



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:57 AM GMT

PDB ID : 2JGU
Title : CRYSTAL STRUCTURE OF DNA-DIRECTED DNA POLYMERASE
Authors : Kim, D.U.; Cho, H.S.
Deposited on : 2007-02-15
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

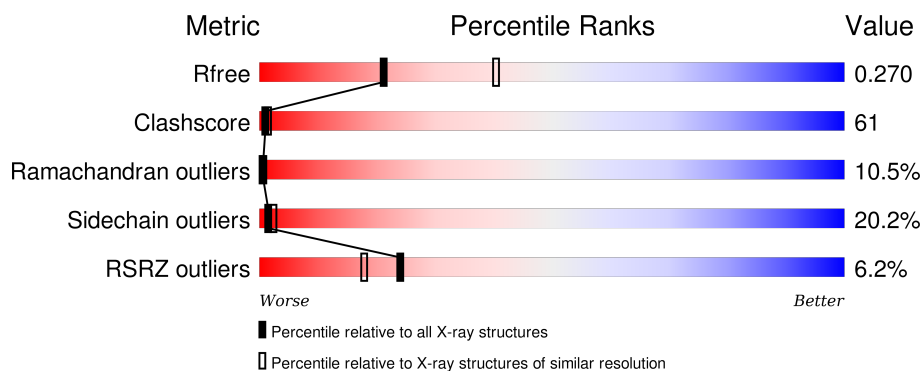
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	775	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5859 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 DNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	712	Total	C	N	O	S	0	0	1
			5826	3777	963	1072	14			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	LEU	ILE	CONFLICT	UNP P61875
A	169	ARG	LYS	CONFLICT	UNP P61875
A	183	SER	VAL	CONFLICT	UNP P61875
A	186	THR	SER	CONFLICT	UNP P61875
A	188	LYS	ARG	CONFLICT	UNP P61875
A	265	ARG	THR	CONFLICT	UNP P61875
A	266	THR	ARG	CONFLICT	UNP P61875
A	406	TYR	PHE	CONFLICT	UNP P61875
A	407	LYS	ARG	CONFLICT	UNP P61875
A	408	SER	ALA	CONFLICT	UNP P61875

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		

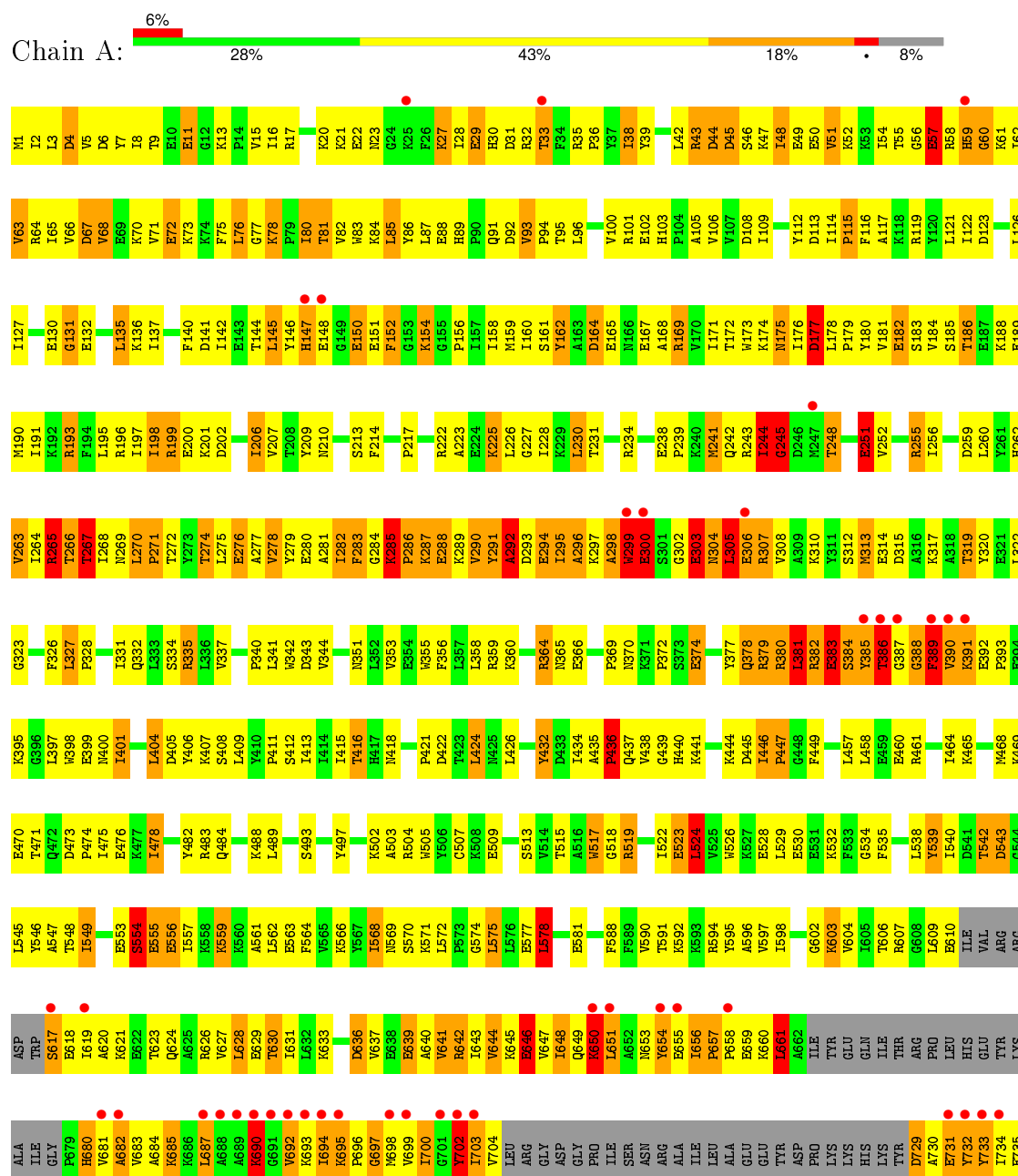
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total	O	0	0
			31	31		

3 Residue-property plots

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

• Molecule 1: DNA POLYMERASE



N736	Q737	V738	L739	P740	A741	V742	L743	R744	I745	L746	E747	G748	F749	G750	Y751	R752	K753	E754	D755	L756	R757	Y758	GLN	LYS	THR	ARG	GLN	VAL	GLY	LEU	THR	SER	TRP	LEU	ASN	ILE	LYS	LYS	SER
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.18 Å 127.92 Å 89.21 Å 90.00° 109.11° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 41.61 – 2.41	Depositor EDS
% Data completeness (in resolution range)	94.2 (15.00-2.60) 90.5 (41.61-2.41)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.42 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.275 , 0.271 0.267 , 0.270	Depositor DCC
R_{free} test set	1403 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 33968 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5859	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.94	11/5953 (0.2%)	1.34	53/8024 (0.7%)

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	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	LYS	C-N	-14.43	1.06	1.34
1	A	251	GLU	CB-CG	12.28	1.75	1.52
1	A	251	GLU	CG-CD	9.50	1.66	1.51
1	A	556	GLU	CB-CG	-6.50	1.39	1.52
1	A	387	GLY	CA-C	5.92	1.61	1.51
1	A	387	GLY	N-CA	5.62	1.54	1.46
1	A	251	GLU	CA-CB	5.31	1.65	1.53
1	A	553	GLU	CB-CG	-5.24	1.42	1.52
1	A	102	GLU	CB-CG	5.21	1.62	1.52
1	A	476	GLU	CG-CD	5.10	1.59	1.51
1	A	505	TRP	CB-CG	5.04	1.59	1.50

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	684	ALA	N-CA-C	-10.50	82.65	111.00
1	A	382	ARG	CA-C-N	-9.62	96.03	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	LYS	C-N-CD	-9.08	100.62	120.60
1	A	305	LEU	CA-CB-CG	8.06	133.84	115.30
1	A	687	LEU	CA-CB-CG	8.05	133.82	115.30
1	A	150	GLU	N-CA-C	7.77	131.99	111.00
1	A	554	SER	N-CA-C	7.76	131.94	111.00
1	A	387	GLY	N-CA-C	7.68	132.31	113.10
1	A	145	LEU	CA-CB-CG	7.61	132.79	115.30
1	A	682	ALA	C-N-CA	-7.07	104.02	121.70
1	A	291	TYR	N-CA-C	6.64	128.94	111.00
1	A	383	GLU	CA-C-N	-6.55	102.80	117.20
1	A	556	GLU	N-CA-CB	-6.53	98.84	110.60
1	A	299	TRP	N-CA-CB	6.47	122.25	110.60
1	A	245	GLY	N-CA-C	-6.46	96.94	113.10
1	A	389	PHE	CB-CA-C	-6.38	97.64	110.40
1	A	543	ASP	CB-CA-C	-6.38	97.64	110.40
1	A	578	LEU	CA-CB-CG	6.36	129.93	115.30
1	A	661	LEU	CA-CB-CG	-6.32	100.76	115.30
1	A	386	THR	CA-C-N	6.30	128.79	116.20
1	A	382	ARG	N-CA-CB	6.19	121.75	110.60
1	A	650	LYS	N-CA-C	-6.17	94.35	111.00
1	A	60	GLY	N-CA-C	-6.15	97.72	113.10
1	A	251	GLU	OE1-CD-OE2	-5.98	116.12	123.30
1	A	381	LEU	CA-CB-CG	-5.95	101.61	115.30
1	A	382	ARG	C-N-CA	5.92	136.49	121.70
1	A	702	TYR	N-CA-C	5.89	126.89	111.00
1	A	386	THR	N-CA-C	5.77	126.59	111.00
1	A	154	LYS	N-CA-C	-5.73	95.52	111.00
1	A	578	LEU	CB-CG-CD1	-5.68	101.34	111.00
1	A	489	LEU	CB-CG-CD1	-5.59	101.50	111.00
1	A	636	ASP	N-CA-C	5.58	126.08	111.00
1	A	387	GLY	C-N-CA	5.57	133.99	122.30
1	A	389	PHE	CB-CG-CD1	-5.52	116.94	120.80
1	A	555	GLU	N-CA-C	-5.51	96.13	111.00
1	A	641	VAL	N-CA-C	-5.49	96.18	111.00
1	A	251	GLU	CA-CB-CG	5.42	125.33	113.40
1	A	299	TRP	N-CA-C	-5.42	96.38	111.00
1	A	299	TRP	CA-CB-CG	-5.41	103.42	113.70
1	A	278	VAL	CB-CA-C	-5.37	101.19	111.40
1	A	135	LEU	CA-CB-CG	-5.34	103.02	115.30
1	A	607	ARG	N-CA-C	-5.33	96.59	111.00
1	A	382	ARG	O-C-N	5.31	131.20	122.70
1	A	389	PHE	C-N-CA	-5.24	108.59	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	GLU	N-CA-CB	-5.21	101.21	110.60
1	A	23	ASN	N-CA-CB	5.18	119.92	110.60
1	A	404	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	305	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	A	292	ALA	N-CA-C	-5.08	97.29	111.00
1	A	44	ASP	CB-CA-C	5.06	120.52	110.40
1	A	299	TRP	CG-CD2-CE3	5.06	138.45	133.90
1	A	690	LYS	N-CA-C	5.06	124.65	111.00
1	A	248	THR	N-CA-CB	-5.03	100.75	110.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	TYR	Sidechain
1	A	389	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5826	0	5919	718	0
2	A	2	0	0	0	0
3	A	31	0	0	5	0
All	All	5859	0	5919	718	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 61.

