



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:36 am GMT

PDB ID : 1PWW
Title : Crystal structure of Anthrax Lethal Factor active site mutant protein complexed with an optimised peptide substrate in the presence of zinc.
Authors : Wong, T.Y.; Schwarzenbacher, R.; Liddington, R.C.
Deposited on : 2003-07-02
Resolution : 2.80 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

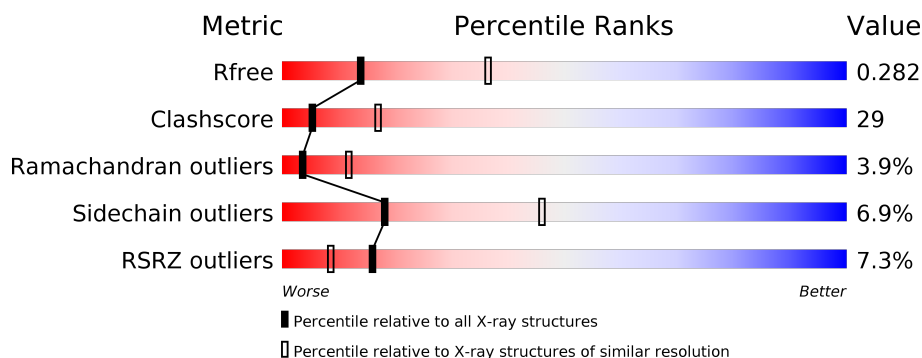
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	776	<div> <div>6%</div> <div>43%</div> <div>44%</div> <div>6%</div> <div>6%</div> </div>
1	B	776	<div> <div>6%</div> <div>48%</div> <div>42%</div> <div>•</div> <div>5%</div> </div>
2	C	20	<div> <div>35%</div> <div>15%</div> <div>15%</div> <div>20%</div> <div>5%</div> <div>45%</div> </div>
2	D	20	<div> <div>40%</div> <div>5%</div> <div>30%</div> <div>10%</div> <div>10%</div> <div>45%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12185 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 Lethal factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5965	3796	1002	1159	8			
1	B	734	Total	C	N	O	S	0	0	0
			6030	3833	1017	1172	8			

There are 2 discrepancies between the modelled and reference sequences:

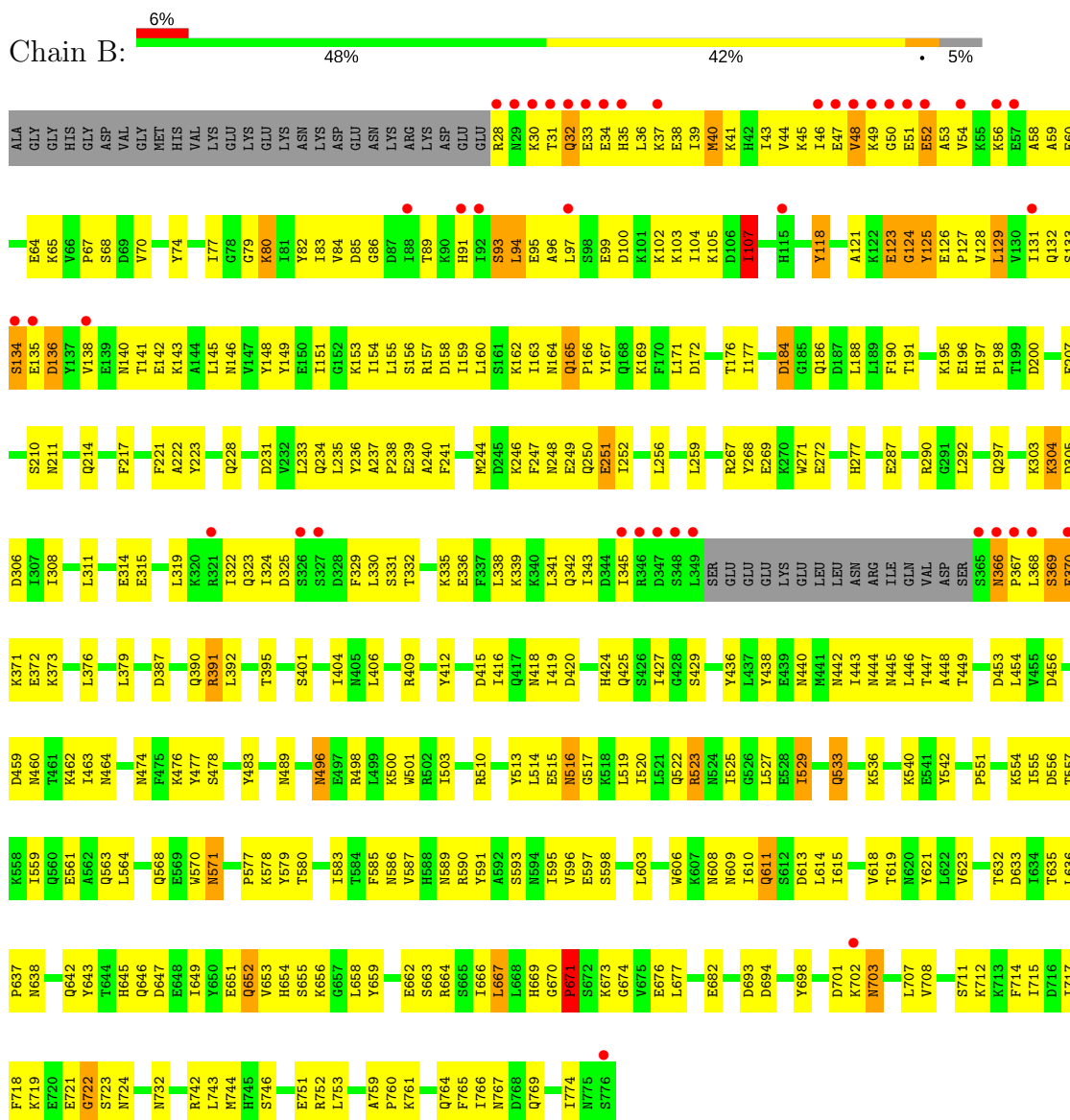
Chain	Residue	Modelled	Actual	Comment	Reference
A	687	CYS	GLU	engineered	UNP P15917
B	687	CYS	GLU	engineered	UNP P15917

- Molecule 2 is a protein called LF20.

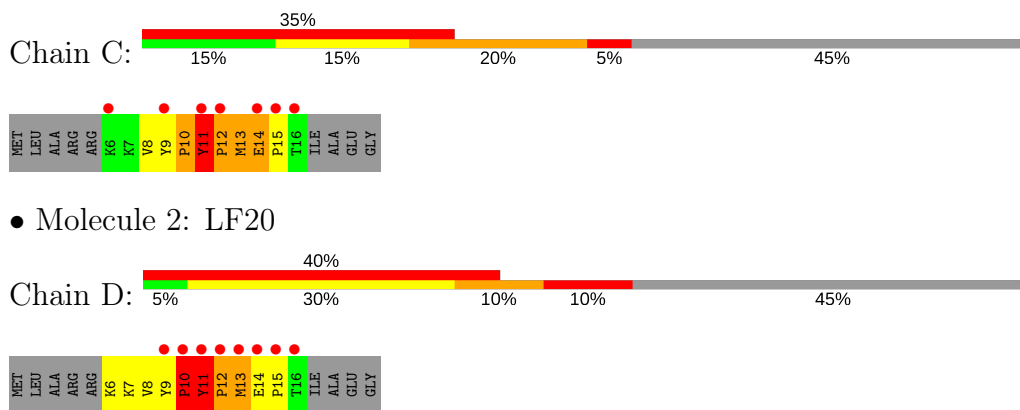
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	S	0	0	0
			94	64	13	16	1			
2	D	11	Total	C	N	O	S	0	0	0
			94	64	13	16	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

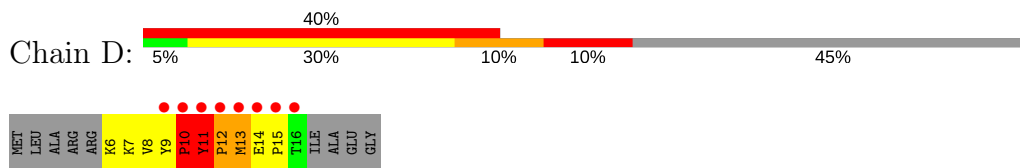
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		



- Molecule 2: LF20



- Molecule 2: LF20



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.70Å 137.40Å 98.30Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	22.69 – 2.80 46.05 – 2.80	Depositor EDS
% Data completeness (in resolution range)	81.7 (22.69-2.80) 81.6 (46.05-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.288 0.237 , 0.282	Depositor DCC
R_{free} test set	2583 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12185	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: ZN

