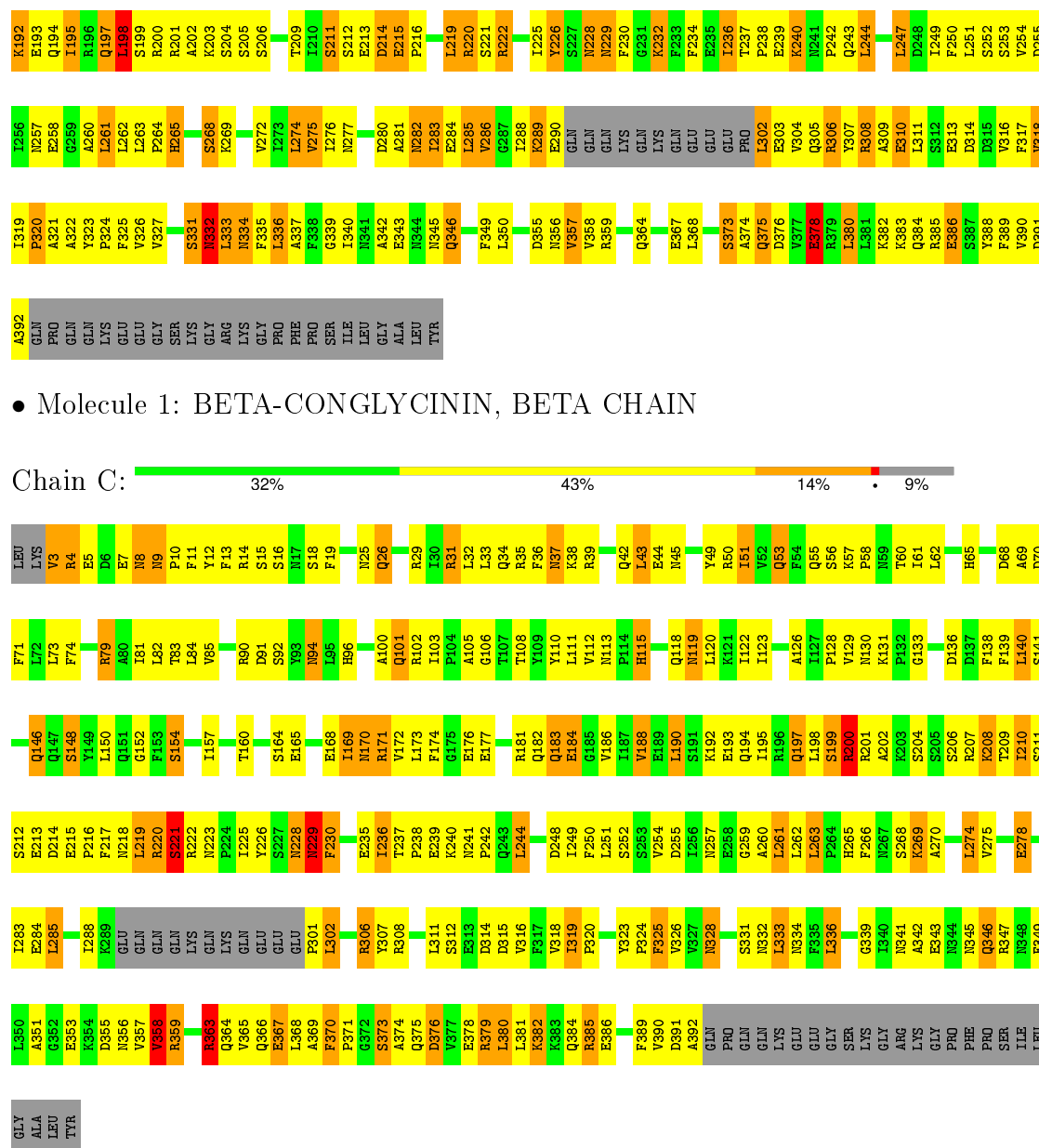
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: BETA-CONGLYCININ, BETA CHAIN



• Molecule 1: BETA-CONGLYCININ, BETA CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.51Å 63.48Å 131.43Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	7.00 – 2.70 8.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.70) 83.5 (8.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.70Å)	Xtriage
Refinement program	?	Depositor
R, R_{free}	0.205 , 0.275 0.204 , 0.280	Depositor DCC
R_{free} test set	2933 reflections (11.33%)	DCC
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 96.6	EDS
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 29543 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9074	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.40	0/3062	0.68	0/4141
1	B	0.39	0/3037	0.66	0/4107
1	C	0.39	0/3158	0.70	2/4270 (0.0%)
All	All	0.39	0/9257	0.68	2/12518 (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	C	200	ARG	N-CA-C	6.33	128.09	111.00
1	C	201	ARG	N-CA-C	-6.15	94.40	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3001	0	2945	263	0
1	B	2977	0	2923	334	0
1	C	3096	0	3026	264	0
All	All	9074	0	8894	803	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 45.

All (803) 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:B:14:ARG:HB3	1:B:17:ASN:HB2	1.30	1.09
1:A:379:ARG:HH11	1:A:379:ARG:HB3	1.20	1.06
1:B:22:LEU:HD12	1:B:30:ILE:HG22	1.37	1.06
1:C:359:ARG:HH22	1:C:382:LYS:HE3	1.20	1.04
1:B:222:ARG:HH21	1:B:240:LYS:HD3	1.26	0.99
1:C:220:ARG:HG2	1:C:220:ARG:HH11	1.24	0.99
1:A:367:GLU:HB2	1:A:374:ALA:HB2	1.44	0.99
1:B:24:GLU:HG3	1:B:29:ARG:HB3	1.45	0.98
1:C:284:GLU:HG2	1:C:308:ARG:HG3	1.45	0.98
1:A:29:ARG:HH11	1:A:55:GLN:HE22	1.10	0.97
1:B:61:ILE:HG13	1:B:112:VAL:HG22	1.46	0.94
1:C:270:ALA:H	1:C:345:ASN:ND2	1.68	0.90
1:A:115:HIS:HD2	1:A:117:HIS:H	1.19	0.89
1:C:184:GLU:HG2	1:C:184:GLU:O	1.71	0.89
1:C:79:ARG:HH21	1:C:94:ASN:HD21	1.13	0.88
1:C:29:ARG:HH21	1:C:55:GLN:HE22	1.21	0.88
1:B:275:VAL:HG12	1:B:316:VAL:HG22	1.55	0.88
1:B:158:LEU:HD23	1:B:162:PHE:HE2	1.38	0.88
1:C:79:ARG:NH2	1:C:94:ASN:HD21	1.70	0.88
1:B:22:LEU:HD21	1:B:32:LEU:HB2	1.56	0.88
1:B:284:GLU:HB2	1:B:326:VAL:HG12	1.56	0.87
1:C:261:LEU:HB2	1:C:328:ASN:ND2	1.90	0.86
1:C:268:SER:HB3	1:C:346:GLN:H	1.41	0.85
1:B:94:ASN:HB2	1:B:203:LYS:O	1.78	0.84
1:C:197:GLN:HE21	1:C:197:GLN:HA	1.42	0.84
1:B:115:HIS:CD2	1:B:118:GLN:H	1.95	0.84
1:B:79:ARG:HH11	1:B:79:ARG:HG2	1.40	0.84
1:B:140:LEU:O	1:B:148:SER:HB2	1.77	0.84
1:C:379:ARG:HG3	1:C:380:LEU:N	1.93	0.83
1:C:261:LEU:HB2	1:C:328:ASN:HD22	1.38	0.83
1:B:281:ALA:HB2	1:B:333:LEU:HD13	1.60	0.83
1:A:85:VAL:HG22	1:A:108:THR:HB	1.60	0.83
1:C:207:ARG:NH1	1:C:222:ARG:HD3	1.92	0.83
1:C:33:LEU:HD12	1:C:34:GLN:H	1.42	0.83
1:C:33:LEU:HD12	1:C:34:GLN:N	1.94	0.83
1:B:25:ASN:HD21	1:B:187:ILE:HB	1.42	0.82
1:C:359:ARG:NH2	1:C:382:LYS:HE3	1.93	0.82
1:A:306:ARG:HD3	1:C:152:GLY:O	1.80	0.82
1:A:29:ARG:HH11	1:A:55:GLN:NE2	1.78	0.82
1:C:288:ILE:HG21	1:C:302:LEU:HD22	1.62	0.81
1:A:29:ARG:HD3	1:A:55:GLN:HE21	1.43	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:VAL:HG12	1:B:122:ILE:HD11	1.62	0.81
1:C:33:LEU:HD22	1:C:316:VAL:HG21	1.61	0.81
1:B:230:PHE:CE1	1:B:391:ASP:HB2	2.15	0.81
1:C:123:ILE:HG21	1:C:336:LEU:CD2	2.10	0.81
1:A:47:ARG:HG3	1:A:48:ASP:OD1	1.82	0.80
1:C:220:ARG:NH1	1:C:220:ARG:HG2	1.96	0.79
1:B:285:LEU:HD23	1:B:325:PHE:HB3	1.62	0.79
1:B:258:GLU:HB2	1:B:332:ASN:H	1.45	0.79
1:C:123:ILE:HG21	1:C:336:LEU:HD21	1.64	0.79
1:A:43:LEU:HD22	1:A:318:VAL:HG21	1.64	0.79
1:C:250:PHE:CE1	1:C:339:GLY:HA3	2.18	0.79
1:B:92:SER:O	1:B:202:ALA:HA	1.83	0.79
1:B:115:HIS:HD2	1:B:118:GLN:H	1.30	0.78
1:C:380:LEU:HD12	1:C:381:LEU:HG	1.63	0.78
1:A:115:HIS:CD2	1:A:118:GLN:H	2.00	0.78
1:A:225:ILE:HG13	1:A:226:TYR:H	1.49	0.78
1:C:61:ILE:HG22	1:C:188:VAL:HG22	1.65	0.78
1:B:219:LEU:HD11	1:B:234:PHE:HB3	1.66	0.78
1:B:115:HIS:CD2	1:B:117:HIS:H	2.02	0.78
1:A:321:ALA:HB3	1:C:130:ASN:HD21	1.47	0.78
1:A:166:PHE:O	1:A:169:ILE:HG12	1.84	0.78
1:C:380:LEU:CD1	1:C:381:LEU:HG	2.14	0.77
1:B:14:ARG:HB3	1:B:17:ASN:CB	2.11	0.77
1:B:61:ILE:HB	1:B:190:LEU:HD13	1.65	0.77
1:A:61:ILE:HG13	1:A:112:VAL:HG22	1.67	0.77
1:B:222:ARG:HH21	1:B:240:LYS:CD	1.98	0.77
1:A:222:ARG:HH22	1:A:240:LYS:HG2	1.49	0.76
1:B:166:PHE:O	1:B:169:ILE:HG12	1.85	0.76
1:A:379:ARG:NH1	1:A:379:ARG:HB3	1.98	0.76
1:A:26:GLN:HG2	1:A:27:ASN:ND2	2.01	0.76
1:B:60:THR:HA	1:B:189:GLU:HA	1.65	0.76
1:B:74:PHE:CE1	1:B:336:LEU:HD13	2.20	0.76
1:C:250:PHE:CD1	1:C:339:GLY:HA3	2.21	0.76
1:B:236:ILE:HD13	1:B:240:LYS:HB3	1.69	0.75
1:B:228:ASN:OD1	1:B:389:PHE:HB2	1.86	0.75
1:B:382:LYS:HE2	1:B:385:ARG:HH21	1.51	0.75
1:B:21:THR:HA	1:B:31:ARG:HG2	1.67	0.75
1:C:79:ARG:HH21	1:C:94:ASN:ND2	1.85	0.75
1:C:226:TYR:OH	1:C:347:ARG:HD2	1.87	0.74
1:B:169:ILE:HG22	1:C:380:LEU:HD21	1.68	0.74
1:B:220:ARG:HH22	1:B:255:ASP:CG	1.90	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:THR:HB	1:A:238:PRO:CD	2.18	0.74
1:C:74:PHE:CD1	1:C:336:LEU:HD13	2.23	0.74
1:C:176:GLU:O	1:C:177:GLU:HB2	1.87	0.74
1:A:32:LEU:HD23	1:A:52:VAL:HG22	1.68	0.74
1:A:115:HIS:CD2	1:A:117:HIS:H	2.06	0.73
1:B:156:ASN:ND2	1:B:156:ASN:H	1.85	0.73
1:B:373:SER:HB3	1:B:376:ASP:OD2	1.88	0.73
1:A:33:LEU:O	1:A:50:ARG:NH2	2.21	0.73