All (718) 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:389:PHE:CE1	1:A:519:ARG:HG2	1.30	1.65
1:A:389:PHE:HE1	1:A:519:ARG:CG	1.08	1.63
1:A:251:GLU:CB	1:A:251:GLU:CG	1.75	1.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:SER:OG	1:A:737:GLN:NE2	1.65	1.26
1:A:389:PHE:O	1:A:390:VAL:HG23	1.40	1.22
1:A:389:PHE:CE1	1:A:519:ARG:CG	2.00	1.22
1:A:384:SER:O	1:A:385:TYR:O	1.65	1.15
1:A:176:ILE:HD11	1:A:305:LEU:CD2	1.76	1.14
1:A:178:LEU:CD2	1:A:179:PRO:HD2	1.76	1.14
1:A:289:LYS:O	1:A:290:VAL:HG23	1.47	1.13
1:A:651:LEU:HD23	1:A:734:ILE:HG13	1.19	1.13
1:A:178:LEU:HD23	1:A:179:PRO:HD2	1.28	1.13
1:A:386:THR:HG22	1:A:386:THR:O	1.39	1.10
1:A:45:ASP:O	1:A:48:ILE:HG23	1.51	1.10
1:A:52:LYS:O	1:A:65:ILE:HG21	1.49	1.10
1:A:377:TYR:HE1	1:A:502:LYS:HG2	1.06	1.10
1:A:176:ILE:HD11	1:A:305:LEU:HD23	1.14	1.08
1:A:528:GLU:OE1	1:A:532:LYS:HD2	1.55	1.06
1:A:244:ILE:CG2	1:A:245:GLY:H	1.67	1.06
1:A:737:GLN:O	1:A:740:PRO:HD2	1.56	1.04
1:A:389:PHE:O	1:A:390:VAL:CG2	2.05	1.03
1:A:377:TYR:CE1	1:A:502:LYS:HG2	1.93	1.02
1:A:383:GLU:HG3	1:A:384:SER:N	1.75	1.02
1:A:639:GLU:O	1:A:643:ILE:HG12	1.59	1.01
1:A:144:THR:HG22	1:A:145:LEU:H	1.25	1.00
1:A:182:GLU:HG2	1:A:193:ARG:HH22	1.26	0.99
1:A:731:GLU:O	1:A:735:GLU:HB2	1.62	0.98
1:A:299:TRP:O	1:A:300:GLU:HB2	1.61	0.98
1:A:303:GLU:C	1:A:305:LEU:H	1.63	0.97
1:A:182:GLU:HG2	1:A:193:ARG:NH2	1.79	0.97
1:A:729:ASP:HB3	1:A:732:TYR:HB2	1.44	0.97
1:A:144:THR:HG22	1:A:145:LEU:N	1.79	0.97
1:A:460:GLU:OE2	1:A:483:ARG:NH2	1.98	0.97
1:A:739:LEU:O	1:A:743:LEU:HB2	1.64	0.96
1:A:176:ILE:CD1	1:A:305:LEU:HD23	1.94	0.96
1:A:45:ASP:O	1:A:48:ILE:CG2	2.13	0.96
1:A:70:LYS:HB2	1:A:83:TRP:CZ3	2.00	0.96
1:A:390:VAL:O	1:A:391:LYS:O	1.84	0.96
1:A:298:ALA:O	1:A:299:TRP:C	2.00	0.95
1:A:231:THR:HG22	1:A:231:THR:O	1.66	0.95
1:A:270:LEU:HD22	1:A:271:PRO:HD2	1.48	0.95
1:A:296:ALA:HB1	1:A:305:LEU:HB2	1.48	0.94
1:A:244:ILE:CG2	1:A:245:GLY:N	2.27	0.94
1:A:303:GLU:O	1:A:305:LEU:N	2.00	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:ILE:HG21	1:A:757:ARG:O	1.68	0.93
1:A:383:GLU:HG3	1:A:384:SER:H	1.33	0.93
1:A:389:PHE:CD2	1:A:540:ILE:HG21	2.02	0.93
1:A:389:PHE:CE1	1:A:519:ARG:HG3	2.04	0.92
1:A:685:LYS:HA	1:A:685:LYS:HE3	1.50	0.92
1:A:223:ALA:C	1:A:225:LYS:H	1.71	0.92
1:A:78:LYS:HD3	1:A:80:ILE:HD12	1.51	0.91
1:A:71:VAL:HG12	1:A:72:GLU:N	1.83	0.91
1:A:78:LYS:HD3	1:A:80:ILE:CD1	2.00	0.91
1:A:244:ILE:HG23	1:A:245:GLY:H	1.31	0.90
1:A:285:LYS:HG2	1:A:286:PRO:HD2	1.53	0.90
1:A:680:HIS:O	1:A:681:VAL:HB	1.71	0.90
1:A:3:LEU:HD22	1:A:256:ILE:HD11	1.54	0.89
1:A:437:GLN:HE22	1:A:519:ARG:HH21	1.16	0.89
1:A:89:HIS:HD2	1:A:91:GLN:HG2	1.38	0.88
1:A:384:SER:O	1:A:385:TYR:C	2.11	0.88
1:A:144:THR:CG2	1:A:145:LEU:H	1.86	0.88
1:A:298:ALA:O	1:A:299:TRP:O	1.91	0.88
1:A:302:GLY:O	1:A:303:GLU:O	1.92	0.87
1:A:360:LYS:O	1:A:364:ARG:HG2	1.74	0.87
1:A:48:ILE:HG13	1:A:49:GLU:N	1.88	0.87
1:A:432:TYR:HD1	1:A:432:TYR:O	1.58	0.87
1:A:383:GLU:CG	1:A:384:SER:N	2.28	0.86
1:A:386:THR:O	1:A:386:THR:CG2	2.16	0.86
1:A:89:HIS:CD2	1:A:91:GLN:HG2	2.11	0.86
1:A:474:PRO:O	1:A:478:ILE:HG22	1.74	0.86
1:A:52:LYS:O	1:A:65:ILE:CG2	2.23	0.86
1:A:89:HIS:HD2	1:A:91:GLN:CG	1.89	0.86
1:A:651:LEU:HD23	1:A:734:ILE:CG1	2.06	0.86
1:A:227:GLY:O	1:A:228:ILE:HD12	1.75	0.85
1:A:244:ILE:HG22	1:A:245:GLY:N	1.89	0.85
1:A:178:LEU:HD23	1:A:179:PRO:CD	2.06	0.85
1:A:147:HIS:CG	1:A:148:GLU:H	1.94	0.85
1:A:379:ARG:O	1:A:382:ARG:N	2.07	0.85
1:A:122:ILE:HA	1:A:359:ARG:HH12	1.41	0.85
1:A:195:LEU:HA	1:A:198:ILE:CD1	2.06	0.85
1:A:378:GLN:HA	1:A:378:GLN:OE1	1.74	0.85
1:A:58:ARG:O	1:A:60:GLY:N	2.08	0.85
1:A:641:VAL:HA	1:A:644:VAL:HG23	1.59	0.84
1:A:437:GLN:HE22	1:A:519:ARG:NH2	1.75	0.84
1:A:42:LEU:CD1	1:A:106:VAL:HG12	2.07	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LYS:O	1:A:49:GLU:N	2.11	0.83
1:A:158:ILE:HG22	1:A:159:MET:HG3	1.58	0.83
1:A:377:TYR:HE1	1:A:502:LYS:CG	1.91	0.83
1:A:745:ILE:HG22	1:A:746:LEU:HD23	1.59	0.83
1:A:51:VAL:O	1:A:51:VAL:HG23	1.78	0.83
1:A:57:GLU:N	1:A:63:VAL:HG23	1.94	0.83
1:A:323:GLY:O	1:A:327:LEU:HB2	1.78	0.82
1:A:289:LYS:HG2	1:A:290:VAL:N	1.93	0.82
1:A:270:LEU:HD22	1:A:271:PRO:CD	2.10	0.82
1:A:680:HIS:O	1:A:682:ALA:N	2.12	0.82
1:A:648:ILE:HD12	1:A:757:ARG:HA	1.60	0.81
1:A:732:TYR:O	1:A:735:GLU:N	2.13	0.81
1:A:653:ASN:O	1:A:654:TYR:HB2	1.79	0.81
1:A:755:ASP:CG	1:A:756:LEU:H	1.84	0.81
1:A:160:ILE:CG2	1:A:171:ILE:HB	2.11	0.81
1:A:461:ARG:HH21	1:A:484:GLN:HE21	1.28	0.81
1:A:266:THR:OG1	1:A:267:THR:N	2.11	0.80
1:A:303:GLU:OE2	1:A:306:GLU:HB3	1.82	0.80
1:A:58:ARG:NH1	1:A:91:GLN:HB2	1.97	0.80
1:A:432:TYR:HA	1:A:444:LYS:HG3	1.63	0.79
1:A:545:LEU:N	1:A:545:LEU:HD23	1.98	0.79
1:A:464:ILE:HD11	1:A:483:ARG:CZ	2.12	0.78
1:A:178:LEU:HD22	1:A:179:PRO:HD2	1.62	0.78
1:A:518:GLY:O	1:A:522:ILE:HG12	1.83	0.78
1:A:284:GLY:O	1:A:285:LYS:O	2.02	0.77
1:A:298:ALA:C	1:A:299:TRP:O	2.20	0.77
1:A:266:THR:O	1:A:267:THR:O	2.03	0.77
1:A:692:VAL:HG12	1:A:692:VAL:O	1.82	0.77
1:A:315:ASP:O	1:A:319:THR:OG1	2.02	0.77
1:A:383:GLU:O	1:A:385:TYR:N	2.19	0.76
1:A:568:ILE:O	1:A:568:ILE:HD13	1.86	0.76
1:A:42:LEU:HD13	1:A:106:VAL:HG12	1.65	0.76
1:A:389:PHE:HD2	1:A:540:ILE:CG2	1.98	0.76
1:A:405:ASP:HB2	1:A:581:GLU:CG	2.15	0.76
1:A:380:ARG:C	1:A:382:ARG:N	2.38	0.76
1:A:380:ARG:C	1:A:382:ARG:H	1.88	0.75
1:A:100:VAL:O	1:A:106:VAL:HG21	1.87	0.75
1:A:432:TYR:CD1	1:A:432:TYR:O	2.40	0.75
1:A:209:TYR:O	1:A:210:ASN:HB3	1.85	0.75
1:A:374:GLU:HA	1:A:374:GLU:OE1	1.85	0.75
1:A:71:VAL:CG1	1:A:72:GLU:N	2.50	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:C	1:A:245:GLY:O	2.21	0.74
1:A:89:HIS:CD2	1:A:91:GLN:CG	2.70	0.74
1:A:389:PHE:CZ	1:A:391:LYS:NZ	2.55	0.74
1:A:252:VAL:HG12	1:A:255:ARG:HG3	1.69	0.74
1:A:20:LYS:NZ	1:A:29:GLU:HG2	2.03	0.74
1:A:389:PHE:CZ	1:A:519:ARG:HG2	2.16	0.74
1:A:473:ASP:OD2	1:A:475:ILE:N	2.17	0.74
1:A:66:VAL:O	1:A:67:ASP:O	2.05	0.74
1:A:641:VAL:HA	1:A:644:VAL:CG2	2.16	0.73
1:A:692:VAL:O	1:A:694:ILE:N	2.20	0.73
1:A:122:ILE:HA	1:A:359:ARG:NH1	2.01	0.73
1:A:372:PRO:HG3	1:A:380:ARG:NH1	2.03	0.73
1:A:36:PRO:HD3	1:A:116:PHE:CE1	2.23	0.73
1:A:263:VAL:O	1:A:266:THR:HG23	1.87	0.73
1:A:682:ALA:O	1:A:685:LYS:HB2	1.89	0.73
1:A:3:LEU:CD2	1:A:256:ILE:HD11	2.18	0.73
1:A:340:PRO:O	1:A:343:ASP:HB2	1.89	0.73
1:A:223:ALA:C	1:A:225:LYS:N	2.40	0.73
1:A:464:ILE:HD11	1:A:483:ARG:NE	2.03	0.72
1:A:630:THR:HG21	1:A:639:GLU:HG3	1.72	0.72
1:A:61:LYS:HG3	1:A:62:ILE:H	1.52	0.72
1:A:169:ARG:HH12	1:A:182:GLU:CD	1.93	0.72
1:A:20:LYS:HE2	3:A:2003:HOH:O	1.89	0.72
1:A:35:ARG:NH1	1:A:67:ASP:OD2	2.23	0.72
1:A:70:LYS:HB2	1:A:83:TRP:CH2	2.25	0.71
1:A:388:GLY:H	1:A:515:THR:HG23	1.54	0.71
1:A:405:ASP:HB2	1:A:581:GLU:HG3	1.70	0.71
1:A:271:PRO:HG2	1:A:272:THR:H	1.54	0.71
1:A:58:ARG:HH11	1:A:91:GLN:HB2	1.53	0.71
1:A:195:LEU:HA	1:A:198:ILE:HD13	1.72	0.71
1:A:437:GLN:NE2	1:A:519:ARG:HH21	1.88	0.71
1:A:568:ILE:CD1	1:A:572:LEU:HG	2.20	0.71
1:A:298:ALA:O	1:A:300:GLU:O	2.08	0.70
1:A:641:VAL:CA	1:A:644:VAL:HG23	2.21	0.70
1:A:289:LYS:HA	1:A:291:TYR:CE2	2.26	0.70
1:A:736:ASN:C	1:A:736:ASN:HD22	1.95	0.70
1:A:172:THR:HA	1:A:190:MET:CE	2.22	0.70
1:A:389:PHE:CD2	1:A:540:ILE:CG2	2.72	0.70
1:A:640:ALA:C	1:A:643:ILE:H	1.95	0.70
1:A:227:GLY:C	1:A:228:ILE:HD12	2.11	0.70
1:A:64:ARG:CG	1:A:65:ILE:N	2.54	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:VAL:O	1:A:282:ILE:HG23	1.91	0.70
1:A:438:VAL:O	1:A:438:VAL:HG22	1.90	0.70
1:A:38:ILE:HG13	1:A:39:TYR:N	2.07	0.70
1:A:378:GLN:O	1:A:381:LEU:HD12	1.92	0.69
1:A:47:LYS:O	1:A:50:GLU:N	2.18	0.69
1:A:303:GLU:C	1:A:305:LEU:N	2.29	0.69
1:A:692:VAL:CG1	1:A:692:VAL:O	2.41	0.69
1:A:230:LEU:O	1:A:238:GLU:HG2	1.92	0.69
1:A:383:GLU:HG3	1:A:384:SER:CA	2.22	0.69
1:A:383:GLU:HG3	1:A:384:SER:CB	2.23	0.69
1:A:64:ARG:HG3	1:A:65:ILE:H	1.55	0.69
