



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:19 am BST

PDB ID : 3D9B
Title : Symmetric structure of E. coli AcrB
Authors : Veesler, D.; Blangy, S.; Cambillau, C.; Sciara, G.
Deposited on : 2008-05-27
Resolution : 3.42 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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

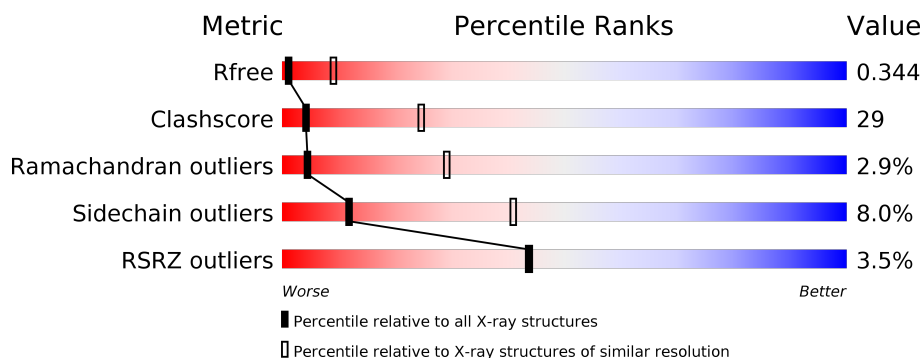
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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 $\leq 5\%$. 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	1049	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7951 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 Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1045	Total	C	N	O	S	84	0	0
			7950	5110	1316	1480	44			

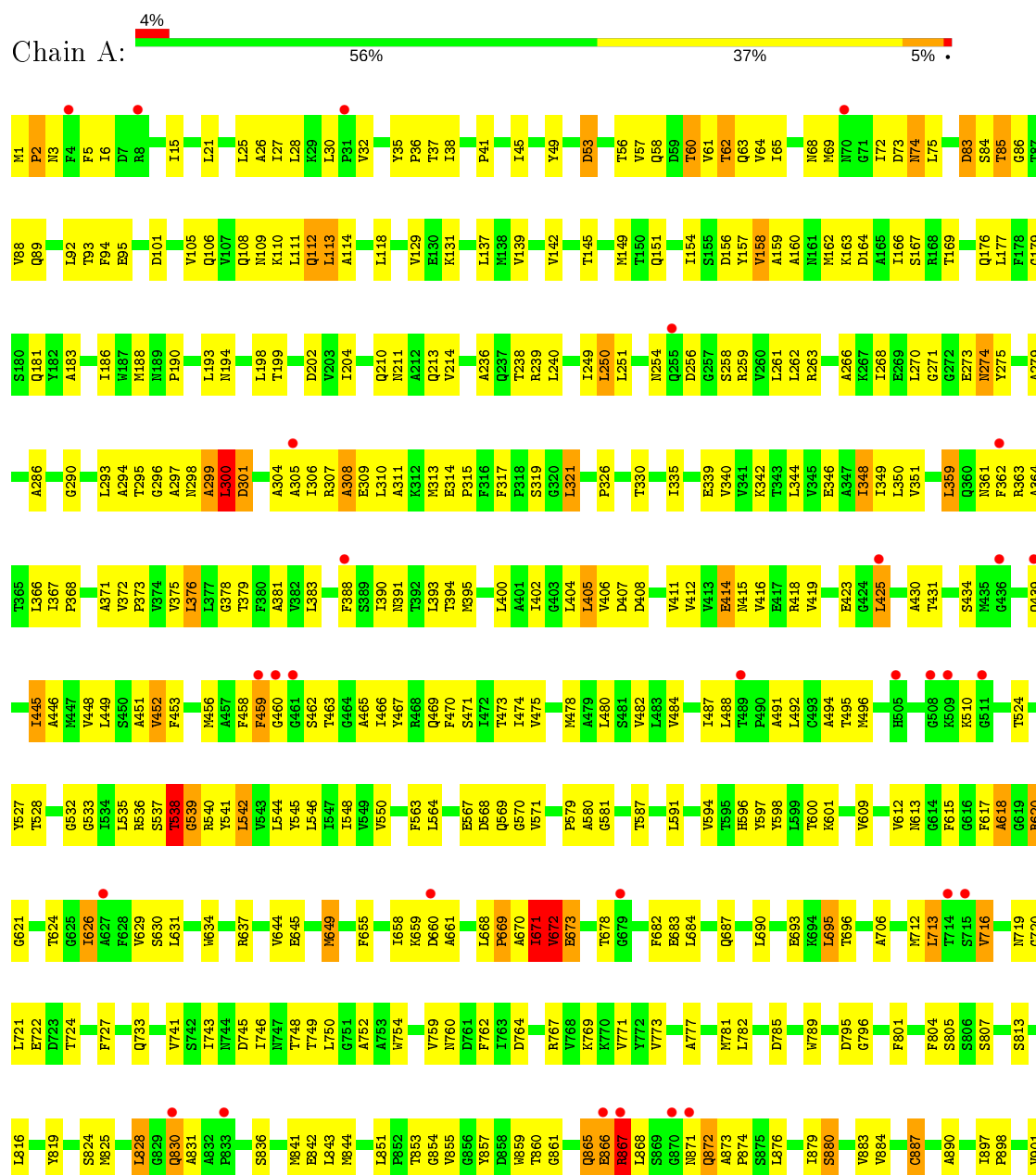
- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

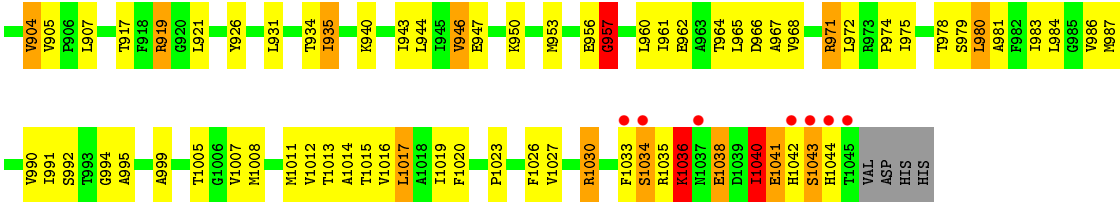
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		

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: Acriflavine resistance protein B





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	145.74Å 145.74Å 514.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 3.42 19.97 – 3.42	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.97-3.42) 99.9 (19.97-3.42)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 3.44Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.289 , 0.355 0.283 , 0.344	Depositor DCC
R_{free} test set	1152 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	86.4	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 79.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7951	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.52	3/8102 (0.0%)	0.72	13/11001 (0.1%)