1:B:115:HIS:HD2	1:B:117:HIS:H	1.36	0.73
1:A:222:ARG:HH21	1:A:236:ILE:HG12	1.53	0.73
1:A:373:SER:C	1:A:375:GLN:H	1.89	0.73
1:B:222:ARG:NH2	1:B:240:LYS:HD3	2.02	0.72
1:A:282:ASN:ND2	1:A:328:ASN:HB3	2.03	0.72
1:A:225:ILE:HD11	1:A:233:PHE:CD1	2.25	0.72
1:A:361:ILE:HG23	1:C:110:TYR:HE1	1.53	0.72
1:B:32:LEU:HD11	1:B:135:TYR:HE1	1.54	0.72
1:B:155:HIS:O	1:B:159:GLU:HB2	1.88	0.72
1:A:193:GLU:HG3	1:A:197:GLN:HE22	1.54	0.72
1:B:33:LEU:HD23	1:B:34:GLN:O	1.89	0.72
1:A:149:TYR:HE1	1:B:350:LEU:HD11	1.55	0.72
1:C:270:ALA:N	1:C:345:ASN:ND2	2.38	0.72
1:C:141:SER:OG	1:C:146:GLN:NE2	2.23	0.72
1:A:259:GLY:O	1:A:392:ALA:HB3	1.90	0.71
1:B:25:ASN:OD1	1:B:27:ASN:N	2.23	0.71
1:A:160:THR:CG2	1:B:392:ALA:HA	2.19	0.71
1:B:65:HIS:HB3	1:B:139:PHE:CD2	2.25	0.71
1:B:228:ASN:HD21	1:B:230:PHE:HD2	1.37	0.71
1:C:218:ASN:HB3	1:C:221:SER:HB2	1.72	0.71
1:B:170:ASN:HD22	1:B:174:PHE:HD1	1.39	0.71
1:C:382:LYS:HE2	1:C:385:ARG:NE	2.05	0.71
1:B:258:GLU:HB2	1:B:332:ASN:N	2.05	0.70
1:B:197:GLN:HE21	1:B:197:GLN:N	1.89	0.70
1:C:207:ARG:HH11	1:C:222:ARG:HD3	1.56	0.70
1:C:367:GLU:OE1	1:C:373:SER:HA	1.91	0.70
1:C:193:GLU:O	1:C:197:GLN:HG2	1.91	0.70
1:C:207:ARG:HH11	1:C:222:ARG:CD	2.05	0.70
1:C:29:ARG:HH21	1:C:55:GLN:NE2	1.89	0.70
1:A:156:ASN:H	1:A:156:ASN:HD22	1.40	0.70
1:B:32:LEU:CD2	1:B:52:VAL:HG22	2.22	0.70
1:A:29:ARG:NH1	1:A:55:GLN:HE22	1.86	0.70
1:C:269:LYS:H	1:C:345:ASN:ND2	1.89	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LEU:HD21	1:A:390:VAL:HG11	1.73	0.70
1:A:263:LEU:HD13	1:A:351:ALA:HB3	1.73	0.69
1:C:357:VAL:HG13	1:C:358:VAL:H	1.57	0.69
1:B:222:ARG:CB	1:B:222:ARG:HH11	2.05	0.69
1:B:367:GLU:OE2	1:B:374:ALA:HB2	1.92	0.69
1:A:238:PRO:O	1:A:245:ARG:HB2	1.93	0.69
1:B:158:LEU:HD23	1:B:162:PHE:CE2	2.24	0.69
1:B:59:ASN:HA	1:B:195:ILE:HD11	1.73	0.69
1:B:166:PHE:CE2	1:B:170:ASN:HB2	2.28	0.69
1:C:363:ARG:HD3	1:C:374:ALA:HB1	1.75	0.68
1:A:168:GLU:O	1:A:172:VAL:HG23	1.92	0.68
1:B:143:THR:HG21	1:B:185:GLY:O	1.93	0.68
1:B:265:HIS:HB3	1:B:349:PHE:CD1	2.28	0.68
1:B:75:VAL:CG1	1:B:122:ILE:HD11	2.23	0.68
1:A:285:LEU:HD21	1:A:323:TYR:HB3	1.75	0.68
1:A:220:ARG:NH2	1:A:255:ASP:OD1	2.27	0.68
1:A:263:LEU:HD22	1:A:264:PRO:HD2	1.74	0.68
1:C:208:LYS:HG3	1:C:208:LYS:O	1.94	0.68
1:C:384:GLN:HE21	1:C:386:GLU:H	1.42	0.68
1:C:119:ASN:H	1:C:119:ASN:HD22	1.42	0.68
1:B:79:ARG:HH11	1:B:79:ARG:CG	2.07	0.67
1:A:160:THR:HG21	1:B:392:ALA:CB	2.25	0.67
1:A:358:VAL:HG12	1:A:381:LEU:HD11	1.77	0.67
1:B:234:PHE:HB2	1:B:253:SER:O	1.95	0.67
1:A:313:GLU:O	1:A:314:ASP:HB2	1.95	0.67
1:B:222:ARG:HB2	1:B:222:ARG:HH11	1.59	0.66
1:A:390:VAL:CG2	1:A:391:ASP:N	2.58	0.66
1:C:190:LEU:HB3	1:C:194:GLN:NE2	2.11	0.66
1:A:13:PHE:CE1	1:A:39:ARG:HG3	2.30	0.66
1:C:13:PHE:HB2	1:C:316:VAL:HB	1.78	0.66
1:B:55:GLN:HA	1:B:120:LEU:O	1.96	0.66
1:A:359:ARG:O	1:A:359:ARG:HG2	1.95	0.65
1:B:274:LEU:HD21	1:B:317:PHE:HB3	1.78	0.65
1:C:220:ARG:HH22	1:C:255:ASP:CG	2.00	0.65
1:C:284:GLU:CG	1:C:308:ARG:HG3	2.24	0.65
1:A:191:SER:H	1:A:194:GLN:HG3	1.61	0.65
1:C:270:ALA:N	1:C:345:ASN:HD22	1.94	0.65
1:A:160:THR:HG21	1:B:392:ALA:HA	1.78	0.65
1:B:25:ASN:O	1:B:27:ASN:N	2.29	0.65
1:C:115:HIS:HD2	1:C:118:GLN:HB3	1.62	0.65
1:B:228:ASN:O	1:B:230:PHE:N	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:PHE:CE1	1:C:391:ASP:HB2	2.32	0.65
1:C:101:GLN:HG3	1:C:102:ARG:N	2.12	0.64
1:B:283:ILE:HG21	1:B:317:PHE:CE1	2.32	0.64
1:A:390:VAL:HG23	1:A:391:ASP:N	2.13	0.64
1:B:333:LEU:HG	1:B:334:ASN:N	2.12	0.64
1:A:306:ARG:HH12	1:C:154:SER:HA	1.61	0.64
1:B:243:GLN:O	1:B:247:LEU:HD12	1.97	0.64
1:C:349:PHE:O	1:C:356:ASN:HA	1.98	0.64
1:C:12:TYR:CE2	1:C:311:LEU:HD23	2.32	0.64
1:A:85:VAL:CG2	1:A:108:THR:HB	2.28	0.64
1:B:82:LEU:HD21	1:B:103:ILE:HD11	1.78	0.64
1:B:284:GLU:O	1:B:325:PHE:HA	1.98	0.64
1:B:75:VAL:HA	1:B:122:ILE:HG12	1.79	0.64
1:B:21:THR:HA	1:B:31:ARG:CG	2.28	0.64
1:B:96:HIS:O	1:B:99:ASP:HB2	1.98	0.63
1:A:115:HIS:HD2	1:A:118:GLN:H	1.44	0.63
1:B:250:PHE:CE1	1:B:339:GLY:HA3	2.34	0.63
1:A:46:LEU:HD21	1:A:340:ILE:HG13	1.80	0.63
1:C:33:LEU:HD23	1:C:51:ILE:HB	1.81	0.62
1:C:190:LEU:HB3	1:C:194:GLN:HE21	1.62	0.62
1:B:236:ILE:CD1	1:B:240:LYS:HB3	2.29	0.62
1:B:275:VAL:CG1	1:B:316:VAL:HG22	2.27	0.62
1:B:254:VAL:O	1:B:334:ASN:HA	1.99	0.62
1:A:281:ALA:HB2	1:A:333:LEU:HD13	1.81	0.62
1:A:392:ALA:HA	1:C:160:THR:CG2	2.29	0.62
1:C:363:ARG:HH11	1:C:374:ALA:HB1	1.64	0.62
1:B:25:ASN:ND2	1:B:187:ILE:HB	2.14	0.62
1:B:283:ILE:O	1:B:308:ARG:HG3	1.99	0.62
1:C:380:LEU:C	1:C:380:LEU:HD13	2.20	0.62
1:B:220:ARG:NH2	1:B:255:ASP:OD2	2.30	0.62
1:C:37:ASN:N	1:C:37:ASN:HD22	1.96	0.62
1:B:382:LYS:HE2	1:B:385:ARG:NH2	2.14	0.61
1:A:390:VAL:HG23	1:A:391:ASP:H	1.64	0.61
1:C:356:ASN:HD22	1:C:359:ARG:HB2	1.65	0.61
1:C:85:VAL:HG22	1:C:108:THR:HB	1.83	0.61
1:C:217:PHE:CD2	1:C:236:ILE:HD12	2.36	0.61
1:A:12:TYR:HE2	1:A:311:LEU:HD23	1.66	0.61
1:A:26:GLN:HG2	1:A:27:ASN:HD22	1.64	0.61
1:A:37:ASN:H	1:A:37:ASN:HD22	1.48	0.61
1:A:32:LEU:HD13	1:A:50:ARG:CZ	2.29	0.61
1:A:361:ILE:HG23	1:C:110:TYR:CE1	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ARG:CD	1:A:55:GLN:HE21	2.13	0.61
1:A:222:ARG:NH2	1:A:240:LYS:HG2	2.15	0.61
1:B:203:LYS:HZ1	1:B:215:GLU:CD	2.04	0.60
1:A:387:SER:O	1:A:389:PHE:N	2.34	0.60
1:B:74:PHE:CD1	1:B:336:LEU:HD13	2.36	0.60
1:A:35:ARG:NH1	1:A:134:ARG:HD3	2.16	0.60
1:B:274:LEU:CD2	1:B:317:PHE:HB3	2.31	0.60