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	0/6072	0.65	0/8178
1	B	0.42	0/6138	0.66	1/8267 (0.0%)
2	C	0.69	0/98	1.01	0/133
2	D	0.44	0/98	1.08	1/133 (0.8%)
All	All	0.41	0/12406	0.66	2/16711 (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	B	671	PRO	CA-N-CD	-10.49	96.81	111.50
2	D	10	PRO	CA-N-CD	-7.20	101.42	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5965	0	5957	368	0
1	B	6030	0	6021	332	0
2	C	94	0	95	23	0
2	D	94	0	95	23	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
All	All	12185	0	12168	706	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 (706) 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:653:VAL:HG11	2:D:10:PRO:HG3	1.34	1.06
1:B:551:PRO:HD2	1:B:554:LYS:HE2	1.36	1.05
1:B:319:LEU:HD23	1:B:345:ILE:HD12	1.39	1.05
1:B:366:ASN:HB3	1:B:367:PRO:HD3	1.38	1.01
1:A:563:GLN:NE2	1:A:585:PHE:H	1.57	1.00
1:A:602:ILE:HD11	1:A:680:ASP:HB3	1.45	0.99
1:B:677:LEU:HD11	2:D:11:TYR:CZ	2.01	0.96
1:A:268:TYR:HB3	1:B:125:TYR:CE2	2.00	0.95
1:B:510:ARG:H	1:B:522:GLN:HE21	0.94	0.92
1:B:496:ASN:H	1:B:496:ASN:HD22	1.13	0.92
2:D:7:LYS:HG2	2:D:8:VAL:H	1.35	0.91
1:B:516:ASN:HD22	1:B:516:ASN:H	1.09	0.90
1:B:510:ARG:H	1:B:522:GLN:NE2	1.70	0.89
1:A:316:LYS:HE3	1:A:345:ILE:HG21	1.55	0.89
1:B:366:ASN:HB3	1:B:367:PRO:CD	2.03	0.89
1:B:176:THR:HG21	1:B:239:GLU:HG3	1.54	0.88
1:B:658:LEU:HD11	2:D:8:VAL:HG12	1.52	0.88
1:B:677:LEU:HD21	2:D:11:TYR:OH	1.73	0.87
1:B:94:LEU:HB3	1:B:97:LEU:HD12	1.56	0.86
1:A:119:VAL:HG21	1:A:147:VAL:HG22	1.56	0.85
1:B:99:GLU:HG3	1:B:100:ASP:H	1.40	0.85
1:B:85:ASP:HB3	1:B:133:SER:OG	1.77	0.84
1:A:176:THR:HG21	1:A:239:GLU:HG3	1.59	0.84
1:A:92:ILE:HD12	1:A:92:ILE:H	1.42	0.83
1:A:714:PHE:HA	1:A:717:ILE:HD13	1.59	0.83
1:B:424:HIS:HA	1:B:510:ARG:HD2	1.59	0.83
1:B:658:LEU:HD11	2:D:8:VAL:CG1	2.08	0.82
1:A:48:VAL:HG11	1:A:55:LYS:HG2	1.61	0.82
1:A:69:ASP:O	1:A:73:MET:HG3	1.80	0.82
1:B:571:ASN:HD21	1:B:580:THR:HB	1.44	0.82
1:B:510:ARG:N	1:B:522:GLN:HE21	1.75	0.82
1:A:435:ILE:H	1:A:435:ILE:HD12	1.45	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:ASN:ND2	1:B:516:ASN:H	1.78	0.82
1:B:585:PHE:CE1	1:B:596:VAL:HG13	2.16	0.81
1:A:308:ILE:HG23	1:A:316:LYS:HE2	1.60	0.80
1:A:771:LYS:HD2	1:A:775:ASN:HD21	1.46	0.80
1:A:314:GLU:O	1:A:318:LEU:HG	1.82	0.79
1:B:516:ASN:HD22	1:B:516:ASN:N	1.71	0.79
1:A:602:ILE:CD1	1:A:680:ASP:HB3	2.12	0.79
1:B:498:ARG:HH21	1:B:540:LYS:HE2	1.48	0.78
1:A:577:PRO:O	1:A:580:THR:HG23	1.83	0.78
1:A:496:ASN:C	1:A:496:ASN:HD22	1.88	0.77
1:B:36:LEU:O	1:B:40:MET:HG2	1.85	0.77
1:A:501:TRP:HB3	1:A:503:ILE:HD11	1.67	0.76
1:A:104:ILE:HG22	1:A:105:LYS:H	1.50	0.76
1:A:435:ILE:HD12	1:A:435:ILE:N	2.01	0.76
1:A:563:GLN:HE21	1:A:585:PHE:H	1.31	0.76
1:B:496:ASN:N	1:B:496:ASN:HD22	1.82	0.76
1:A:233:LEU:HD13	1:A:241:PHE:HB2	1.67	0.76
1:A:636:LEU:HA	1:A:639:ILE:HD13	1.68	0.75
1:B:551:PRO:HD2	1:B:554:LYS:CE	2.15	0.75
1:B:70:VAL:HG13	1:B:155:LEU:HD13	1.68	0.75
1:B:711:SER:O	1:B:715:ILE:HG13	1.86	0.75
1:A:563:GLN:NE2	1:A:584:THR:HA	2.02	0.75
1:A:268:TYR:HB3	1:B:125:TYR:HE2	1.53	0.74
1:B:37:LYS:O	1:B:41:LYS:HG3	1.87	0.74
1:A:566:ILE:HG13	1:A:600:TYR:CE2	2.23	0.74
1:A:581:LYS:HD3	1:A:628:ARG:HH21	1.51	0.74
1:A:648:GLU:HB2	1:A:651:GLU:HG3	1.68	0.74
1:B:387:ASP:HB3	1:B:390:GLN:HB3	1.70	0.74
1:A:113:LEU:HD12	1:A:116:GLU:OE2	1.88	0.73
1:B:156:SER:HB3	1:B:217:PHE:CD2	2.23	0.73
1:A:56:LYS:O	1:A:60:GLU:HG3	1.88	0.73
1:B:49:LYS:HG2	1:B:85:ASP:OD1	1.88	0.73
1:A:449:THR:HA	1:A:673:LYS:HD3	1.70	0.73
1:B:95:GLU:HG3	1:B:96:ALA:H	1.54	0.72
1:B:401:SER:CB	1:B:638:ASN:HD22	2.02	0.72
1:B:77:ILE:HD11	1:B:259:LEU:HD11	1.72	0.72
1:A:686:HIS:HB2	1:A:742:ARG:HD3	1.72	0.72
2:D:7:LYS:HG2	2:D:8:VAL:N	2.04	0.72
1:A:643:TYR:HA	1:A:646:GLN:HG3	1.72	0.71
1:B:483:TYR:HB3	1:B:520:ILE:HD11	1.70	0.71
1:A:368:LEU:N	1:A:373:LYS:HE2	2.05	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:THR:O	1:B:336:GLU:HG2	1.91	0.71
1:B:330:LEU:HD11	1:B:376:LEU:HD22	1.72	0.71
1:A:192:ASN:HA	1:A:195:LYS:HB2	1.72	0.71
1:B:99:GLU:HG3	1:B:100:ASP:N	2.06	0.70
1:B:46:ILE:HG13	1:B:56:LYS:HD3	1.73	0.70
1:A:125:TYR:CD1	1:B:269:GLU:HG3	2.25	0.70
1:B:446:LEU:HG	1:B:591:TYR:HB2	1.73	0.70
1:B:571:ASN:ND2	1:B:580:THR:HB	2.06	0.70
1:A:182:ASP:OD2	1:A:184:ASP:HB2	1.92	0.70
1:A:439:GLU:HB2	1:A:486:VAL:HG12	1.72	0.70
1:B:645:HIS:CD2	1:B:663:SER:HB3	2.27	0.70
1:A:123:GLU:HG2	1:A:124:GLY:H	1.56	0.70
1:B:211:ASN:HA	1:B:214:GLN:HE21	1.55	0.69
1:B:366:ASN:CB	1:B:367:PRO:CD	2.70	0.69
1:B:308:ILE:HG23	1:B:345:ILE:HD11	1.75	0.69
1:B:32:GLN:O	1:B:35:HIS:HB3	1.93	0.69
1:B:501:TRP:HB3	1:B:503:ILE:HD11	1.75	0.69
1:B:60:GLU:O	1:B:64:GLU:HG3	1.92	0.69
1:B:107:ILE:HG21	1:B:145:LEU:CD1	2.23	0.68
1:A:707:LEU:HD11	2:C:9:TYR:OH	1.93	0.68
1:B:330:LEU:HB2	1:B:335:LYS:NZ	2.08	0.68
1:B:693:ASP:OD2	1:B:708:VAL:HG12	1.93	0.68
1:A:440:ASN:ND2	1:A:500:LYS:NZ	2.42	0.68
1:B:658:LEU:CD1	2:D:8:VAL:HG12	2.24	0.68
1:A:102:LYS:HA	1:A:114:LEU:HD12	1.74	0.68
1:A:336:GLU:HG3	1:A:340:LYS:HE3	1.74	0.68
1:B:125:TYR:CE2	1:B:162:LYS:HE3	2.29	0.68
1:B:474:ASN:HB3	1:B:597:GLU:HG3	1.76	0.68
1:A:770:ILE:O	1:A:774:ILE:HG12	1.94	0.67
1:A:49:LYS:HD2	1:A:50:GLY:N	2.10	0.67
1:B:449:THR:HA	1:B:673:LYS:HD2	1.76	0.67
1:A:563:GLN:NE2	1:A:585:PHE:N	2.39	0.67
1:A:674:GLY:HA2	2:C:13:MET:HA	1.76	0.67
1:A:31:THR:HG23	1:A:34:GLU:HG2	1.76	0.67
1:A:57:GLU:HA	1:A:60:GLU:OE2	1.95	0.67
1:B:95:GLU:HG3	1:B:96:ALA:N	2.10	0.66
1:A:753:LEU:O	1:A:757:LYS:HG2	1.95	0.66
1:B:84:VAL:O	1:B:132:GLN:HA	1.94	0.66
1:B:611:GLN:NE2	1:B:614:LEU:H	1.92	0.66
1:A:87:ASP:O	1:A:90:LYS:HB3	1.95	0.66
1:B:446:LEU:O	1:B:671:PRO:HG3	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLU:N	1:A:204:GLU:OE1	2.27	0.66
1:A:379:LEU:O	1:A:383:ILE:HG12	1.96	0.66
1:B:707:LEU:HD11	2:D:9:TYR:CZ	2.31	0.66
1:A:741:PHE:O	1:A:745:HIS:HD2	1.78	0.65
1:A:713:LYS:HE2	1:A:761:LYS:HE2	1.78	0.65
1:A:67:PRO:O	1:A:70:VAL:HG13	1.95	0.65
1:A:94:LEU:HD11	1:A:130:VAL:HG21	1.77	0.65
1:A:272:GLU:HG3	1:B:125:TYR:CD1	2.31	0.65
1:B:707:LEU:HD11	2:D:9:TYR:OH	1.96	0.65
1:B:401:SER:HB3	1:B:638:ASN:HD22	1.62	0.65
1:B:45:LYS:HB2	1:B:82:TYR:HD2	1.62	0.65
1:B:442:ASN:O	1:B:445:ASN:HB2	1.96	0.65
1:B:662:GLU:H	1:B:662:GLU:CD	2.01	0.64
1:B:611:GLN:HE22	1:B:613:ASP:HB2	1.62	0.64
1:A:80:LYS:HB3	1:A:82:TYR:HE1	1.62	0.64
1:B:440:ASN:ND2	1:B:500:LYS:HG2	2.12	0.64
1:A:31:THR:O	1:A:34:GLU:HG3	1.98	0.64
1:A:535:ILE:HD13	1:A:544:ARG:HB2	1.80	0.64
1:B:35:HIS:O	1:B:39:ILE:HG12	1.97	0.64
1:A:298:ILE:O	1:A:298:ILE:HD12	1.98	0.64
1:A:563:GLN:HE22	1:A:585:PHE:H	1.42	0.64
1:B:34:GLU:O	1:B:38:GLU:HB2	1.98	0.64
1:B:769:GLN:NE2	1:B:769:GLN:HA	2.13	0.64
1:A:35:HIS:HD2	1:A:39:ILE:HD11	1.63	0.64
1:A:107:ILE:HG13	1:A:145:LEU:CD1	2.28	0.63
1:B:436:TYR:HA	1:B:503:ILE:O	1.99	0.63
1:A:256:LEU:HD22	1:A:260:LYS:HE3	1.81	0.63
1:A:46:ILE:N	1:A:46:ILE:HD12	2.13	0.63
1:A:163:ILE:HG21	1:A:258:GLU:HG2	1.80	0.63
1:A:327:SER:HB2	1:A:329:PHE:CE2	2.33	0.63
1:A:429:SER:OG	1:A:431:LEU:HG	1.98	0.63
1:B:267:ARG:HB3	1:B:489:ASN:ND2	2.12	0.63
1:B:655:SER:HB2	2:D:11:TYR:C	2.19	0.63
1:A:391:ARG:NH1	1:A:404:ILE:HD12	2.14	0.63
1:B:154:ILE:HD13	1:B:158:ASP:OD1	1.98	0.63
1:B:674:GLY:HA3	1:B:677:LEU:HD12	1.81	0.63
1:B:496:ASN:H	1:B:496:ASN:ND2	1.90	0.63
1:A:443:ILE:HD13	1:A:454:LEU:HD22	1.81	0.63
1:A:87:ASP:OD1	1:A:115:HIS:HB2	1.99	0.63
2:C:11:TYR:N	2:C:12:PRO:HD3	2.14	0.62
1:A:748:ASP:OD2	1:A:750:ALA:HB3	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ASN:ND2	1:A:500:LYS:HZ2	1.97	0.62
1:B:246:LYS:HG3	1:B:250:GLN:HE21	1.64	0.62
1:A:163:ILE:CG2	1:A:258:GLU:HG2	2.29	0.62
1:B:330:LEU:HB2	1:B:335:LYS:HZ2	1.63	0.62
1:A:307:ILE:HG21	1:A:341:LEU:HD11	1.80	0.62
1:B:163:ILE:HG13	1:B:165:GLN:HG3	1.81	0.62
1:B:647:ASP:HB2	1:B:651:GLU:OE2	1.99	0.62
1:A:744:MET:O	1:A:752:ARG:HG2	2.01	0.61
1:B:221:PHE:HD1	1:B:244:MET:HE1	1.65	0.61
1:A:176:THR:CG2	1:A:239:GLU:HG3	2.31	0.61
