



Full wwPDB X-ray Structure Validation Report i

May 17, 2020 – 01:05 am BST

PDB ID : 2X6J
Title : THE CRYSTAL STRUCTURE OF THE DROSOPHILA CLASS III PI3-KINASE VPS34 IN COMPLEX WITH PIK-93
Authors : Miller, S.; Tavshanjian, B.; Oleksy, A.; Perisic, O.; Houseman, B.T.; Shokat, K.M.; Williams, R.L.
Deposited on : 2010-02-17
Resolution : 3.50 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 i symbol.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

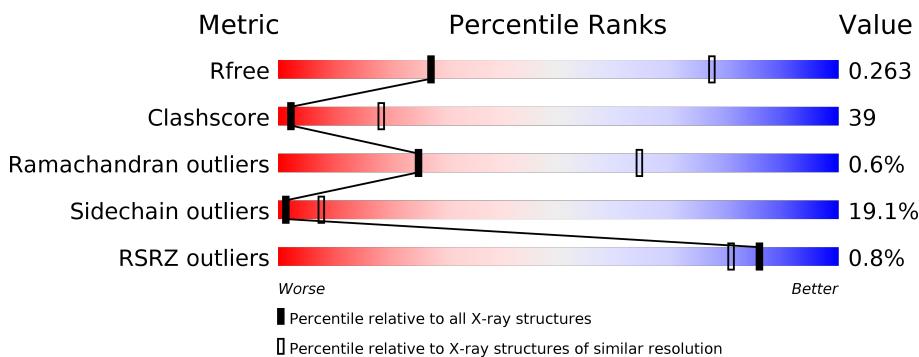
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

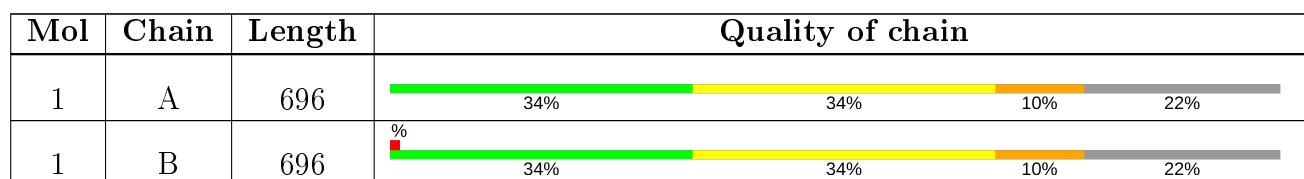
The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.



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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	093	B	1950	-	X	-	-

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 8967 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.

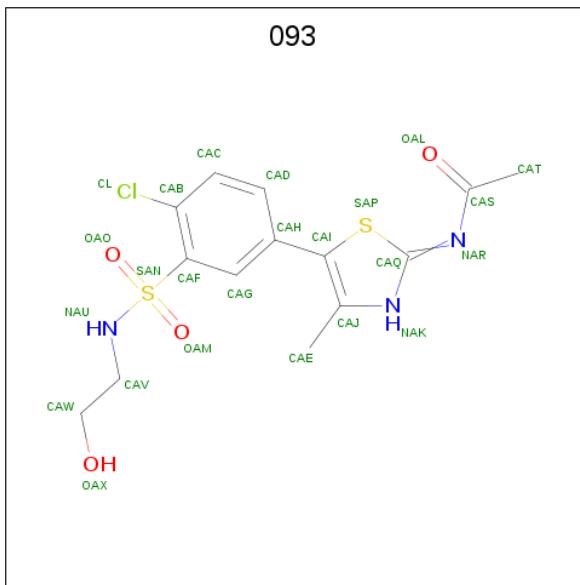
- Molecule 1 is a protein called PHOSPHOTIDYLINOSITOL 3 KINASE 59F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C 4457	N 2882	O 757	S 791	27	0	0
1	B	546	Total	C 4462	N 2886	O 759	S 790	27	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	GLY	-	expression tag	UNP Q9W1M7
A	255	SER	-	expression tag	UNP Q9W1M7
A	256	HIS	-	expression tag	UNP Q9W1M7
A	257	MET	-	expression tag	UNP Q9W1M7
A	455	ALA	GLY	engineered mutation	UNP Q9W1M7
B	254	GLY	-	expression tag	UNP Q9W1M7
B	255	SER	-	expression tag	UNP Q9W1M7
B	256	HIS	-	expression tag	UNP Q9W1M7
B	257	MET	-	expression tag	UNP Q9W1M7
B	455	ALA	GLY	engineered mutation	UNP Q9W1M7

- Molecule 2 is N-(5-(4-CHLORO-3-(2-HYDROXY-ETHYLSULFAMOYL)- PHENYLTHIA ZOLE-2-YL)-ACETAMIDE (three-letter code: 093) (formula: C₁₄H₁₆ClN₃O₄S₂).

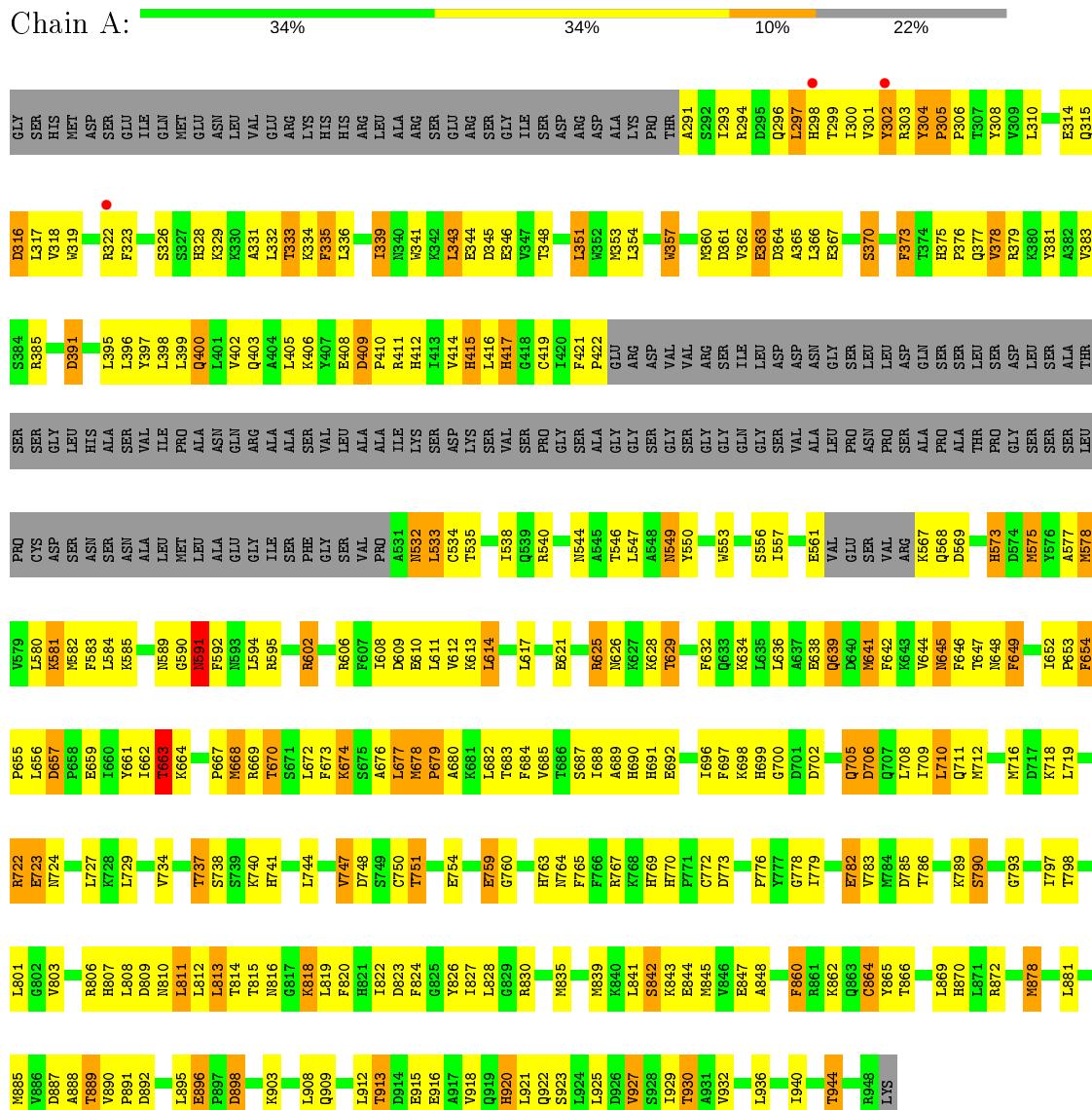


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total		C	Cl	N	O	S	
			24		14	1	3	4	2	0
2	B	1	Total		C	Cl	N	O	S	
			24		14	1	3	4	2	0

3 Residue-property plots

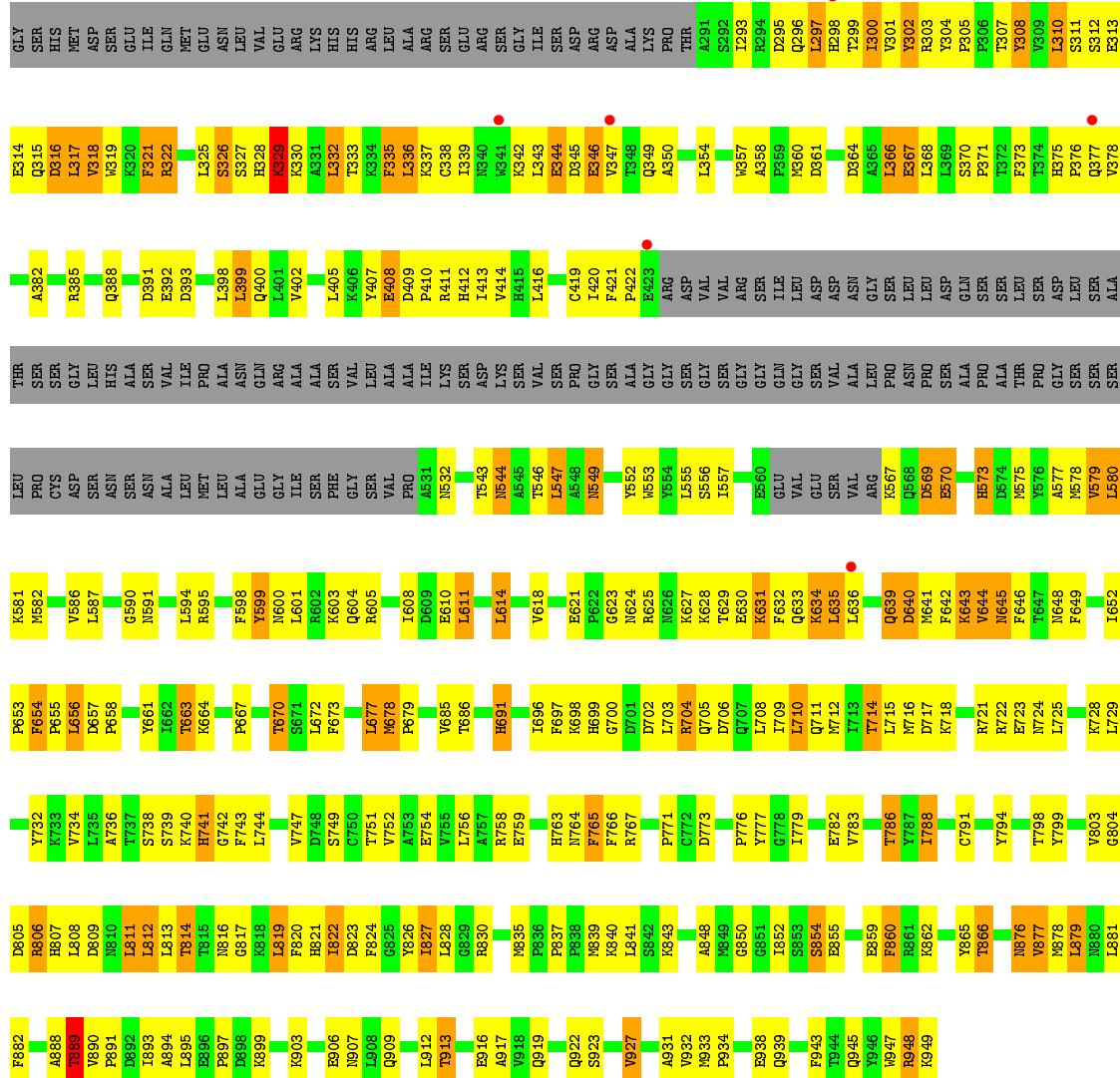
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: PHOSPHOTIDYLINOSITOL 3 KINASE 59F



- Molecule 1: PHOSPHOTIDYLINOSITOL 3 KINASE 59F





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.95 Å 156.33 Å 242.91 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.62 – 3.50 61.62 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (61.62-3.50) 99.5 (61.62-3.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	4.04 (at 3.49 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R , R_{free}	0.230 , 0.272 0.225 , 0.263	Depositor DCC
R_{free} test set	1313 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	93.2	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.2	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	0.92	EDS
Total number of atoms	8967	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:
093

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	0.61	1/4566 (0.0%)	0.84	1/6183 (0.0%)
1	B	0.48	0/4571	0.69	2/6189 (0.0%)
All	All	0.55	1/9137 (0.0%)	0.77	3/12372 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	864	CYS	CB-SG	-6.21	1.71	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329	LYS	CD-CE-NZ	-5.49	99.07	111.70
1	A	818	LYS	N-CA-C	-5.24	96.86	111.00
1	B	710	LEU	CA-CB-CG	-5.02	103.75	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	589	ASN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	591	ASN	Mainchain
1	A	663	THR	Mainchain
1	A	680	ALA	Peptide
1	A	737	THR	Mainchain
1	A	740	LYS	Peptide

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4457	0	4490	348	1
1	B	4462	0	4499	348	1
2	A	24	0	16	8	0
2	B	24	0	16	6	0
All	All	8967	0	9021	697	2

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 39.