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	4	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	659	LYS	CA-CB	-5.99	1.40	1.53
1	A	842	GLU	CG-CD	5.39	1.60	1.51
1	A	1035	ARG	CB-CG	-5.06	1.38	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	866	GLU	N-CA-C	11.37	141.69	111.00
1	A	865	GLN	N-CA-C	10.87	140.36	111.00
1	A	672	VAL	C-N-CA	-8.19	101.22	121.70
1	A	1044	HIS	N-CA-C	7.93	132.41	111.00
1	A	510	LYS	CB-CA-C	7.08	124.55	110.40
1	A	1036	LYS	N-CA-C	-7.01	92.06	111.00
1	A	957	GLY	N-CA-C	-6.84	95.99	113.10
1	A	671	ILE	CB-CA-C	-6.83	97.94	111.60
1	A	510	LYS	N-CA-CB	5.84	121.11	110.60
1	A	956	GLU	N-CA-C	5.62	126.17	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	538	THR	N-CA-CB	5.46	120.67	110.30
1	A	672	VAL	N-CA-C	5.04	124.60	111.00
1	A	112	GLN	CB-CA-C	5.03	120.46	110.40

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	510	LYS	CA
1	A	538	THR	CA
1	A	866	GLU	CA
1	A	956	GLU	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	539	GLY	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	7950	0	8091	464	0
2	A	1	0	0	0	0
All	All	7951	0	8091	464	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 29.