1:B:184:ASP:HB3	1:B:236:TYR:HB3	1.82	0.61
1:A:658:LEU:HD21	2:C:8:VAL:HG12	1.81	0.61
1:A:647:ASP:HB2	1:A:651:GLU:OE1	2.01	0.60
1:B:551:PRO:CD	1:B:554:LYS:HE2	2.22	0.60
1:B:444:ASN:HD22	1:B:448:ALA:HA	1.67	0.60
1:B:308:ILE:HA	1:B:311:LEU:HD12	1.84	0.60
1:B:235:LEU:HD23	1:B:236:TYR:CE2	2.37	0.60
1:A:34:GLU:HG3	1:A:35:HIS:N	2.17	0.60
1:A:677:LEU:HD11	2:C:11:TYR:CE2	2.37	0.60
1:B:319:LEU:HD23	1:B:345:ILE:CD1	2.26	0.60
1:B:415:ASP:O	1:B:419:ILE:HG13	2.02	0.60
2:D:11:TYR:N	2:D:12:PRO:HD3	2.17	0.60
1:A:34:GLU:HG3	1:A:35:HIS:H	1.67	0.59
1:B:188:LEU:HD11	1:B:223:TYR:CE2	2.37	0.59
1:B:442:ASN:ND2	1:B:496:ASN:HB2	2.17	0.59
1:A:415:ASP:O	1:A:419:ILE:HG13	2.02	0.59
1:A:581:LYS:CD	1:A:628:ARG:HH21	2.15	0.59
1:A:123:GLU:HG2	1:A:124:GLY:N	2.18	0.59
1:A:730:ARG:O	1:A:730:ARG:HG2	2.02	0.59
1:B:476:LYS:O	1:B:529:ILE:HB	2.03	0.59
1:A:465:ARG:O	1:A:469:ASN:OD1	2.21	0.59
1:A:759:ALA:N	1:A:760:PRO:HD3	2.16	0.59
1:B:94:LEU:HB3	1:B:97:LEU:CD1	2.31	0.59
1:B:712:LYS:HA	1:B:715:ILE:HD12	1.85	0.59
1:A:154:ILE:HG22	1:A:159:ILE:HD13	1.85	0.58
1:A:584:THR:CG2	1:A:630:VAL:HG22	2.33	0.58
1:B:287:GLU:HA	1:B:290:ARG:NH1	2.18	0.58
1:B:510:ARG:HG3	1:B:510:ARG:HH11	1.68	0.58
1:A:655:SER:HB2	2:C:11:TYR:C	2.23	0.58
1:B:135:GLU:O	1:B:135:GLU:HG3	2.04	0.58
1:B:483:TYR:CB	1:B:520: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:A:410:LYS:HE3	1:A:414:ARG:NH2	2.18	0.58
1:A:277:HIS:CD2	1:A:429:SER:HB2	2.38	0.58
1:B:151:ILE:O	1:B:151:ILE:HG22	2.04	0.58
1:B:160:LEU:HB3	1:B:165:GLN:HB2	1.84	0.58
1:B:176:THR:CG2	1:B:239:GLU:HG3	2.31	0.58
1:B:338:LEU:HD23	1:B:341:LEU:HD12	1.85	0.58
1:A:686:HIS:CD2	1:A:686:HIS:C	2.77	0.58
1:B:564:LEU:O	1:B:568:GLN:HG3	2.04	0.58
1:A:368:LEU:HD13	1:A:372:GLU:CD	2.24	0.57
1:B:513:TYR:HA	1:B:519:LEU:HD23	1.85	0.57
1:B:93:SER:O	1:B:95:GLU:HG2	2.04	0.57
1:B:308:ILE:O	1:B:311:LEU:HB2	2.04	0.57
1:A:256:LEU:CD2	1:A:260:LYS:HE3	2.33	0.57
1:A:612:SER:O	1:A:616:LYS:HG3	2.04	0.57
1:B:391:ARG:O	1:B:391:ARG:HD3	2.05	0.57
1:A:602:ILE:HD11	1:A:680:ASP:CB	2.29	0.57
1:B:292:LEU:HD13	1:B:419:ILE:HG12	1.86	0.57
1:B:80:LYS:HB3	1:B:80:LYS:NZ	2.20	0.57
1:A:97:LEU:HD22	1:A:101:LYS:HD3	1.85	0.57
1:A:487:ASP:OD1	1:A:518:LYS:HG2	2.05	0.57
1:B:682:GLU:HB3	1:B:742:ARG:HD3	1.85	0.57
1:B:774:ILE:O	1:B:774:ILE:HG22	2.05	0.57
1:B:91:HIS:HD2	1:B:93:SER:OG	1.88	0.57
1:A:411:GLN:HE21	1:A:411:GLN:HA	1.70	0.56
1:A:449:THR:HG22	1:A:672:SER:O	2.06	0.56
1:B:420:ASP:OD1	1:B:523:ARG:HD3	2.05	0.56
1:B:395:THR:HG22	1:B:638:ASN:ND2	2.20	0.56
1:A:717:ILE:CG1	1:A:761:LYS:HD2	2.35	0.56
2:D:8:VAL:HG12	2:D:9:TYR:H	1.70	0.56
1:A:322:ILE:HD13	1:A:376:LEU:HD21	1.88	0.56
1:A:90:LYS:HG2	1:A:90:LYS:O	2.05	0.56
1:B:154:ILE:O	1:B:159:ILE:HG12	2.05	0.56
1:B:223:TYR:HB3	1:B:233:LEU:HG	1.87	0.56
1:A:658:LEU:HD11	2:C:8:VAL:HG11	1.87	0.56
1:A:426:SER:HA	1:A:510:ARG:HA	1.87	0.56
1:B:267:ARG:CZ	1:B:489:ASN:HB3	2.36	0.56
1:B:338:LEU:HD22	1:B:379:LEU:HD13	1.86	0.56
1:B:765:PHE:O	1:B:769:GLN:HG2	2.06	0.56
1:B:28:ARG:O	1:B:32:GLN:HB2	2.06	0.56
1:B:67:PRO:HB2	1:B:70:VAL:HG23	1.88	0.56
1:B:759:ALA:N	1:B:760:PRO:HD3	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:11:TYR:H	2:C:12:PRO:HD3	1.70	0.56
1:A:711:SER:O	1:A:715:ILE:HG13	2.06	0.56
1:A:704:GLN:O	1:A:704:GLN:HG3	2.06	0.55
1:A:92:ILE:H	1:A:92:ILE:CD1	2.15	0.55
1:A:80:LYS:HB3	1:A:82:TYR:CE1	2.42	0.55
1:B:118:TYR:CD1	1:B:118:TYR:N	2.75	0.55
1:B:401:SER:CB	1:B:638:ASN:ND2	2.70	0.55
1:B:401:SER:HB2	1:B:638:ASN:ND2	2.22	0.55
1:B:339:LYS:O	1:B:343:ILE:HG12	2.06	0.55
1:B:769:GLN:HA	1:B:769:GLN:HE21	1.72	0.55
1:A:693:ASP:OD1	1:A:709:THR:HB	2.06	0.54
1:A:159:ILE:N	1:A:159:ILE:HD12	2.22	0.54
1:A:176:THR:O	1:A:180:ALA:HB2	2.07	0.54
1:A:296:LEU:O	1:A:296:LEU:HD13	2.06	0.54
1:A:316:LYS:HZ1	1:A:345:ILE:HB	1.72	0.54
1:A:581:LYS:HD3	1:A:628:ARG:NH2	2.19	0.54
1:B:391:ARG:HD3	1:B:391:ARG:C	2.26	0.54
1:A:308:ILE:HD11	1:A:341:LEU:HD22	1.89	0.54
1:B:244:MET:HE3	1:B:248:ASN:ND2	2.22	0.54
1:B:31:THR:O	1:B:34:GLU:HB3	2.07	0.54
1:B:46:ILE:HD13	1:B:83:ILE:HB	1.90	0.54
1:A:171:LEU:HD21	1:A:206:LEU:HB2	1.88	0.54
1:A:392:LEU:HD21	1:A:416:ILE:HD13	1.90	0.54
1:A:691:ALA:O	1:A:694:ASP:HB3	2.08	0.54
1:A:727:SER:O	1:A:730:ARG:HB3	2.08	0.54
1:B:235:LEU:HD23	1:B:236:TYR:CZ	2.42	0.54
1:B:743:LEU:HD22	1:B:751:GLU:OE1	2.08	0.54
1:A:119:VAL:CG2	1:A:147:VAL:HG22	2.31	0.54
1:B:324:ILE:HD13	1:B:338:LEU:HB2	1.89	0.54
1:A:443:ILE:CD1	1:A:454:LEU:HD22	2.37	0.54
1:B:420:ASP:OD2	1:B:523:ARG:NH1	2.41	0.54
1:A:658:LEU:CD2	2:C:8:VAL:HG12	2.37	0.54
1:B:557:THR:O	1:B:561:GLU:HG3	2.08	0.54
1:A:323:GLN:O	1:A:326:SER:N	2.34	0.54
1:A:717:ILE:HG13	1:A:761:LYS:HD2	1.90	0.54
1:A:111:ASP:OD2	1:A:111:ASP:N	2.38	0.53
1:A:178:LYS:HG3	1:A:179:ASN:N	2.22	0.53
1:A:295:LYS:C	1:A:297:GLN:H	2.11	0.53
1:B:237:ALA:N	1:B:238:PRO:HD3	2.23	0.53
1:B:104:ILE:HG13	1:B:105:LYS:N	2.22	0.53
1:B:404:ILE:HD11	1:B:409:ARG:HA	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:TRP:CZ2	1:B:615:ILE:HG23	2.44	0.53
1:A:226:GLU:OE1	1:A:229:HIS:ND1	2.32	0.53
1:B:676:GLU:O	1:B:677:LEU:HG	2.08	0.53
1:A:446:LEU:HG	1:A:591:TYR:HB2	1.90	0.53
1:B:477:TYR:HE1	1:B:559:ILE:HD11	1.74	0.53
1:A:343:ILE:HG23	1:A:344:ASP:N	2.24	0.53
1:A:515:GLU:HB2	1:B:207:GLU:OE1	2.09	0.53
1:A:496:ASN:C	1:A:496:ASN:ND2	2.59	0.53
1:A:563:GLN:HE21	1:A:585:PHE:N	2.04	0.53
1:A:102:LYS:O	1:A:114:LEU:HB2	2.09	0.53
1:A:118:TYR:OH	1:A:143:LYS:HA	2.09	0.53
2:D:7:LYS:CG	2:D:8:VAL:H	2.15	0.53
1:B:191:THR:O	1:B:195:LYS:HG3	2.09	0.53
1:A:100:ASP:C	1:A:102:LYS:H	2.11	0.52
1:A:40:MET:O	1:A:44:VAL:HB	2.08	0.52
1:B:311:LEU:HD22	1:B:315:GLU:HB3	1.90	0.52
1:B:606:TRP:CE2	1:B:615:ILE:HD12	2.44	0.52
1:A:290:ARG:O	1:A:294:LYS:HB2	2.09	0.52
1:A:90:LYS:CG	1:A:90:LYS:O	2.58	0.52
1:B:91:HIS:CD2	1:B:93:SER:H	2.27	0.52
1:A:707:LEU:HD11	2:C:9:TYR:CZ	2.44	0.52
1:A:315:GLU:HB3	1:A:375:PHE:CE1	2.45	0.52
1:A:274:ILE:HD12	1:A:488:ILE:HG23	1.91	0.52
1:B:608:ASN:C	1:B:609:ASN:HD22	2.12	0.52
1:B:721:GLU:HA	1:B:724:ASN:OD1	2.10	0.52
1:A:31:THR:HG23	1:A:34:GLU:CG	2.39	0.52
1:A:501:TRP:HB3	1:A:503:ILE:CD1	2.39	0.52
1:A:761:LYS:HD3	1:A:761:LYS:O	2.10	0.52
1:B:210:SER:O	1:B:214:GLN:HG3	2.10	0.52
1:B:304:LYS:HG2	1:B:305:ASP:N	2.24	0.52
1:A:319:LEU:C	1:A:322:ILE:HG22	2.30	0.52
1:A:679:ASN:ND2	1:A:682:GLU:H	2.08	0.52
1:B:324:ILE:HD13	1:B:338:LEU:CB	2.40	0.52
1:B:51:GLU:C	1:B:53:ALA:H	2.13	0.52
1:A:235:LEU:HD23	1:A:236:TYR:CE2	2.45	0.52
1:A:639:ILE:N	1:A:639:ILE:HD12	2.25	0.52
1:B:93:SER:O	1:B:95:GLU:N	2.43	0.52
1:B:121:ALA:HB1	1:B:154:ILE:HD11	1.93	0.51
1:A:656:LYS:HE3	1:A:680:ASP:OD2	2.10	0.51
1:A:36:LEU:O	1:A:40:MET:HG3	2.10	0.51
1:B:460:ASN:O	1:B:498:ARG:NH2	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:TYR:H	1:B:593:SER:HB3	1.75	0.51
1:A:567:ASN:HD21	1:A:583:ILE:H	1.59	0.51
1:A:132:GLN:HG2	1:A:133:SER:H	1.75	0.51
1:A:380:LYS:O	1:A:384:GLN:HG2	2.11	0.51
1:A:411:GLN:NE2	1:A:411:GLN:HA	2.24	0.51
1:B:319:LEU:CD2	1:B:345:ILE:HD12	2.26	0.51
1:B:701:ASP:C	1:B:703:ASN:H	2.13	0.51
1:A:419:ILE:O	1:A:423:LEU:HG	2.11	0.51
1:A:118:TYR:CD2	1:A:119:VAL:HG23	2.45	0.51
1:A:754:LYS:O	1:A:758:ASN:HB2	2.11	0.51
1:B:40:MET:HA	1:B:44:VAL:HG23	1.91	0.51
1:A:772:PHE:CD2	1:A:772:PHE:C	2.84	0.51
1:A:94:LEU:CD1	1:A:130:VAL:HG21	2.39	0.51
1:B:586:ASN:HB3	1:B:632:THR:HB	1.93	0.51
1:A:270:LYS:O	1:A:274:ILE:HG13	2.11	0.51
1:A:61:LYS:HA	1:A:64:GLU:OE2	2.10	0.51
1:B:65:LYS:HB2	1:B:148:TYR:OH	2.11	0.51
1:B:247:PHE:CE2	1:B:252:ILE:HD13	2.46	0.51
1:B:610:ILE:HB	1:B:615:ILE:HD11	1.93	0.51
1:B:715:ILE:O	1:B:719:LYS:HG2	2.11	0.51
1:A:226:GLU:OE1	1:A:228:GLN:HB2	2.11	0.50
1:A:244:MET:HE3	1:A:244:MET:HA	1.92	0.50
1:A:496:ASN:ND2	1:A:497:GLU:HG3	2.25	0.50
1:A:679:ASN:HD21	1:A:682:GLU:HG3	1.76	0.50
1:B:635:THR:HB	1:B:637:PRO:HD2	1.93	0.50
1:A:372:GLU:O	1:A:375:PHE:HB3	2.11	0.50
1:A:39:ILE:O	1:A:43:ILE:HG12	2.10	0.50
1:A:655:SER:HB2	2:C:11:TYR:O	2.11	0.50