All (697) 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:375:HIS:CD2	1:A:377:GLN:H	1.54	1.24
1:B:311:SER:HB3	1:B:314:GLU:CB	1.76	1.15
1:B:299:THR:HB	1:B:303:ARG:HH11	1.10	1.14
1:A:705:GLN:HG2	1:A:890:VAL:HG13	1.22	1.13
1:A:629:THR:HB	1:A:672:LEU:HD12	1.18	1.10
1:A:421:PHE:HB3	1:A:422:PRO:HD2	1.33	1.10
1:A:322:ARG:HH12	1:A:353:MET:HG3	1.13	1.09
1:B:412:HIS:CE1	1:B:532:ASN:HB3	1.86	1.09
1:A:638:GLU:HG2	1:A:641:MET:HG3	1.32	1.09
1:A:629:THR:HB	1:A:672:LEU:CD1	1.86	1.05
1:A:298:HIS:HB3	1:A:302:TYR:CE1	1.91	1.04
1:A:591:ASN:O	1:A:595:ARG:HD3	1.58	1.04
1:A:645:ASN:HD22	1:A:645:ASN:C	1.62	1.01
1:A:299:THR:HA	1:A:302:TYR:CE2	1.94	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:SER:HB3	1:B:314:GLU:HB3	1.44	1.00
1:A:532:ASN:OD1	1:A:535:THR:HG23	1.63	0.99
1:B:408:GLU:HB3	1:B:409:ASP:HA	1.41	0.98
1:A:737:THR:HG22	1:A:738:SER:H	1.26	0.97
1:A:814:THR:HG23	1:A:818:LYS:H	1.27	0.97
1:B:702:ASP:HB3	1:B:739:SER:HA	1.47	0.95
1:B:570:GLU:CD	1:B:570:GLU:H	1.67	0.95
1:A:830:ARG:HH22	1:A:903:LYS:NZ	1.64	0.95
1:B:667:PRO:O	1:B:670:THR:HG22	1.65	0.95
1:A:335:PHE:HD2	1:A:335:PHE:C	1.69	0.95
1:A:319:TRP:CD1	1:A:323:PHE:HE2	1.84	0.95
1:A:375:HIS:HD2	1:A:377:GLN:N	1.63	0.95
1:B:329:LYS:NZ	1:B:361:ASP:H	1.64	0.94
1:A:734:VAL:HG22	1:A:744:LEU:HD23	1.48	0.94
1:B:654:PHE:HD1	1:B:655:PRO:HD2	1.33	0.93
1:A:561:GLU:CD	1:A:561:GLU:H	1.71	0.93
1:B:421:PHE:HB3	1:B:422:PRO:HD2	1.51	0.92
1:A:577:ALA:O	1:A:581:LYS:HD2	1.69	0.92
1:A:830:ARG:NH2	1:A:903:LYS:HZ1	1.68	0.92
1:B:710:LEU:CD2	1:B:732:TYR:O	2.18	0.92
1:B:634:LYS:HA	1:B:634:LYS:HE2	1.50	0.91
1:A:553:TRP:O	1:A:557:ILE:HG13	1.72	0.90
1:A:322:ARG:NH1	1:A:353:MET:HG3	1.86	0.90
1:A:591:ASN:OD1	1:A:592:PHE:N	2.05	0.90
1:B:710:LEU:HD23	1:B:732:TYR:O	1.72	0.90
1:B:739:SER:O	1:B:740:LYS:HG2	1.71	0.89
1:B:335:PHE:C	1:B:335:PHE:HD2	1.75	0.89
1:A:830:ARG:HH22	1:A:903:LYS:HZ1	0.95	0.89
1:B:412:HIS:CE1	1:B:532:ASN:CB	2.54	0.89
1:A:814:THR:CG2	1:A:818:LYS:H	1.84	0.89
1:B:827:ILE:HG23	1:B:828:LEU:HG	1.55	0.89
1:A:375:HIS:CD2	1:A:377:GLN:N	2.40	0.88
1:B:375:HIS:CD2	1:B:377:GLN:H	1.91	0.88
1:A:298:HIS:HB3	1:A:302:TYR:HE1	1.36	0.88
1:A:698:LYS:NZ	2:A:1949:093:CL	2.42	0.88
1:B:367:GLU:O	1:B:370:SER:OG	1.90	0.88
1:B:311:SER:HB3	1:B:314:GLU:HB2	1.52	0.88
1:A:319:TRP:CD1	1:A:323:PHE:CE2	2.60	0.88
1:A:654:PHE:HD1	1:A:655:PRO:HD2	1.40	0.87
1:B:332:LEU:CD1	1:B:336:LEU:HD11	2.03	0.87
1:A:363:GLU:HA	1:A:366:LEU:HD12	1.55	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:782:GLU:O	1:B:786:THR:HG23	1.74	0.86
1:B:299:THR:HB	1:B:303:ARG:NH1	1.88	0.86
1:A:335:PHE:CD2	1:A:335:PHE:C	2.44	0.86
1:B:678:MET:C	1:B:699:HIS:HE2	1.79	0.85
1:A:678:MET:O	1:A:699:HIS:CD2	2.30	0.84
1:A:647:THR:O	1:A:664:LYS:HB3	1.77	0.84
1:A:922:GLN:HE22	1:B:919:GLN:HB3	1.42	0.84
1:A:842:SER:OG	1:A:844:GLU:OE1	1.94	0.83
1:A:322:ARG:HD2	1:A:335:PHE:CD1	2.12	0.83
1:B:654:PHE:CD1	1:B:655:PRO:HD2	2.13	0.83
1:B:549:ASN:C	1:B:549:ASN:HD22	1.80	0.83
1:A:319:TRP:HE1	1:A:322:ARG:HH21	1.24	0.83
1:A:751:THR:HG22	1:A:754:GLU:HG3	1.61	0.83
1:A:335:PHE:CD1	1:A:357:TRP:CZ3	2.67	0.82
1:B:412:HIS:HE1	1:B:532:ASN:CB	1.92	0.82
1:B:876:ASN:HD22	1:B:876:ASN:H	1.27	0.81
1:B:296:GLN:O	1:B:300:ILE:HG22	1.81	0.81
1:B:654:PHE:HD1	1:B:655:PRO:CD	1.94	0.81
1:B:663:THR:OG1	1:B:664:LYS:HG2	1.81	0.81
1:A:705:GLN:CG	1:A:890:VAL:HG13	2.09	0.81
1:B:326:SER:HA	1:B:357:TRP:CZ2	2.16	0.80
1:B:329:LYS:HZ3	1:B:361:ASP:CG	1.84	0.80
1:B:712:MET:HE1	1:B:878:MET:HG2	1.64	0.80
1:B:734:VAL:HG22	1:B:744:LEU:HD22	1.61	0.80
1:B:627:LYS:O	1:B:630:GLU:HG2	1.82	0.80
1:B:749:SER:HB2	1:B:812:LEU:CD1	2.11	0.80
1:A:673:PHE:HB2	1:A:679:PRO:HD2	1.65	0.79
1:A:638:GLU:HG2	1:A:641:MET:CG	2.10	0.79
1:A:629:THR:CB	1:A:672:LEU:HD12	2.08	0.79
1:B:913:THR:HG23	1:B:916:GLU:HG3	1.65	0.79
1:B:332:LEU:HD12	1:B:336:LEU:HD11	1.65	0.78
1:A:534:CYS:O	1:A:538:ILE:HG13	1.83	0.78
1:A:591:ASN:O	1:A:595:ARG:CD	2.31	0.78
1:B:400:GLN:HE22	1:B:711:GLN:HE22	1.31	0.78
1:B:728:LYS:HD3	1:B:786:THR:HB	1.64	0.78
1:B:310:LEU:HD13	1:B:311:SER:OG	1.82	0.78
1:A:568:GLN:HA	1:A:568:GLN:OE1	1.83	0.78
1:A:737:THR:HG22	1:A:738:SER:N	1.99	0.77
1:A:645:ASN:ND2	1:A:645:ASN:C	2.35	0.77
1:A:294:ARG:HA	1:A:297:LEU:HD21	1.66	0.77
1:B:421:PHE:HB3	1:B:422:PRO:CD	2.14	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:HIS:HE1	1:A:318:VAL:HA	1.49	0.76
1:A:722:ARG:HH11	1:A:722:ARG:CG	1.98	0.76
1:A:322:ARG:NH1	1:A:335:PHE:HE1	1.83	0.76
1:A:678:MET:O	1:A:699:HIS:NE2	2.19	0.76
1:A:667:PRO:O	1:A:670:THR:HG23	1.85	0.75
1:A:322:ARG:HH11	1:A:335:PHE:HE1	1.33	0.75
1:B:315:GLN:HG3	1:B:338:CYS:HB2	1.67	0.75
1:B:791:CYS:SG	1:B:819:LEU:HD23	2.25	0.75
1:B:329:LYS:HZ2	1:B:361:ASP:H	1.34	0.75
1:B:631:LYS:O	1:B:635:LEU:HD23	1.85	0.75
1:A:747:VAL:HG23	2:A:1949:093:HAK	1.52	0.74
1:A:807:HIS:H	1:A:810:ASN:HB2	1.50	0.74
1:B:329:LYS:NZ	1:B:361:ASP:CG	2.40	0.74
1:A:410:PRO:O	1:A:414:VAL:HG23	1.88	0.74
1:A:677:LEU:HD11	1:A:700:GLY:H	1.50	0.74
1:A:706:ASP:O	1:A:710:LEU:HD12	1.87	0.74
1:B:335:PHE:CD2	1:B:335:PHE:C	2.52	0.74
1:A:626:ASN:HA	1:A:629:THR:CG2	2.18	0.74
1:B:332:LEU:HD22	1:B:357:TRP:HB3	1.69	0.74
1:B:302:TYR:HE2	1:B:303:ARG:HE	1.34	0.74
1:B:629:THR:O	1:B:633:GLN:HG3	1.87	0.73
1:A:843:LYS:O	1:A:847:GLU:HG3	1.88	0.73
1:A:335:PHE:HD1	1:A:357:TRP:CH2	2.06	0.73
1:B:299:THR:CB	1:B:303:ARG:HH11	1.96	0.73
1:B:329:LYS:HZ3	1:B:361:ASP:H	1.34	0.73
1:B:667:PRO:O	1:B:670:THR:CG2	2.35	0.73
1:B:703:LEU:HD13	1:B:744:LEU:HD21	1.71	0.73
1:A:319:TRP:NE1	1:A:323:PHE:CE2	2.57	0.73
1:B:311:SER:CB	1:B:314:GLU:HB3	2.18	0.73
1:A:405:LEU:HD23	1:A:533:LEU:HD21	1.68	0.73
1:B:948:ARG:O	1:B:949:LYS:HB2	1.87	0.73
1:A:639:GLN:NE2	1:A:645:ASN:OD1	2.22	0.73
1:A:375:HIS:HD2	1:A:377:GLN:H	0.87	0.72
1:A:638:GLU:CG	1:A:641:MET:HG3	2.16	0.72
1:A:322:ARG:HH12	1:A:353:MET:CG	1.96	0.72
1:A:421:PHE:HB3	1:A:422:PRO:CD	2.15	0.72
1:B:819:LEU:HD12	1:B:820:PHE:N	2.05	0.71
1:B:582:MET:O	1:B:586:VAL:HG23	1.90	0.71
1:B:738:SER:HB3	1:B:741:HIS:CE1	2.25	0.71
1:A:319:TRP:O	1:A:322:ARG:HB3	1.89	0.71
1:B:549:ASN:C	1:B:549:ASN:ND2	2.43	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ILE:O	1:A:304:TYR:HB2	1.90	0.71
1:A:351:LEU:HD13	1:A:377:GLN:HG2	1.70	0.71
1:B:335:PHE:HD1	1:B:357:TRP:CZ3	2.08	0.71
1:A:405:LEU:HD23	1:A:533:LEU:CD2	2.19	0.71
1:A:722:ARG:HH11	1:A:722:ARG:HG3	1.55	0.70
1:A:296:GLN:O	1:A:299:THR:HG22	1.92	0.70
1:B:319:TRP:HA	1:B:322:ARG:NE	2.06	0.70
1:B:749:SER:HB2	1:B:812:LEU:HD12	1.72	0.70
1:A:319:TRP:NE1	1:A:323:PHE:HE2	1.87	0.70
1:A:332:LEU:HD12	1:A:336:LEU:CD2	2.21	0.70
1:A:654:PHE:CD1	1:A:655:PRO:HD2	2.26	0.70
1:A:322:ARG:NH1	1:A:335:PHE:CE1	2.60	0.69
1:A:722:ARG:CB	1:A:722:ARG:HH11	2.05	0.69
1:B:678:MET:O	1:B:699:HIS:NE2	2.21	0.69
1:B:798:THR:HG23	1:B:803:VAL:HB	1.75	0.69
1:B:749:SER:CB	1:B:812:LEU:HD12	2.23	0.69
1:A:798:THR:HG23	1:A:803:VAL:HB	1.73	0.69
1:B:375:HIS:CD2	1:B:377:GLN:N	2.61	0.69
1:A:793:GLY:O	1:A:797:ILE:HG13	1.93	0.69
1:A:718:LYS:O	1:A:722:ARG:HG2	1.92	0.68
1:A:751:THR:HG22	1:A:754:GLU:CG	2.22	0.68
1:A:304:TYR:CB	1:A:305:PRO:HD3	2.24	0.68
1:B:549:ASN:OD1	1:B:658:PRO:HG3	1.93	0.68
1:A:329:LYS:HB3	1:A:360:MET:HA	1.75	0.68
1:A:913:THR:HG23	1:A:916:GLU:CD	2.13	0.68
1:B:314:GLU:O	1:B:318:VAL:HG12	1.93	0.68
1:A:322:ARG:HD2	1:A:335:PHE:CE1	2.27	0.68
1:B:297:LEU:HA	1:B:300:ILE:CG2	2.23	0.68
1:A:909:GLN:HG3	1:A:912:LEU:HG	1.75	0.68
1:A:332:LEU:HD12	1:A:336:LEU:HD23	1.74	0.68
1:B:335:PHE:HE2	1:B:339:ILE:HD13	1.58	0.68
1:B:751:THR:HA	1:B:812:LEU:HB3	1.75	0.67
1:A:629:THR:HA	1:A:672:LEU:HD11	1.76	0.67
1:A:769:HIS:CD2	1:A:815:THR:HG22	2.29	0.67
1:B:765:PHE:CD2	1:B:765:PHE:C	2.67	0.67
1:A:830:ARG:NH2	1:A:903:LYS:NZ	2.34	0.67
1:B:763:HIS:CD2	1:B:848:ALA:HA	2.29	0.67
1:B:876:ASN:HD22	1:B:876:ASN:N	1.92	0.67
1:A:654:PHE:HD1	1:A:655:PRO:CD	2.08	0.67
1:B:578:MET:O	1:B:582:MET:HG3	1.95	0.67
1:B:877:VAL:O	1:B:881:LEU:HG	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:GLN:HB2	1:B:338:CYS:HB3	1.77	0.67
1:B:549:ASN:ND2	1:B:553:TRP:CD1	2.63	0.67
1:A:625:ARG:O	1:A:629:THR:HG22	1.95	0.66
1:B:913:THR:HG23	1:B:916:GLU:CG	2.25	0.66
1:B:705:GLN:OE1	1:B:890:VAL:HG13	1.96	0.66
1:A:335:PHE:HD1	1:A:357:TRP:CZ3	2.13	0.66
1:A:343:LEU:HD13	1:A:345:ASP:H	1.61	0.66
1:B:297:LEU:HD23	1:B:297:LEU:H	1.60	0.66
1:A:326:SER:HB2	1:A:357:TRP:CE2	2.31	0.66
1:A:332:LEU:O	1:A:336:LEU:HD23	1.95	0.66
1:A:629:THR:CB	1:A:672:LEU:CD1	2.71	0.66
1:B:346:GLU:HA	1:B:349:GLN:CD	2.17	0.66
1:B:549:ASN:ND2	1:B:553:TRP:HD1	1.93	0.66
1:B:699:HIS:H	1:B:699:HIS:CD2	2.11	0.66
1:A:294:ARG:HA	1:A:297:LEU:CD2	2.27	0.65
1:B:329:LYS:NZ	1:B:361:ASP:CB	2.59	0.65
1:B:618:VAL:HG21	1:B:632:PHE:CD2	2.31	0.65
1:A:747:VAL:HG22	2:A:1949:093:HAE1	1.77	0.65
1:B:743:PHE:O	1:B:744:LEU:HD23	1.97	0.65
1:B:751:THR:HG23	1:B:754:GLU:H	1.59	0.65
1:B:749:SER:HB2	1:B:812:LEU:HD13	1.77	0.65
1:A:362:VAL:O	1:A:365:ALA:HB3	1.97	0.65
1:B:335:PHE:CD1	1:B:357:TRP:CZ3	2.84	0.65
1:B:827:ILE:CG2	1:B:828:LEU:HG	2.25	0.65
1:B:830:ARG:HH22	1:B:903:LYS:NZ	1.95	0.64
1:A:335:PHE:HD2	1:A:335:PHE:O	1.80	0.64
1:A:751:THR:CG2	1:A:754:GLU:H	2.10	0.64
1:A:363:GLU:HA	1:A:366:LEU:CD1	2.27	0.64
1:B:319:TRP:CD1	1:B:319:TRP:C	2.71	0.64
1:A:785:ASP:OD1	1:A:789:LYS:HE3	1.98	0.64
1:B:912:LEU:HD12	1:B:917:ALA:HA	1.78	0.64
1:A:405:LEU:CD2	1:A:533:LEU:HD21	2.28	0.64
1:A:751:THR:CG2	1:A:754:GLU:HG3	2.27	0.64
1:A:806:ARG:HA	1:A:810:ASN:HD22	1.62	0.64
1:A:827:ILE:CG2	1:A:828:LEU:HG	2.28	0.64
1:A:862:LYS:O	1:A:866:THR:HG23	1.97	0.64
1:B:329:LYS:HZ3	1:B:361:ASP:N	1.95	0.64
1:A:806:ARG:CZ	1:A:810:ASN:ND2	2.61	0.63
1:B:698:LYS:O	1:B:741:HIS:HA	1.98	0.63
1:B:610:GLU:CD	1:B:643:LYS:HG2	2.19	0.63
1:B:332:LEU:HD12	1:B:336:LEU:CD1	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:GLU:CD	1:B:570:GLU:N	2.48	0.63
1:A:533:LEU:HD23	1:A:534:CYS:N	2.14	0.63
1:B:712:MET:CE	1:B:878:MET:HG2	2.28	0.63
1:B:812:LEU:HD21	1:B:822:ILE:HG21	1.81	0.63
1:A:866:THR:O	1:A:870:HIS:HD2	1.82	0.63
1:A:549:ASN:HD22	1:A:550:TYR:N	1.97	0.62
1:A:811:LEU:C	1:A:812:LEU:HD23	2.18	0.62
1:B:314:GLU:O	1:B:317:LEU:HG	1.99	0.62
1:B:329:LYS:NZ	1:B:361:ASP:N	2.43	0.62
1:A:813:LEU:HD12	1:A:818:LYS:O	1.98	0.62
1:B:621:GLU:HG2	1:B:623:GLY:H	1.63	0.62
1:A:319:TRP:HD1	1:A:323:PHE:CE2	2.17	0.62