1:B:285:LEU:O	1:B:306:ARG:HA	2.01	0.60
1:A:169:ILE:HG22	1:B:380:LEU:HD11	1.81	0.60
1:B:319:ILE:HG21	1:B:325:PHE:CD1	2.37	0.60
1:A:225:ILE:HD12	1:A:226:TYR:CE1	2.36	0.60
1:A:230:PHE:HB3	1:A:260:ALA:HB2	1.82	0.60
1:A:237:THR:HB	1:A:238:PRO:HD2	1.82	0.60
1:B:191:SER:HB2	1:B:194:GLN:HE21	1.67	0.59
1:A:289:LYS:HD3	1:A:303:GLU:OE1	2.02	0.59
1:B:258:GLU:H	1:B:332:ASN:ND2	2.00	0.59
1:B:65:HIS:HD2	1:B:137:ASP:OD1	1.85	0.59
1:C:229:ASN:HB3	1:C:230:PHE:CE2	2.38	0.59
1:A:311:LEU:HD22	1:A:315:ASP:HB3	1.84	0.59
1:C:215:GLU:HB3	1:C:216:PRO:HD2	1.85	0.59
1:A:359:ARG:CG	1:A:359:ARG:O	2.50	0.59
1:B:237:THR:HB	1:B:238:PRO:HD2	1.83	0.59
1:B:80:ALA:HB2	1:B:120:LEU:HD22	1.84	0.59
1:A:289:LYS:HB2	1:A:303:GLU:HB3	1.83	0.59
1:B:169:ILE:HG13	1:B:170:ASN:N	2.18	0.59
1:A:127:ILE:O	1:A:127:ILE:HG22	2.03	0.59
1:C:225:ILE:HD13	1:C:235:GLU:HB3	1.84	0.59
1:B:225:ILE:HG13	1:B:226:TYR:H	1.68	0.59
1:B:262:LEU:O	1:B:326:VAL:HG23	2.02	0.59
1:B:228:ASN:ND2	1:B:230:PHE:HD2	2.01	0.59
1:C:74:PHE:HB3	1:C:123:ILE:HG22	1.84	0.59
1:A:225:ILE:HG13	1:A:226:TYR:N	2.17	0.59
1:A:130:ASN:HD21	1:B:321:ALA:H	1.49	0.59
1:C:379:ARG:HG3	1:C:380:LEU:H	1.64	0.59
1:A:32:LEU:CD2	1:A:52:VAL:HG22	2.32	0.59
1:C:50:ARG:HD3	1:C:133:GLY:O	2.02	0.59
1:C:71:PHE:HE2	1:C:126:ALA:HB2	1.68	0.59
1:C:57:LYS:HE2	1:C:58:PRO:HD2	1.83	0.59
1:B:32:LEU:HD23	1:B:52:VAL:HG22	1.84	0.59
1:B:163:HIS:HB2	1:C:384:GLN:HB2	1.85	0.58
1:B:51:ILE:CG2	1:B:123:ILE:HD11	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:HD21	1:B:103:ILE:HG12	1.85	0.58
1:C:57:LYS:CE	1:C:58:PRO:HD2	2.34	0.58
1:B:59:ASN:ND2	1:B:115:HIS:O	2.35	0.58
1:C:139:PHE:CZ	1:C:186:VAL:HG11	2.38	0.58
1:B:101:GLN:OE1	1:B:216:PRO:HB3	2.04	0.58
1:A:254:VAL:O	1:A:334:ASN:HA	2.02	0.58
1:A:161:SER:O	1:B:384:GLN:HG2	2.03	0.58
1:A:281:ALA:CB	1:A:333:LEU:HD13	2.34	0.58
1:B:304:VAL:CG1	1:B:305:GLN:N	2.66	0.58
1:B:170:ASN:HA	1:B:174:PHE:CD1	2.38	0.58
1:B:306:ARG:HG2	1:B:307:TYR:N	2.19	0.58
1:A:281:ALA:HA	1:A:330:THR:HG23	1.84	0.58
1:B:115:HIS:CD2	1:B:118:GLN:N	2.69	0.57
1:C:230:PHE:N	1:C:230:PHE:CD2	2.71	0.57
1:C:349:PHE:HB2	1:C:355:ASP:O	2.03	0.57
1:B:25:ASN:C	1:B:27:ASN:H	2.08	0.57
1:C:283:ILE:HG21	1:C:311:LEU:HD11	1.85	0.57
1:A:23:PHE:CZ	1:A:139:PHE:HE1	2.22	0.57
1:B:283:ILE:CD1	1:B:327:VAL:HG22	2.33	0.57
1:A:35:ARG:NH2	1:A:132:PRO:O	2.37	0.57
1:B:22:LEU:N	1:B:30:ILE:O	2.35	0.57
1:C:301:PRO:O	1:C:302:LEU:HD23	2.04	0.57
1:B:257:ASN:HD22	1:B:257:ASN:N	2.02	0.57
1:A:41:PRO:O	1:A:43:LEU:N	2.37	0.57
1:C:123:ILE:HG21	1:C:336:LEU:HD22	1.84	0.57
1:B:219:LEU:HD21	1:B:253:SER:N	2.18	0.57
1:C:115:HIS:CD2	1:C:118:GLN:HB3	2.40	0.57
1:B:197:GLN:HG2	1:C:364:GLN:NE2	2.20	0.57
1:B:115:HIS:HD2	1:B:117:HIS:N	2.03	0.57
1:B:73:LEU:HD23	1:B:103:ILE:HD12	1.87	0.56
1:A:241:ASN:OD1	1:A:243:GLN:HB2	2.05	0.56
1:C:270:ALA:H	1:C:345:ASN:HD21	1.52	0.56
1:B:357:VAL:CG1	1:B:358:VAL:N	2.68	0.56
1:B:24:GLU:HA	1:B:28:GLY:O	2.04	0.56
1:B:198:LEU:N	1:B:198:LEU:HD23	2.20	0.56
1:B:23:PHE:O	1:B:29:ARG:HA	2.06	0.56
1:C:380:LEU:HD13	1:C:381:LEU:N	2.20	0.56
1:A:373:SER:O	1:A:375:GLN:N	2.38	0.56
1:A:263:LEU:CD2	1:A:390:VAL:HG11	2.34	0.56
1:A:263:LEU:HD13	1:A:351:ALA:CB	2.35	0.56
1:B:306:ARG:HG2	1:B:307:TYR:H	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ILE:HD11	1:A:273:ILE:HG21	1.87	0.56
1:B:313:GLU:O	1:B:314:ASP:HB2	2.04	0.56
1:B:32:LEU:HD21	1:B:52:VAL:HG22	1.86	0.56
1:B:57:LYS:HB3	1:B:58:PRO:HD2	1.87	0.56
1:C:15:SER:HB3	1:C:314:ASP:O	2.05	0.56
1:B:272:VAL:CG1	1:B:319:ILE:HD12	2.35	0.56
1:B:331:SER:O	1:B:332:ASN:C	2.44	0.56
1:C:274:LEU:HD12	1:C:274:LEU:C	2.26	0.56
1:C:265:HIS:HB3	1:C:349:PHE:CD1	2.41	0.56
1:A:80:ALA:HB2	1:A:120:LEU:CD1	2.34	0.56
1:B:359:ARG:HH22	1:B:382:LYS:HE3	1.70	0.56
1:C:250:PHE:HB3	1:C:342:ALA:HB1	1.88	0.56
1:B:174:PHE:O	1:C:371:PRO:HG3	2.06	0.56
1:B:44:GLU:O	1:B:47:ARG:HG2	2.06	0.56
1:A:92:SER:HB3	1:A:202:ALA:HA	1.88	0.56
1:B:190:LEU:HD21	1:B:198:LEU:HD11	1.87	0.56
1:C:250:PHE:HB3	1:C:342:ALA:CB	2.36	0.56
1:A:167:GLU:O	1:A:171:ARG:NH1	2.39	0.56
1:C:220:ARG:NH1	1:C:220:ARG:CG	2.69	0.55
1:B:283:ILE:O	1:B:308:ARG:HA	2.06	0.55
1:A:160:THR:HG21	1:B:392:ALA:CA	2.36	0.55
1:B:283:ILE:HA	1:B:326:VAL:O	2.07	0.55
1:C:363:ARG:O	1:C:366:GLN:HB2	2.07	0.55
1:B:364:GLN:O	1:B:367:GLU:HB3	2.06	0.55
1:C:248:ASP:OD2	1:C:343:GLU:HB2	2.06	0.55
1:A:190:LEU:HD21	1:A:198:LEU:HD11	1.89	0.55
1:C:283:ILE:HD11	1:C:325:PHE:HD2	1.72	0.55
1:B:166:PHE:CZ	1:B:170:ASN:HB2	2.41	0.55
1:A:379:ARG:HH11	1:A:379:ARG:CB	2.07	0.55
1:B:191:SER:CB	1:B:194:GLN:HE21	2.19	0.55
1:A:373:SER:C	1:A:375:GLN:N	2.57	0.55
1:A:21:THR:HA	1:A:31:ARG:HB3	1.88	0.55
1:A:80:ALA:HB2	1:A:120:LEU:HD13	1.89	0.54
1:C:228:ASN:OD1	1:C:389:PHE:HB2	2.08	0.54
1:B:47:ARG:HH11	1:B:132:PRO:HG3	1.72	0.54
1:B:75:VAL:HG22	1:B:99:ASP:O	2.08	0.54
1:B:27:ASN:HD22	1:B:60:THR:HG22	1.72	0.54
1:A:191:SER:O	1:A:194:GLN:N	2.41	0.54
1:A:194:GLN:O	1:A:197:GLN:HB2	2.07	0.54
1:A:164:SER:OG	1:A:168:GLU:OE2	2.26	0.54
1:A:50:ARG:HB2	1:A:126:ALA:HB3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:SER:O	1:B:33:LEU:HA	2.08	0.54
1:A:392:ALA:HA	1:C:160:THR:HG21	1.89	0.54
1:B:197:GLN:HE21	1:B:197:GLN:CA	2.20	0.54
1:B:275:VAL:CG2	1:B:336:LEU:HD23	2.37	0.54
1:C:386:GLU:HB3	1:C:390:VAL:HG12	1.90	0.54
1:B:73:LEU:HD23	1:B:103:ILE:CD1	2.37	0.54
1:C:29:ARG:NH2	1:C:55:GLN:HE22	2.00	0.54