1:A:76:ALA:O	1:A:263:ARG:NH1	2.44	0.50
1:B:653:VAL:CG1	2:D:10:PRO:HG3	2.24	0.50
1:A:274:ILE:HD12	1:A:488:ILE:CG2	2.42	0.50
1:A:467:ILE:HD12	1:A:467:ILE:N	2.26	0.50
1:A:674:GLY:O	1:A:676:GLU:N	2.45	0.50
1:B:103:LYS:O	1:B:103:LYS:HG3	2.11	0.50
1:B:140:ASN:OD1	1:B:143:LYS:HB2	2.11	0.50
1:B:244:MET:CE	1:B:248:ASN:HD21	2.25	0.50
1:A:141:THR:HG21	1:A:228:GLN:HG3	1.92	0.50
1:A:139:GLU:O	1:A:141:THR:N	2.43	0.50
1:B:303:LYS:HB3	1:B:306:ASP:OD2	2.11	0.50
1:B:97:LEU:O	1:B:102:LYS:HE3	2.12	0.50
1:B:169:LYS:O	1:B:172:ASP:HB2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ASP:OD2	1:A:458:THR:N	2.41	0.50
1:A:94:LEU:O	1:A:96:ALA:N	2.45	0.50
1:A:125:TYR:HA	1:B:268:TYR:CE2	2.47	0.50
1:A:43:ILE:HG13	1:A:44:VAL:N	2.27	0.50
1:A:316:LYS:HZ3	1:A:319:LEU:HD23	1.76	0.50
1:A:772:PHE:HD2	1:A:772:PHE:C	2.15	0.50
1:B:677:LEU:HD11	2:D:11:TYR:CE1	2.45	0.50
1:A:140:ASN:HD22	1:A:143:LYS:NZ	2.08	0.50
1:A:31:THR:HA	1:A:34:GLU:HG2	1.94	0.50
1:A:771:LYS:HD2	1:A:775:ASN:ND2	2.22	0.50
1:A:440:ASN:HD21	1:A:500:LYS:NZ	2.10	0.49
1:A:678:ARG:HH11	1:A:678:ARG:HG3	1.76	0.49
1:A:690:HIS:CE1	2:C:9:TYR:HB3	2.46	0.49
1:A:706:ASP:OD1	1:A:707:LEU:N	2.45	0.49
1:A:129:LEU:HD13	1:A:154:ILE:HD11	1.93	0.49
1:A:223:TYR:CD2	1:A:229:HIS:HB3	2.48	0.49
1:A:49:LYS:CD	1:A:50:GLY:N	2.75	0.49
1:A:165:GLN:HB3	1:A:166:PRO:HA	1.95	0.49
1:B:135:GLU:O	1:B:135:GLU:CG	2.60	0.49
1:B:391:ARG:HG3	1:B:412:TYR:CD1	2.47	0.49
1:A:340:LYS:O	1:A:343:ILE:HG22	2.11	0.49
1:A:221:PHE:CE2	1:A:225:ILE:HG13	2.47	0.49
1:A:389:ASN:OD1	1:A:482:ASN:HB2	2.11	0.49
1:B:125:TYR:CZ	1:B:162:LYS:HE3	2.47	0.49
1:B:440:ASN:HD21	1:B:500:LYS:NZ	2.11	0.49
1:A:440:ASN:ND2	1:A:500:LYS:HZ1	2.11	0.49
1:B:323:GLN:HE21	1:B:325:ASP:HB2	1.77	0.49
1:A:173:VAL:HG21	1:A:243:TYR:CD2	2.47	0.49
1:A:658:LEU:HD23	2:C:10:PRO:HA	1.93	0.49
1:A:679:ASN:HD22	1:A:679:ASN:C	2.15	0.49
1:B:167:TYR:O	1:B:171:LEU:HG	2.13	0.49
1:A:103:LYS:O	1:A:103:LYS:HD3	2.13	0.48
1:A:410:LYS:HE3	1:A:414:ARG:HH21	1.76	0.48
1:B:444:ASN:ND2	1:B:448:ALA:HA	2.27	0.48
1:B:54:VAL:O	1:B:58:ALA:HB2	2.12	0.48
1:A:308:ILE:CD1	1:A:341:LEU:HD22	2.42	0.48
2:C:9:TYR:HA	2:C:10:PRO:HD3	1.64	0.48
1:A:33:GLU:O	1:A:37:LYS:HG3	2.12	0.48
1:A:51:GLU:C	1:A:53:ALA:H	2.16	0.48
1:A:739:GLU:OE1	1:A:739:GLU:HA	2.13	0.48
1:A:766:ILE:O	1:A:770:ILE:HG13	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ARG:HA	1:B:214:GLN:OE1	2.11	0.48
1:A:113:LEU:O	1:A:116:GLU:HB2	2.14	0.48
1:A:412:TYR:O	1:A:416:ILE:HG13	2.14	0.48
1:A:479:ILE:O	1:A:590:ARG:HD2	2.13	0.48
1:B:136:ASP:HB3	1:B:140:ASN:HD22	1.79	0.48
1:B:570:TRP:CZ2	1:B:603:LEU:HB3	2.48	0.48
1:A:316:LYS:HE3	1:A:345:ILE:CG2	2.35	0.48
1:A:368:LEU:HD13	1:A:372:GLU:HB3	1.95	0.48
1:A:46:ILE:H	1:A:46:ILE:HD12	1.79	0.48
1:A:745:HIS:N	1:A:745:HIS:CD2	2.82	0.48
1:B:34:GLU:O	1:B:38:GLU:CB	2.62	0.48
1:B:45:LYS:HB2	1:B:82:TYR:CD2	2.46	0.48
1:B:477:TYR:CD1	1:B:555:ILE:HG23	2.49	0.48
1:A:83:ILE:HG22	1:A:83:ILE:O	2.13	0.48
1:A:322:ILE:HG13	1:A:368:LEU:HD12	1.94	0.48
1:A:658:LEU:HD21	2:C:8:VAL:CG1	2.43	0.48
1:B:438:TYR:CD1	1:B:438:TYR:N	2.81	0.48
1:B:392:LEU:HD21	1:B:416:ILE:HD13	1.95	0.48
1:A:119:VAL:HG12	1:A:120:TYR:N	2.29	0.47
1:A:567:ASN:ND2	1:A:582:LEU:H	2.12	0.47
1:B:444:ASN:HA	1:B:448:ALA:HA	1.95	0.47
1:B:677:LEU:HD11	2:D:11:TYR:CE2	2.47	0.47
1:A:100:ASP:O	1:A:102:LYS:N	2.47	0.47
1:A:330:LEU:HD13	1:A:338:LEU:CD1	2.44	0.47
1:A:715:ILE:O	1:A:719:LYS:HD3	2.14	0.47
1:B:636:LEU:HD12	1:B:636:LEU:N	2.29	0.47
2:D:8:VAL:HG12	2:D:9:TYR:N	2.29	0.47
1:A:456:ASP:C	1:A:456:ASP:OD2	2.52	0.47
2:D:11:TYR:H	2:D:12:PRO:HD3	1.78	0.47
1:A:733:GLU:N	1:A:733:GLU:CD	2.67	0.47
1:B:165:GLN:HB3	1:B:166:PRO:HA	1.97	0.47
1:B:249:GLU:O	1:B:250:GLN:HG2	2.14	0.47
1:B:613:ASP:HB2	1:B:774:ILE:HG23	1.97	0.47
1:A:399:ILE:HD12	1:A:413:LYS:HG3	1.97	0.47
1:B:556:ASP:O	1:B:559:ILE:HB	2.15	0.47
1:B:48:VAL:CG2	1:B:52:GLU:HG2	2.45	0.47
1:B:77:ILE:HD13	1:B:259:LEU:HD21	1.95	0.47
1:A:107:ILE:HG13	1:A:145:LEU:HD11	1.97	0.47
1:A:308:ILE:CG2	1:A:316:LYS:HE2	2.39	0.47
1:B:136:ASP:O	1:B:140:ASN:HB2	2.15	0.47
2:C:11:TYR:N	2:C:12:PRO:CD	2.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:TYR:O	1:A:698:TYR:HB3	2.15	0.47
1:A:104:ILE:HD11	1:A:114:LEU:HG	1.95	0.46
1:A:114:LEU:C	1:A:116:GLU:H	2.18	0.46
1:A:234:GLN:O	1:A:238:PRO:HG3	2.15	0.46
1:A:368:LEU:HB3	1:A:372:GLU:CB	2.46	0.46
1:A:722:GLY:HA2	1:A:736:PHE:CZ	2.49	0.46
1:B:427:ILE:O	1:B:427:ILE:HG13	2.15	0.46
1:A:371:LYS:HG3	1:A:372:GLU:N	2.29	0.46
1:A:615:ILE:O	1:A:619:THR:HG23	2.16	0.46
1:A:717:ILE:HG23	1:A:721:GLU:OE1	2.15	0.46
1:B:231:ASP:O	1:B:235:LEU:HB2	2.15	0.46
1:B:619:THR:O	1:B:623:VAL:HG23	2.15	0.46
1:A:659:TYR:O	2:C:8:VAL:CG1	2.63	0.46
1:A:323:GLN:HB3	1:A:326:SER:OG	2.15	0.46
1:A:92:ILE:HD12	1:A:92:ILE:N	2.20	0.46
1:B:287:GLU:HA	1:B:290:ARG:HH12	1.80	0.46
1:A:677:LEU:O	1:A:679:ASN:N	2.47	0.46
1:A:733:GLU:CD	1:A:733:GLU:H	2.18	0.46
1:B:99:GLU:CG	1:B:100:ASP:H	2.19	0.46
2:C:13:MET:CE	2:C:13:MET:H	2.28	0.46
2:D:13:MET:H	2:D:13:MET:CE	2.28	0.46
1:A:154:ILE:HG22	1:A:159:ILE:CD1	2.46	0.46
1:B:463:ILE:HG22	1:B:464:ASN:O	2.15	0.46
1:B:587:VAL:HG22	1:B:595:ILE:HG21	1.97	0.46
1:A:369:SER:O	1:A:373:LYS:HG2	2.15	0.46
1:A:485:ILE:HG12	1:A:520:ILE:HG12	1.97	0.46
1:A:94:LEU:C	1:A:96:ALA:H	2.19	0.46
1:B:107:ILE:HG12	1:B:149:TYR:CG	2.51	0.46
1:B:714:PHE:HA	1:B:717:ILE:HG13	1.98	0.46
1:B:48:VAL:HB	1:B:85:ASP:OD2	2.15	0.46
1:A:146:ASN:O	1:A:149:TYR:HB3	2.16	0.46
1:A:716:ASP:HA	1:A:719:LYS:HB2	1.97	0.46
1:B:236:TYR:C	1:B:238:PRO:HD3	2.36	0.46
1:B:666:ILE:C	1:B:667:LEU:HD23	2.37	0.46
1:B:93:SER:C	1:B:95:GLU:H	2.19	0.46
1:A:228:GLN:OE1	1:A:228:GLN:HA	2.16	0.45
1:A:505:LEU:HD12	1:A:509:THR:HG21	1.97	0.45
1:A:54:VAL:O	1:A:57:GLU:HB3	2.16	0.45
1:A:264:MET:HE2	1:A:264:MET:HB3	1.67	0.45
1:A:318:LEU:O	1:A:322:ILE:HB	2.15	0.45
1:A:625:GLY:HA3	1:A:664:ARG:HD2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLU:C	1:B:250:GLN:HG2	2.37	0.45
1:B:368:LEU:O	1:B:369:SER:O	2.35	0.45
1:B:46:ILE:HG22	1:B:46:ILE:O	2.16	0.45
1:B:578:LYS:O	1:B:579:TYR:HB2	2.15	0.45
1:B:94:LEU:HD22	1:B:97:LEU:HD11	1.98	0.45
1:A:40:MET:HA	1:A:44:VAL:HG23	1.98	0.45
1:B:129:LEU:HD13	1:B:131:ILE:HD11	1.98	0.45
1:B:297:GLN:NE2	1:B:514:LEU:HD13	2.32	0.45
1:A:118:TYR:CZ	1:A:143:LYS:HG2	2.51	0.45
1:A:319:LEU:O	1:A:322:ILE:HG22	2.17	0.45
1:B:583:ILE:N	1:B:583:ILE:HD12	2.32	0.45
1:B:656:LYS:NZ	1:B:670:GLY:O	2.50	0.45
1:A:275:LYS:NZ	1:A:279:GLN:HE22	2.14	0.45
1:A:62:LEU:HD22	1:A:137:TYR:CD1	2.52	0.45
1:B:319:LEU:HD12	1:B:319:LEU:O	2.17	0.45
1:B:746:SER:O	1:B:752:ARG:NH1	2.49	0.45
1:A:112:ALA:O	1:A:113:LEU:HD23	2.17	0.45
1:A:87:ASP:OD2	1:A:115:HIS:HA	2.17	0.45
1:B:135:GLU:OE1	1:B:138:VAL:HG23	2.17	0.45
1:B:501:TRP:HB3	1:B:503:ILE:CD1	2.46	0.45
1:B:718:PHE:O	1:B:722:GLY:HA3	2.17	0.45
1:B:79:GLY:HA2	1:B:127:PRO:HG2	1.98	0.45
1:A:660:VAL:HA	2:C:8:VAL:HG13	1.97	0.45
1:A:331:SER:OG	1:A:334:GLU:HG3	2.17	0.45
1:A:499:LEU:HG	1:A:545:ILE:HD11	1.99	0.45
1:A:59:ALA:HB2	1:A:83:ILE:HG12	1.99	0.45
1:A:679:ASN:HD21	1:A:682:GLU:H	1.63	0.45
1:B:86:GLY:O	1:B:132:GLN:NE2	2.49	0.45
1:B:177:ILE:HD11	1:B:240:ALA:HB2	1.98	0.45
1:A:136:ASP:C	1:A:138:VAL:N	2.70	0.45
1:B:164:ASN:OD1	1:B:536:LYS:HG2	2.17	0.45
1:B:610:ILE:O	1:B:611:GLN:C	2.54	0.45
1:A:97:LEU:HB3	1:A:101:LYS:HB2	1.99	0.45
1:A:221:PHE:O	1:A:225:ILE:HG12	2.17	0.45
1:A:759:ALA:N	1:A:760:PRO:CD	2.80	0.45
1:B:153:LYS:O	1:B:157:ARG:HB3	2.17	0.44
1:A:386:TYR:OH	1:A:411:GLN:HG3	2.17	0.44
1:A:71:LEU:HA	1:A:71:LEU:HD12	1.80	0.44
1:B:246:LYS:O	1:B:251:GLU:HG3	2.17	0.44
1:B:456:ASP:HB3	1:B:462:LYS:O	2.18	0.44
1:B:459:ASP:OD2	1:B:459:ASP:C	2.55	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:LEU:O	1:B:606:TRP:HB3	2.17	0.44
1:B:646:GLN:HE22	1:B:652:GLN:HB3	1.81	0.44
1:A:107:ILE:HG13	1:A:145:LEU:HD12	1.99	0.44
1:A:330:LEU:HD11	1:A:376:LEU:HD13	1.98	0.44
1:B:322:ILE:O	1:B:342:GLN:NE2	2.50	0.44