1:B:806:ARG:NH1	1:B:823:ASP:O	2.29	0.62
1:A:677:LEU:HD21	1:A:699:HIS:HB2	1.80	0.62
1:A:657:ASP:OD2	1:A:657:ASP:C	2.37	0.62
1:A:363:GLU:CA	1:A:366:LEU:HD12	2.29	0.62
1:B:319:TRP:HD1	1:B:319:TRP:O	1.82	0.62
1:B:751:THR:HG22	1:B:754:GLU:HB2	1.82	0.62
1:B:749:SER:CB	1:B:812:LEU:CD1	2.76	0.62
1:A:664:LYS:H	1:A:685:VAL:CG2	2.12	0.62
1:A:578:MET:O	1:A:582:MET:HG3	2.00	0.61
1:B:411:ARG:HA	1:B:414:VAL:HG22	1.81	0.61
1:B:549:ASN:HD21	1:B:553:TRP:HD1	1.46	0.61
1:B:751:THR:HG22	1:B:754:GLU:CG	2.31	0.61
1:B:826:TYR:HB3	1:B:830:ARG:O	2.00	0.61
1:A:813:LEU:CD1	1:A:818:LYS:O	2.49	0.61
1:A:723:GLU:O	1:A:724:ASN:HB3	1.99	0.61
1:B:913:THR:HG23	1:B:916:GLU:CD	2.21	0.61
1:A:335:PHE:CD1	1:A:357:TRP:HZ3	2.17	0.60
1:A:580:LEU:HD22	1:A:581:LYS:HE2	1.82	0.60
1:A:689:ALA:HB3	1:A:691:HIS:CE1	2.34	0.60
1:A:803:VAL:HG12	1:A:806:ARG:HD3	1.83	0.60
1:A:580:LEU:HD22	1:A:581:LYS:CE	2.32	0.60
1:A:716:MET:SD	1:A:797:ILE:HG23	2.42	0.60
1:B:703:LEU:CD1	1:B:744:LEU:HD21	2.31	0.60
1:A:812:LEU:HD11	1:A:822:ILE:CD1	2.31	0.60
1:A:315:GLN:HG3	1:A:316:ASP:OD2	2.01	0.60
1:A:549:ASN:ND2	1:A:549:ASN:C	2.54	0.60
1:B:587:LEU:HB3	1:B:598:PHE:HB2	1.84	0.60
1:B:618:VAL:HG21	1:B:632:PHE:HD2	1.66	0.60
1:A:751:THR:HG22	1:A:754:GLU:CB	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:749:SER:OG	2:B:1950:093:NAR	2.35	0.60
1:B:315:GLN:HG2	1:B:316:ASP:N	2.17	0.60
1:B:722:ARG:HB3	1:B:722:ARG:HH11	1.66	0.60
1:A:722:ARG:HG3	1:A:722:ARG:NH1	2.17	0.60
1:B:412:HIS:HE1	1:B:532:ASN:HB2	1.64	0.60
1:A:649:PHE:HE1	1:A:662:ILE:HG13	1.66	0.60
1:B:807:HIS:CD2	1:B:809:ASP:HB2	2.36	0.60
1:B:339:ILE:O	1:B:342:LYS:HB3	2.01	0.60
1:B:629:THR:HG22	1:B:672:LEU:HB3	1.84	0.60
1:B:573:HIS:C	1:B:573:HIS:CD2	2.75	0.59
1:A:806:ARG:CZ	1:A:810:ASN:HD22	2.14	0.59
1:A:920:HIS:CD2	1:A:920:HIS:C	2.75	0.59
1:B:645:ASN:C	1:B:645:ASN:OD1	2.40	0.59
1:A:297:LEU:O	1:A:301:VAL:HG23	2.03	0.59
1:B:614:LEU:HD21	1:B:636:LEU:HD23	1.84	0.59
1:A:709:ILE:HD12	1:A:801:LEU:HD13	1.83	0.59
1:B:335:PHE:CD1	1:B:357:TRP:HZ3	2.21	0.59
1:A:645:ASN:HD22	1:A:646:PHE:N	2.01	0.58
1:B:412:HIS:NE2	1:B:532:ASN:HB3	2.18	0.58
1:B:814:THR:OG1	1:B:816:ASN:HB3	2.03	0.58
1:A:335:PHE:CD1	1:A:357:TRP:CH2	2.88	0.58
1:A:812:LEU:HD11	1:A:822:ILE:HD12	1.84	0.58
1:A:406:LYS:NZ	1:A:887:ASP:O	2.36	0.58
1:B:319:TRP:HA	1:B:322:ARG:HE	1.66	0.58
1:B:599:TYR:HD2	1:B:599:TYR:O	1.87	0.58
1:B:614:LEU:C	1:B:614:LEU:HD12	2.24	0.58
1:B:862:LYS:O	1:B:866:THR:HG22	2.03	0.58
1:B:799:TYR:O	1:B:907:ASN:ND2	2.37	0.58
1:A:363:GLU:N	1:A:363:GLU:CD	2.57	0.58
1:A:305:PRO:O	1:A:334:LYS:NZ	2.37	0.58
1:B:710:LEU:HD22	1:B:732:TYR:O	2.03	0.58
1:A:373:PHE:N	1:A:373:PHE:CD2	2.71	0.57
1:B:812:LEU:HD12	1:B:820:PHE:CZ	2.39	0.57
1:A:657:ASP:OD2	1:A:659:GLU:N	2.37	0.57
1:B:544:ASN:OD1	1:B:544:ASN:C	2.42	0.57
1:B:634:LYS:CE	1:B:634:LYS:HA	2.21	0.57
1:A:538:ILE:HG23	1:A:583:PHE:HD1	1.69	0.57
1:A:621:GLU:O	1:A:628:LYS:HE2	2.04	0.57
1:B:830:ARG:NH2	1:B:903:LYS:NZ	2.52	0.57
1:B:392:GLU:HG2	1:B:393:ASP:N	2.19	0.57
1:A:373:PHE:HD2	1:A:373:PHE:N	2.02	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:HIS:HD2	1:A:809:ASP:HB2	1.70	0.57
1:B:375:HIS:NE2	1:B:377:GLN:HB2	2.19	0.57
1:B:841:LEU:O	1:B:932:VAL:HG21	2.05	0.57
1:A:335:PHE:CD2	1:A:335:PHE:O	2.57	0.57
1:A:865:TYR:HD1	1:A:921:LEU:HD23	1.69	0.57
1:A:319:TRP:HE1	1:A:322:ARG:NH2	2.00	0.56
1:B:590:GLY:O	1:B:595:ARG:HD3	2.05	0.56
1:A:421:PHE:CB	1:A:422:PRO:HD2	2.22	0.56
1:A:677:LEU:HD11	1:A:700:GLY:N	2.20	0.56
1:A:898:ASP:OD1	1:A:898:ASP:N	2.37	0.56
1:B:344:GLU:O	1:B:347:VAL:HB	2.04	0.56
1:B:702:ASP:HB3	1:B:739:SER:CA	2.30	0.56
1:B:878:MET:O	1:B:882:PHE:HD2	1.88	0.56
1:A:326:SER:HB2	1:A:357:TRP:NE1	2.20	0.56
1:A:375:HIS:HB3	1:A:378:VAL:HG22	1.88	0.56
1:B:332:LEU:O	1:B:336:LEU:HD22	2.06	0.56
1:B:416:LEU:O	1:B:420:ILE:HG12	2.06	0.56
1:B:723:GLU:O	1:B:724:ASN:OD1	2.24	0.56
1:B:318:VAL:HG23	1:B:322:ARG:HB2	1.88	0.56
1:A:335:PHE:CE1	1:A:357:TRP:HZ3	2.24	0.56
1:A:415:HIS:ND1	1:A:415:HIS:C	2.59	0.56
1:A:417:HIS:ND1	1:A:417:HIS:C	2.58	0.56
1:B:335:PHE:HD1	1:B:357:TRP:HZ3	1.50	0.56
1:B:400:GLN:HE22	1:B:711:GLN:NE2	2.02	0.56
1:B:934:PRO:O	1:B:938:GLU:HG3	2.06	0.56
1:B:763:HIS:NE2	1:B:848:ALA:HA	2.21	0.55
1:B:649:PHE:CE2	1:B:664:LYS:HA	2.41	0.55
1:B:876:ASN:N	1:B:876:ASN:ND2	2.54	0.55
1:A:409:ASP:OD1	1:A:411:ARG:N	2.39	0.55
1:B:329:LYS:HZ3	1:B:361:ASP:CB	2.19	0.55
1:A:827:ILE:HG23	1:A:828:LEU:HG	1.87	0.55
1:B:402:VAL:O	1:B:405:LEU:HB2	2.05	0.55
1:A:869:LEU:HD11	1:A:918:VAL:CG2	2.36	0.55
1:B:343:LEU:O	1:B:346:GLU:HG2	2.07	0.55
1:B:325:LEU:O	1:B:327:SER:N	2.40	0.55
1:A:405:LEU:CD2	1:A:533:LEU:CD2	2.85	0.55
1:B:343:LEU:HG	1:B:344:GLU:H	1.71	0.55
1:B:806:ARG:HD2	1:B:806:ARG:N	2.22	0.55
1:A:772:CYS:O	1:A:778:GLY:HA2	2.07	0.54
1:B:333:THR:HA	1:B:336:LEU:CD2	2.38	0.54
1:A:409:ASP:HB3	1:A:412:HIS:CD2	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:THR:HG22	1:A:754:GLU:H	1.72	0.54
1:B:299:THR:O	1:B:302:TYR:HD2	1.90	0.54
1:B:315:GLN:CG	1:B:338:CYS:HB2	2.35	0.54
1:A:930:THR:HA	1:A:936:LEU:HD12	1.90	0.54
1:A:629:THR:CA	1:A:672:LEU:HD11	2.37	0.54
1:A:645:ASN:ND2	1:A:647:THR:H	2.06	0.54
1:B:712:MET:O	1:B:716:MET:HG3	2.07	0.54
1:B:640:ASP:OD1	1:B:640:ASP:C	2.46	0.54
1:A:391:ASP:CG	1:A:540:ARG:HH12	2.10	0.53
1:A:645:ASN:ND2	1:A:647:THR:N	2.56	0.53
1:A:610:GLU:HG3	1:A:644:VAL:HG12	1.90	0.53
1:B:366:LEU:HD12	1:B:881:LEU:HD21	1.91	0.53
1:B:375:HIS:C	1:B:375:HIS:CD2	2.82	0.53
1:A:677:LEU:O	1:A:679:PRO:HD3	2.08	0.53
1:B:767:ARG:O	1:B:771:PRO:HG3	2.09	0.53
1:A:304:TYR:HB2	1:A:305:PRO:HD3	1.89	0.53
1:A:811:LEU:O	1:A:812:LEU:HD23	2.09	0.53
1:A:807:HIS:HA	1:B:947:TRP:CZ3	2.44	0.53
1:A:806:ARG:HA	1:A:810:ASN:ND2	2.23	0.53
1:B:765:PHE:HD2	1:B:766:PHE:N	2.06	0.53
1:A:705:GLN:HG3	1:A:891:PRO:HD2	1.91	0.53
1:B:408:GLU:HB3	1:B:409:ASP:CA	2.29	0.52
1:B:766:PHE:CE1	1:B:817:GLY:HA2	2.44	0.52
1:A:375:HIS:O	1:A:378:VAL:HG23	2.09	0.52
1:B:744:LEU:HD13	2:B:1950:093:CAC	2.39	0.52
1:A:575:MET:C	1:A:575:MET:SD	2.88	0.52
1:A:319:TRP:O	1:A:319:TRP:HD1	1.92	0.52
1:A:723:GLU:O	1:A:724:ASN:CB	2.58	0.52
1:A:567:LYS:HG3	1:A:568:GLN:H	1.75	0.52
1:B:412:HIS:CE1	1:B:532:ASN:HB2	2.39	0.52
1:B:621:GLU:O	1:B:628:LYS:HE2	2.09	0.52
1:B:552:TYR:CG	1:B:601:LEU:HD13	2.45	0.51
1:A:645:ASN:ND2	1:A:648:ASN:H	2.08	0.51
1:A:649:PHE:CE1	1:A:663:THR:O	2.64	0.51
1:A:626:ASN:HA	1:A:629:THR:HG22	1.89	0.51
1:A:763:HIS:NE2	1:A:848:ALA:O	2.35	0.51
1:B:371:PRO:HB3	1:B:407:TYR:CE2	2.45	0.51
2:A:1949:093:CAE	2:A:1949:093:HAD	2.40	0.51
1:A:689:ALA:O	1:A:690:HIS:HB2	2.10	0.51
1:B:315:GLN:HA	1:B:318:VAL:HG13	1.93	0.51
1:B:657:ASP:OD2	1:B:657:ASP:C	2.49	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:751:THR:HG22	1:B:754:GLU:CB	2.41	0.51
2:A:1949:093:SAP	2:A:1949:093:OAL	2.69	0.51
1:B:552:TYR:OH	1:B:605:ARG:NE	2.36	0.51
1:A:944:THR:OG1	1:B:931:ALA:O	2.26	0.51
1:A:367:GLU:O	1:A:370:SER:HB3	2.10	0.51
1:A:375:HIS:HB3	1:A:378:VAL:CG2	2.41	0.51
1:A:764:ASN:OD1	1:A:767:ARG:NH1	2.44	0.51
2:B:1950:093:SAP	2:B:1950:093:CAT	2.99	0.51
1:B:909:GLN:HB3	1:B:912:LEU:HG	1.93	0.51
1:B:843:LYS:HA	1:B:932:VAL:HG13	1.92	0.51
1:B:830:ARG:HH22	1:B:903:LYS:CE	2.24	0.51
1:A:609:ASP:O	1:A:613:LYS:HG3	2.11	0.50
1:B:312:SER:HA	1:B:315:GLN:OE1	2.10	0.50
1:B:409:ASP:OD1	1:B:410:PRO:HD2	2.12	0.50
1:A:722:ARG:CG	1:A:722:ARG:NH1	2.66	0.50
1:B:828:LEU:O	1:B:830:ARG:NH1	2.44	0.50
1:A:305:PRO:HB2	1:A:308:TYR:CD2	2.46	0.50
1:B:807:HIS:NE2	1:B:809:ASP:HB2	2.27	0.50
1:A:661:TYR:HB2	1:A:687:SER:HB3	1.92	0.50
1:B:345:ASP:O	1:B:349:GLN:HG3	2.11	0.50
1:B:375:HIS:HD2	1:B:377:GLN:N	2.10	0.50
1:B:634:LYS:CA	1:B:634:LYS:HE2	2.33	0.50
1:B:677:LEU:HD11	1:B:700:GLY:HA3	1.93	0.50
1:B:807:HIS:HD2	1:B:809:ASP:H	1.59	0.50
1:A:807:HIS:HA	1:B:947:TRP:HZ3	1.77	0.50
1:A:696:ILE:HG22	1:A:697:PHE:N	2.25	0.50
1:A:807:HIS:CD2	1:A:809:ASP:HB2	2.46	0.50
1:A:872:ARG:HH12	1:A:909:GLN:C	2.14	0.50
1:B:318:VAL:O	1:B:322:ARG:N	2.39	0.50
1:A:722:ARG:HH11	1:A:722:ARG:HB2	1.75	0.50
1:B:629:THR:HG22	1:B:672:LEU:CB	2.41	0.50
1:B:806:ARG:HB3	1:B:811:LEU:HD21	1.94	0.50
1:B:673:PHE:HB2	1:B:679:PRO:HD2	1.93	0.50
1:A:544:ASN:OD1	1:A:546:THR:N	2.45	0.49
1:A:827:ILE:HG22	1:A:828:LEU:HG	1.94	0.49
1:B:569:ASP:C	1:B:569:ASP:OD1	2.51	0.49
1:A:360:MET:HE1	1:A:365:ALA:HA	1.95	0.49
1:B:399:LEU:HD22	1:B:399:LEU:H	1.76	0.49
1:B:876:ASN:H	1:B:876:ASN:ND2	2.01	0.49
1:A:360:MET:HG2	1:A:364:ASP:HB2	1.93	0.49
1:A:751:THR:HG23	1:A:754:GLU:H	1.75	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ASP:OD1	1:A:409:ASP:C	2.50	0.49
2:B:1950:093:CL	2:B:1950:093:NAU	2.81	0.49
1:B:321:PHE:O	1:B:325:LEU:HD23	2.12	0.49
1:B:297:LEU:HA	1:B:300:ILE:HG22	1.94	0.49
1:B:329:LYS:O	1:B:332:LEU:HB3	2.12	0.49
1:B:894:ALA:O	1:B:897:PRO:HD3	2.13	0.49
1:B:339:ILE:HD12	1:B:350:ALA:CB	2.42	0.49
1:A:872:ARG:NH1	1:A:909:GLN:O	2.44	0.49
1:B:590:GLY:HA3	1:B:594:LEU:HB2	1.94	0.49
1:B:599:TYR:O	1:B:603:LYS:HG3	2.13	0.49
1:B:577:ALA:O	1:B:581:LYS:HD3	2.13	0.49
1:A:399:LEU:HB3	1:A:400:GLN:NE2	2.28	0.48
1:A:806:ARG:HD2	1:A:806:ARG:N	2.28	0.48
1:B:300:ILE:O	1:B:304:TYR:HD2	1.95	0.48
1:B:335:PHE:O	1:B:335:PHE:HD2	1.94	0.48
1:B:346:GLU:HA	1:B:349:GLN:OE1	2.13	0.48
2:B:1950:093:HAT2	2:B:1950:093:SAP	2.53	0.48
1:B:299:THR:O	1:B:302:TYR:CD2	2.66	0.48
1:B:413:ILE:HD13	1:B:575:MET:HG2	1.95	0.48
1:A:843:LYS:HA	1:A:932:VAL:CG1	2.43	0.48
1:B:329:LYS:NZ	1:B:361:ASP:HB2	2.27	0.48
1:B:648:ASN:HA	1:B:664:LYS:HB3	1.96	0.48
1:A:786:THR:O	1:A:790:SER:OG	2.29	0.48
1:A:807:HIS:O	1:A:810:ASN:HB2	2.13	0.48
1:B:310:LEU:HD22	1:B:311:SER:H	1.78	0.48
1:B:357:TRP:CD1	1:B:358:ALA:N	2.81	0.48
1:B:300:ILE:HA	1:B:304:TYR:CD2	2.49	0.48
1:B:399:LEU:CD2	1:B:399:LEU:H	2.27	0.48
1:A:769:HIS:HB3	1:A:770:HIS:HD2	1.78	0.48
1:B:382:ALA:O	1:B:385:ARG:HB2	2.14	0.48
1:B:823:ASP:OD1	1:B:824:PHE:N	2.46	0.48
1:B:906:GLU:O	1:B:909:GLN:NE2	2.47	0.48
1:B:783:VAL:HG13	1:B:816:ASN:O	2.14	0.48
1:A:544:ASN:C	1:A:544:ASN:OD1	2.52	0.48
1:A:561:GLU:N	1:A:561:GLU:CD	2.53	0.48
1:B:388:GLN:HA	1:B:388:GLN:OE1	2.13	0.48
1:B:656:LEU:HD23	1:B:656:LEU:C	2.34	0.48
1:B:888:ALA:O	1:B:889:THR:HG22	2.14	0.48
1:A:729:LEU:HD21	1:A:793:GLY:HA3	1.96	0.48
1:A:737:THR:HB	1:A:741:HIS:CD2	2.48	0.47
1:B:301:VAL:O	1:B:305:PRO:HD2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:LYS:C	1:B:570:GLU:OE1	2.53	0.47