All (464) 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:957:GLY:HA2	1:A:1042:HIS:CE1	1.58	1.38
1:A:101:ASP:OD1	1:A:131:LYS:NZ	1.72	1.22
1:A:463:THR:HG21	1:A:868:LEU:HD11	1.19	1.16
1:A:672:VAL:HG12	1:A:673:GLU:N	1.57	1.15
1:A:463:THR:HG21	1:A:868:LEU:CD1	1.81	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:THR:CG2	1:A:868:LEU:HD11	1.81	1.10
1:A:990:VAL:HG23	1:A:1005:THR:HG22	1.38	1.06
1:A:672:VAL:CG1	1:A:673:GLU:N	2.15	1.05
1:A:672:VAL:CG1	1:A:673:GLU:H	1.72	1.02
1:A:45:ILE:HG23	1:A:129:VAL:HG22	1.44	0.97
1:A:612:VAL:HG23	1:A:626:ILE:HG23	1.50	0.94
1:A:990:VAL:HG23	1:A:1005:THR:CG2	1.99	0.93
1:A:449:LEU:HD23	1:A:478:MET:HE2	1.47	0.92
1:A:375:VAL:HG22	1:A:484:VAL:HG21	1.51	0.92
1:A:612:VAL:CG2	1:A:626:ILE:HG23	1.99	0.92
1:A:58:GLN:NE2	1:A:816:LEU:HD23	1.85	0.91
1:A:580:ALA:CB	1:A:724:THR:HG21	2.01	0.91
1:A:38:ILE:HD13	1:A:466:ILE:HD11	1.52	0.90
1:A:524:THR:O	1:A:528:THR:HG23	1.73	0.88
1:A:990:VAL:CG2	1:A:1005:THR:HG22	2.04	0.88
1:A:591:LEU:HD12	1:A:613:ASN:HD22	1.36	0.87
1:A:463:THR:HG21	1:A:868:LEU:CG	2.05	0.87
1:A:1016:VAL:HG23	1:A:1017:LEU:HD13	1.57	0.86
1:A:306:ILE:HG23	1:A:310:LEU:HD13	1.55	0.86
1:A:866:GLU:O	1:A:867:ARG:HB2	1.74	0.85
1:A:83:ASP:HB2	1:A:85:THR:HG22	1.58	0.85
1:A:27:ILE:CG2	1:A:28:LEU:HD23	2.07	0.85
1:A:872:GLN:C	1:A:874:PRO:HD2	1.99	0.83
1:A:580:ALA:HB1	1:A:724:THR:HG21	1.61	0.82
1:A:609:VAL:HG22	1:A:629:VAL:HG22	1.59	0.82
1:A:445:ILE:O	1:A:449:LEU:HD13	1.80	0.82
1:A:38:ILE:HD13	1:A:466:ILE:CD1	2.10	0.82
1:A:672:VAL:HG12	1:A:673:GLU:H	1.30	0.81
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.62	0.81
1:A:297:ALA:HB1	1:A:298:ASN:O	1.80	0.81
1:A:204:ILE:HD11	1:A:773:VAL:HG11	1.64	0.79
1:A:214:VAL:CG2	1:A:236:ALA:HB3	2.12	0.79
1:A:458:PHE:HA	1:A:459:PHE:HB3	1.65	0.78
1:A:615:PHE:CD1	1:A:620:ARG:NH1	2.51	0.78
1:A:306:ILE:CG2	1:A:310:LEU:HD13	2.13	0.78
1:A:813:SER:HB3	1:A:816:LEU:HD12	1.66	0.78
1:A:402:ILE:O	1:A:406:VAL:HG22	1.84	0.78
1:A:957:GLY:CA	1:A:1042:HIS:CE1	2.55	0.78
1:A:471:SER:O	1:A:475:VAL:HG23	1.85	0.77
1:A:987:MET:O	1:A:991:ILE:HD13	1.85	0.77
1:A:1:MET:N	1:A:2:PRO:HD3	2.01	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ILE:HD11	1:A:943:ILE:HG21	1.66	0.76
1:A:872:GLN:C	1:A:874:PRO:CD	2.54	0.76
1:A:166:ILE:HD11	1:A:310:LEU:HD12	1.67	0.75
1:A:214:VAL:HG23	1:A:236:ALA:HB3	1.66	0.75
1:A:393:LEU:CD1	1:A:466:ILE:HG23	2.16	0.75
1:A:27:ILE:HG22	1:A:28:LEU:HD23	1.68	0.75
1:A:964:THR:O	1:A:968:VAL:HG23	1.87	0.74
1:A:615:PHE:HE1	1:A:620:ARG:HH12	1.30	0.74
1:A:569:GLN:O	1:A:571:VAL:HG22	1.87	0.74
1:A:612:VAL:HG23	1:A:626:ILE:CG2	2.17	0.74
1:A:1042:HIS:CD2	1:A:1043:SER:H	2.06	0.74
1:A:445:ILE:HD11	1:A:943:ILE:CG2	2.18	0.74
1:A:393:LEU:HD13	1:A:466:ILE:HG23	1.69	0.73
1:A:873:ALA:N	1:A:874:PRO:CD	2.51	0.73
1:A:672:VAL:HG13	1:A:673:GLU:H	1.53	0.73
1:A:259:ARG:HD3	1:A:261:LEU:HD21	1.70	0.72
1:A:110:LYS:HD3	1:A:113:LEU:HD22	1.70	0.72
1:A:45:ILE:HG23	1:A:129:VAL:CG2	2.17	0.72
1:A:587:THR:HB	1:A:613:ASN:HD21	1.52	0.72
1:A:407:ASP:OD2	1:A:978:THR:HG21	1.89	0.71
1:A:297:ALA:HA	1:A:298:ASN:HB2	1.69	0.71
1:A:254:ASN:HD22	1:A:258:SER:HB2	1.55	0.71
1:A:445:ILE:HG21	1:A:940:LYS:NZ	2.06	0.71
1:A:307:ARG:O	1:A:311:ALA:N	2.21	0.70
1:A:35:TYR:HD2	1:A:671:ILE:HD12	1.56	0.70
1:A:445:ILE:CD1	1:A:943:ILE:HG21	2.20	0.70
1:A:159:ALA:HB1	1:A:181:GLN:HB2	1.74	0.69
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.22	0.69
1:A:53:ASP:O	1:A:57:VAL:HG23	1.92	0.69
1:A:394:THR:HG23	1:A:473:THR:HG21	1.74	0.69
1:A:943:ILE:O	1:A:946:VAL:HG13	1.93	0.69
1:A:957:GLY:HA2	1:A:1042:HIS:NE2	2.04	0.69
1:A:690:LEU:HD11	1:A:854:GLY:HA3	1.75	0.68
1:A:866:GLU:O	1:A:867:ARG:CB	2.42	0.68
1:A:451:ALA:HB1	1:A:883:VAL:HG12	1.75	0.68
1:A:111:LEU:HD12	1:A:129:VAL:HG21	1.74	0.68
1:A:137:LEU:HD12	1:A:293:LEU:HD12	1.74	0.68
1:A:669:PRO:O	1:A:670:ALA:HB3	1.93	0.67
1:A:1038:GLU:HB2	1:A:1040:ILE:HG22	1.77	0.67
1:A:972:LEU:HD23	1:A:1019:ILE:HD11	1.77	0.67
1:A:350:LEU:HD23	1:A:984:LEU:HB3	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:MET:HE1	1:A:193:LEU:HD11	1.76	0.67
1:A:204:ILE:HD11	1:A:773:VAL:CG1	2.25	0.67
1:A:3:ASN:HA	1:A:6:ILE:HD12	1.77	0.67
1:A:169:THR:OG1	1:A:309:GLU:HG3	1.94	0.67
1:A:541:TYR:O	1:A:544:LEU:N	2.27	0.67
1:A:615:PHE:HD1	1:A:620:ARG:NH1	1.93	0.66
1:A:671:ILE:HG12	1:A:672:VAL:N	2.10	0.66
1:A:293:LEU:HD21	1:A:297:ALA:CB	2.26	0.66
1:A:524:THR:HG22	1:A:972:LEU:HD12	1.76	0.66
1:A:448:VAL:HG23	1:A:449:LEU:CD1	2.26	0.66
1:A:448:VAL:HG13	1:A:887:CYS:HB2	1.77	0.65
1:A:1016:VAL:O	1:A:1019:ILE:HG22	1.96	0.65
1:A:177:LEU:HD23	1:A:179:GLY:O	1.97	0.65
1:A:75:LEU:HD12	1:A:92:LEU:HD23	1.78	0.65
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.79	0.65
1:A:372:VAL:HG22	1:A:405:LEU:HD13	1.77	0.65
1:A:383:LEU:HD21	1:A:473:THR:HG22	1.78	0.64
1:A:944:LEU:HB3	1:A:971:ARG:HD3	1.80	0.64
1:A:204:ILE:CD1	1:A:773:VAL:HG11	2.27	0.64
1:A:37:THR:HG21	1:A:296:GLY:HA2	1.80	0.63
1:A:5:PHE:CD2	1:A:487:ILE:HG23	2.34	0.63
1:A:580:ALA:CB	1:A:724:THR:CG2	2.77	0.63
1:A:254:ASN:ND2	1:A:258:SER:HB2	2.13	0.63
1:A:72:ILE:HG23	1:A:106:GLN:HB3	1.79	0.63
1:A:431:THR:HG21	1:A:494:ALA:HB2	1.80	0.63
1:A:268:ILE:N	1:A:268:ILE:HD12	2.14	0.62