1:B:214:ASP:OD2	1:B:215:GLU:N	2.41	0.54
1:A:311:LEU:HD22	1:A:315:ASP:CB	2.37	0.54
1:A:321:ALA:O	1:A:322:ALA:HB3	2.08	0.54
1:A:363:ARG:HG2	1:A:374:ALA:HB1	1.89	0.53
1:B:281:ALA:CB	1:B:333:LEU:HD13	2.35	0.53
1:C:130:ASN:N	1:C:130:ASN:HD22	2.05	0.53
1:A:172:VAL:HG13	1:B:376:ASP:HB3	1.90	0.53
1:B:357:VAL:HG13	1:B:358:VAL:N	2.22	0.53
1:C:139:PHE:HB3	1:C:146:GLN:NE2	2.23	0.53
1:C:237:THR:HB	1:C:238:PRO:HD2	1.90	0.53
1:B:173:LEU:C	1:C:371:PRO:HD2	2.29	0.53
1:A:83:THR:HG21	1:A:110:TYR:OH	2.07	0.53
1:A:364:GLN:HB2	1:C:198:LEU:HD21	1.91	0.53
1:A:360:GLN:O	1:C:90:ARG:HD3	2.08	0.53
1:B:189:GLU:HG2	1:B:190:LEU:O	2.08	0.53
1:C:197:GLN:HA	1:C:197:GLN:NE2	2.20	0.53
1:A:30:ILE:HG12	1:A:54:PHE:HD1	1.72	0.53
1:A:331:SER:O	1:A:332:ASN:C	2.45	0.53
1:B:205:SER:N	1:B:216:PRO:HG2	2.24	0.53
1:B:49:TYR:CD1	1:B:125:LEU:HD11	2.44	0.53
1:A:149:TYR:CE1	1:B:350:LEU:HD11	2.41	0.52
1:A:250:PHE:C	1:A:250:PHE:CD2	2.82	0.52
1:B:29:ARG:HD3	1:B:55:GLN:HE21	1.73	0.52
1:A:61:ILE:HG12	1:A:62:LEU:H	1.74	0.52
1:A:367:GLU:CB	1:A:374:ALA:HB2	2.30	0.52
1:C:364:GLN:O	1:C:368:LEU:HD12	2.10	0.52
1:C:12:TYR:HE2	1:C:311:LEU:HD23	1.71	0.52
1:A:269:LYS:H	1:A:345:ASN:HD22	1.58	0.52
1:C:61:ILE:HG13	1:C:112:VAL:HG22	1.91	0.52
1:A:269:LYS:HD3	1:A:343:GLU:O	2.09	0.52
1:A:371:PRO:HG3	1:C:174:PHE:O	2.09	0.52
1:C:25:ASN:C	1:C:25:ASN:OD1	2.48	0.52
1:B:25:ASN:C	1:B:25:ASN:OD1	2.47	0.52
1:B:58:PRO:HB2	1:B:115:HIS:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LYS:O	1:B:204:SER:HB3	2.09	0.52
1:A:122:ILE:CG2	1:A:123:ILE:N	2.73	0.52
1:C:257:ASN:HD22	1:C:257:ASN:N	2.07	0.52
1:B:59:ASN:O	1:B:189:GLU:HG3	2.09	0.52
1:B:190:LEU:HD21	1:B:198:LEU:CD1	2.40	0.52
1:C:230:PHE:HB3	1:C:260:ALA:HB2	1.92	0.52
1:B:70:ASP:HB2	1:B:127:ILE:HB	1.92	0.52
1:A:61:ILE:O	1:A:187:ILE:HA	2.10	0.52
1:B:25:ASN:OD1	1:B:27:ASN:HB2	2.10	0.51
1:A:23:PHE:O	1:A:24:GLU:HB2	2.09	0.51
1:C:262:LEU:HD13	1:C:389:PHE:CE1	2.45	0.51
1:B:272:VAL:HG12	1:B:319:ILE:HD12	1.91	0.51
1:A:236:ILE:HG22	1:A:251:LEU:HB2	1.92	0.51
1:B:73:LEU:HD21	1:B:82:LEU:HD22	1.92	0.51
1:A:18:SER:O	1:A:34:GLN:HG3	2.10	0.51
1:B:191:SER:O	1:B:194:GLN:N	2.43	0.51
1:A:59:ASN:HD22	1:A:195:ILE:CD1	2.23	0.51
1:B:88:ASP:N	1:B:88:ASP:OD2	2.43	0.51
1:A:174:PHE:N	1:A:174:PHE:CD2	2.78	0.51
1:B:280:ASP:HA	1:B:311:LEU:O	2.10	0.51
1:C:81:ILE:O	1:C:111:LEU:HD12	2.10	0.51
1:B:261:LEU:CD2	1:B:390:VAL:HG22	2.41	0.51
1:C:92:SER:O	1:C:202:ALA:HA	2.10	0.51
1:A:363:ARG:CG	1:A:374:ALA:HB1	2.41	0.51
1:B:24:GLU:CG	1:B:29:ARG:HB3	2.31	0.51
1:C:250:PHE:HE2	1:C:252:SER:HG	1.59	0.51
1:A:280:ASP:HB2	1:A:330:THR:OG1	2.11	0.51
1:B:68:ASP:N	1:B:68:ASP:OD2	2.44	0.51
1:B:211:SER:O	1:B:212:SER:C	2.48	0.51
1:B:21:THR:CA	1:B:31:ARG:HG2	2.38	0.51
1:B:359:ARG:HH22	1:B:382:LYS:HG3	1.75	0.51
1:B:170:ASN:ND2	1:B:174:PHE:HD1	2.08	0.51
1:A:166:PHE:O	1:A:168:GLU:N	2.43	0.51
1:C:139:PHE:CE1	1:C:186:VAL:HG11	2.46	0.51
1:B:67:ALA:HB1	1:B:136:ASP:O	2.10	0.51
1:A:359:ARG:HH22	1:A:382:LYS:HD3	1.75	0.51
1:B:265:HIS:HE1	1:B:325:PHE:CZ	2.29	0.51
1:C:229:ASN:HB3	1:C:230:PHE:CD2	2.46	0.51
1:B:101:GLN:HG3	1:B:102:ARG:N	2.25	0.51
1:A:274:LEU:HD23	1:A:319:ILE:HD11	1.93	0.51
1:A:225:ILE:HD12	1:A:226:TYR:CD1	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:LEU:O	1:C:370:PHE:HB3	2.11	0.50
1:B:161:SER:O	1:C:384:GLN:HG2	2.11	0.50
1:A:277:ASN:HB3	1:A:334:ASN:ND2	2.26	0.50
1:C:81:ILE:CD1	1:C:199:SER:HA	2.41	0.50
1:C:210:ILE:HG22	1:C:211:SER:OG	2.10	0.50
1:B:191:SER:O	1:B:192:LYS:C	2.50	0.50
1:B:13:PHE:HE1	1:B:39:ARG:HD3	1.75	0.50
1:B:244:LEU:HD11	1:B:251:LEU:HD11	1.93	0.50
1:B:197:GLN:HB3	1:B:198:LEU:HD23	1.93	0.50
1:B:159:GLU:HG3	1:B:166:PHE:N	2.26	0.50
1:B:257:ASN:N	1:B:257:ASN:ND2	2.59	0.50
1:C:8:ASN:O	1:C:10:PRO:HD3	2.12	0.50
1:B:80:ALA:HB2	1:B:120:LEU:CD2	2.40	0.50
1:A:61:ILE:HG12	1:A:62:LEU:N	2.26	0.50
1:A:213:GLU:HG3	1:A:214:ASP:OD1	2.11	0.50
1:B:373:SER:O	1:B:376:ASP:HB2	2.12	0.50
1:B:168:GLU:O	1:B:172:VAL:HG23	2.12	0.50
1:A:370:PHE:O	1:A:372:GLY:N	2.39	0.50
1:B:69:ALA:CB	1:B:128:PRO:HA	2.42	0.50
1:A:79:ARG:NH1	1:A:94:ASN:OD1	2.45	0.50
1:C:288:ILE:CG2	1:C:302:LEU:HD22	2.39	0.50
1:A:222:ARG:NH2	1:A:240:LYS:HD3	2.27	0.50
1:A:371:PRO:HD2	1:C:173:LEU:O	2.12	0.50
1:A:59:ASN:HD22	1:A:195:ILE:HD11	1.77	0.50
1:C:359:ARG:HH22	1:C:382:LYS:CE	2.08	0.49
1:A:111:LEU:HD21	1:A:122:ILE:HD12	1.94	0.49
1:B:375:GLN:O	1:B:376:ASP:C	2.49	0.49
1:A:54:PHE:CE2	1:A:111:LEU:HD23	2.47	0.49
1:C:206:SER:OG	1:C:209:THR:HG23	2.12	0.49
1:B:75:VAL:HG12	1:B:122:ILE:CD1	2.40	0.49
1:B:286:VAL:O	1:B:324:PRO:HD2	2.12	0.49
1:C:119:ASN:N	1:C:119:ASN:ND2	2.60	0.49
1:A:79:ARG:NH1	1:A:94:ASN:HD21	2.09	0.49
1:A:225:ILE:HG13	1:A:233:PHE:O	2.12	0.49
1:B:130:ASN:O	1:C:45:ASN:HB2	2.11	0.49
1:C:19:PHE:HD2	1:C:31:ARG:HB2	1.78	0.49
1:B:254:VAL:HG21	1:B:335:PHE:CZ	2.47	0.49
1:B:209:THR:HB	1:B:215:GLU:HB3	1.93	0.49
1:A:267:ASN:HB3	1:A:345:ASN:HD21	1.78	0.49
1:A:183:GLN:NE2	1:B:368:LEU:O	2.45	0.49
1:C:37:ASN:H	1:C:37:ASN:HD22	1.58	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LEU:HD23	1:A:319:ILE:CD1	2.41	0.49
1:C:359:ARG:HH12	1:C:382:LYS:HE3	1.77	0.49
1:B:166:PHE:HD2	1:B:169:ILE:HD11	1.78	0.49
1:B:13:PHE:CE1	1:B:39:ARG:HD3	2.47	0.49
1:B:87:ASN:O	1:C:355:ASP:HA	2.13	0.49
1:A:166:PHE:C	1:A:168:GLU:H	2.16	0.49
1:A:159:GLU:HG2	1:A:166:PHE:H	1.78	0.49