1:A:71:VAL:CG1	1:A:72:GLU:H	2.06	0.69
1:A:534:GLY:O	1:A:549:ILE:HG23	1.91	0.69
1:A:523:GLU:O	1:A:526:TRP:N	2.25	0.68
1:A:231:THR:CG2	1:A:231:THR:O	2.38	0.68
1:A:434:ILE:HG12	1:A:441:LYS:HG2	1.74	0.68
1:A:680:HIS:O	1:A:681:VAL:CB	2.39	0.68
1:A:172:THR:HA	1:A:190:MET:HE3	1.76	0.68
1:A:165:GLU:HG2	1:A:320:TYR:OH	1.93	0.68
1:A:736:ASN:C	1:A:736:ASN:ND2	2.47	0.68
1:A:71:VAL:HG12	1:A:72:GLU:H	1.56	0.67
1:A:62:ILE:N	1:A:62:ILE:HD12	2.09	0.67
1:A:263:VAL:O	1:A:266:THR:CG2	2.41	0.67
1:A:184:VAL:HG11	1:A:189:GLU:HB3	1.76	0.67
1:A:171:ILE:O	1:A:190:MET:HE2	1.94	0.67
1:A:5:VAL:HG21	1:A:121:LEU:HD21	1.77	0.67
1:A:119:ARG:NH1	1:A:123:ASP:OD1	2.26	0.67
1:A:168:ALA:HB3	1:A:313:MET:HE1	1.76	0.67
1:A:546:TYR:CD2	1:A:546:TYR:N	2.63	0.67
1:A:36:PRO:HD3	1:A:116:PHE:HE1	1.59	0.67
1:A:680:HIS:CG	1:A:681:VAL:HG23	2.29	0.67
1:A:172:THR:O	1:A:183:SER:HA	1.95	0.67
1:A:184:VAL:HG12	1:A:189:GLU:HB2	1.75	0.66
1:A:389:PHE:CE1	1:A:519:ARG:CD	2.77	0.66
1:A:687:LEU:CD2	1:A:692:VAL:HG11	2.25	0.66
1:A:389:PHE:HD2	1:A:540:ILE:HG21	1.48	0.66
1:A:398:TRP:HB2	1:A:401:ILE:HD11	1.76	0.66
1:A:661:LEU:CD2	1:A:733:TYR:CE2	2.79	0.66
1:A:295:ILE:O	1:A:300:GLU:O	2.12	0.66
1:A:27:LYS:C	1:A:28:ILE:HG13	2.15	0.66
1:A:147:HIS:CG	1:A:148:GLU:N	2.63	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ILE:HD11	1:A:602:GLY:HA2	1.78	0.66
1:A:144:THR:O	1:A:158:ILE:HD12	1.95	0.66
1:A:294:GLU:CG	1:A:294:GLU:O	2.44	0.66
1:A:64:ARG:CG	1:A:65:ILE:H	2.09	0.65
1:A:680:HIS:C	1:A:681:VAL:HG23	2.15	0.65
1:A:51:VAL:O	1:A:51:VAL:CG2	2.44	0.65
1:A:661:LEU:HD23	1:A:733:TYR:HE2	1.61	0.65
1:A:70:LYS:HD2	1:A:83:TRP:CZ2	2.32	0.65
1:A:248:THR:O	1:A:248:THR:HG23	1.96	0.65
1:A:52:LYS:HA	1:A:65:ILE:HD13	1.78	0.65
1:A:389:PHE:HE1	1:A:519:ARG:HG2	0.48	0.65
1:A:754:GLU:O	1:A:755:ASP:C	2.35	0.65
1:A:468:MET:O	1:A:471:THR:HG22	1.96	0.65
1:A:624:GLN:HG2	1:A:624:GLN:O	1.97	0.65
1:A:21:LYS:O	1:A:22:GLU:HG2	1.97	0.65
1:A:755:ASP:CG	1:A:756:LEU:N	2.50	0.64
1:A:446:ILE:O	1:A:446:ILE:HG12	1.97	0.64
1:A:335:ARG:HG2	1:A:335:ARG:NH1	2.11	0.64
1:A:169:ARG:CG	1:A:169:ARG:HH11	2.10	0.64
1:A:181:VAL:HG12	1:A:182:GLU:N	2.12	0.64
1:A:289:LYS:HG2	1:A:290:VAL:H	1.62	0.64
1:A:645:LYS:C	1:A:647:VAL:H	1.99	0.64
1:A:360:LYS:O	1:A:364:ARG:CG	2.46	0.64
1:A:66:VAL:HG12	1:A:67:ASP:N	2.13	0.64
1:A:244:ILE:HG22	1:A:245:GLY:H	1.51	0.64
1:A:737:GLN:O	1:A:740:PRO:CD	2.41	0.64
1:A:386:THR:O	1:A:515:THR:HG21	1.98	0.64
1:A:528:GLU:CD	1:A:532:LYS:HD2	2.18	0.63
1:A:647:VAL:C	1:A:649:GLN:N	2.49	0.63
1:A:568:ILE:HD12	1:A:572:LEU:HG	1.80	0.63
1:A:460:GLU:CD	1:A:483:ARG:NH2	2.52	0.63
1:A:754:GLU:OE1	1:A:754:GLU:HA	1.99	0.63
1:A:147:HIS:ND1	1:A:148:GLU:N	2.46	0.63
1:A:657:PRO:HB3	1:A:659:GLU:HG3	1.80	0.63
1:A:262:HIS:HA	3:A:2014:HOH:O	1.98	0.63
1:A:66:VAL:HG12	1:A:67:ASP:H	1.62	0.63
1:A:390:VAL:O	1:A:390:VAL:HG12	1.97	0.63
1:A:383:GLU:CG	1:A:384:SER:H	1.80	0.63
1:A:202:ASP:OD1	1:A:255:ARG:NH2	2.32	0.63
1:A:184:VAL:CG1	1:A:189:GLU:CB	2.77	0.63
1:A:285:LYS:CG	1:A:286:PRO:HD2	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:HD11	1:A:116:PHE:CE2	2.34	0.63
1:A:653:ASN:HB2	1:A:655:GLU:OE2	1.99	0.62
1:A:648:ILE:CD1	1:A:757:ARG:HA	2.29	0.62
1:A:45:ASP:HB2	1:A:83:TRP:HZ2	1.64	0.62
1:A:372:PRO:HB2	1:A:377:TYR:HB2	1.81	0.62
1:A:687:LEU:HG	1:A:692:VAL:HG11	1.82	0.62
1:A:112:TYR:CE1	1:A:370:ASN:OD1	2.53	0.62
1:A:265:ARG:HD3	3:A:2014:HOH:O	1.99	0.62
1:A:151:GLU:O	1:A:152:PHE:HB3	2.00	0.62
1:A:390:VAL:HG12	1:A:592:LYS:HD2	1.82	0.62
1:A:405:ASP:HB2	1:A:581:GLU:HG2	1.82	0.61
1:A:44:ASP:C	1:A:46:SER:N	2.51	0.61
1:A:530:GLU:HG2	1:A:535:PHE:O	2.00	0.61
1:A:160:ILE:HG22	1:A:171:ILE:HB	1.82	0.61
1:A:298:ALA:O	1:A:300:GLU:C	2.39	0.61
1:A:42:LEU:CD1	1:A:106:VAL:CG1	2.78	0.61
1:A:647:VAL:C	1:A:649:GLN:H	2.03	0.61
1:A:209:TYR:O	1:A:210:ASN:CB	2.48	0.61
1:A:7:TYR:HA	1:A:15:VAL:O	2.00	0.61
1:A:264:ILE:HA	1:A:326:PHE:CE2	2.35	0.61
1:A:159:MET:HE1	1:A:308:VAL:HG12	1.82	0.60
1:A:364:ARG:CD	1:A:449:PHE:HE1	2.14	0.60
1:A:655:GLU:N	1:A:655:GLU:OE2	2.34	0.60
1:A:680:HIS:CB	1:A:681:VAL:HG23	2.31	0.60
1:A:58:ARG:NH1	1:A:91:GLN:CB	2.64	0.60
1:A:43:ARG:HB2	1:A:105:ALA:O	2.02	0.60
1:A:650:LYS:HE2	1:A:655:GLU:O	2.02	0.60
1:A:660:LYS:C	1:A:661:LEU:HG	2.07	0.60
1:A:269:ASN:O	1:A:270:LEU:HD23	2.02	0.60
1:A:598:ILE:HA	1:A:603:LYS:O	2.02	0.60
1:A:294:GLU:OE1	1:A:294:GLU:O	2.19	0.60
1:A:78:LYS:CD	1:A:80:ILE:CD1	2.76	0.60
1:A:287:LYS:O	1:A:288:GLU:HG2	2.02	0.60
1:A:380:ARG:O	1:A:382:ARG:N	2.35	0.60
1:A:61:LYS:HG3	1:A:62:ILE:N	2.16	0.60
1:A:538:LEU:O	1:A:539:TYR:HB2	2.02	0.60
1:A:289:LYS:HA	1:A:291:TYR:HE2	1.64	0.59
1:A:609:LEU:O	1:A:610:GLU:C	2.39	0.59
1:A:335:ARG:CG	1:A:335:ARG:HH11	2.14	0.59
1:A:114:ILE:HG22	1:A:115:PRO:O	2.03	0.59
1:A:438:VAL:HG13	1:A:440:HIS:CD2	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ALA:HA	1:A:302:GLY:O	2.02	0.59
1:A:661:LEU:HD23	1:A:733:TYR:CE2	2.37	0.59
1:A:31:ASP:C	1:A:31:ASP:OD1	2.40	0.59
1:A:657:PRO:C	1:A:659:GLU:H	2.05	0.59
1:A:9:THR:HG23	1:A:13:LYS:O	2.02	0.59
1:A:20:LYS:HZ3	1:A:29:GLU:HG2	1.67	0.59
1:A:184:VAL:CG1	1:A:189:GLU:HB3	2.32	0.59
1:A:390:VAL:O	1:A:390:VAL:CG1	2.51	0.58
1:A:545:LEU:N	1:A:545:LEU:CD2	2.66	0.58
1:A:244:ILE:O	1:A:245:GLY:O	2.21	0.58
1:A:58:ARG:N	1:A:61:LYS:O	2.36	0.58
1:A:595:TYR:C	1:A:595:TYR:CD1	2.76	0.58
1:A:234:ARG:HG3	1:A:255:ARG:NH1	2.18	0.58
1:A:17:ARG:HG2	1:A:30:HIS:CD2	2.38	0.58
1:A:390:VAL:HG12	1:A:592:LYS:CD	2.33	0.58
1:A:661:LEU:HD22	1:A:733:TYR:CE2	2.38	0.58
1:A:214:PHE:O	1:A:217:PRO:HD2	2.03	0.58
1:A:169:ARG:NH2	1:A:182:GLU:OE1	2.37	0.58
1:A:746:LEU:O	1:A:747:GLU:C	2.41	0.58
1:A:754:GLU:OE1	1:A:754:GLU:CA	2.50	0.58
1:A:729:ASP:CB	1:A:732:TYR:HB2	2.28	0.58
1:A:100:VAL:O	1:A:106:VAL:CG2	2.52	0.58
1:A:733:TYR:O	1:A:737:GLN:HB3	2.03	0.58
1:A:1:MET:HG2	1:A:2:ILE:N	2.19	0.58
1:A:687:LEU:CG	1:A:692:VAL:HG11	2.33	0.58
1:A:196:ARG:HA	1:A:199:ARG:CZ	2.34	0.58
1:A:569:ASN:HD21	1:A:578:LEU:H	1.50	0.57
1:A:206:ILE:HD12	1:A:207:VAL:N	2.19	0.57
1:A:644:VAL:HG13	1:A:742:VAL:HG11	1.86	0.57
1:A:7:TYR:HB2	1:A:15:VAL:O	2.04	0.57
1:A:184:VAL:CG1	1:A:189:GLU:HB2	2.33	0.57
1:A:294:GLU:HG2	1:A:294:GLU:O	2.04	0.57
1:A:440:HIS:CE1	1:A:509:GLU:HG2	2.38	0.57
1:A:264:ILE:HG12	1:A:326:PHE:CZ	2.39	0.57
1:A:176:ILE:CD1	1:A:305:LEU:CD2	2.63	0.57
1:A:159:MET:CE	1:A:308:VAL:HG12	2.35	0.57
1:A:752:ARG:HD2	1:A:753:LYS:HG2	1.86	0.57
1:A:680:HIS:C	1:A:682:ALA:H	2.05	0.57
1:A:618:GLU:HB3	1:A:660:LYS:HB3	1.87	0.57
1:A:377:TYR:O	1:A:377:TYR:CD2	2.58	0.57
1:A:145:LEU:HG	1:A:156:PRO:HD2	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:HD11	1:A:322:LEU:HB2	1.86	0.56
1:A:244:ILE:O	1:A:245:GLY:C	2.42	0.56
1:A:119:ARG:HD2	1:A:123:ASP:OD2	2.05	0.56
1:A:529:LEU:HD13	1:A:564:PHE:CE2	2.40	0.56
1:A:175:ASN:N	1:A:175:ASN:OD1	2.37	0.56
1:A:289:LYS:O	1:A:290:VAL:CG2	2.38	0.56
1:A:685:LYS:CA	1:A:685:LYS:HE3	2.30	0.56
1:A:294:GLU:CB	3:A:2016:HOH:O	2.53	0.56
1:A:122:ILE:HG12	1:A:359:ARG:NH1	2.20	0.56
1:A:252:VAL:CG1	1:A:255:ARG:HG3	2.35	0.56
1:A:299:TRP:O	1:A:300:GLU:CB	2.38	0.56
1:A:641:VAL:C	1:A:643:ILE:N	2.59	0.56
1:A:196:ARG:HA	1:A:199:ARG:NH2	2.21	0.56
1:A:168:ALA:HB3	1:A:313:MET:CE	2.36	0.56
1:A:432:TYR:CE2	1:A:441:LYS:HD2	2.40	0.56
1:A:446:ILE:O	1:A:447:PRO:O	2.24	0.56
1:A:87:LEU:HD21	1:A:96:LEU:HG	1.87	0.56
1:A:620:ALA:O	1:A:623:THR:N	2.39	0.56
1:A:389:PHE:CD1	1:A:519:ARG:HG3	2.40	0.55
1:A:169:ARG:HG3	1:A:169:ARG:HH11	1.71	0.55
1:A:58:ARG:HH12	1:A:91:GLN:HG3	1.70	0.55
1:A:137:ILE:N	1:A:137:ILE:HD12	2.21	0.55
1:A:755:ASP:O	1:A:757:ARG:N	2.39	0.55
1:A:335:ARG:HG2	1:A:335:ARG:HH11	1.68	0.55
1:A:274:THR:HB	1:A:276:GLU:HG2	1.88	0.55
1:A:735:GLU:CD	1:A:757:ARG:HH21	2.10	0.55
1:A:735:GLU:O	1:A:740:PRO:HD3	2.07	0.55
1:A:122:ILE:HG12	1:A:359:ARG:HH11	1.70	0.55