1:A:614:LEU:HD21	1:A:636:LEU:CD2	2.44	0.47
1:A:608:ILE:HG21	1:A:737:THR:HG21	1.96	0.47
1:A:776:PRO:HD2	1:A:779:ILE:O	2.14	0.47
1:B:555:LEU:HB3	1:B:580:LEU:HG	1.96	0.47
1:B:752:VAL:HG12	1:B:808:LEU:HD23	1.96	0.47
1:A:308:TYR:CD1	1:A:310:LEU:HD13	2.49	0.47
1:A:399:LEU:HB3	1:A:400:GLN:HE22	1.78	0.47
1:B:364:ASP:O	1:B:367:GLU:HB3	2.14	0.47
1:A:737:THR:CG2	1:A:741:HIS:CD2	2.98	0.47
1:A:790:SER:CB	1:A:819:LEU:H	2.27	0.47
1:B:598:PHE:C	1:B:598:PHE:CD2	2.87	0.47
1:A:329:LYS:HG3	1:A:329:LYS:H	1.32	0.47
1:A:614:LEU:HD21	1:A:636:LEU:HD23	1.96	0.47
1:A:737:THR:CG2	1:A:738:SER:N	2.69	0.47
1:B:322:ARG:HG3	1:B:335:PHE:CD1	2.50	0.47
1:A:343:LEU:HD13	1:A:345:ASP:N	2.28	0.47
1:B:312:SER:O	1:B:315:GLN:HG2	2.14	0.47
1:B:408:GLU:CB	1:B:409:ASP:HA	2.18	0.47
1:B:717:ASP:HB2	1:B:729:LEU:HD12	1.97	0.47
1:B:777:TYR:CD1	1:B:777:TYR:N	2.83	0.47
1:B:879:LEU:HD23	1:B:879:LEU:N	2.29	0.47
1:A:747:VAL:CG2	2:A:1949:093:HAK	2.25	0.46
1:A:332:LEU:HD12	1:A:336:LEU:HD21	1.93	0.46
1:A:915:GLU:OE2	1:A:915:GLU:N	2.46	0.46
1:B:329:LYS:HZ1	1:B:361:ASP:HB2	1.79	0.46
1:A:291:ALA:O	1:A:294:ARG:NE	2.48	0.46
1:B:696:ILE:O	1:B:743:PHE:HA	2.15	0.46
1:B:697:PHE:HA	1:B:742:GLY:O	2.16	0.46
1:A:402:VAL:O	1:A:405:LEU:HB2	2.15	0.46
1:A:827:ILE:N	1:A:892:ASP:OD2	2.39	0.46
1:A:303:ARG:O	1:A:304:TYR:CD2	2.69	0.46
1:A:708:LEU:HD12	1:A:890:VAL:HG21	1.97	0.46
1:A:814:THR:CG2	1:A:818:LYS:N	2.66	0.46
1:B:354:LEU:HD23	1:B:354:LEU:C	2.35	0.46
1:B:678:MET:HA	1:B:679:PRO:HD3	1.63	0.46
1:B:764:ASN:HA	1:B:767:ARG:NH1	2.30	0.46
1:A:708:LEU:O	1:A:708:LEU:HD23	2.15	0.46
1:A:922:GLN:HE22	1:B:919:GLN:CB	2.21	0.46
1:B:319:TRP:CG	1:B:322:ARG:CZ	2.98	0.46
1:B:948:ARG:O	1:B:949:LYS:CB	2.62	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:HIS:CE1	1:A:318:VAL:HA	2.39	0.46
1:A:375:HIS:CD2	1:A:376:PRO:N	2.83	0.46
1:A:590:GLY:HA3	1:A:594:LEU:HD12	1.98	0.46
1:B:752:VAL:CG1	1:B:808:LEU:HD23	2.46	0.46
1:A:654:PHE:HB3	1:A:657:ASP:O	2.16	0.46
1:B:642:PHE:HB2	1:B:644:VAL:O	2.16	0.46
1:B:788:ILE:HG13	1:B:860:PHE:HB2	1.96	0.46
1:A:391:ASP:CG	1:A:540:ARG:NH1	2.68	0.46
1:A:649:PHE:CD1	1:A:663:THR:O	2.69	0.46
1:B:367:GLU:O	1:B:367:GLU:HG3	2.14	0.46
1:B:763:HIS:NE2	1:B:848:ALA:O	2.49	0.46
1:A:332:LEU:HD23	1:A:360:MET:HB2	1.98	0.46
1:A:408:GLU:OE2	1:A:533:LEU:N	2.48	0.46
1:B:302:TYR:CZ	1:B:303:ARG:HG3	2.50	0.46
1:B:756:LEU:HA	1:B:759:GLU:O	2.16	0.46
1:B:776:PRO:HG2	1:B:777:TYR:H	1.81	0.46
1:B:891:PRO:O	1:B:895:LEU:HD12	2.14	0.46
1:A:375:HIS:C	1:A:375:HIS:CD2	2.88	0.46
1:A:629:THR:HB	1:A:672:LEU:HD11	1.90	0.46
1:B:360:MET:O	1:B:385:ARG:NH2	2.48	0.46
1:B:625:ARG:HG3	1:B:672:LEU:HD22	1.97	0.46
1:A:785:ASP:O	1:A:789:LYS:HG3	2.16	0.45
1:B:544:ASN:OD1	1:B:547:LEU:HB2	2.16	0.45
1:B:664:LYS:HG3	1:B:685:VAL:HG23	1.98	0.45
1:A:319:TRP:NE1	1:A:322:ARG:NH2	2.53	0.45
1:B:594:LEU:HD23	1:B:594:LEU:N	2.30	0.45
1:B:899:LYS:O	1:B:903:LYS:HG3	2.16	0.45
1:A:363:GLU:H	1:A:363:GLU:CD	2.18	0.45
1:B:366:LEU:HD12	1:B:881:LEU:CD2	2.46	0.45
1:A:814:THR:CG2	1:A:818:LYS:HB2	2.47	0.45
1:A:319:TRP:CD1	1:A:322:ARG:NE	2.74	0.45
1:A:734:VAL:CG2	1:A:744:LEU:HD23	2.34	0.45
1:A:878:MET:HA	1:A:881:LEU:HD12	1.99	0.45
1:B:339:ILE:CD1	1:B:350:ALA:HB1	2.46	0.45
1:B:939:GLN:HG2	1:B:943:PHE:CZ	2.52	0.45
1:A:718:LYS:O	1:A:722:ARG:CG	2.63	0.45
1:A:723:GLU:OE1	1:A:723:GLU:N	2.50	0.45
1:B:710:LEU:O	1:B:714:THR:OG1	2.34	0.45
1:B:314:GLU:O	1:B:318:VAL:CG1	2.61	0.45
1:B:357:TRP:HD1	1:B:358:ALA:N	2.15	0.45
1:B:821:HIS:CD2	1:B:821:HIS:N	2.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:CD1	1:A:336:LEU:HD21	2.47	0.45
1:A:553:TRP:O	1:A:557:ILE:CG1	2.55	0.45
1:A:689:ALA:CB	1:A:691:HIS:CE1	2.99	0.44
1:A:782:GLU:O	1:A:786:THR:HG23	2.17	0.44
1:A:549:ASN:C	1:A:549:ASN:HD22	2.18	0.44
1:A:783:VAL:HG13	1:A:816:ASN:O	2.17	0.44
1:B:664:LYS:HG3	1:B:685:VAL:CG2	2.47	0.44
1:B:747:VAL:HG12	2:B:1950:093:HAE1	2.00	0.44
1:B:308:TYR:HD2	1:B:308:TYR:HA	1.69	0.44
1:B:794:TYR:CD1	1:B:821:HIS:CD2	3.05	0.44
1:A:649:PHE:CE1	1:A:662:ILE:HG13	2.48	0.44
1:A:335:PHE:HE2	1:A:339:ILE:HD12	1.81	0.44
1:A:896:GLU:OE1	1:A:898:ASP:OD1	2.36	0.44
1:B:366:LEU:CD1	1:B:881:LEU:HD21	2.47	0.44
1:A:397:TYR:O	1:A:398:LEU:C	2.56	0.44
1:A:709:ILE:O	1:A:712:MET:HB2	2.17	0.44
1:B:699:HIS:N	1:B:699:HIS:CD2	2.82	0.44
1:B:739:SER:O	1:B:740:LYS:CG	2.56	0.44
1:A:759:GLU:O	1:A:760:GLY:C	2.56	0.44
1:A:719:LEU:O	1:A:723:GLU:HG2	2.17	0.44
1:A:747:VAL:HG23	2:A:1949:093:NAK	2.26	0.44
1:B:302:TYR:CE2	1:B:303:ARG:HG3	2.52	0.44
1:B:600:ASN:HA	1:B:603:LYS:HD3	2.00	0.44
1:B:636:LEU:HD12	1:B:670:THR:HG21	2.00	0.43
1:B:766:PHE:HE1	1:B:817:GLY:HA2	1.83	0.43
1:A:328:HIS:O	1:A:331:ALA:HB3	2.17	0.43
1:A:395:LEU:C	1:A:395:LEU:HD23	2.38	0.43
1:A:811:LEU:HD23	1:A:811:LEU:N	2.33	0.43
1:B:664:LYS:HE3	1:B:685:VAL:HG21	2.01	0.43
1:A:532:ASN:ND2	1:A:534:CYS:SG	2.89	0.43
1:A:396:LEU:HD12	1:A:718:LYS:HE3	2.00	0.43
1:B:325:LEU:C	1:B:327:SER:N	2.71	0.43
1:B:865:TYR:OH	1:B:922:GLN:HG3	2.17	0.43
1:A:319:TRP:NE1	1:A:323:PHE:CZ	2.85	0.43
1:A:344:GLU:O	1:A:348:THR:HG23	2.18	0.43
1:A:625:ARG:HG3	1:A:626:ASN:N	2.27	0.43
1:A:668:MET:N	1:A:668:MET:SD	2.85	0.43
1:A:888:ALA:O	1:A:889:THR:HG23	2.19	0.43
1:B:310:LEU:HD13	1:B:311:SER:HG	1.83	0.43
1:B:350:ALA:O	1:B:354:LEU:N	2.44	0.43
1:B:368:LEU:C	1:B:370:SER:H	2.22	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:HIS:O	1:B:378:VAL:HG22	2.18	0.43
1:B:686:THR:OG1	1:B:691:HIS:HB2	2.18	0.43
1:A:652:ILE:HG22	1:A:653:PRO:O	2.19	0.43
1:A:723:GLU:OE1	1:A:723:GLU:CA	2.67	0.43
1:B:575:MET:O	1:B:579:VAL:HG23	2.18	0.43
1:B:704:ARG:H	1:B:704:ARG:HG3	1.60	0.43
1:A:547:LEU:HD23	1:A:547:LEU:HA	1.85	0.43
1:B:311:SER:HB3	1:B:314:GLU:CD	2.39	0.43
1:A:381:TYR:O	1:A:385:ARG:HG2	2.18	0.43
1:A:822:ILE:HD13	1:A:822:ILE:HG21	1.77	0.43
1:A:865:TYR:CD1	1:A:921:LEU:HD23	2.52	0.43
1:B:370:SER:HB3	1:B:371:PRO:HD2	2.01	0.43
1:A:684:PHE:O	1:A:692:GLU:HA	2.17	0.43
1:B:368:LEU:HD22	1:B:373:PHE:CE2	2.54	0.43
1:A:335:PHE:HD2	1:A:336:LEU:N	2.15	0.43
1:A:391:ASP:N	1:A:391:ASP:OD2	2.52	0.43
1:A:908:LEU:HD23	1:A:908:LEU:HA	1.81	0.43
1:B:343:LEU:CG	1:B:344:GLU:H	2.31	0.43
1:B:888:ALA:O	1:B:889:THR:CB	2.67	0.43
1:B:893:ILE:O	1:B:897:PRO:HA	2.18	0.43
1:A:602:ARG:NH1	1:A:606:ARG:HD2	2.33	0.42
1:A:641:MET:HE2	1:A:642:PHE:CE1	2.54	0.42
1:A:820:PHE:CD2	1:A:820:PHE:N	2.87	0.42
1:A:845:MET:O	1:A:848:ALA:HB3	2.19	0.42
1:A:843:LYS:HE2	1:A:847:GLU:OE2	2.18	0.42
1:B:300:ILE:HA	1:B:304:TYR:HD2	1.84	0.42
1:B:300:ILE:HG12	1:B:304:TYR:CD2	2.54	0.42
1:B:717:ASP:OD1	1:B:721:ARG:HG3	2.19	0.42
1:A:673:PHE:HE2	1:A:696:ILE:HG12	1.84	0.42
1:A:830:ARG:NH1	1:A:903:LYS:HZ2	2.17	0.42
1:B:611:LEU:HG	1:B:646:PHE:CE2	2.54	0.42
1:B:837:PRO:O	1:B:840:LYS:HE3	2.19	0.42
1:B:912:LEU:HB3	1:B:916:GLU:HB2	2.00	0.42
1:A:826:TYR:HB3	1:A:830:ARG:O	2.20	0.42
1:A:830:ARG:HH12	1:A:903:LYS:HZ2	1.66	0.42
1:B:656:LEU:HD23	1:B:657:ASP:N	2.35	0.42
1:A:823:ASP:O	1:A:823:ASP:CG	2.58	0.42
1:B:314:GLU:HA	1:B:317:LEU:HD23	2.02	0.42
1:B:329:LYS:HZ1	1:B:361:ASP:CB	2.32	0.42
1:B:614:LEU:HD21	1:B:636:LEU:CD2	2.47	0.42
1:A:580:LEU:HD23	1:A:584:LEU:HG	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:LEU:O	1:A:932:VAL:HG21	2.20	0.42
1:A:860:PHE:CE1	1:A:864:CYS:SG	3.13	0.42
1:B:741:HIS:ND1	1:B:741:HIS:N	2.68	0.42
1:A:400:GLN:N	1:A:400:GLN:NE2	2.68	0.41
1:A:747:VAL:HG21	1:A:820:PHE:CZ	2.55	0.41
1:B:375:HIS:CD2	1:B:376:PRO:N	2.88	0.41
1:B:570:GLU:OE1	1:B:570:GLU:N	2.51	0.41
1:A:375:HIS:NE2	1:A:377:GLN:CB	2.84	0.41
1:A:923:SER:O	1:A:927:VAL:HG22	2.20	0.41
1:A:403:GLN:NE2	1:A:888:ALA:HA	2.35	0.41
1:A:405:LEU:HA	1:A:405:LEU:HD23	1.75	0.41
1:B:375:HIS:NE2	1:B:377:GLN:CB	2.82	0.41
1:B:743:PHE:C	1:B:744:LEU:HD23	2.40	0.41
1:A:293:ILE:O	1:A:297:LEU:HD23	2.20	0.41
1:A:319:TRP:HH2	1:A:346:GLU:HG3	1.85	0.41
1:A:636:LEU:CD1	1:A:670:THR:HG21	2.51	0.41
1:B:368:LEU:HD22	1:B:373:PHE:HE2	1.85	0.41
1:B:933:MET:HA	1:B:934:PRO:HD3	1.89	0.41
1:B:639:GLN:N	1:B:639:GLN:OE1	2.54	0.41
1:B:625:ARG:HB2	1:B:678:MET:HE1	2.02	0.41
1:A:573:HIS:CD2	1:A:573:HIS:C	2.94	0.41
1:A:709:ILE:HA	1:A:709:ILE:HD13	1.77	0.41
1:B:608:ILE:HA	1:B:608:ILE:HD13	1.89	0.41
1:B:653:PRO:HB3	1:B:661:TYR:CE1	2.55	0.41
1:B:794:TYR:HB3	1:B:821:HIS:NE2	2.35	0.41
1:A:299:THR:HA	1:A:302:TYR:CZ	2.48	0.41
1:B:804:GLY:O	1:B:805:ASP:CB	2.69	0.41
1:A:641:MET:HB3	1:A:641:MET:HE3	1.92	0.41
1:A:727:LEU:N	1:A:727:LEU:HD23	2.35	0.41
1:B:400:GLN:HG2	1:B:881:LEU:HD22	2.02	0.41
1:B:333:THR:O	1:B:337:LYS:HG3	2.21	0.41
1:B:342:LYS:HG3	1:B:346:GLU:CD	2.41	0.41
1:B:751:THR:HG22	1:B:754:GLU:HG3	2.02	0.41
1:B:830:ARG:NH2	1:B:903:LYS:HZ2	2.19	0.41
1:A:298:HIS:HB3	1:A:302:TYR:CZ	2.51	0.41
1:A:585:LYS:HA	1:A:585:LYS:HD2	1.78	0.41
1:A:828:LEU:O	1:A:830:ARG:NH1	2.54	0.41
1:B:302:TYR:CE2	1:B:303:ARG:NE	2.86	0.41
1:B:302:TYR:HD1	1:B:330:LYS:HB2	1.86	0.41
1:B:307:THR:O	1:B:308:TYR:HD2	2.04	0.41
2:A:1949:093:NAU	2:A:1949:093:CL	2.91	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:THR:HG21	1:A:364:ASP:OD2	2.21	0.41
1:B:806:ARG:HH22	1:B:823:ASP:H	1.69	0.41
1:B:923:SER:O	1:B:927:VAL:HG22	2.21	0.41
1:A:303:ARG:O	1:A:304:TYR:HD2	2.03	0.40
1:A:580:LEU:O	1:A:580:LEU:HD23	2.21	0.40
1:A:676:ALA:O	1:A:677:LEU:C	2.59	0.40
1:A:400:GLN:OE1	1:A:711:GLN:OE1	2.38	0.40
1:A:841:LEU:HD23	1:A:845:MET:HE2	2.02	0.40
1:B:678:MET:C	1:B:699:HIS:NE2	2.60	0.40
1:B:709:ILE:HA	1:B:709:ILE:HD13	1.93	0.40
1:B:850:GLY:O	1:B:854:SER:HB3	2.21	0.40
1:A:810:ASN:HB3	1:A:811:LEU:HD23	2.03	0.40
1:B:610:GLU:HG3	1:B:644:VAL:H	1.87	0.40
1:A:314:GLU:HG3	1:A:314:GLU:H	1.76	0.40
1:A:379:ARG:O	1:A:383:VAL:HG23	2.21	0.40
1:A:824:PHE:HB3	1:A:827:ILE:HD11	2.03	0.40
1:A:888:ALA:O	1:A:889:THR:CG2	2.70	0.40
1:B:604:GLN:HE21	1:B:653:PRO:HG2	1.86	0.40
1:A:305:PRO:HA	1:A:306:PRO:HD3	1.91	0.40
1:A:674:LYS:HD3	1:A:674:LYS:H	1.86	0.40
1:A:885:MET:O	1:A:888:ALA:HB2	2.21	0.40
1:B:318:VAL:O	1:B:319:TRP:C	2.58	0.40
1:B:718:LYS:O	1:B:722:ARG:HG3	2.21	0.40
1:A:925:LEU:O	1:A:929:ILE:HG13	2.21	0.40
1:B:557:ILE:HD11	1:B:736:ALA:O	2.21	0.40
1:B:603:LYS:HE3	1:B:652:ILE:HG12	2.04	0.40
1:B:843:LYS:HA	1:B:932:VAL:CG1	2.51	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:TYR:OH	1:A:782:GLU:OE1[6_555]	2.07	0.13
1:B:391:ASP:OD2	1:B:724:ASN:ND2[8_565]	2.18	0.02