1:C:278:GLU:O	1:C:333:LEU:HA	2.12	0.49
1:A:24:GLU:CD	1:A:29:ARG:HB2	2.32	0.49
1:C:228:ASN:O	1:C:230:PHE:N	2.45	0.49
1:A:66:HIS:CD2	1:B:322:ALA:HB1	2.48	0.49
1:A:154:SER:OG	1:A:157:ILE:HB	2.13	0.49
1:A:26:GLN:NE2	1:A:26:GLN:H	2.11	0.48
1:B:161:SER:HB3	1:C:263:LEU:HD22	1.95	0.48
1:A:55:GLN:HA	1:A:120:LEU:O	2.12	0.48
1:B:203:LYS:NZ	1:B:215:GLU:CD	2.67	0.48
1:C:65:HIS:HB2	1:C:138:PHE:O	2.13	0.48
1:B:157:ILE:O	1:B:161:SER:OG	2.31	0.48
1:C:119:ASN:N	1:C:119:ASN:HD22	2.08	0.48
1:A:153:PHE:CZ	1:B:264:PRO:HB3	2.49	0.48
1:C:356:ASN:ND2	1:C:359:ARG:HB2	2.28	0.48
1:B:79:ARG:O	1:B:120:LEU:HD13	2.12	0.48
1:A:29:ARG:HD3	1:A:55:GLN:NE2	2.21	0.48
1:B:265:HIS:CE1	1:B:325:PHE:CZ	3.02	0.48
1:C:331:SER:O	1:C:332:ASN:C	2.52	0.48
1:C:83:THR:HA	1:C:91:ASP:O	2.12	0.48
1:A:263:LEU:HG	1:A:390:VAL:HG12	1.94	0.48
1:C:382:LYS:HE2	1:C:385:ARG:HE	1.76	0.48
1:C:319:ILE:HD13	1:C:325:PHE:CD1	2.49	0.48
1:A:392:ALA:HA	1:C:160:THR:HG23	1.94	0.48
1:C:57:LYS:O	1:C:60:THR:HG23	2.13	0.48
1:C:69:ALA:HB2	1:C:128:PRO:HA	1.95	0.48
1:B:159:GLU:HG3	1:B:166:PHE:H	1.79	0.48
1:C:263:LEU:HD13	1:C:351:ALA:O	2.13	0.48
1:C:164:SER:OG	1:C:168:GLU:HB3	2.13	0.48
1:B:61:ILE:HA	1:B:111:LEU:O	2.13	0.48
1:C:269:LYS:HE2	1:C:341:ASN:OD1	2.14	0.48
1:A:371:PRO:HG3	1:C:174:PHE:C	2.34	0.48
1:B:172:VAL:HG11	1:C:376:ASP:O	2.14	0.48
1:A:236:ILE:HD11	1:A:240:LYS:HB3	1.94	0.48
1:B:141:SER:HB2	1:C:369:ALA:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ILE:HG21	1:A:336:LEU:CD2	2.43	0.48
1:A:368:LEU:HD12	1:C:183:GLN:OE1	2.13	0.48
1:C:312:SER:O	1:C:315:ASP:HB2	2.14	0.48
1:B:12:TYR:HB2	1:B:317:PHE:HE2	1.79	0.48
1:A:225:ILE:HD12	1:A:226:TYR:CZ	2.49	0.48
1:A:112:VAL:O	1:A:114:PRO:HD3	2.12	0.48
1:A:156:ASN:H	1:A:156:ASN:ND2	2.08	0.48
1:A:349:PHE:O	1:A:356:ASN:HA	2.14	0.48
1:C:71:PHE:CE2	1:C:126:ALA:HB2	2.49	0.48
1:A:217:PHE:CD1	1:A:241:ASN:ND2	2.82	0.48
1:B:49:TYR:CZ	1:B:340:ILE:HD12	2.49	0.48
1:C:9:ASN:HD22	1:C:9:ASN:C	2.17	0.48
1:A:29:ARG:CD	1:A:55:GLN:NE2	2.77	0.47
1:B:65:HIS:CD2	1:B:137:ASP:OD1	2.67	0.47
1:B:310:GLU:O	1:B:311:LEU:HD23	2.13	0.47
1:B:269:LYS:H	1:B:345:ASN:HD22	1.61	0.47
1:A:23:PHE:CE1	1:B:302:LEU:HD13	2.49	0.47
1:C:120:LEU:HD11	1:C:122:ILE:HD11	1.96	0.47
1:C:197:GLN:HE21	1:C:197:GLN:CA	2.13	0.47
1:C:244:LEU:HG	1:C:249:ILE:O	2.14	0.47
1:C:3:VAL:HG13	1:C:4:ARG:N	2.29	0.47
1:C:129:VAL:C	1:C:130:ASN:HD22	2.17	0.47
1:C:36:PHE:HB3	1:C:43:LEU:CD1	2.45	0.47
1:A:210:ILE:HD11	1:A:221:SER:OG	2.15	0.47
1:B:75:VAL:HG21	1:B:96:HIS:O	2.14	0.47
1:A:166:PHE:HA	1:A:169:ILE:HD11	1.95	0.47
1:B:95:LEU:N	1:B:95:LEU:HD23	2.29	0.47
1:C:213:GLU:HG2	1:C:242:PRO:CB	2.44	0.47
1:B:34:GLN:NE2	1:B:39:ARG:HD3	2.30	0.47
1:A:228:ASN:O	1:A:230:PHE:N	2.46	0.47
1:A:273:ILE:HB	1:A:338:PHE:HB2	1.96	0.47
1:B:140:LEU:HG	1:B:149:TYR:OH	2.15	0.47
1:C:359:ARG:CZ	1:C:382:LYS:HE3	2.45	0.47
1:B:23:PHE:HZ	1:B:145:ALA:CB	2.28	0.47
1:C:55:GLN:HA	1:C:120:LEU:O	2.15	0.47
1:B:284:GLU:HB2	1:B:326:VAL:CG1	2.39	0.47
1:A:305:GLN:HE21	1:A:306:ARG:H	1.62	0.47
1:A:147:GLN:O	1:A:148:SER:C	2.53	0.47
1:A:268:SER:HB3	1:A:346:GLN:H	1.79	0.47
1:A:333:LEU:HG	1:A:334:ASN:N	2.30	0.47
1:A:57:LYS:HA	1:A:119:ASN:OD1	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:LEU:HD22	1:B:162:PHE:HZ	1.79	0.47
1:C:154:SER:OG	1:C:157:ILE:HD13	2.15	0.47
1:A:14:ARG:HG2	1:A:16:SER:H	1.79	0.47
1:A:84:LEU:HD21	1:A:103:ILE:HG12	1.96	0.47
1:B:197:GLN:NE2	1:B:197:GLN:CA	2.78	0.46
1:B:86:ASN:HD22	1:B:86:ASN:N	2.11	0.46
1:B:69:ALA:HB2	1:B:128:PRO:HA	1.98	0.46
1:B:319:ILE:O	1:B:320:PRO:O	2.33	0.46
1:B:283:ILE:HD11	1:B:327:VAL:HG22	1.97	0.46
1:C:218:ASN:O	1:C:221:SER:HB2	2.15	0.46
1:A:228:ASN:OD1	1:A:389:PHE:HB2	2.15	0.46
1:B:51:ILE:HG23	1:B:123:ILE:HD11	1.97	0.46
1:B:228:ASN:C	1:B:228:ASN:ND2	2.67	0.46
1:C:384:GLN:HE21	1:C:386:GLU:N	2.09	0.46
1:B:79:ARG:CG	1:B:79:ARG:NH1	2.71	0.46
1:C:319:ILE:CD1	1:C:325:PHE:CD1	2.98	0.46
1:B:230:PHE:HB3	1:B:260:ALA:HB2	1.96	0.46
1:B:375:GLN:O	1:B:378:GLU:N	2.48	0.46
1:C:366:GLN:O	1:C:369:ALA:N	2.48	0.46
1:A:219:LEU:HD23	1:A:253:SER:HB2	1.97	0.46
1:A:157:ILE:HG22	1:A:158:LEU:N	2.30	0.46
1:B:225:ILE:HG13	1:B:226:TYR:N	2.31	0.46
1:C:236:ILE:O	1:C:236:ILE:HG23	2.15	0.46
1:B:258:GLU:H	1:B:332:ASN:HD22	1.63	0.46
1:A:191:SER:O	1:A:193:GLU:N	2.48	0.46
1:C:230:PHE:HE1	1:C:391:ASP:OD1	1.98	0.46
1:B:73:LEU:HD11	1:B:95:LEU:HD12	1.98	0.46
1:B:282:ASN:O	1:B:327:VAL:HA	2.13	0.46
1:B:184:GLU:O	1:B:185:GLY:O	2.34	0.46
1:A:37:ASN:H	1:A:37:ASN:ND2	2.12	0.46
1:B:47:ARG:HH11	1:B:132:PRO:CG	2.29	0.46
1:A:257:ASN:ND2	1:A:257:ASN:N	2.62	0.46
1:C:68:ASP:OD2	1:C:68:ASP:O	2.34	0.46
1:B:197:GLN:HE21	1:B:197:GLN:H	1.62	0.46
1:A:65:HIS:HB3	1:A:139:PHE:CD2	2.50	0.46
1:B:349:PHE:O	1:B:356:ASN:HA	2.16	0.46
1:A:12:TYR:CE2	1:A:311:LEU:HD23	2.50	0.46
1:B:54:PHE:CE2	1:B:111:LEU:HD23	2.50	0.46
1:B:25:ASN:HD21	1:B:187:ILE:CB	2.19	0.46
1:B:308:ARG:CG	1:B:309:ALA:N	2.78	0.46
1:B:349:PHE:CE2	1:B:388:TYR:HD2	2.34	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:ILE:O	1:C:236:ILE:CG2	2.63	0.46
1:B:250:PHE:HD1	1:B:342:ALA:CB	2.29	0.46
1:B:173:LEU:O	1:C:371:PRO:HD2	2.14	0.46
1:A:183:GLN:HG2	1:A:188:VAL:HG11	1.97	0.46
1:B:244:LEU:HD21	1:B:251:LEU:HD12	1.98	0.46
1:C:83:THR:HB	1:C:110:TYR:CE2	2.51	0.45
1:C:146:GLN:OE1	1:C:186:VAL:HG12	2.16	0.45
1:A:234:PHE:HB2	1:A:253:SER:O	2.16	0.45