1:A:68:VAL:O	1:A:68:VAL:HG12	2.05	0.55
1:A:407:LYS:HG3	1:A:577:GLU:HG2	1.87	0.55
1:A:72:GLU:O	1:A:72:GLU:OE2	2.24	0.55
1:A:264:ILE:HA	1:A:326:PHE:HE2	1.72	0.55
1:A:31:ASP:OD1	1:A:32:ARG:N	2.39	0.55
1:A:645:LYS:O	1:A:647:VAL:N	2.35	0.55
1:A:182:GLU:CG	1:A:193:ARG:HH22	2.11	0.54
1:A:270:LEU:CD2	1:A:271:PRO:HD2	2.31	0.54
1:A:188:LYS:HE3	1:A:226:LEU:HG	1.89	0.54
1:A:695:LYS:O	1:A:697:GLY:N	2.36	0.54
1:A:687:LEU:HD23	1:A:692:VAL:CG1	2.38	0.54
1:A:293:ASP:C	1:A:295:ILE:H	2.10	0.54
1:A:617:SER:CB	1:A:737:GLN:HE21	2.17	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:VAL:HG12	1:A:67:ASP:OD2	2.07	0.54
1:A:596:ALA:O	1:A:597:VAL:HG12	2.08	0.54
1:A:620:ALA:O	1:A:621:LYS:C	2.46	0.53
1:A:416:THR:CG2	1:A:574:GLY:HA3	2.39	0.53
1:A:464:ILE:HD11	1:A:483:ARG:NH2	2.22	0.53
1:A:8:ILE:HG13	1:A:15:VAL:HB	1.90	0.53
1:A:497:TYR:CZ	1:A:503:ALA:HB1	2.43	0.53
1:A:48:ILE:O	1:A:52:LYS:HG3	2.08	0.53
1:A:64:ARG:HG2	1:A:65:ILE:N	2.23	0.53
1:A:195:LEU:HA	1:A:198:ILE:HD11	1.88	0.53
1:A:559:LYS:O	1:A:563:GLU:HG3	2.08	0.53
1:A:639:GLU:O	1:A:642:ARG:HB3	2.08	0.53
1:A:264:ILE:C	1:A:266:THR:H	2.12	0.53
1:A:753:LYS:O	1:A:754:GLU:O	2.26	0.53
1:A:45:ASP:OD1	1:A:45:ASP:N	2.41	0.53
1:A:144:THR:CG2	1:A:145:LEU:N	2.47	0.53
1:A:169:ARG:NH1	1:A:182:GLU:OE1	2.42	0.53
1:A:432:TYR:C	1:A:432:TYR:CD1	2.79	0.53
1:A:264:ILE:HG22	1:A:265:ARG:N	2.23	0.53
1:A:66:VAL:HG12	1:A:67:ASP:CG	2.28	0.53
1:A:549:ILE:CG1	1:A:557:ILE:HG12	2.38	0.53
1:A:538:LEU:O	1:A:539:TYR:CB	2.55	0.53
1:A:130:GLU:O	1:A:131:GLY:O	2.27	0.53
1:A:335:ARG:NH1	1:A:335:ARG:CG	2.72	0.53
1:A:424:LEU:C	1:A:424:LEU:HD22	2.29	0.52
1:A:388:GLY:H	1:A:515:THR:CG2	2.22	0.52
1:A:78:LYS:CD	1:A:80:ILE:HD12	2.31	0.52
1:A:169:ARG:HH22	1:A:182:GLU:CD	2.12	0.52
1:A:364:ARG:HD2	1:A:449:PHE:HE1	1.73	0.52
1:A:473:ASP:OD2	1:A:473:ASP:C	2.47	0.52
1:A:195:LEU:CA	1:A:198:ILE:HD13	2.40	0.52
1:A:63:VAL:HG21	1:A:95:THR:HG21	1.91	0.52
1:A:745:ILE:HG22	1:A:746:LEU:CD2	2.35	0.52
1:A:146:TYR:O	1:A:147:HIS:O	2.26	0.52
1:A:264:ILE:O	1:A:266:THR:N	2.33	0.52
1:A:460:GLU:CD	1:A:483:ARG:HH21	2.13	0.52
1:A:241:MET:N	1:A:241:MET:SD	2.82	0.52
1:A:81:THR:O	1:A:82:VAL:CG1	2.58	0.52
1:A:81:THR:O	1:A:82:VAL:HG13	2.10	0.52
1:A:169:ARG:CB	1:A:169:ARG:HH11	2.23	0.52
1:A:222:ARG:HG3	1:A:222:ARG:O	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ASP:HB2	1:A:83:TRP:CZ2	2.44	0.52
1:A:464:ILE:HG22	1:A:468:MET:HE2	1.92	0.52
1:A:434:ILE:HG23	1:A:441:LYS:HG2	1.92	0.52
1:A:148:GLU:OE1	1:A:148:GLU:HA	2.10	0.52
1:A:122:ILE:CA	1:A:359:ARG:HH12	2.18	0.52
1:A:328:PRO:O	1:A:332:GLN:HG2	2.10	0.52
1:A:438:VAL:CG2	1:A:438:VAL:O	2.58	0.51
1:A:141:ASP:OD1	1:A:315:ASP:HB3	2.10	0.51
1:A:84:LYS:HD3	1:A:86:TYR:CZ	2.45	0.51
1:A:700:ILE:HD12	1:A:700:ILE:O	2.10	0.51
1:A:313:MET:HE2	1:A:313:MET:O	2.11	0.51
1:A:687:LEU:HD23	1:A:692:VAL:HG11	1.92	0.51
1:A:169:ARG:HB3	1:A:169:ARG:HH11	1.76	0.51
1:A:650:LYS:O	1:A:656:ILE:CD1	2.58	0.51
1:A:436:PRO:HG2	1:A:517:TRP:HA	1.93	0.51
1:A:378:GLN:HA	1:A:381:LEU:HD12	1.92	0.51
1:A:446:ILE:C	1:A:447:PRO:O	2.47	0.51
1:A:264:ILE:HD13	1:A:278:VAL:HG21	1.93	0.50
1:A:184:VAL:HG11	1:A:189:GLU:CB	2.40	0.50
1:A:732:TYR:O	1:A:733:TYR:C	2.49	0.50
1:A:7:TYR:CA	1:A:15:VAL:O	2.58	0.50
1:A:401:ILE:HD13	1:A:538:LEU:CD1	2.41	0.50
1:A:703:ILE:HG13	1:A:704:VAL:H	1.76	0.50
1:A:523:GLU:O	1:A:526:TRP:HB3	2.11	0.50
1:A:289:LYS:HG3	1:A:291:TYR:CE2	2.46	0.50
1:A:750:GLY:O	1:A:751:TYR:O	2.30	0.50
1:A:48:ILE:CG1	1:A:49:GLU:N	2.67	0.50
1:A:20:LYS:HZ2	1:A:29:GLU:HG2	1.72	0.50
1:A:142:ILE:HD12	1:A:142:ILE:C	2.32	0.50
1:A:264:ILE:HG12	1:A:326:PHE:CE2	2.46	0.50
1:A:303:GLU:OE2	1:A:306:GLU:CB	2.54	0.50
1:A:151:GLU:O	1:A:152:PHE:CB	2.59	0.50
1:A:754:GLU:O	1:A:757:ARG:HB2	2.12	0.50
1:A:644:VAL:CG1	1:A:742:VAL:HG11	2.41	0.50
1:A:377:TYR:C	1:A:377:TYR:CD2	2.86	0.50
1:A:225:LYS:HD3	1:A:226:LEU:HD13	1.94	0.50
1:A:280:GLU:HG3	1:A:284:GLY:O	2.11	0.50
1:A:89:HIS:CD2	1:A:91:GLN:HG3	2.46	0.50
1:A:314:GLU:O	1:A:315:ASP:C	2.49	0.50
1:A:730:ALA:C	1:A:732:TYR:H	2.14	0.49
1:A:640:ALA:O	1:A:643:ILE:N	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:VAL:O	1:A:694:ILE:HB	2.12	0.49
1:A:76:LEU:O	1:A:422:ASP:HB2	2.12	0.49
1:A:735:GLU:OE1	1:A:757:ARG:NE	2.42	0.49
1:A:569:ASN:HD22	1:A:572:LEU:HD12	1.77	0.49
1:A:619:ILE:HD11	1:A:651:LEU:HD11	1.93	0.49
1:A:57:GLU:H	1:A:63:VAL:HG23	1.77	0.49
1:A:313:MET:CE	1:A:317:LYS:HD2	2.42	0.49
1:A:44:ASP:C	1:A:46:SER:H	2.15	0.49
1:A:404:LEU:HB3	1:A:578:LEU:HD13	1.94	0.49
1:A:16:ILE:O	1:A:30:HIS:HA	2.12	0.49
1:A:617:SER:HG	1:A:737:GLN:NE2	2.02	0.49
1:A:377:TYR:O	1:A:381:LEU:CD1	2.61	0.49
1:A:528:GLU:OE1	1:A:532:LYS:CD	2.44	0.49
1:A:409:LEU:HD11	1:A:413:ILE:HD11	1.94	0.49
1:A:288:GLU:O	1:A:289:LYS:HB2	2.13	0.49
1:A:2:ILE:CG2	1:A:3:LEU:N	2.74	0.49
1:A:191:ILE:O	1:A:195:LEU:HG	2.13	0.49
1:A:20:LYS:CE	3:A:2003:HOH:O	2.57	0.49
1:A:415:ILE:CD1	1:A:458:LEU:HD12	2.42	0.49
1:A:645:LYS:C	1:A:647:VAL:N	2.65	0.49
1:A:312:SER:C	1:A:314:GLU:N	2.64	0.49
1:A:661:LEU:HB3	1:A:733:TYR:OH	2.13	0.49
1:A:91:GLN:O	1:A:94:PRO:HD2	2.12	0.49
1:A:657:PRO:HB3	1:A:659:GLU:OE2	2.13	0.48
1:A:745:ILE:HG22	1:A:746:LEU:N	2.26	0.48
1:A:63:VAL:HG11	1:A:92:ASP:HA	1.93	0.48
1:A:295:ILE:O	1:A:297:LYS:N	2.46	0.48
1:A:392:GLU:OE2	1:A:591:THR:HG22	2.13	0.48
1:A:680:HIS:HB2	1:A:681:VAL:HG23	1.95	0.48
1:A:43:ARG:HD2	1:A:105:ALA:HA	1.95	0.48
1:A:264:ILE:CG1	1:A:326:PHE:CE2	2.97	0.48
1:A:140:PHE:HB2	1:A:161:SER:O	2.12	0.48
1:A:93:VAL:HB	1:A:94:PRO:HD3	1.94	0.48
1:A:702:TYR:HD2	1:A:702:TYR:H	1.59	0.48
1:A:353:VAL:O	1:A:356:PHE:HB3	2.14	0.48
1:A:127:ILE:HD13	1:A:359:ARG:HH21	1.78	0.48
1:A:160:ILE:HG23	1:A:171:ILE:HB	1.92	0.48
1:A:656:ILE:O	1:A:657:PRO:C	2.51	0.48
1:A:468:MET:HA	1:A:471:THR:HG22	1.95	0.48
1:A:468:MET:O	1:A:470:GLU:N	2.47	0.48
1:A:76:LEU:HG	1:A:422:ASP:HB3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:VAL:HG12	1:A:628:LEU:N	2.29	0.48
1:A:694:ILE:HA	1:A:698:MET:HG3	1.94	0.47
1:A:694:ILE:HG12	1:A:698:MET:HG3	1.95	0.47
1:A:478:ILE:HG13	1:A:482:TYR:CE1	2.49	0.47
1:A:230:LEU:O	1:A:238:GLU:HA	2.14	0.47
1:A:596:ALA:O	1:A:597:VAL:CG1	2.62	0.47
1:A:732:TYR:CD1	1:A:736:ASN:HB3	2.50	0.47
1:A:435:ALA:HA	1:A:436:PRO:HD2	1.73	0.47
1:A:405:ASP:CB	1:A:581:GLU:HG3	2.42	0.47
1:A:4:ASP:C	1:A:5:VAL:HG23	2.34	0.47
1:A:289:LYS:C	1:A:290:VAL:HG23	2.30	0.47
1:A:95:THR:O	1:A:95:THR:CG2	2.62	0.47
1:A:271:PRO:CG	1:A:272:THR:H	2.26	0.47
1:A:136:LYS:C	1:A:137:ILE:HD12	2.35	0.47
1:A:369:PRO:O	1:A:504:ARG:HD3	2.13	0.47
1:A:182:GLU:HG2	1:A:193:ARG:CZ	2.40	0.47
1:A:181:VAL:CG1	1:A:182:GLU:N	2.78	0.47
1:A:549:ILE:HG12	1:A:557:ILE:HG12	1.97	0.47
1:A:703:ILE:HG13	1:A:704:VAL:N	2.30	0.47
1:A:287:LYS:O	1:A:288:GLU:CB	2.63	0.47
1:A:731:GLU:O	1:A:735:GLU:CB	2.50	0.47
1:A:113:ASP:OD2	1:A:113:ASP:N	2.46	0.47
1:A:47:LYS:O	1:A:48:ILE:C	2.53	0.47
1:A:432:TYR:OH	1:A:441:LYS:NZ	2.40	0.47
1:A:523:GLU:O	1:A:524:LEU:C	2.53	0.46
1:A:59:HIS:CD2	1:A:59:HIS:O	2.68	0.46
1:A:264:ILE:HD13	1:A:278:VAL:HG11	1.97	0.46
1:A:341:LEU:HA	1:A:344:VAL:HB	1.97	0.46
1:A:468:MET:C	1:A:470:GLU:H	2.19	0.46
1:A:62:ILE:HD12	1:A:62:ILE:H	1.77	0.46
1:A:408:SER:HB2	1:A:411:PRO:HG2	1.97	0.46
1:A:283:PHE:N	1:A:283:PHE:CD1	2.83	0.46
1:A:445:ASP:N	1:A:445:ASP:OD1	2.48	0.46
1:A:202:ASP:HA	1:A:255:ARG:NH2	2.30	0.46
1:A:649:GLN:O	1:A:653:ASN:OD1	2.33	0.46
1:A:148:GLU:CA	1:A:148:GLU:OE1	2.63	0.46
1:A:731:GLU:HG3	1:A:735:GLU:HG3	1.97	0.46
1:A:178:LEU:HD13	1:A:180:TYR:CZ	2.50	0.46
1:A:160:ILE:HG23	1:A:160:ILE:O	2.15	0.46
1:A:400:ASN:OD1	1:A:554:SER:HB2	2.16	0.46
1:A:655:GLU:N	1:A:655:GLU:CD	2.69	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:ALA:C	1:A:732:TYR:N	2.68	0.46
1:A:641:VAL:C	1:A:643:ILE:H	2.17	0.46
1:A:513:SER:O	1:A:517:TRP:HB2	2.15	0.46