1:A:720:GLY:O	1:A:721:LEU:HD23	1.99	0.62
1:A:965:LEU:HA	1:A:968:VAL:HG23	1.80	0.62
1:A:27:ILE:HG23	1:A:28:LEU:HD23	1.81	0.62
1:A:372:VAL:HG13	1:A:376:LEU:HD22	1.81	0.62
1:A:335:ILE:O	1:A:335:ILE:HG22	1.99	0.62
1:A:907:LEU:HD13	1:A:1017:LEU:HB3	1.81	0.62
1:A:211:ASN:HA	1:A:240:LEU:HD13	1.82	0.62
1:A:83:ASP:C	1:A:85:THR:H	2.03	0.62
1:A:190:PRO:HB3	1:A:789:TRP:CZ3	2.35	0.61
1:A:448:VAL:HG23	1:A:449:LEU:HD13	1.81	0.61
1:A:371:ALA:O	1:A:375:VAL:HG23	2.01	0.61
1:A:449:LEU:HD23	1:A:478:MET:CE	2.25	0.61
1:A:931:LEU:O	1:A:935:ILE:HG23	2.01	0.61
1:A:3:ASN:HA	1:A:6:ILE:HB	1.83	0.61
1:A:393:LEU:HD22	1:A:470:PHE:CE2	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:VAL:HG12	1:A:88:VAL:HG22	1.81	0.61
1:A:38:ILE:HG12	1:A:465:ALA:HB3	1.83	0.60
1:A:533:GLY:HA2	1:A:536:ARG:NE	2.16	0.60
1:A:684:LEU:HD23	1:A:695:LEU:CD2	2.31	0.60
1:A:527:TYR:OH	1:A:968:VAL:CG1	2.49	0.60
1:A:1:MET:H3	1:A:2:PRO:HD3	1.66	0.60
1:A:706:ALA:HB1	1:A:716:VAL:HG21	1.83	0.60
1:A:463:THR:HG23	1:A:563:PHE:CE2	2.37	0.60
1:A:706:ALA:CB	1:A:716:VAL:HG21	2.31	0.60
1:A:188:MET:CE	1:A:193:LEU:HD11	2.32	0.60
1:A:990:VAL:O	1:A:990:VAL:HG22	2.02	0.60
1:A:181:GLN:NE2	1:A:769:LYS:HG2	2.17	0.59
1:A:897:ILE:N	1:A:898:PRO:HD2	2.17	0.59
1:A:35:TYR:CD2	1:A:671:ILE:HD12	2.37	0.59
1:A:75:LEU:CD1	1:A:92:LEU:HD23	2.32	0.59
1:A:1011:MET:HE3	1:A:1015:THR:HG21	1.85	0.58
1:A:972:LEU:HD23	1:A:1019:ILE:CD1	2.33	0.58
1:A:480:LEU:O	1:A:484:VAL:HG23	2.03	0.58
1:A:210:GLN:NE2	1:A:249:ILE:HG23	2.18	0.58
1:A:830:GLN:HA	1:A:830:GLN:HE21	1.66	0.58
1:A:458:PHE:CA	1:A:459:PHE:HB3	2.33	0.58
1:A:32:VAL:O	1:A:299:ALA:HB1	2.04	0.58
1:A:449:LEU:O	1:A:452:VAL:HG22	2.03	0.58
1:A:873:ALA:N	1:A:874:PRO:HD3	2.19	0.58
1:A:684:LEU:O	1:A:824:SER:HB2	2.04	0.57
1:A:537:SER:O	1:A:538:THR:C	2.42	0.57
1:A:570:GLY:O	1:A:571:VAL:HG13	2.03	0.57
1:A:3:ASN:CA	1:A:6:ILE:HD12	2.34	0.57
1:A:669:PRO:O	1:A:670:ALA:CB	2.53	0.57
1:A:111:LEU:HD23	1:A:111:LEU:O	2.04	0.57
1:A:259:ARG:CD	1:A:261:LEU:HD21	2.33	0.57
1:A:372:VAL:HG22	1:A:405:LEU:CD1	2.33	0.57
1:A:719:ASN:HB2	1:A:828:LEU:HD13	1.85	0.57
1:A:307:ARG:HG3	1:A:311:ALA:HB2	1.85	0.57
1:A:580:ALA:HB3	1:A:724:THR:CG2	2.34	0.56
1:A:960:LEU:HD13	1:A:1027:VAL:HG12	1.87	0.56
1:A:111:LEU:HD12	1:A:129:VAL:CG2	2.35	0.56
1:A:61:VAL:CG1	1:A:88:VAL:HG21	2.35	0.56
1:A:105:VAL:O	1:A:108:GLN:N	2.36	0.56
1:A:162:MET:O	1:A:166:ILE:HG12	2.06	0.56
1:A:186:ILE:HB	1:A:773:VAL:HG23	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:THR:HG23	1:A:563:PHE:HE2	1.69	0.56
1:A:300:LEU:HD23	1:A:304:ALA:HB2	1.87	0.55
1:A:149:MET:SD	1:A:321:LEU:HD23	2.46	0.55
1:A:1042:HIS:CG	1:A:1043:SER:H	2.24	0.55
1:A:750:LEU:HD12	1:A:754:TRP:CD1	2.42	0.55
1:A:957:GLY:HA2	1:A:1042:HIS:ND1	2.12	0.55
1:A:131:LYS:HG3	1:A:131:LYS:O	2.06	0.55
1:A:400:LEU:HD21	1:A:1007:VAL:HG21	1.87	0.55
1:A:596:HIS:NE2	1:A:600:THR:HG21	2.21	0.55
1:A:160:ALA:HB1	1:A:767:ARG:HD2	1.88	0.55
1:A:383:LEU:HD21	1:A:473:THR:CG2	2.37	0.55
1:A:383:LEU:HD22	1:A:388:PHE:HB2	1.89	0.55
1:A:539:GLY:C	1:A:541:TYR:N	2.59	0.55
1:A:631:LEU:HD11	1:A:644:VAL:HG12	1.89	0.55
1:A:293:LEU:HD21	1:A:297:ALA:HB3	1.88	0.55
1:A:449:LEU:HB3	1:A:478:MET:HE1	1.89	0.54
1:A:713:LEU:HD13	1:A:843:LEU:HD23	1.88	0.54
1:A:1038:GLU:H	1:A:1038:GLU:CD	2.10	0.54
1:A:972:LEU:HA	1:A:975:ILE:HD12	1.90	0.54
1:A:451:ALA:CB	1:A:883:VAL:HG12	2.37	0.54
1:A:533:GLY:HA2	1:A:536:ARG:HE	1.72	0.54
1:A:142:VAL:HG12	1:A:154:ILE:CG2	2.38	0.54
1:A:176:GLN:CD	1:A:620:ARG:HH22	2.12	0.54
1:A:305:ALA:O	1:A:308:ALA:HB3	2.08	0.54
1:A:880:SER:O	1:A:884:VAL:HG23	2.08	0.54
1:A:274:ASN:OD1	1:A:274:ASN:C	2.47	0.54
1:A:299:ALA:C	1:A:301:ASP:N	2.61	0.54
1:A:631:LEU:HD13	1:A:637:ARG:NH2	2.23	0.54
1:A:984:LEU:HD23	1:A:987:MET:CE	2.37	0.54
1:A:720:GLY:C	1:A:721:LEU:HD23	2.27	0.54
1:A:990:VAL:HG11	1:A:1008:MET:CE	2.38	0.53
1:A:617:PHE:O	1:A:618:ALA:CB	2.56	0.53
1:A:658:ILE:HG22	1:A:661:ALA:HB3	1.90	0.53
1:A:394:THR:HG23	1:A:473:THR:CG2	2.38	0.53
1:A:960:LEU:O	1:A:964:THR:HG23	2.08	0.53
1:A:598:TYR:CE2	1:A:629:VAL:HG21	2.44	0.53
1:A:1:MET:H2	1:A:2:PRO:HD3	1.73	0.53
1:A:615:PHE:CE1	1:A:620:ARG:NH1	2.61	0.53
1:A:1:MET:N	1:A:2:PRO:CD	2.69	0.53
1:A:463:THR:HG21	1:A:868:LEU:HG	1.89	0.52
1:A:68:ASN:HB2	1:A:114:ALA:HB2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:MET:HG3	1:A:467:TYR:HB3	1.90	0.52
1:A:58:GLN:O	1:A:63:GLN:HG3	2.09	0.52
1:A:297:ALA:CA	1:A:298:ASN:HB2	2.38	0.52
1:A:533:GLY:CA	1:A:536:ARG:HE	2.23	0.52
1:A:546:LEU:O	1:A:550:VAL:HG23	2.10	0.52
1:A:306:ILE:O	1:A:309:GLU:N	2.44	0.51
1:A:26:ALA:O	1:A:30:LEU:HB2	2.09	0.51
1:A:539:GLY:O	1:A:542:LEU:HB2	2.10	0.51
1:A:190:PRO:HB3	1:A:789:TRP:CE3	2.45	0.51
1:A:983:ILE:HD13	1:A:1012:VAL:HG22	1.93	0.51
1:A:142:VAL:HG12	1:A:154:ILE:HG23	1.91	0.51
1:A:539:GLY:HA3	1:A:542:LEU:HD13	1.92	0.51
1:A:72:ILE:HG23	1:A:106:GLN:CB	2.41	0.51
1:A:564:LEU:HD22	1:A:926:TYR:CE1	2.46	0.51
1:A:960:LEU:HD12	1:A:961:ILE:N	2.26	0.51
1:A:527:TYR:CE2	1:A:1019:ILE:HG13	2.45	0.51
1:A:831:ALA:HB1	1:A:836:SER:O	2.10	0.51
1:A:214:VAL:CG2	1:A:236:ALA:CB	2.88	0.51
1:A:300:LEU:CD2	1:A:304:ALA:HB2	2.41	0.51
1:A:45:ILE:HD11	1:A:92:LEU:HD11	1.92	0.51
1:A:38:ILE:O	1:A:38:ILE:HG22	2.10	0.50