1:B:36:PHE:CD2	1:B:46:LEU:HB3	2.51	0.45
1:C:374:ALA:O	1:C:378:GLU:N	2.49	0.45
1:C:210:ILE:HG22	1:C:211:SER:N	2.30	0.45
1:C:219:LEU:HD13	1:C:236:ILE:HB	1.98	0.45
1:C:384:GLN:NE2	1:C:386:GLU:H	2.11	0.45
1:B:250:PHE:CD2	1:B:250:PHE:C	2.90	0.45
1:A:61:ILE:HG22	1:A:188:VAL:HG22	1.98	0.45
1:A:156:ASN:ND2	1:A:156:ASN:N	2.63	0.45
1:C:140:LEU:O	1:C:148:SER:OG	2.29	0.45
1:A:379:ARG:HG2	1:A:379:ARG:O	2.16	0.45
1:B:283:ILE:HG13	1:B:327:VAL:HG22	1.99	0.45
1:A:236:ILE:O	1:A:236:ILE:CG2	2.63	0.45
1:C:37:ASN:ND2	1:C:37:ASN:N	2.64	0.45
1:B:261:LEU:HD23	1:B:390:VAL:HG22	1.98	0.45
1:A:58:PRO:HA	1:A:113:ASN:ND2	2.32	0.45
1:B:112:VAL:O	1:B:114:PRO:HD3	2.16	0.45
1:B:25:ASN:C	1:B:27:ASN:N	2.69	0.45
1:B:226:TYR:HB3	1:B:388:TYR:CD1	2.52	0.45
1:C:130:ASN:N	1:C:130:ASN:ND2	2.65	0.45
1:C:171:ARG:O	1:C:181:ARG:NH2	2.50	0.45
1:C:195:ILE:O	1:C:199:SER:CB	2.64	0.45
1:C:241:ASN:HA	1:C:242:PRO:HD2	1.83	0.45
1:B:63:LEU:HD12	1:B:186:VAL:HA	1.99	0.45
1:B:140:LEU:HD13	1:C:358:VAL:HG13	1.99	0.45
1:B:283:ILE:HG13	1:B:326:VAL:O	2.17	0.45
1:C:81:ILE:HD13	1:C:199:SER:HA	1.98	0.45
1:B:63:LEU:HA	1:B:63:LEU:HD23	1.78	0.45
1:B:289:LYS:HB2	1:B:303:GLU:O	2.17	0.45
1:C:306:ARG:H	1:C:306:ARG:HG2	1.56	0.45
1:C:12:TYR:CD2	1:C:311:LEU:HD23	2.51	0.45
1:B:356:ASN:HB3	1:B:359:ARG:HB3	1.98	0.45
1:A:183:GLN:OE1	1:B:368:LEU:HD12	2.17	0.45
1:C:65:HIS:HB3	1:C:139:PHE:CD2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:TYR:HE2	1:A:311:LEU:CD2	2.28	0.45
1:A:289:LYS:C	1:A:290:GLU:HG3	2.37	0.45
1:A:87:ASN:O	1:B:355:ASP:HA	2.17	0.45
1:C:11:PHE:HB3	1:C:318:VAL:O	2.17	0.44
1:B:304:VAL:HG12	1:B:305:GLN:N	2.32	0.44
1:C:146:GLN:OE1	1:C:186:VAL:CG1	2.65	0.44
1:B:84:LEU:O	1:B:90:ARG:HA	2.18	0.44
1:A:166:PHE:HA	1:A:169:ILE:CD1	2.48	0.44
1:B:232:LYS:HE3	1:B:232:LYS:HB2	1.72	0.44
1:B:11:PHE:HB3	1:B:318:VAL:O	2.17	0.44
1:A:308:ARG:HG2	1:A:309:ALA:N	2.32	0.44
1:A:73:LEU:O	1:A:100:ALA:HA	2.17	0.44
1:C:172:VAL:HG12	1:C:172:VAL:O	2.17	0.44
1:B:174:PHE:C	1:C:371:PRO:HG3	2.38	0.44
1:B:234:PHE:O	1:B:252:SER:HA	2.17	0.44
1:A:165:GLU:O	1:A:166:PHE:C	2.56	0.44
1:B:356:ASN:HB3	1:B:359:ARG:HD2	2.00	0.44
1:A:193:GLU:CG	1:A:197:GLN:HE22	2.26	0.44
1:B:268:SER:HB3	1:B:346:GLN:H	1.82	0.44
1:C:359:ARG:NH1	1:C:382:LYS:HE3	2.33	0.44
1:C:84:LEU:HD21	1:C:103:ILE:HG12	1.99	0.44
1:B:263:LEU:HG	1:B:390:VAL:HG13	2.00	0.44
1:B:81:ILE:HG13	1:B:114:PRO:HD3	2.00	0.44
1:B:254:VAL:HG23	1:B:254:VAL:O	2.18	0.44
1:A:357:VAL:HG13	1:A:358:VAL:N	2.33	0.44
1:B:12:TYR:HB2	1:B:317:PHE:CE2	2.53	0.44
1:B:166:PHE:O	1:B:169:ILE:CG1	2.62	0.44
1:A:43:LEU:CD2	1:A:318:VAL:HG21	2.40	0.44
1:A:45:ASN:HB2	1:C:130:ASN:O	2.18	0.44
1:A:35:ARG:HB2	1:A:38:LYS:HB3	2.00	0.44
1:C:3:VAL:CG1	1:C:4:ARG:N	2.79	0.44
1:B:288:ILE:HG22	1:B:289:LYS:O	2.17	0.44
1:B:236:ILE:HD13	1:B:240:LYS:CB	2.43	0.43
1:A:79:ARG:O	1:A:120:LEU:HD13	2.17	0.43
1:C:74:PHE:CE2	1:C:219:LEU:HD23	2.53	0.43
1:A:47:ARG:HG3	1:A:48:ASP:N	2.33	0.43
1:B:263:LEU:HA	1:B:263:LEU:HD23	1.68	0.43
1:C:12:TYR:HD2	1:C:311:LEU:HD21	1.83	0.43
1:A:115:HIS:CD2	1:A:118:GLN:N	2.78	0.43
1:B:284:GLU:OE1	1:B:306:ARG:HD3	2.19	0.43
1:A:236:ILE:CD1	1:A:240:LYS:HB3	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ASP:CG	1:C:171:ARG:HH21	2.20	0.43
1:A:149:TYR:O	1:B:286:VAL:HG21	2.19	0.43
1:A:220:ARG:HA	1:A:234:PHE:CD2	2.53	0.43
1:A:230:PHE:CD2	1:A:230:PHE:N	2.85	0.43
1:A:66:HIS:HD2	1:A:106:GLY:HA2	1.83	0.43
1:A:93:TYR:HA	1:A:203:LYS:O	2.17	0.43
1:C:285:LEU:HD21	1:C:323:TYR:HB3	2.00	0.43
1:B:258:GLU:HG3	1:B:331:SER:HA	2.00	0.43
1:A:41:PRO:C	1:A:43:LEU:N	2.72	0.43
1:A:277:ASN:HB3	1:A:334:ASN:O	2.18	0.43
1:A:250:PHE:HD1	1:A:342:ALA:CB	2.32	0.43
1:C:220:ARG:NH2	1:C:255:ASP:OD2	2.51	0.43
1:B:190:LEU:HB3	1:B:191:SER:H	1.64	0.43
1:A:156:ASN:HD22	1:A:156:ASN:N	2.12	0.43
1:A:358:VAL:CG1	1:A:381:LEU:HD11	2.45	0.43
1:C:257:ASN:ND2	1:C:257:ASN:N	2.66	0.43
1:C:357:VAL:HG13	1:C:358:VAL:N	2.27	0.43
1:B:19:PHE:HD2	1:B:31:ARG:CZ	2.32	0.43
1:B:336:LEU:HG	1:B:337:ALA:N	2.33	0.43
1:C:170:ASN:HA	1:C:170:ASN:HD22	1.63	0.43
1:C:197:GLN:CA	1:C:197:GLN:NE2	2.80	0.43
1:A:143:THR:HB	1:A:183:GLN:O	2.18	0.43
1:B:286:VAL:O	1:B:286:VAL:HG22	2.19	0.43
1:A:218:ASN:HB3	1:A:221:SER:HB3	2.00	0.43
1:C:266:PHE:HB3	1:C:324:PRO:HA	1.99	0.43
1:C:218:ASN:HB3	1:C:221:SER:CB	2.45	0.43
1:C:49:TYR:O	1:C:50:ARG:HD2	2.19	0.43
1:B:244:LEU:HG	1:B:249:ILE:O	2.19	0.43
1:C:359:ARG:HH12	1:C:382:LYS:CE	2.32	0.43
1:C:169:ILE:CG2	1:C:173:LEU:HD12	2.49	0.43
1:A:250:PHE:CE1	1:A:339:GLY:HA3	2.53	0.43
1:B:285:LEU:HD23	1:B:325:PHE:CB	2.42	0.43
1:B:320:PRO:HB2	1:B:323:TYR:CG	2.54	0.43
1:B:359:ARG:HH22	1:B:382:LYS:CG	2.32	0.43
1:B:219:LEU:HD21	1:B:253:SER:HB2	2.01	0.43
1:A:19:PHE:HA	1:A:32:LEU:O	2.18	0.43
1:B:73:LEU:HB2	1:B:124:LYS:HG2	2.01	0.43
1:B:19:PHE:HE2	1:B:53:GLN:HE21	1.65	0.43
1:B:349:PHE:CE2	1:B:388:TYR:CD2	3.07	0.43
1:A:306:ARG:HH12	1:C:154:SER:CA	2.31	0.43
1:A:330:THR:O	1:A:331:SER:HB3	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:THR:O	1:A:211:SER:N	2.52	0.43
1:A:146:GLN:HA	1:B:302:LEU:HB3	2.01	0.42
1:C:248:ASP:OD1	1:C:341:ASN:HA	2.19	0.42
1:B:275:VAL:HG21	1:B:336:LEU:HD23	2.01	0.42
1:B:285:LEU:HD21	1:B:319:ILE:HG23	2.01	0.42
1:B:151:GLN:HE21	1:B:151:GLN:HB3	1.59	0.42
1:B:151:GLN:OE1	1:B:174:PHE:CD1	2.72	0.42
1:A:60:THR:O	1:A:112:VAL:HG13	2.19	0.42
1:A:220:ARG:H	1:A:220:ARG:HG3	1.53	0.42