1:A:703:ILE:CG1	1:A:704:VAL:N	2.79	0.46
1:A:295:ILE:O	1:A:296:ALA:C	2.53	0.46
1:A:169:ARG:CG	1:A:169:ARG:NH1	2.78	0.46
1:A:223:ALA:O	1:A:225:LYS:N	2.48	0.46
1:A:61:LYS:CG	1:A:62:ILE:N	2.79	0.45
1:A:461:ARG:HE	1:A:484:GLN:HG2	1.80	0.45
1:A:426:LEU:HA	1:A:426:LEU:HD12	1.63	0.45
1:A:631:ILE:CD1	1:A:637:VAL:HA	2.46	0.45
1:A:735:GLU:OE1	1:A:757:ARG:NH2	2.48	0.45
1:A:56:GLY:C	1:A:63:VAL:HG23	2.36	0.45
1:A:656:ILE:HG12	1:A:656:ILE:O	2.16	0.45
1:A:661:LEU:HD22	1:A:733:TYR:CZ	2.51	0.45
1:A:263:VAL:O	1:A:266:THR:HG21	2.16	0.45
1:A:4:ASP:O	1:A:5:VAL:CG2	2.64	0.45
1:A:119:ARG:O	1:A:119:ARG:HD3	2.16	0.45
1:A:313:MET:HE2	1:A:317:LYS:HD2	1.99	0.45
1:A:73:LYS:NZ	1:A:365:ASN:OD1	2.28	0.45
1:A:58:ARG:NH1	1:A:91:GLN:HG3	2.32	0.45
1:A:359:ARG:HG3	1:A:359:ARG:NH1	2.30	0.45
1:A:75:PHE:O	1:A:77:GLY:N	2.49	0.45
1:A:355:TRP:CZ3	1:A:358:LEU:HD13	2.51	0.45
1:A:327:LEU:O	1:A:331:ILE:HG12	2.17	0.45
1:A:7:TYR:CB	1:A:15:VAL:O	2.64	0.45
1:A:322:LEU:HA	1:A:322:LEU:HD23	1.70	0.45
1:A:653:ASN:O	1:A:654:TYR:CB	2.53	0.45
1:A:591:THR:HB	1:A:592:LYS:H	1.37	0.45
1:A:176:ILE:HA	1:A:176:ILE:HD13	1.61	0.45
1:A:287:LYS:O	1:A:288:GLU:CG	2.64	0.45
1:A:432:TYR:CZ	1:A:441:LYS:HD2	2.51	0.45
1:A:135:LEU:HD23	1:A:135:LEU:HA	1.65	0.45
1:A:646:GLU:O	1:A:646:GLU:HG2	2.17	0.45
1:A:412:SER:HB2	1:A:575:LEU:HD13	1.99	0.45
1:A:392:GLU:HA	1:A:393:PRO:HD3	1.72	0.45
1:A:162:TYR:CE1	1:A:169:ARG:HG2	2.52	0.45
1:A:294:GLU:CD	1:A:294:GLU:O	2.55	0.45
1:A:214:PHE:C	1:A:217:PRO:HD2	2.36	0.45
1:A:568:ILE:C	1:A:568:ILE:HD13	2.36	0.45
1:A:177:ASP:O	1:A:177:ASP:OD2	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:TYR:O	1:A:381:LEU:HD11	2.16	0.44
1:A:464:ILE:HG21	1:A:484:GLN:HB2	1.99	0.44
1:A:1:MET:HG2	1:A:2:ILE:H	1.79	0.44
1:A:327:LEU:CD2	1:A:331:ILE:HD11	2.47	0.44
1:A:5:VAL:HG12	1:A:117:ALA:HB1	1.99	0.44
1:A:399:GLU:HG3	1:A:400:ASN:ND2	2.33	0.44
1:A:561:ALA:O	1:A:562:LEU:C	2.56	0.44
1:A:650:LYS:O	1:A:656:ILE:HD12	2.17	0.44
1:A:296:ALA:HB1	1:A:305:LEU:CB	2.34	0.44
1:A:378:GLN:CA	1:A:378:GLN:OE1	2.56	0.44
1:A:267:THR:HB	1:A:268:ILE:H	1.41	0.44
1:A:468:MET:C	1:A:470:GLU:N	2.71	0.44
1:A:461:ARG:NH2	1:A:484:GLN:HE21	2.07	0.44
1:A:17:ARG:HG2	1:A:30:HIS:HD2	1.80	0.44
1:A:596:ALA:C	1:A:597:VAL:CG1	2.86	0.44
1:A:279:TYR:CE1	1:A:283:PHE:CE1	3.06	0.44
1:A:327:LEU:N	1:A:328:PRO:HD3	2.33	0.44
1:A:327:LEU:N	1:A:328:PRO:CD	2.80	0.44
1:A:164:ASP:HA	1:A:320:TYR:CE1	2.52	0.44
1:A:702:TYR:N	1:A:702:TYR:CD2	2.86	0.44
1:A:736:ASN:HD22	1:A:737:GLN:N	2.16	0.44
1:A:70:LYS:HD2	1:A:83:TRP:CH2	2.53	0.44
1:A:421:PRO:O	1:A:424:LEU:HB3	2.18	0.44
1:A:141:ASP:OD1	1:A:315:ASP:CB	2.66	0.44
1:A:4:ASP:O	1:A:5:VAL:HG23	2.18	0.44
1:A:294:GLU:CD	1:A:294:GLU:C	2.76	0.44
1:A:276:GLU:O	1:A:277:ALA:C	2.54	0.44
1:A:636:ASP:OD1	1:A:639:GLU:N	2.48	0.43
1:A:186:THR:OG1	1:A:188:LYS:N	2.50	0.43
1:A:285:LYS:HG2	1:A:286:PRO:CD	2.36	0.43
1:A:744:ARG:O	1:A:745:ILE:C	2.56	0.43
1:A:588:PHE:HE1	1:A:590:VAL:HG23	1.82	0.43
1:A:754:GLU:O	1:A:757:ARG:N	2.32	0.43
1:A:57:GLU:N	1:A:63:VAL:CG2	2.75	0.43
1:A:7:TYR:HB3	1:A:16:ILE:HD13	1.98	0.43
1:A:285:LYS:CB	1:A:286:PRO:HD2	2.49	0.43
1:A:2:ILE:HG22	1:A:3:LEU:N	2.32	0.43
1:A:20:LYS:HD2	1:A:29:GLU:HG2	2.01	0.43
1:A:529:LEU:HD13	1:A:564:PHE:CD2	2.53	0.43
1:A:144:THR:HG22	1:A:145:LEU:O	2.18	0.43
1:A:39:TYR:O	1:A:109:ILE:HA	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:THR:O	1:A:248:THR:CG2	2.65	0.43
1:A:21:LYS:O	1:A:22:GLU:CG	2.65	0.43
1:A:755:ASP:O	1:A:756:LEU:C	2.56	0.43
1:A:195:LEU:O	1:A:198:ILE:HD13	2.17	0.43
1:A:265:ARG:C	1:A:266:THR:HG22	2.39	0.43
1:A:416:THR:HG23	1:A:574:GLY:HA3	1.99	0.43
1:A:389:PHE:HD2	1:A:540:ILE:HG22	1.80	0.43
1:A:289:LYS:CA	1:A:291:TYR:HE2	2.31	0.43
1:A:122:ILE:CG1	1:A:359:ARG:NH1	2.82	0.43
1:A:752:ARG:O	1:A:755:ASP:OD1	2.37	0.43
1:A:47:LYS:C	1:A:49:GLU:N	2.72	0.43
1:A:626:ARG:O	1:A:630:THR:OG1	2.35	0.43
1:A:464:ILE:O	1:A:465:LYS:C	2.56	0.43
1:A:457:LEU:O	1:A:458:LEU:C	2.58	0.43
1:A:251:GLU:HA	1:A:342:TRP:CD1	2.53	0.42
1:A:648:ILE:O	1:A:734:ILE:HD11	2.19	0.42
1:A:175:ASN:O	1:A:176:ILE:HD13	2.19	0.42
1:A:45:ASP:O	1:A:48:ILE:HG22	2.10	0.42
1:A:651:LEU:HD12	1:A:656:ILE:CD1	2.49	0.42
1:A:285:LYS:HA	1:A:286:PRO:HD3	1.38	0.42
1:A:177:ASP:O	1:A:177:ASP:CG	2.58	0.42
1:A:619:ILE:CD1	1:A:651:LEU:HD11	2.50	0.42
1:A:176:ILE:O	1:A:178:LEU:N	2.44	0.42
1:A:103:HIS:HB3	1:A:106:VAL:HG22	2.01	0.42
1:A:63:VAL:HG12	1:A:92:ASP:HB3	2.01	0.42
1:A:160:ILE:CG2	1:A:160:ILE:O	2.68	0.42
1:A:264:ILE:C	1:A:266:THR:N	2.72	0.42
1:A:588:PHE:CE1	1:A:590:VAL:HG23	2.54	0.42
1:A:378:GLN:CA	1:A:381:LEU:HD12	2.50	0.42
1:A:690:LYS:O	1:A:692:VAL:HG23	2.19	0.42
1:A:445:ASP:C	1:A:446:ILE:HG23	2.40	0.42
1:A:44:ASP:O	1:A:46:SER:N	2.52	0.42
1:A:145:LEU:CG	1:A:156:PRO:HD2	2.49	0.42
1:A:383:GLU:C	1:A:385:TYR:N	2.72	0.42
1:A:641:VAL:O	1:A:644:VAL:HG23	2.20	0.42
1:A:142:ILE:HG22	1:A:160:ILE:HG13	2.01	0.42
1:A:293:ASP:C	1:A:295:ILE:N	2.73	0.42
1:A:464:ILE:HG22	1:A:468:MET:CE	2.49	0.42
1:A:58:ARG:HG2	1:A:59:HIS:H	1.85	0.42
1:A:337:VAL:O	1:A:359:ARG:HD2	2.19	0.42
1:A:266:THR:C	1:A:267:THR:O	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:ARG:O	1:A:595:TYR:HB3	2.20	0.42
1:A:750:GLY:C	1:A:751:TYR:O	2.56	0.42
1:A:522:ILE:O	1:A:523:GLU:O	2.38	0.42
1:A:55:THR:OG1	1:A:56:GLY:N	2.53	0.42
1:A:66:VAL:CG1	1:A:67:ASP:N	2.82	0.42
1:A:270:LEU:HD13	1:A:271:PRO:HD2	2.02	0.42
1:A:81:THR:C	1:A:82:VAL:HG13	2.40	0.42
1:A:732:TYR:CE1	1:A:736:ASN:HB3	2.55	0.41
1:A:657:PRO:HA	1:A:658:PRO:HD3	1.67	0.41
1:A:58:ARG:CG	1:A:59:HIS:H	2.33	0.41
1:A:65:ILE:O	1:A:65:ILE:HG23	2.20	0.41
1:A:522:ILE:O	1:A:523:GLU:C	2.58	0.41
1:A:732:TYR:O	1:A:734:ILE:N	2.54	0.41
1:A:568:ILE:O	1:A:571:LYS:N	2.41	0.41
1:A:657:PRO:CB	1:A:659:GLU:HG3	2.49	0.41
1:A:197:ILE:C	1:A:199:ARG:N	2.73	0.41
1:A:497:TYR:CE2	1:A:503:ALA:HB1	2.56	0.41
1:A:334:SER:HA	1:A:344:VAL:HG21	2.02	0.41
1:A:629:GLU:O	1:A:633:LYS:HB3	2.20	0.41
1:A:658:PRO:HA	1:A:661:LEU:CD1	2.51	0.41
1:A:372:PRO:HG3	1:A:380:ARG:HH12	1.84	0.41
1:A:377:TYR:CD2	1:A:381:LEU:HD11	2.56	0.41
1:A:209:TYR:HB2	1:A:319:THR:HG23	2.03	0.41
1:A:9:THR:CG2	1:A:13:LYS:O	2.68	0.41
1:A:421:PRO:HD2	1:A:422:ASP:H	1.86	0.41
1:A:464:ILE:HD13	1:A:483:ARG:HB2	2.02	0.41
1:A:228:ILE:HG22	1:A:228:ILE:O	2.20	0.41
1:A:438:VAL:CG1	1:A:440:HIS:CD2	3.02	0.41
1:A:292:ALA:C	1:A:294:GLU:H	2.24	0.41
1:A:31:ASP:OD1	1:A:33:THR:N	2.48	0.41
1:A:389:PHE:HZ	1:A:523:GLU:HG3	1.86	0.41
1:A:126:LEU:O	1:A:359:ARG:NH2	2.54	0.41
1:A:630:THR:HG21	1:A:639:GLU:CG	2.46	0.41
1:A:252:VAL:HG12	1:A:252:VAL:O	2.21	0.41
1:A:749:PHE:CD1	1:A:749:PHE:N	2.88	0.41
1:A:437:GLN:NE2	1:A:519:ARG:NH2	2.53	0.40
1:A:651:LEU:HD12	1:A:656:ILE:HD11	2.03	0.40
1:A:598:ILE:HB	1:A:604:VAL:HG22	2.02	0.40
1:A:307:ARG:O	1:A:310:LYS:HB3	2.21	0.40
1:A:303:GLU:HB3	1:A:304:ASN:H	1.54	0.40
1:A:169:ARG:HG3	1:A:169:ARG:NH1	2.32	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ASP:OD2	1:A:475:ILE:HB	2.20	0.40
1:A:569:ASN:HA	1:A:569:ASN:HD22	1.62	0.40
1:A:547:ALA:O	1:A:548:THR:HB	2.22	0.40
1:A:390:VAL:HG12	1:A:592:LYS:HD3	2.03	0.40
1:A:291:TYR:CD2	1:A:291:TYR:N	2.88	0.40
1:A:473:ASP:OD2	1:A:474:PRO:N	2.54	0.40
1:A:95:THR:O	1:A:95:THR:HG22	2.20	0.40
1:A:391:LYS:HE2	1:A:526:TRP:HZ3	1.86	0.40
1:A:657:PRO:C	1:A:659:GLU:N	2.73	0.40
1:A:196:ARG:O	1:A:196:ARG:HG2	2.20	0.40
1:A:303:GLU:O	1:A:304:ASN:C	2.59	0.40
1:A:83:TRP:O	1:A:85:LEU:HD23	2.22	0.40
1:A:461:ARG:NE	1:A:488:LYS:HB2	2.36	0.40
1:A:3:LEU:HD22	1:A:256:ILE:CD1	2.38	0.40
1:A:364:ARG:HD3	1:A:449:PHE:CE1	2.56	0.40
1:A:173:TRP:CD1	1:A:173:TRP:N	2.90	0.40
1:A:173:TRP:HB3	1:A:184:VAL:O	2.22	0.40
1:A:259:ASP:O	1:A:260:LEU:C	2.57	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	704/775 (91%)	521 (74%)	109 (16%)	74 (10%)	1 0