1:A:367:ILE:HB	1:A:368:PRO:CD	2.41	0.50
1:A:463:THR:HA	1:A:466:ILE:HD13	1.94	0.50
1:A:393:LEU:HD22	1:A:470:PHE:HE2	1.72	0.50
1:A:872:GLN:O	1:A:874:PRO:N	2.44	0.50
1:A:972:LEU:HD22	1:A:972:LEU:O	2.12	0.50
1:A:62:THR:HG23	1:A:88:VAL:CG1	2.42	0.50
1:A:162:MET:HA	1:A:313:MET:SD	2.52	0.50
1:A:453:PHE:CE2	1:A:474:ILE:HG21	2.46	0.50
1:A:533:GLY:O	1:A:536:ARG:HB2	2.12	0.49
1:A:733:GLN:HE22	1:A:743:ILE:HG21	1.76	0.49
1:A:139:VAL:O	1:A:326:PRO:HD2	2.12	0.49
1:A:156:ASP:O	1:A:157:TYR:C	2.50	0.49
1:A:405:LEU:C	1:A:405:LEU:HD23	2.33	0.49
1:A:404:LEU:HD13	1:A:478:MET:HE3	1.94	0.49
1:A:407:ASP:CB	1:A:978:THR:HG21	2.42	0.49
1:A:1038:GLU:HG2	1:A:1040:ILE:H	1.76	0.49
1:A:1042:HIS:O	1:A:1043:SER:CB	2.60	0.49
1:A:405:LEU:C	1:A:405:LEU:CD2	2.80	0.49
1:A:88:VAL:HG12	1:A:89:GLN:N	2.28	0.49
1:A:57:VAL:HG21	1:A:86:GLY:HA2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:LEU:O	1:A:880:SER:HB2	2.12	0.49
1:A:1036:LYS:HD2	1:A:1036:LYS:O	2.13	0.49
1:A:65:ILE:HG13	1:A:118:LEU:HD21	1.94	0.49
1:A:378:GLY:O	1:A:381:ALA:HB3	2.13	0.49
1:A:412:VAL:O	1:A:416:VAL:HG23	2.11	0.49
1:A:448:VAL:CG1	1:A:887:CYS:HB2	2.42	0.49
1:A:682:PHE:HD1	1:A:859:TRP:CH2	2.31	0.48
1:A:83:ASP:OD2	1:A:83:ASP:N	2.45	0.48
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.95	0.48
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.95	0.48
1:A:879:ILE:O	1:A:883:VAL:HG23	2.14	0.48
1:A:463:THR:CG2	1:A:868:LEU:HD21	2.43	0.48
1:A:631:LEU:HD11	1:A:644:VAL:CG1	2.43	0.48
1:A:964:THR:O	1:A:967:ALA:HB3	2.13	0.48
1:A:193:LEU:HB3	1:A:198:LEU:O	2.13	0.48
1:A:423:GLU:HB3	1:A:425:LEU:HD13	1.94	0.48
1:A:213:GLN:HB2	1:A:239:ARG:HG2	1.96	0.47
1:A:746:ILE:HD13	1:A:804:PHE:CE2	2.49	0.47
1:A:58:GLN:HA	1:A:62:THR:OG1	2.14	0.47
1:A:453:PHE:CD2	1:A:474:ILE:HG21	2.49	0.47
1:A:693:GLU:O	1:A:696:THR:HB	2.15	0.47
1:A:860:THR:OG1	1:A:861:GLY:N	2.46	0.47
1:A:965:LEU:HD12	1:A:966:ASP:N	2.29	0.47
1:A:294:ALA:O	1:A:295:THR:C	2.53	0.47
1:A:414:GLU:HG2	1:A:974:PRO:HB3	1.96	0.47
1:A:617:PHE:O	1:A:618:ALA:HB2	2.15	0.47
1:A:488:LEU:O	1:A:492:LEU:HD13	2.15	0.47
1:A:56:THR:O	1:A:60:THR:HG22	2.15	0.47
1:A:372:VAL:HG12	1:A:373:PRO:N	2.29	0.47
1:A:743:ILE:HD12	1:A:743:ILE:H	1.80	0.47
1:A:35:TYR:HB3	1:A:36:PRO:HD2	1.97	0.46
1:A:1011:MET:CE	1:A:1015:THR:HG21	2.46	0.46
1:A:1040:ILE:HG23	1:A:1041:GLU:N	2.30	0.46
1:A:112:GLN:O	1:A:113:LEU:C	2.53	0.46
1:A:445:ILE:HD11	1:A:943:ILE:HG22	1.95	0.46
1:A:445:ILE:HG21	1:A:940:LYS:HZ1	1.75	0.46
1:A:795:ASP:OD1	1:A:796:GLY:N	2.48	0.46
1:A:960:LEU:HD22	1:A:1030:ARG:HB3	1.96	0.46
1:A:348:ILE:HG22	1:A:349:ILE:N	2.30	0.46
1:A:670:ALA:O	1:A:671:ILE:HB	2.15	0.46
1:A:1033:PHE:O	1:A:1034:SER:CB	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:HD21	1:A:297:ALA:HB2	1.98	0.46
1:A:727:PHE:CE2	1:A:807:SER:HB2	2.49	0.46
1:A:35:TYR:HD2	1:A:671:ILE:CD1	2.27	0.46
1:A:671:ILE:HG12	1:A:672:VAL:H	1.80	0.46
1:A:407:ASP:HB2	1:A:978:THR:HG21	1.97	0.46
1:A:383:LEU:HD11	1:A:473:THR:HG22	1.98	0.46
1:A:157:TYR:CD2	1:A:157:TYR:C	2.89	0.46
1:A:256:ASP:OD1	1:A:258:SER:OG	2.30	0.46
1:A:38:ILE:CD1	1:A:466:ILE:CD1	2.89	0.46
1:A:363:ARG:NE	1:A:496:MET:O	2.48	0.46
1:A:56:THR:HG22	1:A:56:THR:O	2.16	0.46
1:A:326:PRO:O	1:A:630:SER:HB2	2.15	0.46
1:A:158:VAL:HG23	1:A:177:LEU:HD11	1.98	0.46
1:A:451:ALA:HB1	1:A:883:VAL:CG1	2.43	0.46
1:A:407:ASP:CG	1:A:978:THR:HG21	2.36	0.46
1:A:411:VAL:HG22	1:A:971:ARG:HH22	1.81	0.45
1:A:567:GLU:OE2	1:A:999:ALA:N	2.45	0.45
1:A:946:VAL:O	1:A:947:GLU:C	2.54	0.45
1:A:211:ASN:O	1:A:211:ASN:CG	2.54	0.45
1:A:274:ASN:OD1	1:A:275:TYR:N	2.50	0.45
1:A:62:THR:HG23	1:A:88:VAL:HG13	1.98	0.45
1:A:950:LYS:HA	1:A:953:MET:HE2	1.97	0.45
1:A:979:SER:OG	1:A:1015:THR:HG21	2.17	0.45
1:A:314:GLU:N	1:A:315:PRO:HD3	2.32	0.45
1:A:760:ASN:OD1	1:A:760:ASN:O	2.34	0.45
1:A:984:LEU:HD23	1:A:987:MET:HE2	1.97	0.45
1:A:314:GLU:N	1:A:315:PRO:CD	2.79	0.45
1:A:672:VAL:HG13	1:A:673:GLU:N	2.15	0.45
1:A:760:ASN:O	1:A:771:VAL:HG23	2.16	0.45
1:A:527:TYR:OH	1:A:968:VAL:HG11	2.16	0.45
1:A:72:ILE:HD11	1:A:110:LYS:HG3	1.98	0.45
1:A:204:ILE:HD12	1:A:759:VAL:HG22	1.97	0.45
1:A:139:VAL:HG22	1:A:290:GLY:HA2	1.97	0.45
1:A:393:LEU:HD11	1:A:466:ILE:HG23	1.95	0.45
1:A:527:TYR:CE1	1:A:968:VAL:HG12	2.51	0.45
1:A:782:LEU:O	1:A:785:ASP:HB2	2.17	0.45
1:A:68:ASN:O	1:A:110:LYS:HB3	2.17	0.45
1:A:68:ASN:CB	1:A:114:ALA:HB2	2.46	0.45
1:A:314:GLU:HA	1:A:317:PHE:CE2	2.52	0.45
1:A:532:GLY:HA2	1:A:535:LEU:HD12	1.98	0.45
1:A:568:ASP:OD2	1:A:637:ARG:NH2	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:LEU:HD23	1:A:695:LEU:HD22	1.97	0.45
1:A:872:GLN:O	1:A:873:ALA:C	2.54	0.45
1:A:658:ILE:CG2	1:A:661:ALA:HB3	2.47	0.45
1:A:266:ALA:O	1:A:268:ILE:HD12	2.17	0.45
1:A:404:LEU:HD22	1:A:478:MET:CE	2.46	0.45
1:A:527:TYR:CZ	1:A:1019:ILE:HG13	2.52	0.45
1:A:535:LEU:HD22	1:A:1027:VAL:HG11	1.98	0.45
1:A:748:THR:O	1:A:752:ALA:CB	2.65	0.45
1:A:980:LEU:HD23	1:A:984:LEU:HD12	1.98	0.45
1:A:1020:PHE:O	1:A:1023:PRO:HD2	2.17	0.45
1:A:390:ILE:HG22	1:A:390:ILE:O	2.17	0.45
1:A:391:ASN:HD21	1:A:469:GLN:CD	2.21	0.45
1:A:745:ASP:O	1:A:749:THR:HG23	2.17	0.45
1:A:594:VAL:HG13	1:A:655:PHE:CZ	2.51	0.44
1:A:307:ARG:O	1:A:311:ALA:HB3	2.17	0.44