1:A:567:ASN:O	1:A:571:ASN:HB2	2.17	0.44
1:A:748:ASP:OD2	1:A:751:GLU:HG3	2.17	0.44
1:B:613:ASP:CB	1:B:774:ILE:HG23	2.48	0.44
1:A:118:TYR:N	1:A:118:TYR:CD1	2.85	0.44
1:A:144:ALA:O	1:A:148:TYR:CD1	2.71	0.44
1:A:246:LYS:O	1:A:250:GLN:HG2	2.17	0.44
1:B:719:LYS:HA	1:B:719:LYS:HD3	1.76	0.44
1:B:80:LYS:O	1:B:128:VAL:HA	2.17	0.44
1:A:269:GLU:HG2	1:A:273:LYS:HE3	1.99	0.44
1:B:304:LYS:N	1:B:304:LYS:HD2	2.33	0.44
1:A:100:ASP:C	1:A:102:LYS:N	2.71	0.44
1:A:259:LEU:HD23	1:A:259:LEU:HA	1.83	0.44
1:A:261:ASP:O	1:A:267:ARG:HD2	2.18	0.44
1:B:406:LEU:HD12	1:B:406:LEU:O	2.18	0.44
1:B:443:ILE:CD1	1:B:454:LEU:HD22	2.47	0.44
1:A:592:ALA:O	1:A:595:ILE:N	2.50	0.44
1:A:268:TYR:CB	1:B:125:TYR:HE2	2.25	0.44
1:B:247:PHE:HE2	1:B:252:ILE:HD13	1.83	0.44
1:A:741:PHE:CD2	1:A:741:PHE:C	2.92	0.44
2:D:11:TYR:N	2:D:12:PRO:CD	2.80	0.44
1:A:197:HIS:ND1	1:A:198:PRO:HD2	2.33	0.43
1:A:322:ILE:HG13	1:A:368:LEU:CD1	2.48	0.43
1:A:606:TRP:CD1	1:A:610:ILE:HD12	2.53	0.43
1:B:271:TRP:CZ2	1:B:517:GLY:HA3	2.53	0.43
1:B:477:TYR:CZ	1:B:593:SER:HA	2.53	0.43
1:B:636:LEU:HD11	1:B:669:HIS:HB2	2.00	0.43
1:B:718:PHE:CZ	1:B:732:ASN:HA	2.53	0.43
1:A:135:GLU:N	1:A:135:GLU:OE1	2.49	0.43
1:A:295:LYS:C	1:A:297:GLN:N	2.72	0.43
1:A:458:THR:OG1	1:A:459:ASP:N	2.51	0.43
1:A:662:GLU:OE2	1:A:662:GLU:N	2.38	0.43
1:A:701:ASP:O	1:A:703:ASN:N	2.50	0.43
1:A:169:LYS:NZ	1:A:251:GLU:OE2	2.51	0.43
1:A:33:GLU:O	1:A:36:LEU:HB3	2.18	0.43
1:A:368:LEU:HB3	1:A:369:SER:H	1.69	0.43
1:A:767:ASN:HD22	1:A:767:ASN:HA	1.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ILE:O	1:B:107:ILE:HD13	2.18	0.43
1:B:211:ASN:HA	1:B:214:GLN:HG3	2.00	0.43
1:B:56:LYS:C	1:B:58:ALA:N	2.71	0.43
1:B:658:LEU:HD11	2:D:8:VAL:HG11	1.96	0.43
1:A:155:LEU:O	1:A:160:LEU:HG	2.19	0.43
1:A:31:THR:O	1:A:34:GLU:CG	2.64	0.43
1:A:70:VAL:HG12	1:A:252:ILE:HD11	1.99	0.43
1:A:91:HIS:ND1	1:A:92:ILE:N	2.67	0.43
1:B:85:ASP:HB3	1:B:133:SER:HG	1.78	0.43
1:A:199:THR:OG1	1:A:200:ASP:N	2.50	0.43
1:A:672:SER:HB2	1:A:673:LYS:H	1.61	0.43
1:A:697:GLY:N	1:A:708:VAL:HB	2.34	0.43
1:A:174:LEU:HD11	1:A:213:VAL:HG13	2.00	0.43
1:B:149:TYR:HA	1:B:222:ALA:HB2	2.00	0.43
1:B:234:GLN:HB2	1:B:241:PHE:CD2	2.54	0.43
1:B:370:GLU:HG3	1:B:371:LYS:N	2.33	0.43
1:B:368:LEU:O	1:B:373:LYS:HG3	2.18	0.43
1:B:637:PRO:HA	1:B:642:GLN:NE2	2.34	0.43
1:A:159:ILE:CD1	1:A:159:ILE:N	2.81	0.43
1:A:295:LYS:O	1:A:297:GLN:N	2.51	0.43
1:A:322:ILE:HD11	1:A:376:LEU:HD11	2.00	0.43
1:A:37:LYS:O	1:A:41:LYS:N	2.49	0.43
1:B:444:ASN:HD22	1:B:448:ALA:CA	2.29	0.43
1:A:30:LYS:HB3	1:A:31:THR:H	1.58	0.43
1:B:462:LYS:HE2	1:B:462:LYS:HB3	1.78	0.43
1:B:74:TYR:CE2	1:B:79:GLY:HA3	2.54	0.43
1:A:298:ILE:HA	1:A:299:PRO:HD3	1.84	0.43
1:A:320:LYS:HA	1:A:320:LYS:HD2	1.84	0.43
1:A:435:ILE:CD1	1:A:435:ILE:N	2.66	0.43
1:A:581:LYS:HE2	1:A:628:ARG:HE	1.84	0.43
1:B:136:ASP:O	1:B:140:ASN:CB	2.67	0.43
1:B:277:HIS:CD2	1:B:429:SER:HB2	2.53	0.43
1:B:563:GLN:HE21	1:B:585:PHE:HB2	1.83	0.43
1:B:611:GLN:HE21	1:B:614:LEU:H	1.64	0.43
1:B:135:GLU:CD	1:B:138:VAL:HG23	2.40	0.42
1:A:308:ILE:HA	1:A:311:LEU:HD12	2.01	0.42
1:A:267:ARG:NH1	1:A:489:ASN:HB3	2.34	0.42
1:B:39:ILE:O	1:B:43:ILE:HG12	2.18	0.42
1:A:327:SER:OG	1:A:330:LEU:HD12	2.19	0.42
1:B:744:MET:SD	1:B:766:ILE:HG21	2.59	0.42
1:B:96:ALA:O	1:B:97:LEU:C	2.57	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ILE:HG12	1:A:149:TYR:CG	2.54	0.42
1:B:34:GLU:O	1:B:38:GLU:N	2.52	0.42
1:B:721:GLU:OE1	1:B:761:LYS:HB2	2.19	0.42
1:A:440:ASN:HD21	1:A:500:LYS:HZ1	1.66	0.42
1:B:304:LYS:CG	1:B:305:ASP:N	2.82	0.42
1:A:87:ASP:CG	1:A:115:HIS:HB2	2.40	0.42
1:A:114:LEU:HD21	1:A:120:TYR:HB2	2.01	0.42
1:A:39:ILE:HD13	1:A:72:GLU:HB2	2.00	0.42
1:B:268:TYR:O	1:B:272:GLU:HG2	2.19	0.42
1:A:125:TYR:CE1	1:B:269:GLU:HG3	2.55	0.42
1:A:233:LEU:HD13	1:A:241:PHE:CB	2.42	0.42
1:A:627:GLY:HA3	1:A:664:ARG:O	2.20	0.42
1:B:151:ILE:CG2	1:B:151:ILE:O	2.66	0.42
1:B:33:GLU:O	1:B:37:LYS:HG2	2.20	0.42
1:B:498:ARG:HA	1:B:498:ARG:HD3	1.73	0.42
1:B:589:ASN:HB3	1:B:590:ARG:H	1.68	0.42
1:B:632:THR:OG1	1:B:633:ASP:N	2.53	0.42
1:B:89:THR:HG21	1:B:102:LYS:NZ	2.34	0.42
1:B:329:PHE:O	1:B:330:LEU:HD23	2.19	0.42
1:B:107:ILE:HG21	1:B:145:LEU:HD12	1.99	0.42
1:B:186:GLN:HG3	1:B:190:PHE:CD1	2.55	0.42
1:A:50:GLY:O	1:A:51:GLU:C	2.57	0.42
1:B:292:LEU:HD11	1:B:418:ASN:HB2	2.01	0.42
1:B:698:TYR:CD1	1:B:698:TYR:C	2.94	0.42
1:A:322:ILE:HG23	1:A:322:ILE:O	2.19	0.41
1:A:339:LYS:O	1:A:339:LYS:HD2	2.20	0.41
1:A:573:ALA:O	1:A:574:LEU:HD12	2.19	0.41
1:A:94:LEU:C	1:A:96:ALA:N	2.74	0.41
1:B:701:ASP:C	1:B:703:ASN:N	2.73	0.41
1:A:149:TYR:HA	1:A:222:ALA:HB2	2.01	0.41
1:A:247:PHE:O	1:A:252:ILE:HB	2.20	0.41
1:B:515:GLU:C	1:B:517:GLY:H	2.23	0.41
1:B:621:TYR:CE1	1:B:664:ARG:CZ	3.03	0.41
2:C:13:MET:HE2	2:C:13:MET:H	1.83	0.41
1:A:343:ILE:CG2	1:A:344:ASP:N	2.82	0.41
1:A:621:TYR:CE1	1:A:664:ARG:NH2	2.89	0.41
1:A:628:ARG:O	1:A:665:SER:HB3	2.21	0.41
1:A:649:ILE:O	1:A:652:GLN:HG2	2.20	0.41
1:B:653:VAL:HG12	1:B:654:HIS:N	2.35	0.41
1:A:209:ASN:O	1:A:212:GLU:HB2	2.19	0.41
1:A:496:ASN:HD22	1:A:497:GLU:HG3	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:ASN:HD22	1:A:571:ASN:HA	1.58	0.41
1:B:369:SER:OG	1:B:372:GLU:HG3	2.20	0.41
1:B:453:ASP:O	1:B:464:ASN:ND2	2.45	0.41
1:A:659:TYR:O	2:C:8:VAL:HG12	2.20	0.41
1:A:151:ILE:O	1:A:154:ILE:HB	2.21	0.41
1:A:307:ILE:HG21	1:A:341:LEU:CD1	2.49	0.41
1:A:368:LEU:CD1	1:A:372:GLU:HB3	2.51	0.41
1:A:505:LEU:CD1	1:A:509:THR:HG21	2.51	0.41
1:B:250:GLN:HB2	1:B:251:GLU:H	1.63	0.41
1:B:498:ARG:NH2	1:B:540:LYS:HE2	2.24	0.41
1:A:673:LYS:HG3	2:C:14:GLU:OE2	2.21	0.41
1:A:584:THR:HG23	1:A:630:VAL:HG22	2.03	0.41
1:A:717:ILE:N	1:A:717:ILE:HD12	2.35	0.41
1:B:163:ILE:CG1	1:B:165:GLN:HG3	2.50	0.41
1:A:131:ILE:O	1:A:132:GLN:O	2.39	0.41
1:A:592:ALA:O	1:A:593:SER:C	2.59	0.41
1:A:675:VAL:HG23	2:C:12:PRO:O	2.20	0.41
1:B:129:LEU:HD22	1:B:131:ILE:HD11	2.03	0.41
1:B:197:HIS:HA	1:B:198:PRO:HD2	1.86	0.41
1:B:330:LEU:HB2	1:B:335:LYS:HZ3	1.83	0.41
1:B:250:GLN:O	1:B:252:ILE:N	2.53	0.41
1:B:478:SER:HB3	1:B:527:LEU:HB2	2.03	0.41
1:B:563:GLN:NE2	1:B:585:PHE:H	2.19	0.41
1:A:34:GLU:CG	1:A:35:HIS:N	2.84	0.41
1:A:375:PHE:CE2	1:A:379:LEU:HD11	2.56	0.41
1:B:331:SER:O	1:B:332:THR:C	2.59	0.41
1:B:694:ASP:OD1	1:B:694:ASP:O	2.39	0.41
1:A:333:GLU:O	1:A:336:GLU:HB3	2.21	0.41
1:A:636:LEU:C	1:A:638:ASN:H	2.24	0.41
1:A:666:ILE:HG23	1:A:687:CYS:HB3	2.03	0.41
1:B:123:GLU:O	1:B:124:GLY:C	2.58	0.41
1:B:214:GLN:O	1:B:217:PHE:HB3	2.20	0.41
1:A:125:TYR:CG	1:B:269:GLU:HG3	2.55	0.41
1:B:500:LYS:HD2	1:B:542:TYR:CG	2.56	0.41
1:B:659:TYR:O	2:D:8:VAL:HG13	2.20	0.41
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.92	0.40
1:A:433:ASN:O	1:A:435:ILE:HG13	2.21	0.40
1:A:648:GLU:HB3	1:A:650:TYR:CD2	2.56	0.40
1:A:769:GLN:O	1:A:772:PHE:HB3	2.21	0.40
1:B:221:PHE:HA	1:B:244:MET:HE2	2.03	0.40
1:B:589:ASN:HB2	1:B:633:ASP:OD2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:O	1:A:114:LEU:HD12	2.21	0.40
1:A:46:ILE:N	1:A:46:ILE:CD1	2.84	0.40
1:A:74:TYR:HD2	1:A:74:TYR:HA	1.78	0.40
1:B:118:TYR:CE2	1:B:143:LYS:HG2	2.56	0.40
1:B:48:VAL:O	1:B:49:LYS:HD3	2.21	0.40
1:B:133:SER:O	1:B:134:SER:HB3	2.22	0.40
1:B:424:HIS:CA	1:B:510:ARG:HD2	2.42	0.40
1:B:58:ALA:O	1:B:59:ALA:C	2.60	0.40
1:B:589:ASN:N	1:B:633:ASP:OD2	2.50	0.40
1:B:721:GLU:O	1:B:723:SER:N	2.55	0.40
1:B:47:GLU:O	1:B:84:VAL:HG23	2.20	0.40
1:A:690:HIS:CE1	1:A:735:GLU:OE2	2.75	0.40
1:B:50:GLY:O	1:B:51:GLU:HB2	2.22	0.40
1:B:533:GLN:HE21	1:B:533:GLN:HB2	1.73	0.40
1:B:597:GLU:O	1:B:598:SER:C	2.59	0.40
1:B:618:VAL:O	1:B:621:TYR:HB3	2.21	0.40
1:B:649:ILE:O	1:B:649:ILE:HG22	2.21	0.40
1:B:676:GLU:HA	1:B:676:GLU:OE1	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	722/776 (93%)	617 (86%)	74 (10%)	31 (4%)	3	10
1	B	730/776 (94%)	635 (87%)	76 (10%)	19 (3%)	6	21
2	C	9/20 (45%)	4 (44%)	1 (11%)	4 (44%)	0	0
2	D	9/20 (45%)	4 (44%)	1 (11%)	4 (44%)	0	0
All	All	1470/1592 (92%)	1260 (86%)	152 (10%)	58 (4%)	3	12