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	539/696 (77%)	505 (94%)	30 (6%)	4 (1%)	22 61
1	B	540/696 (78%)	517 (96%)	20 (4%)	3 (1%)	25 64
All	All	1079/1392 (78%)	1022 (95%)	50 (5%)	7 (1%)	25 64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	326	SER
1	A	305	PRO
1	B	408	GLU
1	A	304	TYR
1	A	591	ASN
1	B	889	THR
1	A	679	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	490/612 (80%)	398 (81%)	92 (19%)	1 8
1	B	490/612 (80%)	395 (81%)	95 (19%)	1 7
All	All	980/1224 (80%)	793 (81%)	187 (19%)	1 8

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	LEU
1	A	302	TYR
1	A	316	ASP
1	A	317	LEU
1	A	333	THR
1	A	335	PHE
1	A	339	ILE
1	A	341	TRP
1	A	343	LEU
1	A	351	LEU
1	A	354	LEU
1	A	357	TRP
1	A	361	ASP
1	A	363	GLU
1	A	370	SER
1	A	373	PHE
1	A	378	VAL
1	A	391	ASP
1	A	400	GLN
1	A	409	ASP
1	A	415	HIS
1	A	416	LEU
1	A	417	HIS
1	A	419	CYS
1	A	532	ASN
1	A	533	LEU
1	A	549	ASN
1	A	556	SER
1	A	569	ASP
1	A	573	HIS
1	A	575	MET
1	A	578	MET
1	A	581	LYS
1	A	602	ARG
1	A	611	LEU
1	A	612	VAL
1	A	614	LEU
1	A	617	LEU
1	A	625	ARG
1	A	629	THR
1	A	632	PHE
1	A	634	LYS
1	A	639	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	641	MET
1	A	645	ASN
1	A	649	PHE
1	A	654	PHE
1	A	656	LEU
1	A	657	ASP
1	A	663	THR
1	A	668	MET
1	A	669	ARG
1	A	670	THR
1	A	674	LYS
1	A	677	LEU
1	A	678	MET
1	A	682	LEU
1	A	683	THR
1	A	688	ILE
1	A	702	ASP
1	A	705	GLN
1	A	706	ASP
1	A	710	LEU
1	A	722	ARG
1	A	723	GLU
1	A	747	VAL
1	A	748	ASP
1	A	750	CYS
1	A	751	THR
1	A	759	GLU
1	A	765	PHE
1	A	773	ASP
1	A	782	GLU
1	A	790	SER
1	A	808	LEU
1	A	811	LEU
1	A	813	LEU
1	A	835	MET
1	A	839	MET
1	A	842	SER
1	A	860	PHE
1	A	878	MET
1	A	889	THR
1	A	895	LEU
1	A	896	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	898	ASP
1	A	913	THR
1	A	920	HIS
1	A	927	VAL
1	A	930	THR
1	A	940	ILE
1	A	944	THR
1	B	293	ILE
1	B	295	ASP
1	B	297	LEU
1	B	298	HIS
1	B	300	ILE
1	B	302	TYR
1	B	308	TYR
1	B	310	LEU
1	B	313	GLU
1	B	316	ASP
1	B	317	LEU
1	B	318	VAL
1	B	321	PHE
1	B	322	ARG
1	B	328	HIS
1	B	329	LYS
1	B	332	LEU
1	B	335	PHE
1	B	336	LEU
1	B	344	GLU
1	B	346	GLU
1	B	366	LEU
1	B	367	GLU
1	B	398	LEU
1	B	399	LEU
1	B	419	CYS
1	B	543	THR
1	B	544	ASN
1	B	546	THR
1	B	547	LEU
1	B	549	ASN
1	B	556	SER
1	B	569	ASP
1	B	570	GLU
1	B	573	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	579	VAL
1	B	580	LEU
1	B	591	ASN
1	B	599	TYR
1	B	611	LEU
1	B	614	LEU
1	B	624	ASN
1	B	631	LYS
1	B	634	LYS
1	B	635	LEU
1	B	639	GLN
1	B	640	ASP
1	B	641	MET
1	B	643	LYS
1	B	644	VAL
1	B	645	ASN
1	B	654	PHE
1	B	656	LEU
1	B	663	THR
1	B	670	THR
1	B	677	LEU
1	B	678	MET
1	B	691	HIS
1	B	704	ARG
1	B	706	ASP
1	B	708	LEU
1	B	714	THR
1	B	715	LEU
1	B	725	LEU
1	B	741	HIS
1	B	758	ARG
1	B	765	PHE
1	B	773	ASP
1	B	779	ILE
1	B	786	THR
1	B	788	ILE
1	B	806	ARG
1	B	811	LEU
1	B	812	LEU
1	B	813	LEU
1	B	814	THR
1	B	819	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	822	ILE
1	B	827	ILE
1	B	835	MET
1	B	839	MET
1	B	852	ILE
1	B	854	SER
1	B	855	GLU
1	B	859	GLU
1	B	860	PHE
1	B	866	THR
1	B	876	ASN
1	B	877	VAL
1	B	879	LEU
1	B	889	THR
1	B	913	THR
1	B	927	VAL
1	B	945	GLN
1	B	948	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	HIS
1	A	375	HIS
1	A	403	GLN
1	A	412	HIS
1	A	549	ASN
1	A	573	HIS
1	A	639	GLN
1	A	645	ASN
1	A	691	HIS
1	A	711	GLN
1	A	741	HIS
1	A	769	HIS
1	A	770	HIS
1	A	807	HIS
1	A	810	ASN
1	A	870	HIS
1	A	922	GLN
1	B	403	GLN
1	B	549	ASN
1	B	568	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	573	HIS
1	B	633	GLN
1	B	711	GLN
1	B	724	ASN
1	B	807	HIS
1	B	870	HIS
1	B	876	ASN
1	B	907	ASN
1	B	939	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 [\(i\)](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	093	A	1949	-	20,25,25	3.32	12 (60%)	23,36,36	2.85	11 (47%)
2	093	B	1950	-	20,25,25	3.57	13 (65%)	23,36,36	3.10	10 (43%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	093	A	1949	-	-	4/17/19/19	0/2/2/2
2	093	B	1950	-	-	11/17/19/19	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1949	093	SAN-NAU	7.62	1.73	1.61
2	B	1950	093	SAN-NAU	7.25	1.72	1.61
2	B	1950	093	CAG-CAF	6.82	1.49	1.39
2	A	1949	093	CAG-CAF	6.07	1.48	1.39
2	B	1950	093	CAD-CAC	5.00	1.47	1.38
2	B	1950	093	CAH-CAI	4.51	1.52	1.48
2	A	1949	093	CAD-CAC	4.47	1.46	1.38
2	A	1949	093	CAQ-NAR	4.34	1.45	1.33
2	B	1950	093	CAQ-NAR	4.27	1.45	1.33
2	B	1950	093	CAS-NAR	4.07	1.47	1.37
2	A	1949	093	CAS-NAR	3.85	1.46	1.37
2	A	1949	093	OAO-SAN	3.81	1.47	1.43
2	B	1950	093	OAO-SAN	3.55	1.47	1.43
2	B	1950	093	CAT-CAS	3.52	1.54	1.49
2	B	1950	093	OAM-SAN	3.40	1.47	1.43
2	A	1949	093	CAH-CAI	3.37	1.51	1.48
2	B	1950	093	CAF-SAN	3.36	1.82	1.77
2	B	1950	093	CAC-CAB	2.92	1.44	1.38
2	A	1949	093	OAM-SAN	2.83	1.46	1.43
2	A	1949	093	CAT-CAS	2.75	1.53	1.49
2	A	1949	093	CAF-SAN	2.74	1.81	1.77
2	B	1950	093	CAB-CAF	-2.68	1.36	1.40
2	A	1949	093	CAB-CAF	-2.63	1.36	1.40
2	A	1949	093	CAC-CAB	2.50	1.44	1.38
2	B	1950	093	CAB-CL	2.44	1.79	1.73