1:A:307:ARG:O	1:A:311:ALA:CB	2.65	0.44
1:A:45:ILE:HD11	1:A:92:LEU:CD1	2.48	0.44
1:A:372:VAL:HA	1:A:405:LEU:HD11	1.99	0.44
1:A:415:ASN:O	1:A:419:VAL:HG23	2.17	0.44
1:A:1016:VAL:C	1:A:1019:ILE:HG22	2.37	0.44
1:A:431:THR:HA	1:A:434:SER:HB3	2.00	0.44
1:A:383:LEU:HD22	1:A:388:PHE:CB	2.48	0.44
1:A:597:TYR:HD1	1:A:601:LYS:HD2	1.83	0.44
1:A:621:GLY:O	1:A:624:THR:HG22	2.16	0.44
1:A:668:LEU:O	1:A:670:ALA:N	2.51	0.44
1:A:990:VAL:HG11	1:A:1008:MET:HE2	1.99	0.44
1:A:1011:MET:HE3	1:A:1015:THR:CG2	2.47	0.44
1:A:151:GLN:HA	1:A:154:ILE:HD12	1.99	0.44
1:A:762:PHE:CZ	1:A:764:ASP:HB2	2.52	0.44
1:A:819:TYR:CE1	1:A:860:THR:HB	2.52	0.44
1:A:964:THR:HG22	1:A:1026:PHE:CD2	2.53	0.44
1:A:213:GLN:NE2	1:A:238:THR:HA	2.32	0.44
1:A:57:VAL:HG12	1:A:88:VAL:CG2	2.48	0.44
1:A:990:VAL:C	1:A:991:ILE:HD12	2.38	0.44
1:A:198:LEU:HD23	1:A:202:ASP:OD2	2.17	0.44
1:A:307:ARG:HA	1:A:310:LEU:HB2	1.99	0.44
1:A:335:ILE:CG2	1:A:335:ILE:O	2.65	0.44
1:A:596:HIS:CE1	1:A:600:THR:HG21	2.52	0.44
1:A:748:THR:O	1:A:752:ALA:HB2	2.16	0.44
1:A:580:ALA:HA	1:A:581:GLY:C	2.37	0.44
1:A:342:LYS:HG2	1:A:346:GLU:OE2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:TYR:OH	1:A:968:VAL:HG12	2.18	0.43
1:A:263:ARG:HA	1:A:268:ILE:HD11	2.00	0.43
1:A:38:ILE:CG2	1:A:38:ILE:O	2.66	0.43
1:A:408:ASP:O	1:A:412:VAL:HG23	2.17	0.43
1:A:425:LEU:O	1:A:430:ALA:HB2	2.17	0.43
1:A:919:ARG:C	1:A:921:LEU:H	2.22	0.43
1:A:445:ILE:HG23	1:A:449:LEU:HD22	2.00	0.43
1:A:297:ALA:CB	1:A:298:ASN:O	2.58	0.43
1:A:415:ASN:O	1:A:418:ARG:HB3	2.18	0.43
1:A:781:MET:HB2	1:A:781:MET:HE2	1.94	0.43
1:A:1011:MET:CE	1:A:1015:THR:CG2	2.96	0.43
1:A:137:LEU:HD23	1:A:137:LEU:C	2.38	0.43
1:A:671:ILE:O	1:A:671:ILE:HG23	2.19	0.43
1:A:307:ARG:CG	1:A:311:ALA:HB2	2.49	0.43
1:A:363:ARG:O	1:A:366:LEU:N	2.47	0.43
1:A:541:TYR:O	1:A:542:LEU:C	2.57	0.43
1:A:866:GLU:O	1:A:866:GLU:HG2	2.18	0.43
1:A:402:ILE:O	1:A:406:VAL:N	2.36	0.43
1:A:545:TYR:HA	1:A:548:ILE:HD12	2.00	0.43
1:A:645:GLU:O	1:A:649:MET:HB2	2.19	0.42
1:A:61:VAL:HG11	1:A:88:VAL:HG21	2.00	0.42
1:A:904:VAL:O	1:A:905:VAL:C	2.58	0.42
1:A:466:ILE:HD12	1:A:466:ILE:H	1.84	0.42
1:A:612:VAL:CG2	1:A:626:ILE:CG2	2.82	0.42
1:A:65:ILE:CG1	1:A:118:LEU:HD21	2.50	0.42
1:A:851:LEU:HD13	1:A:855:VAL:HG11	2.02	0.42
1:A:986:VAL:HG11	1:A:1007:VAL:HG11	2.01	0.42
1:A:394:THR:CG2	1:A:473:THR:HG21	2.46	0.42
1:A:712:MET:HG3	1:A:843:LEU:HD22	2.01	0.42
1:A:263:ARG:HA	1:A:268:ILE:CD1	2.50	0.42
1:A:183:ALA:N	1:A:271:GLY:O	2.52	0.42
1:A:364:ALA:O	1:A:368:PRO:HD2	2.19	0.42
1:A:591:LEU:HD12	1:A:613:ASN:ND2	2.19	0.42
1:A:609:VAL:O	1:A:609:VAL:HG12	2.19	0.42
1:A:108:GLN:O	1:A:109:ASN:C	2.57	0.42
1:A:279:ALA:HB3	1:A:286:ALA:O	2.20	0.42
1:A:359:LEU:HD23	1:A:359:LEU:N	2.35	0.42
1:A:463:THR:HG21	1:A:868:LEU:CD2	2.48	0.42
1:A:984:LEU:HD23	1:A:987:MET:HE3	2.00	0.42
1:A:108:GLN:HA	1:A:111:LEU:HB2	2.02	0.42
1:A:198:LEU:CD2	1:A:202:ASP:OD2	2.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:VAL:HG22	1:A:981:ALA:HB1	2.02	0.42
1:A:541:TYR:O	1:A:545:TYR:N	2.45	0.42
1:A:74:ASN:HB3	1:A:95:GLU:HG2	2.02	0.42
1:A:367:ILE:HG22	1:A:368:PRO:N	2.35	0.42
1:A:73:ASP:O	1:A:75:LEU:N	2.53	0.42
1:A:841:MET:HG2	1:A:859:TRP:CH2	2.55	0.42
1:A:901:VAL:HG11	1:A:943:ILE:HG13	2.02	0.42
1:A:250:LEU:HD12	1:A:251:LEU:N	2.35	0.41
1:A:777:ALA:O	1:A:781:MET:HE2	2.20	0.41
1:A:841:MET:O	1:A:844:MET:N	2.53	0.41
1:A:367:ILE:CB	1:A:368:PRO:CD	2.97	0.41
1:A:64:VAL:O	1:A:64:VAL:HG22	2.20	0.41
1:A:695:LEU:HD13	1:A:825:MET:HG3	2.01	0.41
1:A:713:LEU:HD21	1:A:844:MET:HG2	2.01	0.41
1:A:361:ASN:HB3	1:A:364:ALA:HB3	2.02	0.41
1:A:535:LEU:CD2	1:A:1027:VAL:HG11	2.50	0.41
1:A:166:ILE:HD11	1:A:310:LEU:CD1	2.45	0.41
1:A:991:ILE:N	1:A:991:ILE:HD12	2.35	0.41
1:A:183:ALA:HB2	1:A:273:GLU:HG2	2.03	0.41
1:A:887:CYS:O	1:A:890:ALA:HB3	2.20	0.41
1:A:158:VAL:CG2	1:A:177:LEU:HD11	2.51	0.41
1:A:154:ILE:O	1:A:158:VAL:HG13	2.20	0.41
1:A:741:VAL:CG2	1:A:746:ILE:HD11	2.51	0.41
1:A:142:VAL:HG13	1:A:321:LEU:HD13	2.03	0.41
1:A:872:GLN:O	1:A:874:PRO:HD2	2.20	0.41
1:A:176:GLN:NE2	1:A:620:ARG:NH2	2.69	0.41
1:A:580:ALA:HB3	1:A:724:THR:HG22	2.01	0.41
1:A:452:VAL:HA	1:A:880:SER:OG	2.20	0.41
1:A:452:VAL:HG12	1:A:884:VAL:HG21	2.02	0.41
1:A:1013:THR:OG1	1:A:1014:ALA:N	2.54	0.41
1:A:15:ILE:HD12	1:A:487:ILE:HD13	2.03	0.41
1:A:56:THR:O	1:A:60:THR:CG2	2.69	0.41
1:A:871:ASN:O	1:A:872:GLN:NE2	2.54	0.41
1:A:112:GLN:C	1:A:114:ALA:N	2.74	0.40
1:A:163:LYS:HD3	1:A:177:LEU:HD13	2.03	0.40
1:A:176:GLN:NE2	1:A:620:ARG:HH22	2.19	0.40
1:A:983:ILE:HG23	1:A:1008:MET:HG3	2.02	0.40
1:A:69:MET:HE1	1:A:111:LEU:N	2.37	0.40
1:A:21:LEU:O	1:A:25:LEU:HD13	2.20	0.40
1:A:38:ILE:HG12	1:A:465:ALA:CB	2.49	0.40
1:A:462:SER:HB3	1:A:865:GLN:HE22	1.84	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ILE:O	1:A:491:ALA:HB2	2.21	0.40
1:A:539:GLY:O	1:A:540:ARG:C	2.56	0.40
1:A:872:GLN:O	1:A:874:PRO:CD	2.68	0.40
1:A:921:LEU:CD2	1:A:1005:THR:OG1	2.69	0.40
1:A:631:LEU:HD13	1:A:637:ARG:CZ	2.51	0.40
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.57	0.40
1:A:873:ALA:O	1:A:876:LEU:HB2	2.22	0.40
1:A:41:PRO:HD2	1:A:94:PHE:O	2.22	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	1043/1049 (99%)	870 (83%)	143 (14%)	30 (3%)	4	29