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ILE
1	A	59	HIS
1	A	67	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	76	LEU
1	A	131	GLY
1	A	147	HIS
1	A	177	ASP
1	A	185	SER
1	A	265	ARG
1	A	267	THR
1	A	285	LYS
1	A	286	PRO
1	A	288	GLU
1	A	290	VAL
1	A	292	ALA
1	A	298	ALA
1	A	303	GLU
1	A	304	ASN
1	A	383	GLU
1	A	384	SER
1	A	385	TYR
1	A	391	LYS
1	A	436	PRO
1	A	523	GLU
1	A	539	TYR
1	A	542	THR
1	A	690	LYS
1	A	693	LYS
1	A	738	VAL
1	A	748	GLY
1	A	754	GLU
1	A	51	VAL
1	A	164	ASP
1	A	244	ILE
1	A	299	TRP
1	A	395	LYS
1	A	447	PRO
1	A	524	LEU
1	A	646	GLU
1	A	733	TYR
1	A	751	TYR
1	A	753	LYS
1	A	755	ASP
1	A	756	LEU
1	A	45	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	439	GLY
1	A	507	CYS
1	A	654	TYR
1	A	657	PRO
1	A	757	ARG
1	A	11	GLU
1	A	54	ILE
1	A	152	PHE
1	A	296	ALA
1	A	379	ARG
1	A	380	ARG
1	A	469	LYS
1	A	696	PRO
1	A	57	GLU
1	A	245	GLY
1	A	281	ALA
1	A	300	GLU
1	A	381	LEU
1	A	386	THR
1	A	390	VAL
1	A	639	GLU
1	A	732	TYR
1	A	556	GLU
1	A	692	VAL
1	A	745	ILE
1	A	68	VAL
1	A	388	GLY
1	A	697	GLY
1	A	271	PRO