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	181	SER
1	A	370	GLU
1	A	473	LYS
1	A	675	VAL
1	A	678	ARG
1	B	30	LYS
1	B	94	LEU
1	B	200	ASP
1	B	366	ASN
1	B	369	SER
2	C	15	PRO
2	D	15	PRO
1	A	31	THR
1	A	98	SER
1	A	101	LYS
1	A	140	ASN
1	A	296	LEU
1	A	592	ALA
1	A	676	GLU
1	A	696	ALA
1	A	700	LEU
1	A	702	LYS
1	B	48	VAL
1	B	93	SER
1	B	123	GLU
1	B	134	SER
1	B	251	GLU
1	B	722	GLY
2	C	10	PRO
1	A	52	GLU
1	A	87	ASP
1	A	95	GLU
1	A	209	ASN
1	A	250	GLN
1	A	641	GLU
1	B	141	THR
1	B	652	GLN
2	D	10	PRO
1	A	198	PRO
1	A	251	GLU
1	A	324	ILE
1	A	672	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	52	GLU
1	B	196	GLU
1	B	702	LYS
2	C	11	TYR
1	A	760	PRO
1	B	124	GLY
2	D	11	TYR
2	D	12	PRO
1	A	722	GLY
1	B	577	PRO
1	A	92	ILE
1	A	88	ILE
2	C	12	PRO
1	A	383	ILE
1	B	107	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	665/710 (94%)	616 (93%)	49 (7%)	16	42
1	B	673/710 (95%)	636 (94%)	37 (6%)	25	57
2	C	11/17 (65%)	8 (73%)	3 (27%)	0	1
2	D	11/17 (65%)	6 (54%)	5 (46%)	0	0
All	All	1360/1454 (94%)	1266 (93%)	94 (7%)	18	46