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	300	LEU
1	A	459	PHE
1	A	579	PRO
1	A	618	ALA
1	A	620	ARG
1	A	669	PRO
1	A	671	ILE
1	A	867	ARG
1	A	1034	SER
1	A	1043	SER
1	A	538	THR
1	A	672	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	299	ALA
1	A	301	ASP
1	A	439	GLN
1	A	634	TRP
1	A	678	THR
1	A	713	LEU
1	A	992	SER
1	A	995	ALA
1	A	84	SER
1	A	330	THR
1	A	308	ALA
1	A	994	GLY
1	A	2	PRO
1	A	113	LEU
1	A	957	GLY
1	A	460	GLY
1	A	1040	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	851/855 (100%)	783 (92%)	68 (8%)	12 41

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	TYR
1	A	53	ASP
1	A	60	THR
1	A	62	THR
1	A	83	ASP
1	A	85	THR
1	A	93	THR
1	A	145	THR
1	A	158	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	164	ASP
1	A	167	SER
1	A	194	ASN
1	A	199	THR
1	A	250	LEU
1	A	262	LEU
1	A	270	LEU
1	A	274	ASN
1	A	300	LEU
1	A	319	SER
1	A	321	LEU
1	A	339	GLU
1	A	348	ILE
1	A	359	LEU
1	A	362	PHE
1	A	376	LEU
1	A	379	THR
1	A	405	LEU
1	A	414	GLU
1	A	425	LEU
1	A	445	ILE
1	A	452	VAL
1	A	495	THR
1	A	538	THR
1	A	542	LEU
1	A	626	ILE
1	A	649	MET
1	A	660	ASP
1	A	671	ILE
1	A	673	GLU
1	A	683	GLU
1	A	687	GLN
1	A	695	LEU
1	A	716	VAL
1	A	722	GLU
1	A	801	PHE
1	A	805	SER
1	A	828	LEU
1	A	830	GLN
1	A	853	THR
1	A	867	ARG
1	A	872	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	880	SER
1	A	887	CYS
1	A	904	VAL
1	A	917	THR
1	A	919	ARG
1	A	934	THR
1	A	935	ILE
1	A	946	VAL
1	A	962	GLU
1	A	971	ARG
1	A	980	LEU
1	A	1017	LEU
1	A	1030	ARG
1	A	1036	LYS
1	A	1038	GLU
1	A	1040	ILE
1	A	1041	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	161	ASN
1	A	210	GLN
1	A	213	GLN
1	A	254	ASN
1	A	298	ASN
1	A	613	ASN
1	A	687	GLN
1	A	733	GLN
1	A	830	GLN
1	A	872	GLN
1	A	1042	HIS