1:A:192:LYS:HA	1:A:195:ILE:HG13	2.01	0.42
1:C:36:PHE:HB3	1:C:43:LEU:HD12	2.01	0.42
1:A:96:HIS:N	1:A:96:HIS:CD2	2.86	0.42
1:C:265:HIS:HB3	1:C:349:PHE:CE1	2.54	0.42
1:A:263:LEU:HD23	1:A:263:LEU:HA	1.80	0.42
1:A:358:VAL:O	1:A:358:VAL:HG12	2.18	0.42
1:C:225:ILE:CD1	1:C:235:GLU:HB3	2.48	0.42
1:A:161:SER:HB3	1:B:263:LEU:HD22	2.01	0.42
1:C:269:LYS:HE2	1:C:269:LYS:HB2	1.84	0.42
1:B:165:GLU:O	1:B:166:PHE:C	2.58	0.42
1:B:141:SER:HB2	1:C:369:ALA:HA	2.00	0.42
1:C:259:GLY:O	1:C:392:ALA:N	2.49	0.42
1:A:373:SER:HB3	1:A:376:ASP:CG	2.39	0.42
1:A:53:GLN:HG3	1:A:123:ILE:HD12	2.02	0.42
1:C:68:ASP:HB3	1:C:136:ASP:H	1.84	0.42
1:C:357:VAL:O	1:C:359:ARG:N	2.52	0.42
1:B:25:ASN:ND2	1:B:187:ILE:HG13	2.35	0.42
1:A:159:GLU:CG	1:A:166:PHE:H	2.32	0.42
1:B:226:TYR:CD1	1:B:226:TYR:N	2.87	0.42
1:C:154:SER:OG	1:C:157:ILE:CD1	2.68	0.42
1:C:230:PHE:HB3	1:C:260:ALA:CB	2.50	0.42
1:C:73:LEU:O	1:C:100:ALA:HA	2.20	0.42
1:B:80:ALA:HA	1:B:112:VAL:O	2.19	0.42
1:A:244:LEU:HD11	1:A:251:LEU:CD1	2.50	0.42
1:A:333:LEU:HD21	1:A:335:PHE:HD1	1.85	0.42
1:B:140:LEU:CD1	1:C:358:VAL:HG13	2.50	0.42
1:B:27:ASN:HD22	1:B:60:THR:CG2	2.32	0.42
1:C:37:ASN:ND2	1:C:37:ASN:H	2.16	0.42
1:C:164:SER:HB2	1:C:168:GLU:OE2	2.20	0.42
1:B:54:PHE:CZ	1:B:56:SER:HB3	2.55	0.42
1:B:284:GLU:OE1	1:B:306:ARG:NH1	2.51	0.42
1:B:276:ILE:HD12	1:B:333:LEU:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LEU:CD2	1:B:253:SER:HB2	2.50	0.42
1:B:286:VAL:HG13	1:B:324:PRO:HD2	2.01	0.42
1:C:384:GLN:O	1:C:384:GLN:HG3	2.19	0.42
1:A:250:PHE:HE2	1:A:252:SER:OG	2.03	0.42
1:B:211:SER:O	1:B:242:PRO:HG3	2.20	0.42
1:B:269:LYS:H	1:B:345:ASN:ND2	2.18	0.42
1:C:285:LEU:HD11	1:C:320:PRO:HD2	2.00	0.42
1:A:376:ASP:OD1	1:C:171:ARG:NH2	2.48	0.42
1:A:76:LEU:HD13	1:A:277:ASN:CG	2.41	0.42
1:A:122:ILE:HG22	1:A:123:ILE:N	2.34	0.42
1:A:370:PHE:C	1:A:372:GLY:H	2.23	0.42
1:B:86:ASN:N	1:B:86:ASN:ND2	2.68	0.42
1:B:35:ARG:O	1:B:38:LYS:HB3	2.20	0.42
1:C:12:TYR:CD2	1:C:311:LEU:CD2	3.03	0.41
1:B:391:ASP:OD2	1:B:392:ALA:N	2.53	0.41
1:A:371:PRO:O	1:C:181:ARG:NH2	2.53	0.41
1:A:101:GLN:HG3	1:A:102:ARG:H	1.85	0.41
1:C:31:ARG:HH11	1:C:53:GLN:HE22	1.68	0.41
1:B:305:GLN:HG3	1:B:306:ARG:N	2.34	0.41
1:B:359:ARG:NH2	1:B:382:LYS:HE3	2.34	0.41
1:A:150:LEU:C	1:A:152:GLY:N	2.69	0.41
1:B:191:SER:H	1:B:194:GLN:HB2	1.85	0.41
1:A:191:SER:N	1:A:194:GLN:HG3	2.31	0.41
1:C:56:SER:HB2	1:C:60:THR:OG1	2.21	0.41
1:C:199:SER:O	1:C:200:ARG:HG2	2.20	0.41
1:C:31:ARG:HH11	1:C:53:GLN:NE2	2.18	0.41
1:A:373:SER:O	1:A:376:ASP:N	2.52	0.41
1:C:366:GLN:O	1:C:367:GLU:C	2.58	0.41
1:C:35:ARG:HG3	1:C:50:ARG:CZ	2.51	0.41
1:C:25:ASN:O	1:C:26:GLN:C	2.58	0.41
1:B:29:ARG:NH1	1:B:31:ARG:CZ	2.83	0.41
1:A:198:LEU:HG	1:A:198:LEU:H	1.58	0.41
1:A:34:GLN:HG3	1:A:34:GLN:H	1.57	0.41
1:B:14:ARG:CB	1:B:17:ASN:HB2	2.22	0.41
1:C:236:ILE:HG22	1:C:251:LEU:HB2	2.03	0.41
1:A:376:ASP:CG	1:C:171:ARG:NH2	2.74	0.41
1:B:205:SER:CA	1:B:216:PRO:HG2	2.51	0.41
1:C:210:ILE:O	1:C:241:ASN:HB2	2.21	0.41
1:C:169:ILE:HG22	1:C:173:LEU:HD12	2.03	0.41
1:B:128:PRO:HB3	1:B:135:TYR:HB3	2.03	0.41
1:C:359:ARG:HH12	1:C:382:LYS:NZ	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ASN:HB2	1:B:26:GLN:NE2	2.36	0.41
1:C:53:GLN:HE21	1:C:55:GLN:HE21	1.69	0.41
1:A:244:LEU:HD21	1:A:251:LEU:HD12	2.03	0.41
1:B:386:GLU:OE1	1:B:386:GLU:HA	2.20	0.41
1:C:12:TYR:OH	1:C:14:ARG:HG3	2.21	0.41
1:B:173:LEU:HA	1:C:370:PHE:HB3	2.03	0.41
1:C:380:LEU:HD13	1:C:381:LEU:HG	1.97	0.41
1:B:83:THR:HG23	1:B:92:SER:OG	2.20	0.41
1:C:119:ASN:H	1:C:119:ASN:ND2	2.12	0.41
1:A:340:ILE:H	1:A:340:ILE:HG12	1.76	0.41
1:B:25:ASN:ND2	1:B:187:ILE:O	2.54	0.40
1:B:237:THR:HB	1:B:238:PRO:CD	2.51	0.40
1:A:83:THR:O	1:A:109:TYR:HB2	2.21	0.40
1:B:110:TYR:CZ	1:C:365:VAL:HG21	2.56	0.40
1:C:283:ILE:HG12	1:C:284:GLU:N	2.36	0.40
1:C:269:LYS:H	1:C:345:ASN:HD22	1.64	0.40
1:A:263:LEU:CD2	1:A:390:VAL:CG1	2.97	0.40
1:C:84:LEU:HD11	1:C:101:GLN:HE21	1.86	0.40
1:A:354:LYS:HB2	1:A:387:SER:HB3	2.02	0.40
1:B:49:TYR:O	1:B:50:ARG:HD2	2.20	0.40
1:C:285:LEU:HB3	1:C:307:TYR:HB2	2.03	0.40
1:B:380:LEU:HD23	1:B:383:LYS:HD2	2.03	0.40
1:A:131:LYS:HD2	1:A:134:ARG:O	2.22	0.40
1:A:353:GLU:O	1:A:353:GLU:HG2	2.21	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	362/416 (87%)	307 (85%)	39 (11%)	16 (4%)	3 6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	359/416 (86%)	293 (82%)	55 (15%)	11 (3%)	5	12
1	C	375/416 (90%)	325 (87%)	42 (11%)	8 (2%)	9	23
All	All	1096/1248 (88%)	925 (84%)	136 (12%)	35 (3%)	5	12

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	PHE
1	A	229	ASN
1	A	388	TYR
1	B	26	GLN
1	B	185	GLY
1	B	229	ASN
1	B	320	PRO
1	C	199	SER
1	C	221	SER
1	C	229	ASN
1	A	42	GLN
1	A	141	SER
1	A	167	GLU
1	A	374	ALA
1	A	192	LYS
1	A	220	ARG
1	A	320	PRO
1	A	331	SER
1	B	34	GLN
1	A	206	SER
1	A	332	ASN
1	B	198	LEU
1	B	332	ASN
1	B	378	GLU
1	C	105	ALA
1	A	199	SER
1	B	331	SER
1	C	263	LEU
1	C	363	ARG
1	A	371	PRO
1	C	106	GLY
1	C	358	VAL
1	B	104	PRO
1	A	210	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	195	ILE

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	333/375 (89%)	244 (73%)	89 (27%)	0	2
1	B	330/375 (88%)	229 (69%)	101 (31%)	0	1
1	C	343/375 (92%)	250 (73%)	93 (27%)	0	1
All	All	1006/1125 (89%)	723 (72%)	283 (28%)	0	1

All (283) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	16	SER
1	A	17	ASN