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1949	093	OAO-SAN-OAM	-8.80	108.74	119.55
2	B	1950	093	OAO-SAN-OAM	-7.04	110.90	119.55
2	B	1950	093	CAT-CAS-NAR	6.49	124.91	114.85
2	B	1950	093	CAB-CAF-SAN	-5.83	119.44	123.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1950	093	CAF-CAB-CL	-5.18	117.70	121.49
2	A	1949	093	CAF-CAB-CL	-3.63	118.83	121.49
2	A	1949	093	CAT-CAS-NAR	3.55	120.35	114.85
2	B	1950	093	OAL-CAS-NAR	-3.54	116.88	123.67
2	A	1949	093	CAW-CAV-NAU	3.51	118.88	111.02
2	A	1949	093	CAB-CAF-SAN	-3.43	121.01	123.25
2	A	1949	093	OAM-SAN-NAU	3.08	111.85	107.04
2	B	1950	093	OAO-SAN-NAU	2.78	111.39	107.04
2	B	1950	093	CAQ-NAR-CAS	2.78	123.33	116.11
2	A	1949	093	CAV-NAU-SAN	-2.75	111.52	120.41
2	A	1949	093	CAD-CAH-CAG	2.75	122.06	118.16
2	B	1950	093	CAW-CAV-NAU	2.72	117.10	111.02
2	B	1950	093	CAV-NAU-SAN	-2.63	111.92	120.41
2	A	1949	093	OAO-SAN-NAU	2.60	111.10	107.04
2	A	1949	093	OAM-SAN-CAF	-2.14	104.14	107.66
2	B	1950	093	CAC-CAB-CL	2.09	122.59	118.41
2	A	1949	093	OAO-SAN-CAF	2.07	111.06	107.66