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	624/682 (92%)	498 (80%)	126 (20%)	1 2

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	6	ASP
1	A	11	GLU
1	A	27	LYS
1	A	29	GLU
1	A	33	THR
1	A	38	ILE
1	A	43	ARG
1	A	57	GLU
1	A	63	VAL
1	A	72	GLU
1	A	78	LYS
1	A	80	ILE
1	A	81	THR
1	A	85	LEU
1	A	88	GLU
1	A	93	VAL
1	A	101	ARG
1	A	108	ASP
1	A	115	PRO
1	A	132	GLU
1	A	150	GLU
1	A	154	LYS
1	A	167	GLU
1	A	169	ARG
1	A	174	LYS
1	A	175	ASN
1	A	177	ASP
1	A	182	GLU
1	A	186	THR
1	A	193	ARG
1	A	198	ILE
1	A	199	ARG
1	A	200	GLU
1	A	201	LYS
1	A	206	ILE
1	A	213	SER
1	A	225	LYS
1	A	230	LEU
1	A	239	PRO
1	A	241	MET
1	A	242	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	243	ARG
1	A	244	ILE
1	A	251	GLU
1	A	255	ARG
1	A	263	VAL
1	A	265	ARG
1	A	266	THR
1	A	267	THR
1	A	270	LEU
1	A	274	THR
1	A	275	LEU
1	A	276	GLU
1	A	282	ILE
1	A	283	PHE
1	A	287	LYS
1	A	294	GLU
1	A	295	ILE
1	A	300	GLU
1	A	303	GLU
1	A	305	LEU
1	A	306	GLU
1	A	307	ARG
1	A	313	MET
1	A	319	THR
1	A	327	LEU
1	A	335	ARG
1	A	351	ASN
1	A	364	ARG
1	A	374	GLU
1	A	378	GLN
1	A	397	LEU
1	A	401	ILE
1	A	406	TYR
1	A	416	THR
1	A	418	ASN
1	A	424	LEU
1	A	432	TYR
1	A	436	PRO
1	A	446	ILE
1	A	478	ILE
1	A	493	SER
1	A	517	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	519	ARG
1	A	524	LEU
1	A	542	THR
1	A	543	ASP
1	A	549	ILE
1	A	554	SER
1	A	555	GLU
1	A	559	LYS
1	A	566	LYS
1	A	568	ILE
1	A	570	SER
1	A	575	LEU
1	A	578	LEU
1	A	603	LYS
1	A	606	THR
1	A	617	SER
1	A	628	LEU
1	A	630	THR
1	A	642	ARG
1	A	644	VAL
1	A	646	GLU
1	A	648	ILE
1	A	650	LYS
1	A	651	LEU
1	A	656	ILE
1	A	661	LEU
1	A	680	HIS
1	A	683	VAL
1	A	685	LYS
1	A	694	ILE
1	A	695	LYS
1	A	699	VAL
1	A	700	ILE
1	A	702	TYR
1	A	703	ILE
1	A	729	ASP
1	A	731	GLU
1	A	736	ASN
1	A	743	LEU
1	A	744	ARG
1	A	745	ILE
1	A	752	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	59	HIS
1	A	89	HIS
1	A	257	HIS
1	A	417	HIS
1	A	418	ASN
1	A	437	GLN
1	A	484	GLN
1	A	569	ASN
1	A	736	ASN
1	A	737	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](#)