5.3.3 RNA ⓘ

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1045/1049 (99%)	-0.02	37 (3%) 44 44	25, 52, 84, 110	19 (1%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	PRO	6.5
1	A	866	GLU	5.7
1	A	715	SER	4.6
1	A	436	GLY	4.0
1	A	870	GLY	3.9
1	A	1033	PHE	3.8
1	A	1044	HIS	3.7
1	A	255	GLN	3.5
1	A	459	PHE	3.4
1	A	1045	THR	3.3
1	A	461	GLY	3.3
1	A	871	ASN	3.2
1	A	833	PRO	3.0
1	A	8	ARG	3.0
1	A	1043	SER	3.0
1	A	70	ASN	3.0
1	A	1042	HIS	2.8
1	A	714	THR	2.8
1	A	1034	SER	2.8
1	A	660	ASP	2.8
1	A	679	GLY	2.8
1	A	867	ARG	2.7
1	A	460	GLY	2.7
1	A	439	GLN	2.6
1	A	505	HIS	2.6
1	A	1037	ASN	2.5
1	A	305	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	362	PHE	2.4
1	A	489	THR	2.3
1	A	4	PHE	2.3
1	A	425	LEU	2.3
1	A	508	GLY	2.2
1	A	511	GLY	2.1
1	A	509	LYS	2.1
1	A	627	ALA	2.1
1	A	388	PHE	2.0
1	A	830	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(\AA^2)	Q<0.9
2	NI	A	1201	1/1	0.99	0.22	24,24,24,24	1

6.5 Other polymers [i](#)

There are no such residues in this entry.