There are no chirality outliers.

All (15) torsion outliers are listed below:

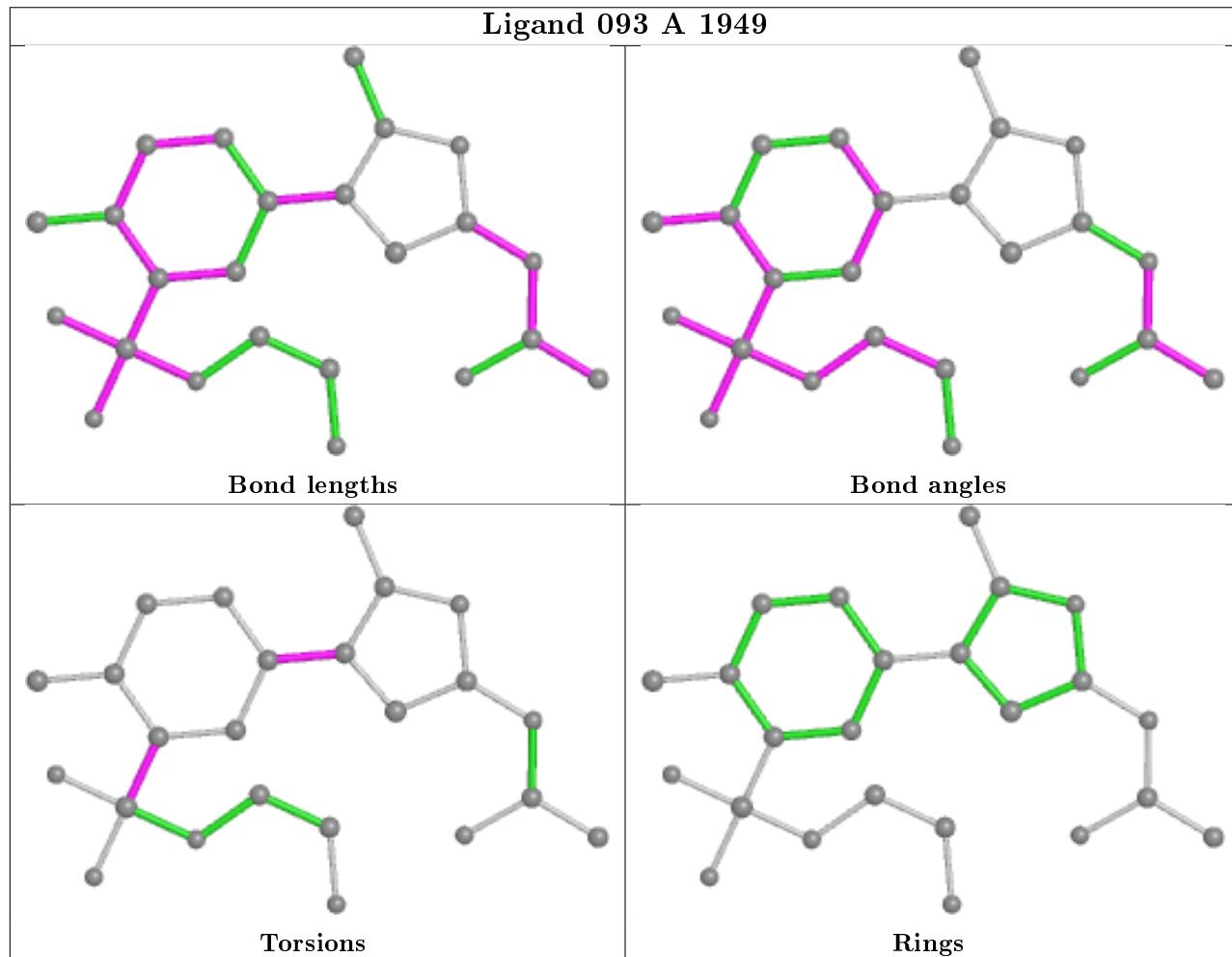
Mol	Chain	Res	Type	Atoms
2	B	1950	093	OAL-CAS-NAR-CAQ
2	B	1950	093	CAT-CAS-NAR-CAQ
2	A	1949	093	CAD-CAH-CAI-CAJ
2	A	1949	093	CAG-CAH-CAI-CAJ
2	B	1950	093	CAD-CAH-CAI-CAJ
2	B	1950	093	CAG-CAH-CAI-CAJ
2	B	1950	093	NAU-CAV-CAW-OAX
2	B	1950	093	CAV-NAU-SAN-OAM
2	B	1950	093	CAG-CAF-SAN-OAM
2	B	1950	093	CAV-NAU-SAN-OAO
2	A	1949	093	CAG-CAF-SAN-OAM
2	B	1950	093	CAV-NAU-SAN-CAF
2	B	1950	093	CAG-CAF-SAN-NAU
2	B	1950	093	CAB-CAF-SAN-OAM
2	A	1949	093	CAB-CAF-SAN-OAM