1	A	26	GLN
1	A	29	ARG
1	A	31	ARG
1	A	34	GLN
1	A	37	ASN
1	A	38	LYS
1	A	39	ARG
1	A	44	GLU
1	A	47	ARG
1	A	50	ARG
1	A	53	GLN
1	A	55	GLN
1	A	56	SER
1	A	62	LEU
1	A	70	ASP
1	A	73	LEU
1	A	77	SER
1	A	82	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	92	SER
1	A	94	ASN
1	A	96	HIS
1	A	102	ARG
1	A	117	HIS
1	A	123	ILE
1	A	131	LYS
1	A	140	LEU
1	A	142	SER
1	A	146	GLN
1	A	156	ASN
1	A	157	ILE
1	A	160	THR
1	A	167	GLU
1	A	171	ARG
1	A	174	PHE
1	A	183	GLN
1	A	187	ILE
1	A	188	VAL
1	A	191	SER
1	A	194	GLN
1	A	196	ARG
1	A	197	GLN
1	A	198	LEU
1	A	200	ARG
1	A	207	ARG
1	A	214	ASP
1	A	215	GLU
1	A	220	ARG
1	A	222	ARG
1	A	227	SER
1	A	229	ASN
1	A	230	PHE
1	A	232	LYS
1	A	236	ILE
1	A	240	LYS
1	A	244	LEU
1	A	245	ARG
1	A	250	PHE
1	A	254	VAL
1	A	257	ASN
1	A	261	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	277	ASN
1	A	280	ASP
1	A	282	ASN
1	A	285	LEU
1	A	289	LYS
1	A	290	GLU
1	A	291	GLN
1	A	310	GLU
1	A	312	SER
1	A	318	VAL
1	A	326	VAL
1	A	333	LEU
1	A	334	ASN
1	A	336	LEU
1	A	343	GLU
1	A	346	GLN
1	A	354	LYS
1	A	363	ARG
1	A	375	GLN
1	A	378	GLU
1	A	379	ARG
1	A	380	LEU
1	A	382	LYS
1	A	385	ARG
1	A	386	GLU
1	A	390	VAL
1	B	15	SER
1	B	18	SER
1	B	19	PHE
1	B	20	GLN
1	B	23	PHE
1	B	26	GLN
1	B	29	ARG
1	B	32	LEU
1	B	37	ASN
1	B	39	ARG
1	B	42	GLN
1	B	43	LEU
1	B	44	GLU
1	B	48	ASP
1	B	53	GLN
1	B	61	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	62	LEU
1	B	70	ASP
1	B	73	LEU
1	B	75	VAL
1	B	79	ARG
1	B	84	LEU
1	B	86	ASN
1	B	90	ARG
1	B	94	ASN
1	B	95	LEU
1	B	117	HIS
1	B	119	ASN
1	B	123	ILE
1	B	131	LYS
1	B	137	ASP
1	B	140	LEU
1	B	146	GLN
1	B	148	SER
1	B	151	GLN
1	B	154	SER
1	B	156	ASN
1	B	157	ILE
1	B	158	LEU
1	B	161	SER
1	B	164	SER
1	B	165	GLU
1	B	167	GLU
1	B	171	ARG
1	B	183	GLN
1	B	186	VAL
1	B	187	ILE
1	B	192	LYS
1	B	193	GLU
1	B	197	GLN
1	B	198	LEU
1	B	199	SER
1	B	200	ARG
1	B	201	ARG
1	B	206	SER
1	B	211	SER
1	B	213	GLU
1	B	214	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	215	GLU
1	B	219	LEU
1	B	220	ARG
1	B	221	SER
1	B	222	ARG
1	B	226	TYR
1	B	228	ASN
1	B	229	ASN
1	B	232	LYS
1	B	236	ILE
1	B	239	GLU
1	B	240	LYS
1	B	244	LEU
1	B	247	LEU
1	B	261	LEU
1	B	265	HIS
1	B	268	SER
1	B	274	LEU
1	B	275	VAL
1	B	277	ASN
1	B	282	ASN
1	B	283	ILE
1	B	285	LEU
1	B	286	VAL
1	B	289	LYS
1	B	290	GLU
1	B	302	LEU
1	B	306	ARG
1	B	308	ARG
1	B	310	GLU
1	B	318	VAL
1	B	332	ASN
1	B	333	LEU
1	B	334	ASN
1	B	336	LEU
1	B	343	GLU
1	B	346	GLN
1	B	357	VAL
1	B	373	SER
1	B	375	GLN
1	B	378	GLU
1	B	380	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	386	GLU
1	C	3	VAL
1	C	4	ARG
1	C	5	GLU
1	C	7	GLU
1	C	8	ASN
1	C	9	ASN
1	C	16	SER
1	C	18	SER
1	C	26	GLN
1	C	31	ARG
1	C	32	LEU
1	C	37	ASN
1	C	38	LYS
1	C	39	ARG
1	C	42	GLN
1	C	43	LEU
1	C	44	GLU
1	C	51	ILE
1	C	53	GLN
1	C	62	LEU
1	C	70	ASP
1	C	79	ARG
1	C	82	LEU
1	C	94	ASN
1	C	96	HIS
1	C	101	GLN
1	C	113	ASN
1	C	115	HIS
1	C	119	ASN
1	C	131	LYS
1	C	140	LEU
1	C	146	GLN
1	C	148	SER
1	C	150	LEU
1	C	154	SER
1	C	165	GLU
1	C	169	ILE
1	C	170	ASN
1	C	171	ARG
1	C	182	GLN
1	C	183	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	184	GLU
1	C	188	VAL
1	C	190	LEU
1	C	192	LYS
1	C	197	GLN
1	C	200	ARG
1	C	204	SER
1	C	208	LYS
1	C	210	ILE
1	C	212	SER
1	C	214	ASP
1	C	219	LEU
1	C	220	ARG
1	C	221	SER
1	C	223	ASN
1	C	228	ASN
1	C	229	ASN
1	C	230	PHE
1	C	236	ILE
1	C	239	GLU
1	C	240	LYS
1	C	244	LEU
1	C	254	VAL
1	C	261	LEU
1	C	269	LYS
1	C	274	LEU
1	C	275	VAL
1	C	278	GLU
1	C	285	LEU
1	C	302	LEU
1	C	306	ARG
1	C	319	ILE
1	C	325	PHE
1	C	326	VAL
1	C	328	ASN
1	C	333	LEU
1	C	334	ASN
1	C	336	LEU
1	C	346	GLN
1	C	353	GLU
1	C	358	VAL
1	C	359	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	363	ARG
1	C	367	GLU
1	C	370	PHE
1	C	373	SER
1	C	375	GLN
1	C	376	ASP
1	C	379	ARG
1	C	380	LEU
1	C	382	LYS
1	C	385	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	17	ASN
1	A	26	GLN
1	A	27	ASN
1	A	37	ASN
1	A	55	GLN
1	A	59	ASN
1	A	65	HIS
1	A	96	HIS
1	A	115	HIS
1	A	118	GLN
1	A	130	ASN
1	A	156	ASN
1	A	197	GLN
1	A	277	ASN
1	A	282	ASN
1	A	305	GLN
1	A	328	ASN
1	A	334	ASN
1	A	345	ASN
1	A	366	GLN
1	B	20	GLN
1	B	27	ASN
1	B	34	GLN
1	B	55	GLN
1	B	59	ASN
1	B	65	HIS
1	B	86	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	115	HIS
1	B	118	GLN
1	B	119	ASN
1	B	151	GLN
1	B	156	ASN
1	B	170	ASN
1	B	183	GLN
1	B	194	GLN
1	B	197	GLN
1	B	228	ASN
1	B	257	ASN
1	B	265	HIS
1	B	277	ASN
1	B	282	ASN
1	B	328	ASN
1	B	332	ASN
1	B	334	ASN
1	B	344	ASN
1	B	345	ASN
1	C	9	ASN
1	C	37	ASN
1	C	42	GLN
1	C	53	GLN
1	C	55	GLN
1	C	94	ASN
1	C	113	ASN
1	C	115	HIS
1	C	119	ASN
1	C	130	ASN
1	C	146	GLN
1	C	170	ASN
1	C	194	GLN
1	C	197	GLN
1	C	257	ASN
1	C	277	ASN
1	C	328	ASN
1	C	334	ASN
1	C	344	ASN
1	C	345	ASN
1	C	356	ASN
1	C	360	GLN
1	C	375	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	384	GLN

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 carbohydrates 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 [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	368/416 (88%)	-0.54	0 100 100	5, 20, 41, 55	0
1	B	365/416 (87%)	-0.19	1 (0%) 94 95	9, 31, 49, 59	0
1	C	379/416 (91%)	-0.50	0 100 100	5, 21, 43, 55	0
All	All	1112/1248 (89%)	-0.41	1 (0%) 95 97	5, 24, 45, 59	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	26	GLN	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 carbohydrates 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.