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	34	GLU
1	A	45	LYS
1	A	49	LYS
1	A	71	LEU
1	A	74	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	85	ASP
1	A	100	ASP
1	A	107	ILE
1	A	111	ASP
1	A	136	ASP
1	A	193	GLN
1	A	200	ASP
1	A	203	VAL
1	A	226	GLU
1	A	233	LEU
1	A	256	LEU
1	A	288	GLU
1	A	294	LYS
1	A	301	GLU
1	A	305	ASP
1	A	321	ARG
1	A	343	ILE
1	A	374	GLU
1	A	404	ILE
1	A	431	LEU
1	A	433	ASN
1	A	435	ILE
1	A	446	LEU
1	A	447	THR
1	A	449	THR
1	A	470	GLU
1	A	475	PHE
1	A	494	LEU
1	A	496	ASN
1	A	523	ARG
1	A	582	LEU
1	A	620	ASN
1	A	636	LEU
1	A	656	LYS
1	A	678	ARG
1	A	679	ASN
1	A	686	HIS
1	A	701	ASP
1	A	730	ARG
1	A	733	GLU
1	A	739	GLU
1	A	767	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	772	PHE
1	B	32	GLN
1	B	40	MET
1	B	68	SER
1	B	80	LYS
1	B	107	ILE
1	B	118	TYR
1	B	125	TYR
1	B	126	GLU
1	B	129	LEU
1	B	136	ASP
1	B	142	GLU
1	B	146	ASN
1	B	165	GLN
1	B	184	ASP
1	B	228	GLN
1	B	256	LEU
1	B	304	LYS
1	B	314	GLU
1	B	370	GLU
1	B	391	ARG
1	B	425	GLN
1	B	447	THR
1	B	496	ASN
1	B	516	ASN
1	B	523	ARG
1	B	525	ILE
1	B	529	ILE
1	B	533	GLN
1	B	571	ASN
1	B	611	GLN
1	B	643	TYR
1	B	667	LEU
1	B	671	PRO
1	B	703	ASN
1	B	753	LEU
1	B	764	GLN
1	B	767	ASN
2	C	11	TYR
2	C	13	MET
2	C	14	GLU
2	D	6	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	10	PRO
2	D	11	TYR
2	D	13	MET
2	D	14	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	35	HIS
1	A	140	ASN
1	A	164	ASN
1	A	186	GLN
1	A	193	GLN
1	A	214	GLN
1	A	242	ASN
1	A	248	ASN
1	A	276	GLN
1	A	277	HIS
1	A	279	GLN
1	A	411	GLN
1	A	440	ASN
1	A	496	ASN
1	A	504	GLN
1	A	524	ASN
1	A	560	GLN
1	A	563	GLN
1	A	567	ASN
1	A	571	ASN
1	A	589	ASN
1	A	608	ASN
1	A	646	GLN
1	A	679	ASN
1	A	745	HIS
1	A	767	ASN
1	A	775	ASN
1	B	35	HIS
1	B	91	HIS
1	B	132	GLN
1	B	165	GLN
1	B	186	GLN
1	B	193	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	197	HIS
1	B	209	ASN
1	B	214	GLN
1	B	228	GLN
1	B	248	ASN
1	B	250	GLN
1	B	253	ASN
1	B	277	HIS
1	B	297	GLN
1	B	309	HIS
1	B	313	GLN
1	B	323	GLN
1	B	390	GLN
1	B	424	HIS
1	B	440	ASN
1	B	444	ASN
1	B	496	ASN
1	B	504	GLN
1	B	516	ASN
1	B	522	GLN
1	B	524	ASN
1	B	533	GLN
1	B	537	GLN
1	B	563	GLN
1	B	571	ASN
1	B	608	ASN
1	B	609	ASN
1	B	611	GLN
1	B	638	ASN
1	B	645	HIS
1	B	710	ASN
1	B	745	HIS
1	B	756	GLN
1	B	767	ASN
1	B	769	GLN