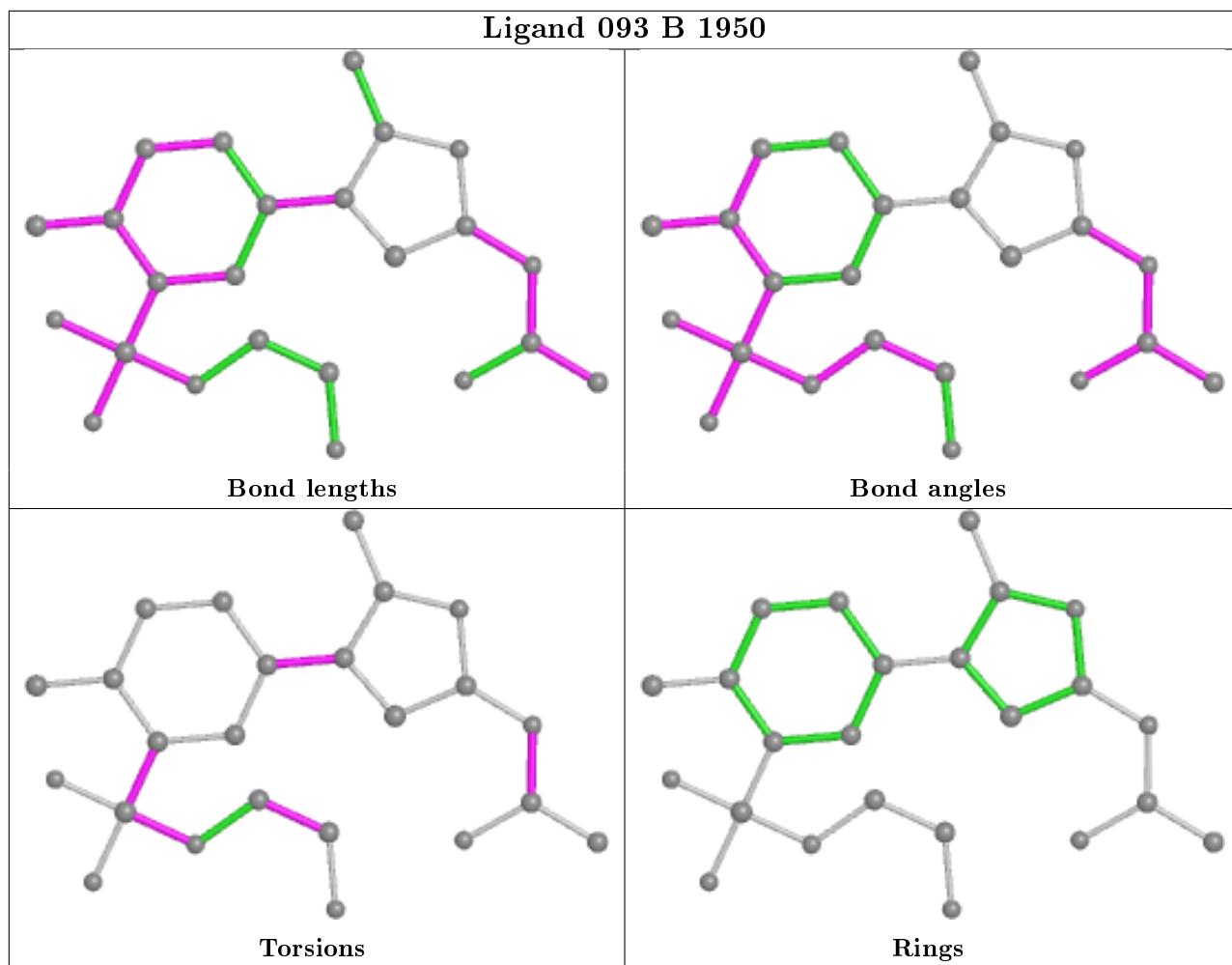
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1949	093	8	0
2	B	1950	093	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	545/696 (78%)	-0.29	3 (0%) 89 86	32, 55, 105, 116	0
1	B	546/696 (78%)	-0.18	6 (1%) 80 75	43, 65, 116, 123	0
All	All	1091/1392 (78%)	-0.23	9 (0%) 86 81	32, 61, 107, 123	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	341	TRP	3.1
1	A	302	TYR	2.7
1	B	636	LEU	2.5
1	A	322	ARG	2.2
1	A	298	HIS	2.2
1	B	423	GLU	2.2
1	B	347	VAL	2.2
1	B	298	HIS	2.0
1	B	377	GLN	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 carbohydrates in this entry.

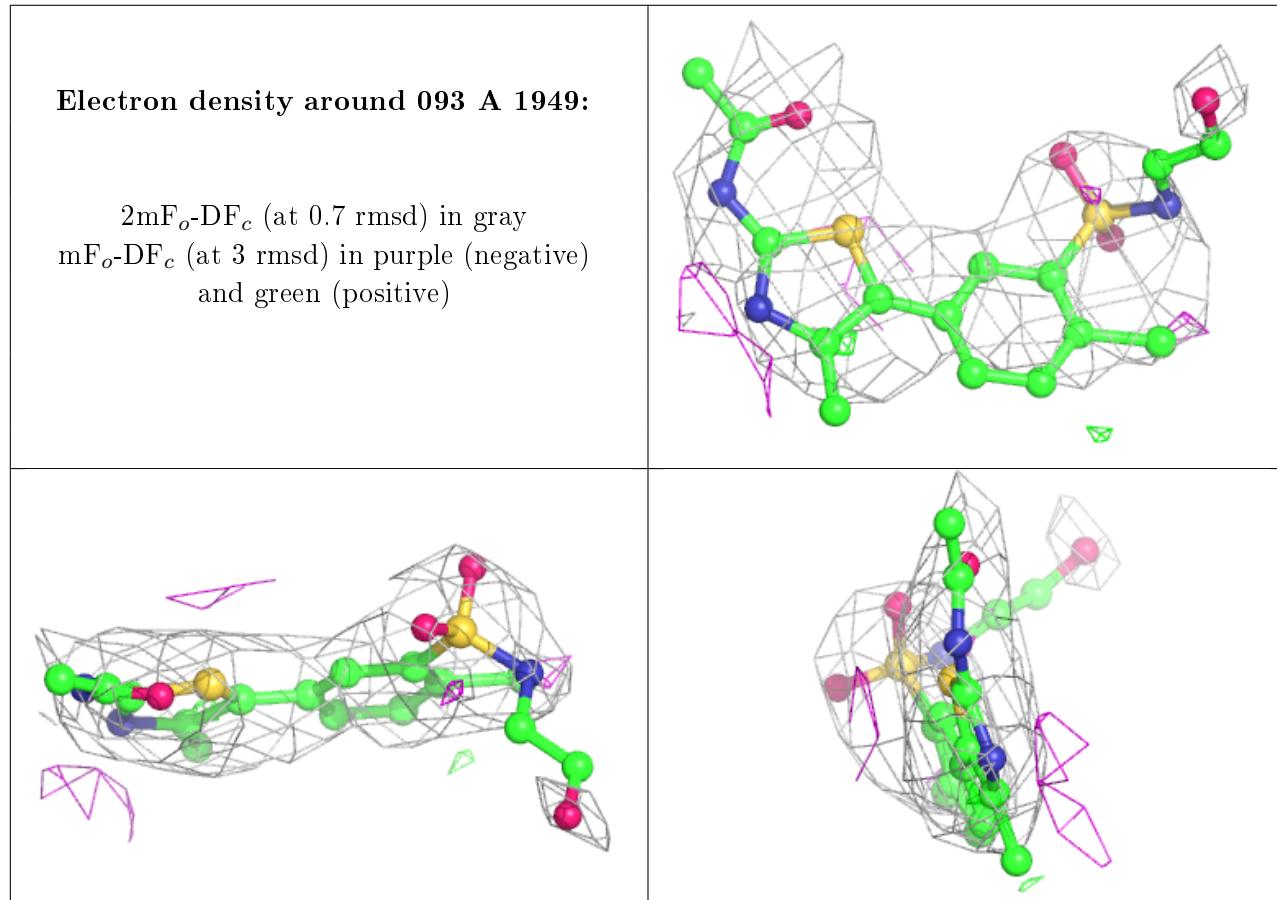
6.4 Ligands i

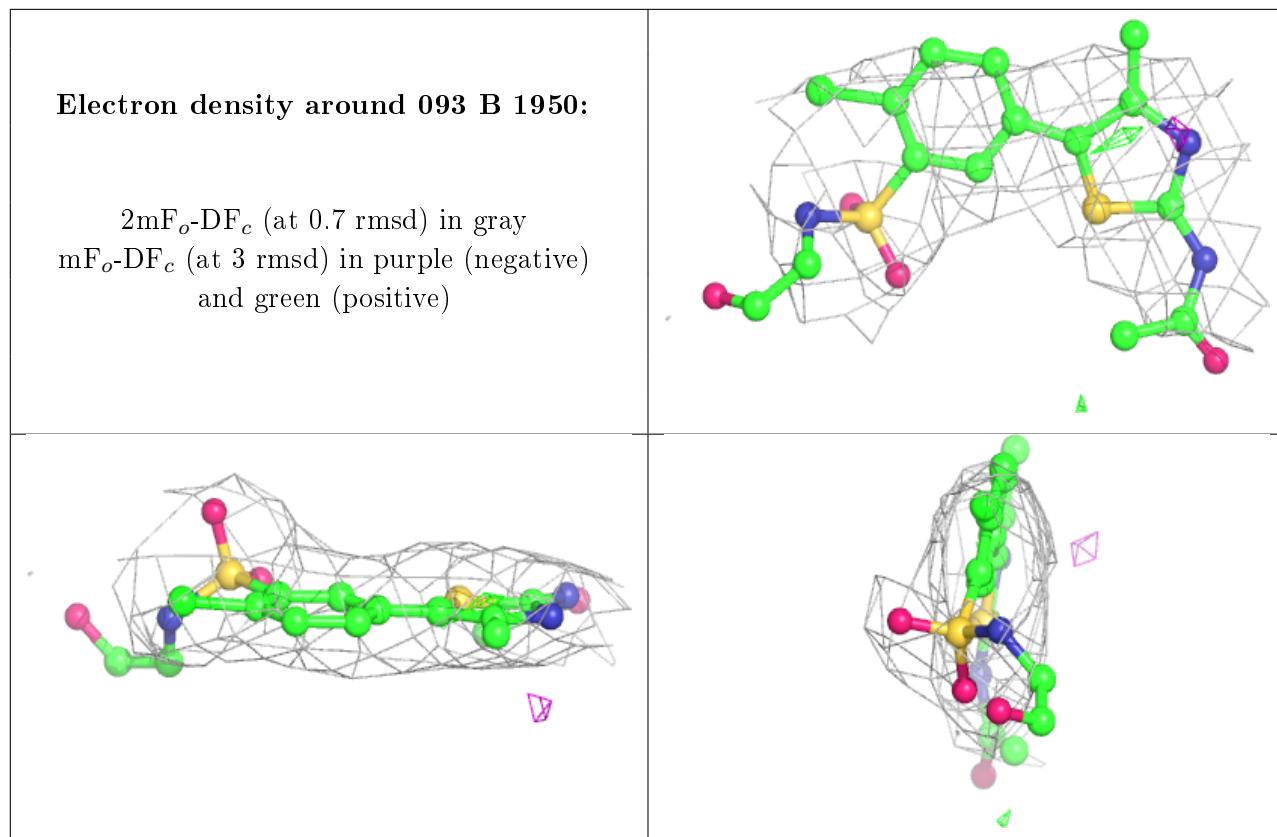
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	093	A	1949	24/24	0.89	0.31	87,97,104,107	0
2	093	B	1950	24/24	0.91	0.35	101,108,117,119	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.