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	712/775 (91%)	0.27	44 (6%) 24 18	21, 59, 91, 101	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	694	ILE	7.4
1	A	687	LEU	6.4
1	A	702	TYR	6.2
1	A	703	ILE	6.0
1	A	299	TRP	5.3
1	A	385	TYR	4.6
1	A	692	VAL	4.2
1	A	148	GLU	4.2
1	A	699	VAL	4.0
1	A	691	GLY	3.9
1	A	389	PHE	3.8
1	A	650	LYS	3.7
1	A	693	LYS	3.7
1	A	701	GLY	3.6
1	A	733	TYR	3.6
1	A	619	ILE	3.5
1	A	25	LYS	3.4
1	A	681	VAL	3.4
1	A	734	ILE	3.3
1	A	386	THR	3.3
1	A	390	VAL	3.2
1	A	698	MET	3.2
1	A	690	LYS	3.1
1	A	658	PRO	3.0
1	A	654	TYR	2.9
1	A	617	SER	2.9
1	A	689	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	147	HIS	2.5
1	A	387	GLY	2.4
1	A	59	HIS	2.4
1	A	732	TYR	2.3
1	A	651	LEU	2.3
1	A	655	GLU	2.3
1	A	743	LEU	2.3
1	A	682	ALA	2.2
1	A	745	ILE	2.2
1	A	731	GLU	2.2
1	A	306	GLU	2.2
1	A	695	LYS	2.2
1	A	300	GLU	2.1
1	A	688	ALA	2.1
1	A	247	MET	2.1
1	A	391	LYS	2.1
1	A	33	THR	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
2	MN	A	1758	1/1	0.89	0.22	1.30	61,61,61,61	0
2	MN	A	1759	1/1	0.85	0.07	-	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.