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 2 ligands modelled in this entry, 2 are 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	726/776 (93%)	0.16	50 (6%) 18 10	14, 40, 88, 94	0
1	B	734/776 (94%)	0.07	43 (5%) 23 15	13, 39, 85, 123	0
2	C	11/20 (55%)	3.00	7 (63%) 0 0	89, 98, 108, 108	0
2	D	11/20 (55%)	3.28	8 (72%) 0 0	88, 98, 108, 108	0
All	All	1482/1592 (93%)	0.16	108 (7%) 16 8	13, 40, 88, 123	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	29	ASN	8.8
2	D	16	THR	7.6
2	C	11	TYR	5.9
2	D	11	TYR	5.5
1	A	321	ARG	5.1
1	B	48	VAL	5.0
1	A	319	LEU	4.9
1	A	703	ASN	4.9
1	A	343	ILE	4.8
1	A	309	HIS	4.7
1	B	54	VAL	4.7
2	D	14	GLU	4.5
2	C	14	GLU	4.5
1	A	322	ILE	4.3
1	B	30	LYS	4.3
2	C	16	THR	4.2
1	A	368	LEU	4.2
1	A	308	ILE	4.2
1	B	367	PRO	4.1
1	A	307	ILE	4.0
1	B	29	ASN	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	31	THR	3.9
1	B	46	ILE	3.9
1	A	328	ASP	3.9
1	A	324	ILE	3.9
1	B	349	LEU	3.9
1	A	344	ASP	3.8
2	C	15	PRO	3.7
1	A	316	LYS	3.7
1	A	54	VAL	3.6
2	C	12	PRO	3.6
2	D	12	PRO	3.5
2	D	15	PRO	3.5
1	A	345	ILE	3.4
1	B	50	GLY	3.4
1	B	115	HIS	3.4
1	B	321	ARG	3.4
1	A	320	LYS	3.3
1	B	28	ARG	3.3
1	A	30	LYS	3.2
1	B	37	LYS	3.2
1	A	371	LYS	3.2
1	B	52	GLU	3.2
1	A	48	VAL	3.1
1	B	366	ASN	3.1
2	D	9	TYR	3.1
1	A	318	LEU	3.0
2	D	13	MET	3.0
1	B	35	HIS	3.0
1	A	313	GLN	3.0
1	A	34	GLU	3.0
1	B	368	LEU	3.0
1	A	338	LEU	2.9
1	A	315	GLU	2.9
1	B	32	GLN	2.9
1	B	131	ILE	2.9
1	A	372	GLU	2.9
1	B	31	THR	2.8
1	A	36	LEU	2.8
1	A	323	GLN	2.8
1	B	327	SER	2.8
1	A	327	SER	2.8
1	B	57	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	326	SER	2.7
1	A	53	ALA	2.7
1	B	135	GLU	2.7
2	C	6	LYS	2.7
1	A	52	GLU	2.7
1	B	702	LYS	2.7
1	B	348	SER	2.6
1	B	776	SER	2.6
2	C	9	TYR	2.6
1	B	51	GLU	2.6
1	A	51	GLU	2.6
1	A	310	SER	2.6
1	A	317	GLU	2.5
1	B	370	GLU	2.5
1	B	49	LYS	2.5
1	A	341	LEU	2.5
1	A	337	PHE	2.5
1	A	32	GLN	2.4
1	A	33	GLU	2.4
1	B	34	GLU	2.4
1	B	92	ILE	2.3
1	A	375	PHE	2.3
1	A	306	ASP	2.3
1	A	311	LEU	2.3
1	B	345	ILE	2.3
1	B	134	SER	2.3
1	B	33	GLU	2.3
1	A	35	HIS	2.3
1	A	99	GLU	2.2
1	B	138	VAL	2.2
1	B	346	ARG	2.2
1	B	347	ASP	2.2
1	B	365	SER	2.2
1	B	47	GLU	2.2
1	A	49	LYS	2.2
1	A	340	LYS	2.2
1	A	650	TYR	2.2
1	B	91	HIS	2.1
2	D	10	PRO	2.1
1	A	305	ASP	2.1
1	B	88	ILE	2.1
1	B	56	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	97	LEU	2.1
1	A	94	LEU	2.0
1	A	704	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	A	9001	1/1	0.99	0.21	-0.57	45,45,45,45	0
3	ZN	B	9002	1/1	0.98	0.19	-0.59	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.